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# Study of Chemical Constituents and Traditional Usage of Neem Plant

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**Abstract:** ***Neem (Azadirachta indica) is an evergreen tree native to the Indian subcontinent with a long history of traditional medicinal use for a wide range of ailments. Its various parts contain a complex array of compounds, including limonoids like azadirachtin, nimbidin, and nimbolide, which exhibit potent antibacterial, antifungal, and insecticidal properties. The plant is also known for its antioxidant, anti-inflammatory, and potential anticancer activities, and its use has expanded from traditional remedies to modern pharmaceuticals and biopesticides.***

**Keywords:** Neem (Azadirachta indica), antioxidant, anti-inflammatory

## 1. Introduction

Aromatic plants[1] have been used for centuries for their pleasant fragrances and therapeutic properties. Aromatic plants, also known as herbs or fragrant plants, are a diverse group of plant species that are valued for their pleasant fragrances[1]and essential oils[2]. These plants have been used for thousands of years in various cultures for culinary, medicinal[3], cosmetic[4], and spiritual purposes[5]. The importance of aromatic plants are vast, ranging from flavoring foods[6] to treating ailments and providing aromatherapy[7],due to various parts of the plant, such as leaves, flowers, seeds, and roots.

Aromatic compounds are organic molecules that contain one or more rings of atoms with a conjugated system of pi electrons, which confer them stability, resonance[8], and distinctive properties, such as odour, colour, and reactivity[8]. Plants produce a wide variety of organic compounds, including many aromatic ones. These compounds serve different functions within the plant such as defence against pathogens, attracting pollinators, or acting as signalling molecules. Here are a few examples:

- **Phenols:** These are aromatic compounds containing a hydroxyl group (OH) attached to an aromatic ring. Phenols can act as antioxidants[9], antimicrobials and UV protectants in plants.
- **Flavonoids:** These areas diverse group of aromatic that often contribute to the coloration of flowers, fruits and leaves. Flavonoids play roles in UV protection, signaling and defence against pathogens and herbivores.
- **Terpenes:** Many terpenes contain aromatic rings within their structures. Terpenes[10] are responsible for the characteristic scents of many plants and play roles in defence , communication and attraction of pollinators and dispersal.
- **Alkaloids:** These are nitrogen –containing aromatic compounds with diverse biological activities. They can have toxic or pharmacological effects and are often involved in plant defence against herbivores and pathogens.

Neem oil, rich in fatty acids and vitamin E[11] is prized for its benefits in skin and hair care[12]. Moreover, neem's potential in sustainable agriculture and environmental conservation is increasingly recognized, as it enhances soil fertility and reduces reliance on synthetic pesticides.

**Active Compounds of Azadirachta Indica (Neem)**

Azadirachta indica(neem) shows therapeutics role in health most important active constituent is azadirachtin and the others are nimbolinin, nimbin, nimbidin, nimbidol, sodium nimbinate, gedunin, salannin, and quercetin. Leaves contain ingredients such as nimbin,nimbanene, 6-desacetylnimbinene, nimbandiol, nimbolide, ascorbic acid, n-hexacosanol and amino acid, 7- desacetyl-7-benzoylazadiradione, 7-desacetyl-7-benzoylgedunin, 17-hydroxyazadiradione, and nimbiol. Quercetin and ß-sitosterol, polyphenolic flavonoids, were purified from neem fresh leaves and were known to have antibacterial[13]and antifungal properties and seeds hold valuable constituents including gedunin and azadirachtin.

**Uses of Neem**

- **Medicinal Purposes[14]:** Neem is used to treat a wide range of ailments in traditional medicine, including kindisorders, digestive issues and infections. It's antifungal, and anti-inflammatory properties make it valuable in wound healing and skin care.
- **Oral Health[15]:** Neem twigs have been traditionally used as toothbrushes in many parts of the world. Chewing neem twigs is believed to promote oral hygiene and prevent dental diseases.
- **Insecticidal Properties[16]:** Neem extracts have been employed as natural insecticides for centuries. They are effective against a wide range of pests and insects, making neem a valuable tool in pest control.
- **Contraceptive**: In some traditional systems of medicine, neem is used as a contraceptive agent. Neem oil and extracts are believed to have spermicidal[17] properties although further research is needed to validate this claim.
- Neem extracts and compounds may be used to treat various inflammatory diseases such as arthritis, asthma and promote wound healing and reduce inflammation[18].

- Neem twigs are used for cough, asthma, hemorrhoids [19], intestinal worms, low sperm levels inside vaginitis used for birth control.
- Early research suggests that applying extract of neem root or leaf to skin helps repel black flies. Also, applying neem oil cream to the skin seems to protect against some types of mosquitos.
- It is used as fragrance in soaps, detergents, perfumes and as a flavouring in food.
- **Pain Relief:** Neem oil is often used topically to help relieve muscle and joint pain. It can also be found in creams and ointments for this purpose.

## 2. Methodology

**Collection of Neem Leaves Sample-**
The sampling of neem leaves was done from the neem tree. Around 400 grams of neem leaves were taken for sampling purposes. The neem leaves are later grinded into smaller fragments for oil extraction purpose.

**Extraction of Neem Leaves Oil:**

**Clevenger Apparatus:** Clevenger apparatus is a laboratory device used to carry out the extraction of essential oils from the plant materials. It functions on the principle of steam distillation. The apparatus usually consists of round bottom flask, a heating mantle with regulator to regulate temperature, water cooled condenser, water supply and a collection tube which has a knob fitted on it. A diagrammatic representation of Clevenger apparatus is shown below.

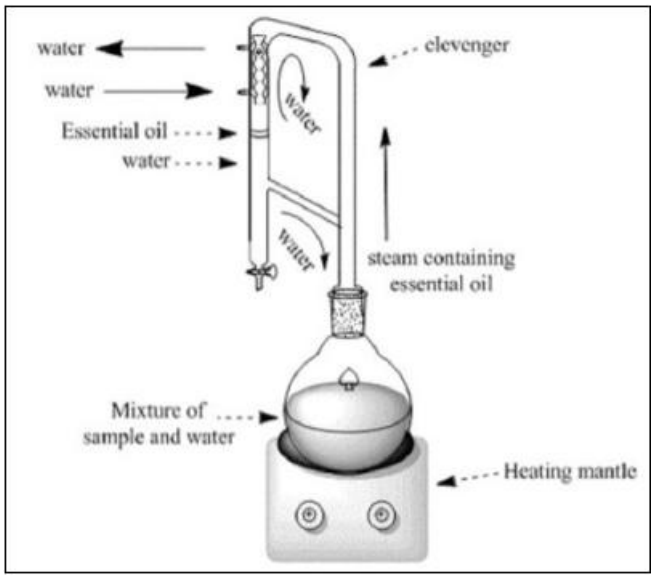


**Figure 1:** Diagrammatic Representation of Clevenger Apparatus

The extraction of neem oil using Clevenger apparatus is done through following steps:

a) **Preparation of the neem oil sample:** The collected sample of neem leaves is crushed or grinded into smaller pieces. The process of crushing/grinding is very necessary as it increases the surface area of neem leaves for easy extraction. It helps to release the essential oil more effectively. For our research we have took 400gm of fresh leaves neem leaves sample.
b) **Addition of water:** Fill the round bottom flask with grinded neem leaves and then water is added to the sample. Before putting the sample, it is checked whether the round bottom flask is clean or not in order to reduce the chances of impurities in the sample. For a 400 grams sample of neem approximately 1200ml of water is added to cover the plant material.

**Figure 2:** Actualism age of the apparatus used during the extraction of neem oil

c) **Setting up the apparatus:** After mixing water i the neem sample the Clevenger apparatus is assembled. The round bottom flask is placed on the heating mantle and the condenser tube and collection tube are fitted above it. It is ensured that cold water supply is maintained in the cooling condenser tube.
d) **Heat application:** Once the assembly of apparatus done, the heating mantle is turned on and the

temperature is slightly increased. The mixture of neem leaves and water started to boil and evaporate after some time. The steam carries the extract of neem oil.

e) **Collection and storage of neem oil extract:** The steam containing the neem oil extract starts evaporating, it rises and goes through the water- cooled condenser tube and gets cooled and condenses. The condensed droplets of neem oil start accumulating on the collection tube of the apparatus. With the droplets of neem oil there is little amount of water is also present. The oil droplets and water are immiscible due to their different densities. The neem oil obtained is collected carefully using the knob present in collection tube in air tight bottles in order to maintain their purity. The neem oil extracted from the above process must be stored in cold, dry and dark place.

**Figure 3:** Neem oil extracted using Clevenger apparatus

**FTIR Analysis of Neem Oil**

- **Sample Preparation:** Neem oil can be analysed directly as a liquid sample without extensive preparation. A small drop of oil is placed on an ATR (Attenuated Total Reflectance) crystal or mixed with KBr and compressed into a pellet if transmission mode is used.
- **Instrument Settings:** Ensure the FTIR spectrometer is properly calibrated. Set the background spectrum using an empty ATR crystal or a KBr pellet.
- **Scanning and Data Collection:** The sample is placed in the instrument and infrared light is passed through it.

## 3. Result and Discussion

The FTIR spectra obtained for neem leaves samples reveal significant insights into the chemical composition and the functional groups present in the extracts. The interpretation of the FTIR spectra was carried out by analyzing the absorption bands corresponding to various functional groups.

**Identification of functional groups:**

The spectra show the distinct peak. These indicate the presence of functional groups- N-H stretching vibrations: (around 3500cm$^{-1}$)

C=O stretching vibrations: (around1650 cm$^{-1}$) C-H stretching: (around 1250 cm$^{-1}$)

C-N stretching and N-H bending (around 800 cm$^{-1}$)

O-H Stretching: The broad peak near3200 – 3500 cm$^{-1}$ indicate the presence of Hydroxyl groups (O-H).

C-H stretching: The sharp peaks around 2900 cm $^{-1}$are characteristics of C-H stretching vibration.

C-H Bending: The sharp peak around 2000cm$^{-1}$are characteristics of C-H Bending vibration Fingerprint Region(1000-1500cm$^{-1}$): complex peaks in this region suggest the presence of multiple organic compounds, including esters, ethers and phenolic compound.

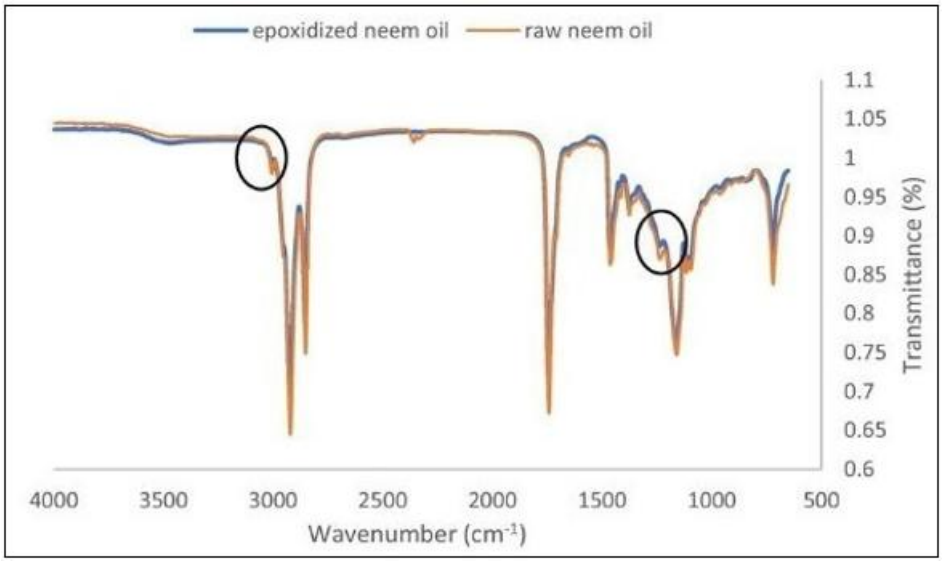


**Figure 4:** FTIR in Neem

The image shows an FTIR spectrum of neem leaves with label indicating key functional group and a list of compound found in neem.

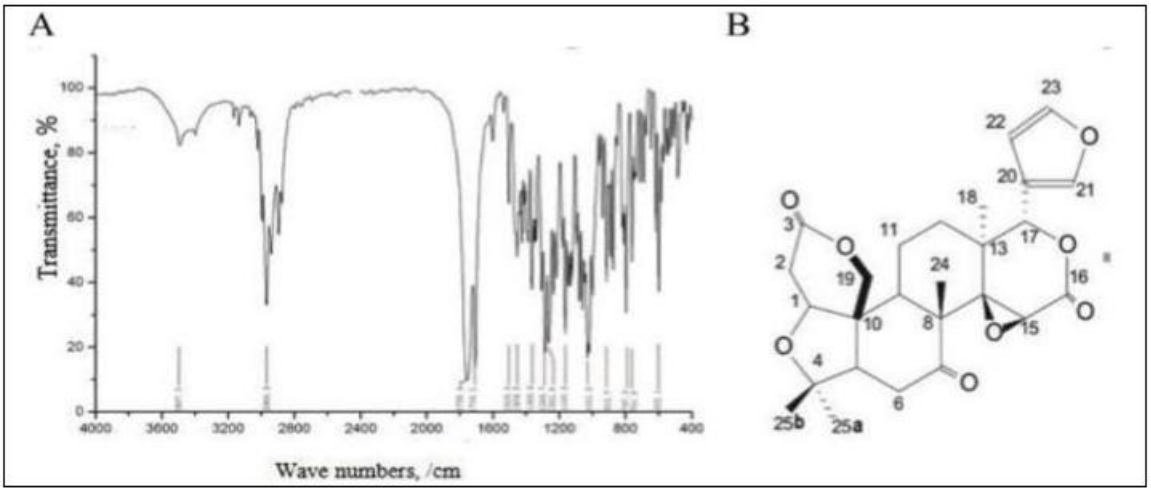


**Figure 5:** FTIR in limonoids compound

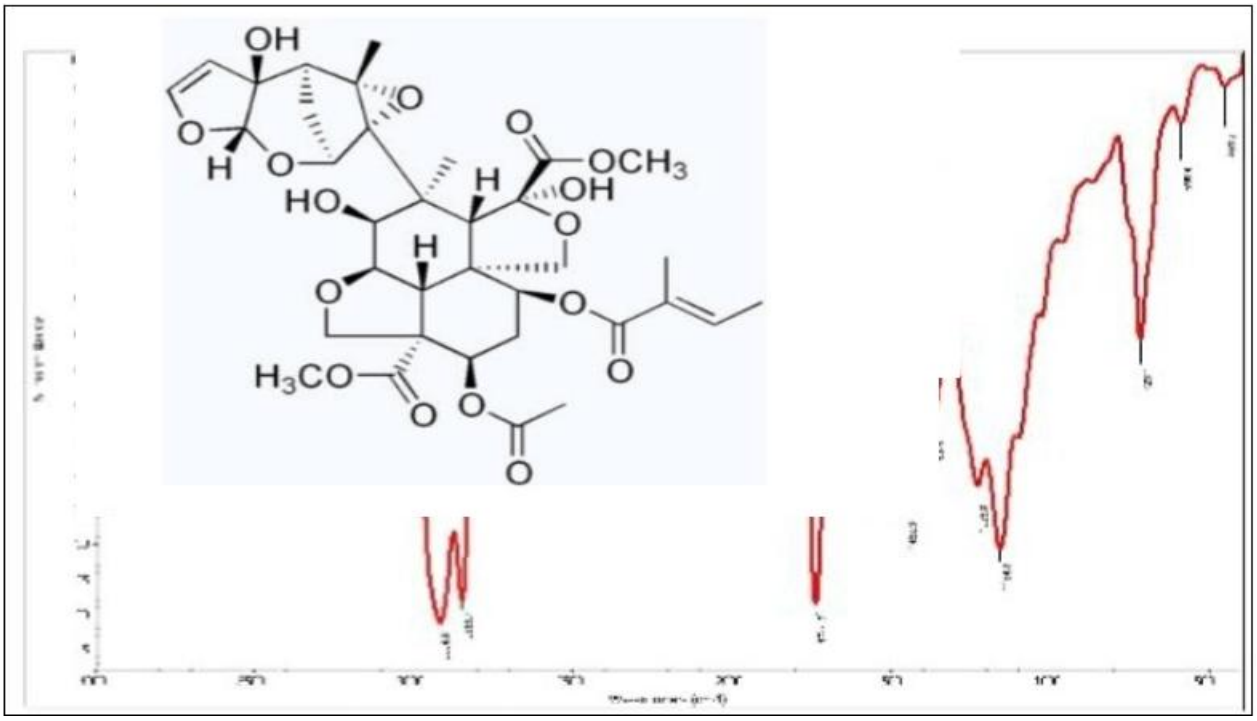

**Figure 6:** Transmittance in Neem oil

**Identification of major compounds**

**Triterpenes:** These are members of isoprenoids that are derived from a C30 precursor, Squatene. These are the most representative groups of phytochemical as over 30,000 of such compunds are recognized to exist. About 40 cyclic triterpenes of formula C30H50O are known. Almost all triterpenes induce apoptosis in tumor cells; they are preferred drugs in the treatment of cancer, because eliminating tumor cells by apoptosis his helpful in lowering side ffects in patients by avoiding necrosis.

**Chemical formula: C30H50O**

**Azardirachtin:** Azardirachtin, a chemical compound belonging to the limenoid group, is a secondary metabolite present in neem seeds. It is highly oxidized tetranortriterpenoid which boasts a plethora of oxygen bearing functional groups, including an enol ether, acetal, hemi acetal, tetra – substituted epoxide and a variety of carboxylic esters.

**Chemical Formulae:C35H44O16**

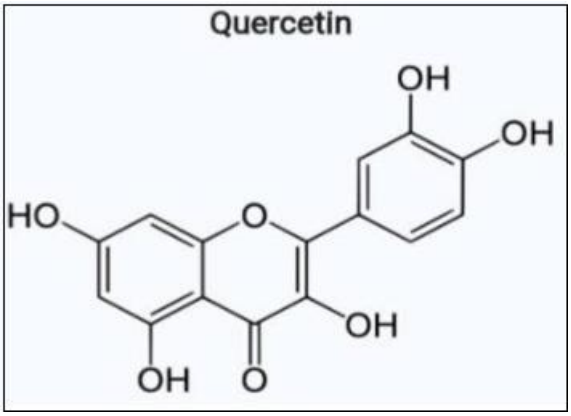


**Figure 7:** Structure of triterpenes

**Quercetin:** it is a plant flavanol from the flavonoid group of polyphenol. It has a bitter flavour and used as an ingredient in dietary supplements, the beverages and foods. It is a

pentahydroxy flavone having the five hydroxyl groups. It has a role as an antibacterial agent, an antioxidant, a protein kinase inhibitor, an antineoplastic agent.

**Chemical Formulae:$C_{15}H_{10}O_7$**

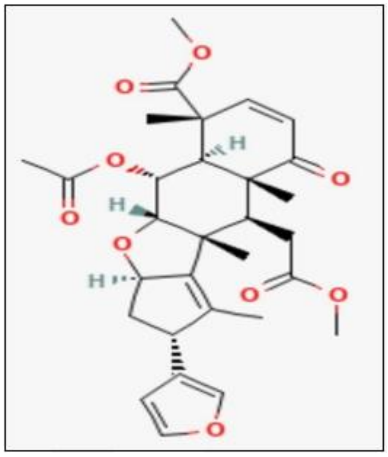

**Figure 8:** Structure of Nimbin

**Nimbidin:** It is the first bitter compound isolated from neem oil which enhances the immune system of the body and helps to fight all kinds of infections. It have anti – inflammatory, antipyretic, fungicidal, antihistamine and antiseptic properties.

**Chemical Formulae: $C_{30}H_{36}O_9$**

**Acid (3, 4, 5 – Tri hydroxy benzoic acid):** It is naturally occurring phenolic compound, a tri hydroxy benzoic acid, found in many plants, particularly in gallnuts, sumac, tea leaves and oak bark. Its known for its antioxidant and anti – inflammatory properties, as well as its potential to inhibit the growth of certain bacteria and cancer cells.

**Chemical Formulae:$C_7H_6O_5$**

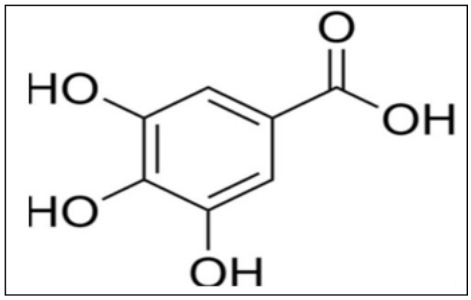


**Figure 9:** Molecular Structure of Gallic acid

**Catechins:** It is a flavan-3-ol, a type of secondary metabolite providing antioxidant roles in plants. It belongs to the subgroup of polyphenols called flavonoids.

**Molecular structure – $C_{15}H_{14}O_6$**

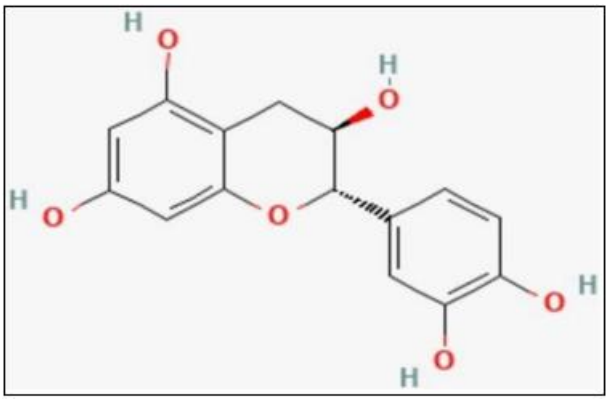

**Figure 10:** Structure of Catechins

**14,15-Epoxy Azadiradione:** It is a limenoid compound isolated from the seeds of neem and may in due mitochondrial apoptosis and inhibition of NFKB in human cervical cancer cells. MIF (Macrophage migration inhibitory factor) is responsible for pro-inflammatory reactions in various infectious and non – infectious diseases.

**Molecular structure: $C_{28}H_{34}O_6$**

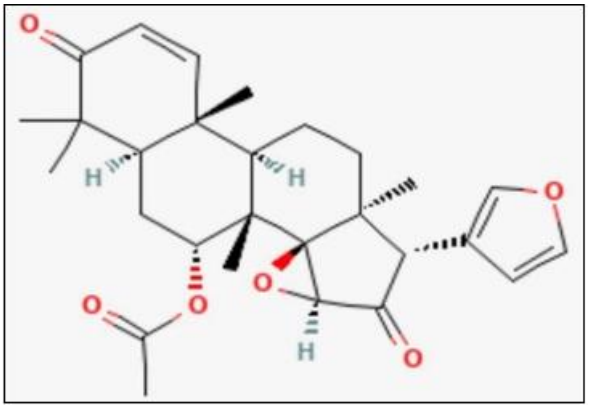

**Figure 11:** Structure of Epoxy 14,15-Azadiradion

**Nimbolide:** Nimbolide is a natural compound from the neem tree with potent anti- inflammatory, anti-microbial, and anti-cancer properties. It has shown therapeutic potential for various chronic diseases by modulating multiple cellular signaling pathways, such as suppressing cancer cell proliferation and inducing apoptosis. While pre-clinical studies show promise, further clinical research is needed to confirm its effectiveness and safety in humans.

**Molecular structure: $C_{27}H_{30}O_7$**

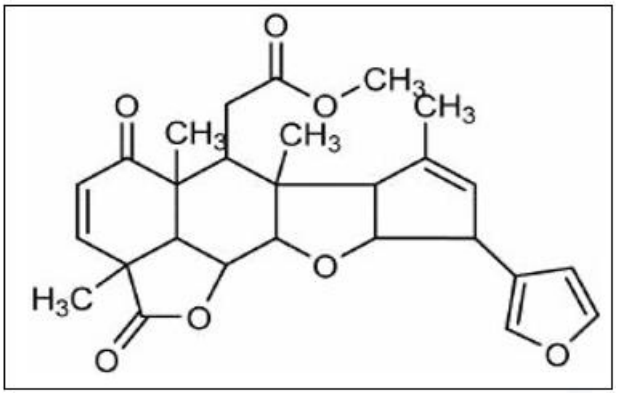

**Figure 12:** Structure of nimbolide

## 4. Conclusion

In conclusion, our study shows the profound significance of neem oil as a valuable natural resource with multifaceted applications. From traditional remedies to modern pharmaceutical formulations, neem oil emerges as a potent agent with the potential to enhance health and well- being across diverse populations. Through a comprehensive quantitative analysis utilizing FTIR, we have conducted a detailed analysis of the essential oil extracted from Neem (Azardirachta indica ) leaves. Employing the steam distillation method with the Clevenger apparatus, we obtained a pure Neem oil extract, which underwent rigorous analysis to elucidate its chemical composition. The FTIR analysis unveiled a rich array of constituents within Neem oil, highlighting key compounds such as Triterpenes, Azardirachtin, limenoids and quercetin, among others. These compounds contribute not only to the characteristic fragrance but also to the therapeutic properties associated with Neem oil.

The Triterpenes content of our neem oil sample is about 40-50 % while some other studies conclude that the Triterpenes concentration of neem essential oil ranges from 60-70%.

It is noteworthy that the concentration of neem, a predominant constituent in neem oil, may vary depending on factors such as geographical location, cultivation practices, and extraction methods. Our findings contribute to the understanding of these variations and underscore the importance of standardization in neem oil production.

In conclusion, our study underscores the profound significance of neem oil as a valuable natural resource with multifaceted applications. From traditional remedies to modern pharmaceutical formulations, neem oil emerges as a potent agent with the potential to enhance health and well-being across diverse populations.

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