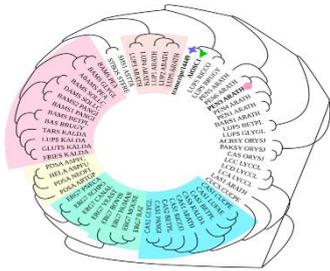


# Neem Research Newsletter

## Volume 5, Issue 9, 2025



**WORLD NEEM ORGANISATION (WNO)**



From

The Editor's Desk.....

In this Issue of the Neem Newsletter, we see interesting research findings on the effect of neem in agriculture, sustainable development, and human health. In the agriculture sector, tomato' graft plants enriched with bio-inputs of neem cake outperformed the non-grafted tomato in growth and yield metrics supporting its use in effectively combating root-knot disease in tomato, caused by *Meloidogyne incognita*. Kaolin-based treatments, particularly when combined with neem soap and microbial amendments, synergistically alleviated sunburn stress in dragon fruit and significantly improved yield. In another study, an amphiphile-assisted nanoprecipitation method to imbibe azadirachtin-rich neem seed extract (NSE) within a glycine carrier matrix, yielded a stable nanocomposite biopesticide. This approach offers a practical method for improving the stability, delivery, and efficacy of biopesticides for sustainable agriculture, enhanced stability, and larvicidal efficacy against fall armyworm. On the sustainable environmental front, a biodiesel blend from castor and neem oils was shown to be a viable alternative fuel for diesel engines. Neem and ginkgo leaves hold great promise for cost-effective and sustainable electrocatalysis for enhancing hydrogen evolution reaction performance in green energy technology. A one-step, green synthesis of silver-micro cellulose nanocomposite using neem leaf extract provided an inexpensive, eco-friendly, and reuseable platform for treating binary mixtures of methylene blue and safranin O dyes. Metal NPs were generated through green synthesis using herbal extracts of tea and neem.

The therapeutic potential of neem against various human ailments has been comprehensively reviewed. In a study from Ethiopia, the ethanolic extract of neem was demonstrated to have a significant effect on the mortality of the malarial parasite *Anopheles pharoensis*. Further, in another study *A. indica* essential oils, particularly at higher concentrations and longer exposures, was found to exhibit superior potency both in laboratory and field trials against the malarial parasite *Anopheles gambiae*. A curated set of 124 neem-derived phytochemicals was screened and shown to possess potential anti-caries properties. Neem exhibited potent anti-microbial efficacy when used as a root canal irrigant after activation with gamma radiation. The protective effect of azadirachtin against iron-induced liver damage was demonstrated. A case report of severe increase in blood sodium levels following saltwater-induced vomiting in a young woman with suspected neem powder poisoning highlighted the adverse effects of neem as well as the inappropriateness in treating with salt water.

S. Nagini

Core Founding Member, WNO  
Chief Scientific Coordinator &  
Regional Director, South India



# Neem in Agriculture

[Integrating grafting and bio-inputs for sustainable management of root knot nematode, \*Meloidogyne incognita\*, in tomato cultivation.](#)

Nagachandrabose S, Shanthi M, Shanmugam SP, Elaiyabharathi T, Sharmila R, Devrajan K, Manickam R, Srinivasan R. *Front Plant Sci.* 2025 Aug 29;16:1623444. doi: 10.3389/fpls.2025.1623444. eCollection 2025. PMID: 40949544

**Introduction:** Root-knot disease in tomato, caused by *Meloidogyne incognita*, presents a major challenge to global tomato production. This study explored a sustainable management approach by evaluating host-plant resistance through grafting combined with bio-inputs in farmers' fields with high natural infestations of *M. incognita*.

**Methods:** The commercial F1 hybrid Shivam® tomato was grafted onto bacterial wilt-resistant eggplant rootstocks, EG 203 and TS 03. Two field experiments were conducted with six treatment groups to compare the performance of 'EG 203-tomato' and 'TS 03-tomato' grafts against the non-grafted hybrid tomato, both with and without bio-input applications. The bio-input protocol included soil application of neem cake (250 kg/ha) and soil and seedling drenching at nursery and transplant stages using biocontrol agents (*Bacillus subtilis*, *Trichoderma asperellum*, and *Purpureocillium lilacinum*, each at 5 g/L).



**Results:** Results indicated that the 'EG 203-tomato' graft demonstrated strong resistance to *M. incognita*, while the 'TS 03-tomato' graft remained susceptible, akin to the non-grafted Shivam® hybrid. The EG 203-tomato graft treated with the bio-inputs achieved the highest suppression of *M. incognita*, with reductions of 76.8-77.7% juvenile populations in the soil, 62.0-66.1% in female populations within roots, 73.6-77.3% in egg masses per female, and 38.1-40.0% in eggs per egg mass. This treatment also resulted in the lowest root gall index, measured at 2.0-2.1.

**Discussion:** In both trial locations, 'EG 203-tomato' graft plants enriched with bio-inputs outperformed the non-grafted tomato in growth and yield metrics, achieving greater plant height (54.6-54.7 cm), leaf count (81.3-84.3 per plant), branch count (3.1-3.7) and fruit yield (10.8-11.5 kg/plant). These findings support the recommendation of EG 203-tomato grafts with bio-input management as an effective large-scale strategy for tomato growers combating *M. incognita* infestations.

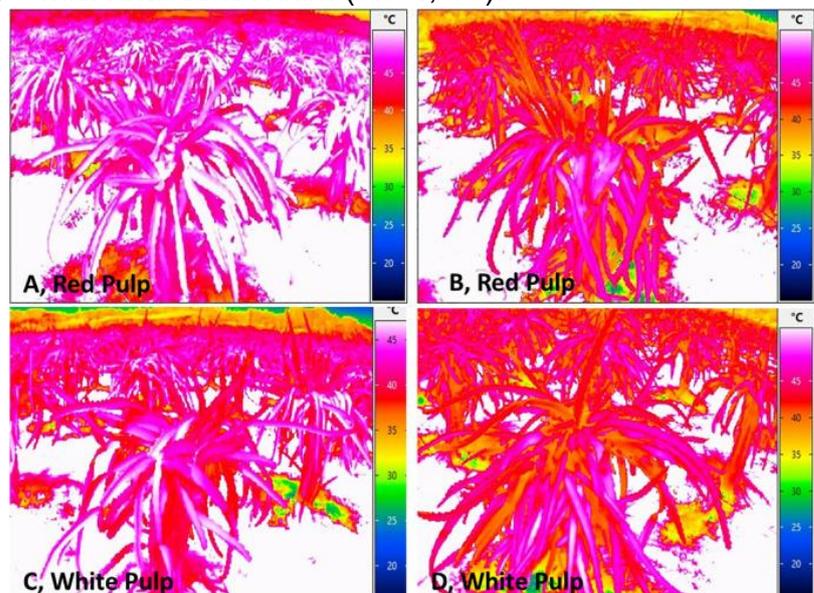
### [Sunburn mitigation in dragon fruit \(\*Hylocereus\* spp.\): unravelling genotype-specific physiological and biochemical responses.](#)

**Karunakaran G, Kanupriya C, Arivalagan M, Laxman RH, Prakash K, Manjunath BL, Ruchitha T, Abhilash K, Hazarika TK.** *Front Plant Sci.* 2025 Sep 11;16:1661147. doi: 10.3389/fpls.2025.1661147. eCollection 2025. PMID: 41019725

**Introduction:** Sunburn is a major abiotic stress affecting dragon fruit (*Hylocereus* spp.), impairing tissue integrity, disrupting physiological functions, and significantly reducing yield. Developing effective mitigation strategies is critical for sustaining productivity under high radiation conditions.

**Methods:** This study evaluated the efficacy of eleven treatments combining kaolin (5%) with shade net, seaweed extract (0.5%), and various biostimulants in red (*H. costaricensis* 'CHESH-D1') and white (*H. undatus* 'CHESH-W1') genotypes. Treatments included T1 (water spray control), T2 (kaolin 5% + green monofilament shade net 30%), and T3-T11 involving kaolin (5%) + seaweed extract (0.5%) combined individually with silica (0.5%, T4), micronutrients (0.5%, T5), petroleum oil (0.5%, T6), salicylic acid (0.5%, T7), neem soap (0.5%, T8), microbial consortium (0.5%, T10), brassinosteroids (0.5%, T11), and both neem soap (0.5%) + microbial consortium (0.5%, T9).

**Results:** Neem soap (T8) and neem soap + microbial consortium (T9) were the most effective treatments, reducing canopy temperature by 4.2-5.1 °C and malondialdehyde (MDA) content by 32-38% compared to the control. These treatments also showed lower phenolic, flavonoid, and antioxidant enzyme (SOD, POD, CAT) activities, indicating reduced oxidative stress. Shade net + kaolin (T2) retained the highest chlorophyll content (1.82 mg g<sup>-1</sup> FW), while microbial augmentation in T9 improved nutrient uptake. The red genotype exhibited higher tolerance to sunburn, with 12% lower MDA levels and 18% higher SOD activity than the white genotype.



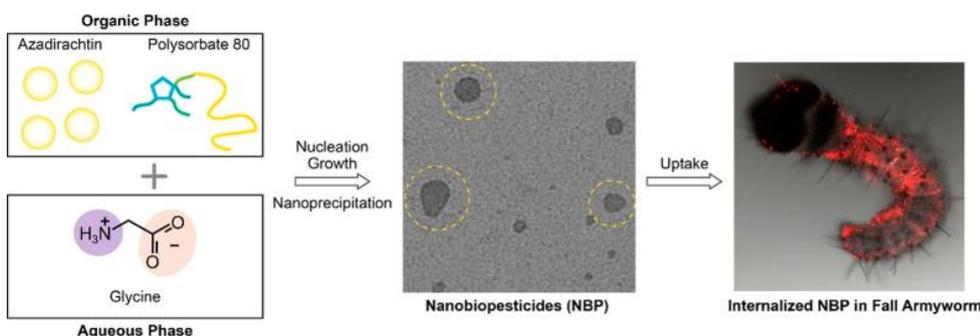
**Discussion:** Kaolin-based treatments, particularly when combined with neem soap and microbial amendments, synergistically alleviated sunburn stress by reducing oxidative damage, improving antioxidant enzyme activity, and enhancing nutrient homeostasis. Genotype-specific responses highlight the potential for precision management strategies to improve dragon fruit resilience under high radiation environments.



[Tailoring Biopesticides: Amphiphile-Assisted Nanoprecipitation of Azadirachtin within a Glycine Matrix for Sustainable Agriculture, Enhanced Stability, and Larvicidal Efficacy against Fall Armyworm.](#)

Bae M, Lewis A, Liu S, Arcot Y, Lin YT, Viswanadha LS, Bernal JS, Akbulut M, Cisneros-Zevallos L. ACS Omega. 2025 Aug 19;10(34):38766-38779. doi: 10.1021/acsomega.5c04028. eCollection 2025 Sep 2. PMID: 40918365

The limited water solubility and environmental instability of natural pesticidal compounds impede their broader agricultural use. This study reports an amphiphile-assisted nanoprecipitation method to imbibe azadirachtin-rich neem seed extract (NSE) within a glycine carrier matrix, yielding a stable nanocomposite biopesticide. The formulation, prepared using polyoxyethylene sorbitan monooleate as a stabilizer and glycine as the matrix former, followed by lyophilization, exhibited a hydrodynamic diameter of ~8 nm when redispersed in water. This glycine nanopesticide (GNP) significantly improved the photostability of azadirachtin under UV-AB irradiation (2000  $\mu\text{W}/\text{cm}^2$ ); spectrophotometric analysis revealed a 27.7% reduction in photodegradation over a 4 day period compared to unformulated NSE powder demonstrated dialysis-based in vitro release assay showed sustained release, with  $68.2 \pm 2.1\%$  released over 7 days, fitting an exponential model with a time constant of 37.6 h. Contact bioassays against *Spodoptera frugiperda* larvae revealed enhanced larvicidal potency.  $\text{LC}_{50}$  values showed a 1.5- to 6.6-fold improvement compared to unformulated NSE over 11 days. On day 7, GNP had an  $\text{LC}_{50}$  of 0.13 mg/mL, compared to 0.86 mg/mL for NSE powder. The nanoformulation also improved wettability on tomato leaves, reducing the contact angle from  $99.0^\circ \pm 1.6^\circ$  (DI water) to  $\sim 60^\circ$  at a concentration of 100 mg/mL GNP. This approach offers a practical method for improving the stability, delivery, and efficacy of hydrophobic biopesticides.



# Neem for Sustainable Environment & Green Synthesis

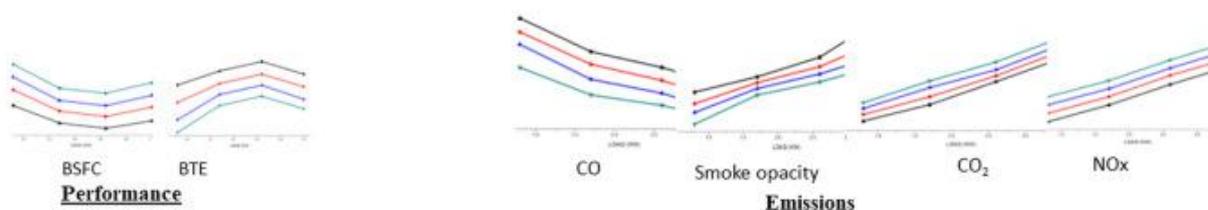
[Production, performance and emission of biodiesel from a mixture of castor oil and neem oil.](#)

Arslan M, Ayyub H, Jamshaid M, Arslan A, Kalam MA, Ahmad F. RSC Adv. 2025 Sep 24;15(42):35296-35311. doi: 10.1039/d5ra04004c. eCollection 2025 Sep 22. PMID: 41000608

The elimination of reserves of petroleum and their consequential environmental impact prompts the development of alternative fuels. This study aimed to blend castor and neem oils (at an 80 : 20 ratio) to address the drawbacks present in castor oil biodiesel, such as elevated kinematic viscosity and density. We propose that this new blending with a highly effective heterogeneous calcium oxide catalyst is the novelty of this work. This study employed a response surface approach to optimize biodiesel production. Biodiesel blends (B10, B20, and B30) were examined *via* standards EN 14214 and ASTM D6751. The performance of the biodiesel blends was scrutinized under experimental conditions, operating at a steady 2000 rpm with engine loads in the 25-100% range. Biodiesel production was optimized at an 8.75 : 1 methanol-to-oil ratio, 3.01 wt% calcium oxide, 56.6 °C, and 800 rpm, achieving a 95% methyl ester yield. The engine performance results indicated that brake thermal efficiency was lower than that of petroleum diesel. Conversely, brake-specific fuel consumption exhibited higher values than those observed with petroleum diesel. In terms of emissions, carbon monoxide and smoke opacity were less common than when using petroleum diesel, as the average smoke opacity for diesel was 10.46%, 18.43%, and 26.93% greater than that of the B10, B20, and B30 blends, respectively. However, the carbon dioxide and nitrogen oxide emissions were greater than those of petroleum diesel. Thus, a biodiesel blend from castor and neem oils can be a viable substitute fuel for internal combustion engines.



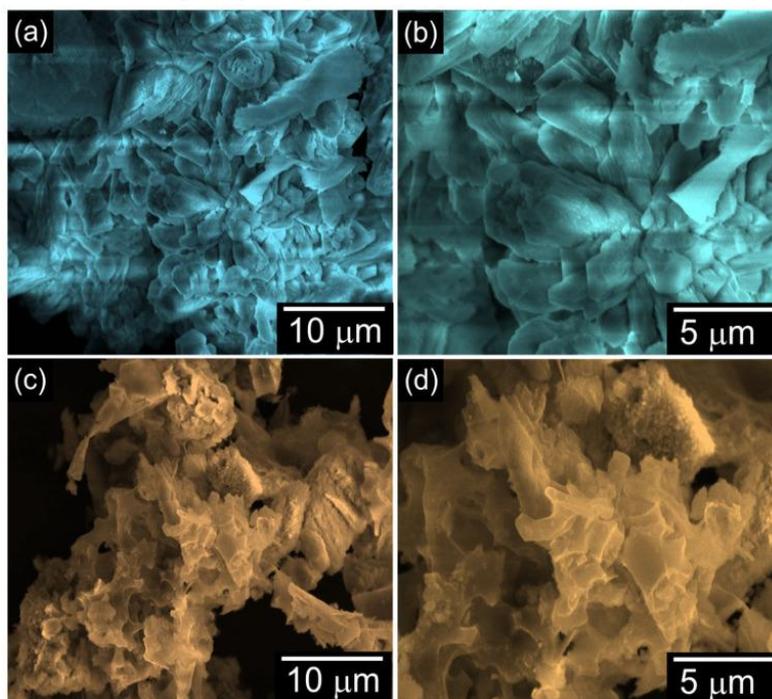
 Castor-neem biodiesel blend is a viable alternative fuel for diesel engines



## [Boosted Hydrogen Evolution Catalysis Using Biomass-Derived Mesoporous Carbon Nanosponges.](#)

Sekar S, Sadhasivam S, Shanmugam A, Sekar S, Lee Y, Lee S. *Int J Mol Sci.* 2025 Sep 1;26(17):8502. doi: 10.3390/ijms26178502.PMID: 40943422

Carbon-based metal-free catalysts, particularly those such as biomass-derived mesoporous activated carbon (AC) nanostructures, hold great promises for cost-effective and sustainable electrocatalysis for enhancing hydrogen evolution reaction (HER) performance in green energy technology. Neem and ginkgo leaves are rich in bioactive compounds and self-doping heteroatoms with naturally porous structures and act as a low-cost, sustainable biomass precursors for high-performance HER catalysts. In this study, mesoporous AC nanoflakes and nanosponges were synthesized using biomass precursors of neem and ginkgo leaves through a KOH activation process. Notably, AC nanosponges derived from ginkgo leaves exhibited outstanding physicochemical characteristics, including a sponge-like porous morphology with a large specific surface area of 1025 m<sup>2</sup>/g. For electrochemical evaluation in 0.5 M H<sub>2</sub>SO<sub>4</sub>, the G-AC sample revealed superior electrocatalytic HER performance, with a remarkably low overpotential of 26 mV at -10 mA/cm<sup>2</sup>, a small Tafel slope of 24 mV/dec, and long-term durability over 30 h. These results depict biomass-derived mesoporous AC nanosponges to hold substantial potential for highly efficient hydrogen production, contributing significantly to the advancement of eco-friendly energy solutions.



### [Eco-Friendly Synthesis of Silver-Cellulose Nanocomposite Adsorbent from Agricultural Residues for Binary Dye System Remediation.](#)

Al-Raimi DS, Alghanmi RM, Aljeddani GS, Hamouda RA. *Polymers* (Basel). 2025 Sep 22;17(18):2555. doi: 10.3390/polym17182555. PMID: 41012319

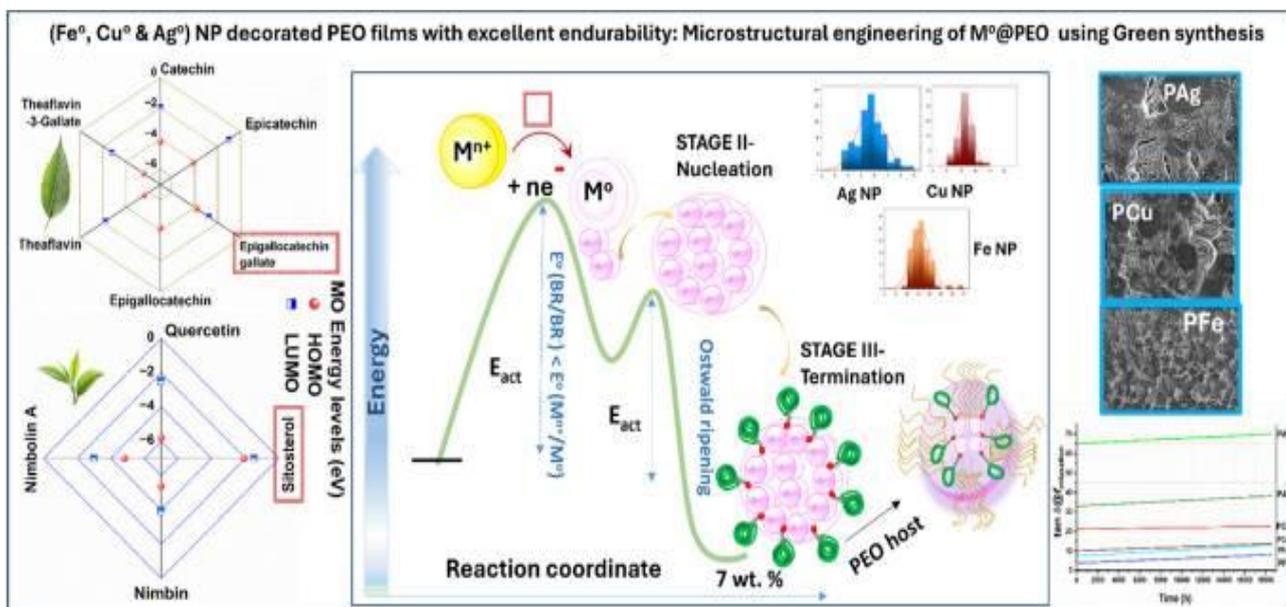
This work reports a one-step, green synthesis of silver-micro cellulose nanocomposite (Ag@Ce NCs) using *Azadirachta indica* A. Juss leaf extract to load micro-cellulose isolated from peanut shells with silver nanoparticles, followed by comprehensive physicochemical characterization (FTIR, TEM, EDX-SEM, zeta potential, and XRD). The composite has  $pH_{PZC} \approx 5.0$  and was tested for simultaneous removal of methylene blue (MB) and safranin O (SO) under batch conditions across various pH levels, doses, contact times, initial concentrations, ionic strengths, and temperatures. The high removal efficiencies observed at pH 10 for MB and 6.0 for SO. The adsorption reached the maximum at 45 min before partially declining, indicating reversible binding on saturated surfaces. Isotherm study favored the Langmuir model, with similar affinities ( $K_L \approx 0.106$ , and  $0.110$  L/mg) and monolayer capacities of  $17.99$  mg/g for MB and  $14.90$  mg/g for SO, suggesting non-selective competition on uniform sites. Kinetic data fitted the pseudo-second-order model, while thermodynamic analysis indicated mainly exothermic and physisorption interactions. Higher ionic strength reduced removal efficiency (at  $1.0$  M NaCl,  $\%RE \approx 33-48\%$ ), highlighting salt sensitivity typical of electrostatic attraction. The adsorbent maintained about 90% of its initial performance after five adsorption-desorption cycles in  $0.1$  M  $H_2SO_4$ , indicating excellent reusability. Overall, Ag@Ce NCs provide an inexpensive, eco-friendly, and reuseable platform for treating binary mixtures of cationic dyes.

### [Green Chemistry-Assisted Synthesis of Metal Nanoparticles and Fabrication of Microstructurally Engineered Conductive and Endurable \$M^0\$ @PEO Functional Films.](#)

Das A, Chatterjee R, Sarkar S, Ninave G, Bose D, Dutta AK, Biswas S, Mukherjee M, Venkatesan R, Majee R, Dasgupta S, Mukhopadhyay J, Mukhopadhyay M. *ACS Omega*. 2025 Aug 19;10(34):38609-38628. doi: 10.1021/acsomega.5c03323. eCollection 2025 Sep 2. PMID: 40918325

The present research reports the synthesis of poly-[ethylene oxide]-based composite films ( $500$   $\mu$ m) containing metal nanoparticles (NPs) [ $Ag^0$  ( $d_p \sim 6$  nm),  $Cu^0$  ( $d_p \sim 25$  nm), and  $Fe^0$  ( $d_p \sim 35$  nm)] as the mobile phase. The novelty of the study is in the corroboration of a plausible mechanism for the generation of metal NPs through green synthesis using herbal extracts of *Camellia sinensis* (Tea) and *Azadirachta indica* (Neem). Density functional theory (DFT) is used to optimize the phyto-reductants present in both biosources, wherein the reducing and/or stabilizing functional entities are primarily hydroxyl groups (-OH). The transition energy (band gap,  $\Delta E_{|LUMO-HOMO|}$ ) is found to be minimum for Epicatechin gallate ( $1.05$  eV, tea) and Sitosterol ( $0.58$  eV, neem), which could act as potent phyto-reductants for initiating a redox reaction, followed by subsequent capping through secondary bond formation. Upon increasing the loading of metal NPs from  $1$  to  $7$  wt %, the ionic conductivity of a PEO composite increases ( $0.1$   $S \cdot cm^{-1}$ ) for  $PAg_N$  (N: neem). With a subsequent increase in loading ( $10$  wt %), the crystalline region within PEO

is enhanced ( $\geq 83\%$  using DSC), which restricts the ion migration and lowers the charge storage capacity, as studied using dielectric constants and complex relaxation processes (EIS and DRT). Among all of the compositions, PCu<sub>N</sub> is observed to exhibit negligible performance deterioration ( $\Delta \tan \delta$  for 18,500 h  $\rightarrow$  0). However, PAg system(s) are good ion conductors with significant dielectric nature, but they suffer from particle ripening. Hence, metal NPs, which functionalize PEO films, could be effectively synthesized using a green synthesis route and applied as a solid electrolyte for device application.



## Neem for Human Health

### [Insecticidal Activities of Plants Extract Against Malaria Vectors in Hadiya Zone, Ethiopia.](#)

Assemie A, Mulu D, Getahun A, Awoke N, Muluken W, Enyew T, Gebremariam A, Aynalem Y.J Parasitol Res. 2025 Aug 28;2025:9980264. doi: 10.1155/japr/9980264. eCollection 2025.PMID: 40917103

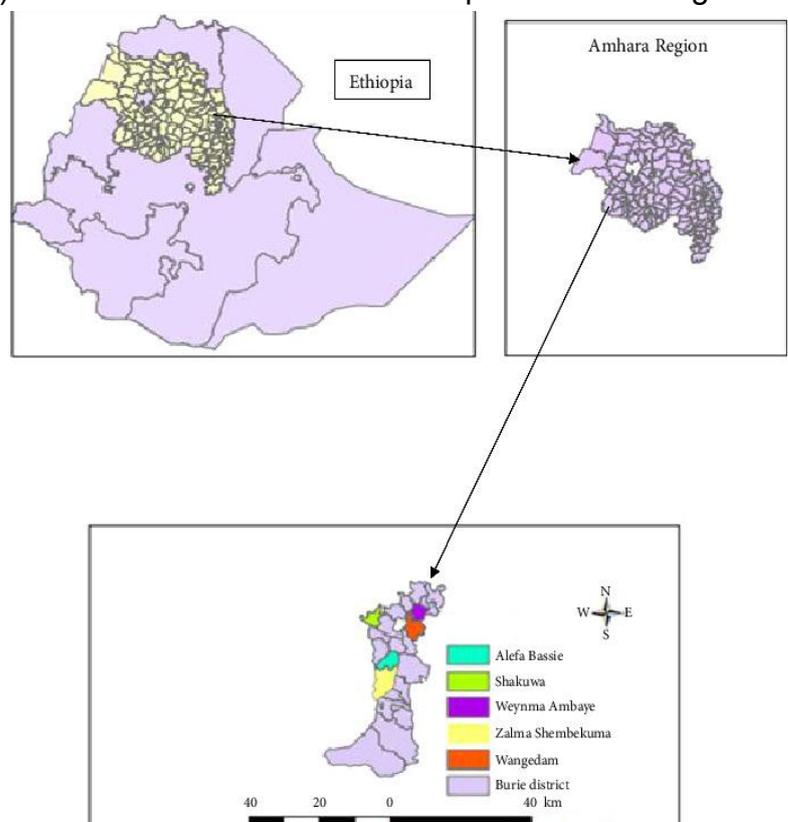
Environmental changes due to global warming and human activities have negatively impacted malaria vector control in Hadiya zone, Ethiopia. Plants contain anthraquinones, flavonoids, glycosides, phenol, saponin, steroids, tannin, and terpenes that are target specific, rapidly biodegradable, ecofriendly, and less toxic to human health. The objective of the study was to evaluate the insecticidal activities of *Azadirachta indica* (neem) and *Allium sativum* L. (garlic) ethanol extracts against malaria vectors in the study area. Then, 20 g from each (*A. indica* and *A. sativum* L.) were extracted separately by ethanol solvents. The phytochemical analysis was evaluated from the crude sample based on standard methods. Then, insecticidal activities were evaluated by introducing the fourth instar larva at 50, 100, 150, 200, and 250 ppm concentrations, and data were subjected to probit analysis to determine the LC<sub>50</sub> and chi-square test to check the significance of the mortality by R statistical software. The presence of phytochemical tests such as alkaloids, saponin, tannin, phenol, anthraquinones, flavonoids, glycosides, steroids, terpenes, and flavonoids was obtained. The mortality of malaria vectors due to ethanol extract of *A.*

*indica* and *A. sativum* was observed. The highest (90.66%) mortality was observed in the ethanol extract of *A. sativum* at 250 ppm concentration. *A. sativum* extracts have a significant effect only on the mortality of *Anopheles gambiae s.l* ( $X^2 = 13.6, p = 0.008687$ ) and *Anopheles pharoensis* ( $X^2 = 11.002, p = 0.02655$ ), but *A. indica* have a significant effect only on the mortality of *An.pharoensis* ( $X^2 = 14.26, p = 0.00651$ ). The lowest LC<sub>50</sub> (39 ppm) was observed in the ethanol extract of *A. sativum*. So, *A. sativum* extract was highly toxic than *A. indica* extract and more effective in the reduction of malaria vectors but further studies will be conducted to determine the insecticidal activities at pupa and adult stages.

### [Efficacy of Seed Oils From \*Azadirachta indica\* and \*Schinus molle\* and Their Combination Against \*Anopheles gambiae s.l.\*](#)

Atenafu G, Atnaf N.J Trop Med. 2025 Sep 15;2025:4460220. doi: 10.1155/jotm/4460220. eCollection 2025.PMID: 40989894

Due to the increasing resistance to synthetic insecticides and the proliferation of resistant strains of malaria vectors, plant-derived essential oils (EOs) are gaining prominence as an alternative for controlling *Anopheles gambiae s.l.* larvae. This study evaluated the larvicidal efficacy of EOs from *Azadirachta indica* and *Schinus molle*, both individually and in combination, against early 4<sup>th</sup>-instar *Anopheles gambiae s.l.* larvae under laboratory and semifield conditions. The EOs were extracted using ethanol in a Soxhlet apparatus. Twenty-five treatments were arranged in a completely randomized design for experimentation. Temephos (Abate) and distilled water served as positive and negative controls, respectively. Each treatment contained 20 larvae, which were acclimatized for 2 h prior to exposure to EOs. Treatment cups were covered with muslin cloth to prevent debris contamination. Larval mortality was assessed at 24, 48, and 72 h postexposure at concentrations of 25, 50, and 75 ppm. In the laboratory, *A. indica* oil exhibited the highest larvicidal activity among plant treatments, with 71.66% mortality at 75 ppm after 72 h, while *S. molle* and the combined treatment produced moderate effects. LC<sub>50</sub> and LC<sub>90</sub> values confirmed *A. indica*'s superior potency, with significantly lower lethal concentrations across all exposure times ( $p < 0.05$ ). In simulated field trials, *A. indica* oil also demonstrated time- and dose-dependent larvicidal activity, achieving 68.33% mortality at 75 ppm after 72 h.

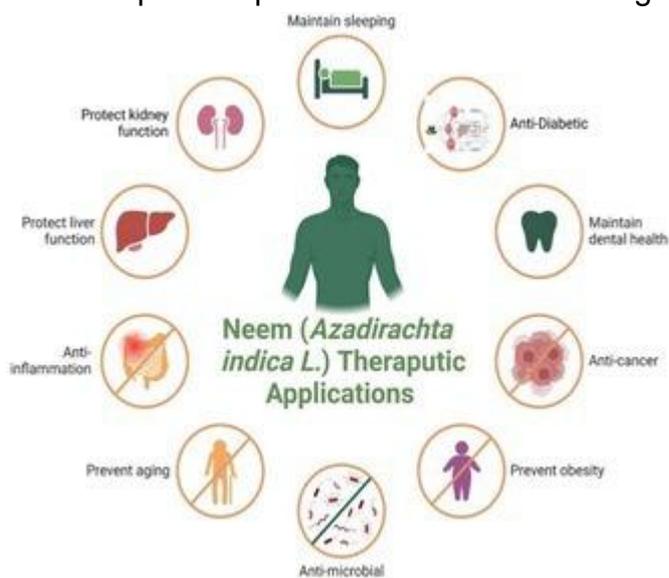


Synthetic larvicide Temephos (Abate) consistently caused 100% mortality within 24 h at all concentrations in both settings. These findings suggest that *A. indica* EO, particularly at higher concentrations and longer exposures, may serve as an effective botanical alternative for larval control in integrated vector management programs.

### [Neem \(Azadirachta indica\): A Miracle Herb; Panacea for All Ailments.](#)

Tufail T, Bader Ul Ain H, Ijaz A, Nasir MA, Ikram A, Noreen S, Arshad MT, Abdullahi MA. *Food Sci Nutr.* 2025 Sep 1;13(9):e70820. doi: 10.1002/fsn3.70820. eCollection 2025 Sep. PMID: 40901661

The neem tree (*Azadirachta indica*), native to the Indian subcontinent, has recently gained global recognition because of its extensive therapeutic qualities. It contains a high concentration of antioxidants and other valuable active substances including azadirachtin, salannin, nimbidin, nimbolin, nimbidol, nimbin, and quercetin, which are extracted from various plant parts. It has been widely utilized in Ayurveda, Unani, and Homeopathic treatments and has gained significant attention in modern medicine. Traditionally, neem leaves, flowers, seeds, fruits, roots, twigs, and bark have been used to treat fever, infection, skin conditions, and dental problems. The immunomodulatory, antiviral, anti-ulcer, antioxidant, anti-inflammatory, antihyperglycemic, antifungal, and anti-carcinogenic properties of neem and its components are well known. This comprehensive review highlights the diverse phytochemicals derived from neem leaves, extraction techniques, and their medicinal value in treating of multiple medical conditions. This miraculous plant has significant potential for enhancing its effectiveness. People have appropriately referred to it as a "natural remedy for numerous illnesses."



### [Integrated Virtual Screening for Anti-Caries Compounds from Neem: Dual-Target Inhibition of Biofilm Formation and Bacterial DNA Replication.](#)

Agboola OE, Agboola O, Ayinla ZA, Agboola SS, Olaiya OE, Oyinloye OM, Fajana OM, Idowu OT, Omotuyi OI, Ilesanmi OS, Oyinloye BE. *Biomedicines.* 2025 Sep 8;13(9):2202. doi: 10.3390/biomedicines13092202. PMID: 41007765

**Background:** Dental caries arise from polymicrobial biofilms and require interventions that address both local virulence and systemic burden. **Methods:** A curated set of 124 neem-derived phytochemicals was screened against *Streptococcus mutans* glucansucrase (3AIC) and *Staphylococcus aureus* DNA gyrase B (3U2D) using harmonized AutoDock Vina parameters. Ligand standardization and receptor preparation followed conventional protocols. **Results:** The most favorable docking scores reached  $-10.7 \text{ kcal}\cdot\text{mol}^{-1}$  for 3AIC

and  $-8.9 \text{ kcal}\cdot\text{mol}^{-1}$  for 3U2D. Redocking produced pose RMSD values of  $1.52 \text{ \AA}$  (3AIC) and  $0.96 \text{ \AA}$  (3U2D). Per-receptor ADMET profiles for the six top-ranked compounds indicated median logP values of 4.93 (3AIC) and 4.52 (3U2D), median TPSA values of 80.3 and  $62.9 \text{ \AA}^2$ , median rotatable bonds of 2.5 and 1.0, and median QED values of 0.41 and 0.76, respectively. **Conclusions:** An integrated, dual-target screen prioritized neem constituents with plausible local anti-cariogenic activity and physicochemical features compatible with systemic disposition. These *in silico* findings motivate targeted experimental validation.

[In vitro evaluation of the anti-microbial efficacy of natural root canal irrigants activated with gamma radiation.](#)

Priya S, Kaur Sohi H, Behera S, Pandey P, Chakrabarti B, Nanda S, Mehta M. *Bioinformation*. 2025 Jun 30;21(6):1471-1474. doi: 10.6026/973206300211471. eCollection 2025. PMID: 40978588

Neem and Tulsi were investigated as natural root canal irrigants with and without gamma radiation activation to evaluate their performance against *Enterococcus faecalis*. In total, 60 affected teeth were divided into six groups and each group was treated with a different irrigant. Neem that received gamma-irradiation had the top reduction of bacteria (96.5%), followed by Tulsi and sodium hypochlorite. The effectiveness of non-irradiated extracts was moderate, compared to the mild results found from saline. Gamma radiation made herbal irrigants much more effective, showing their potential for use as biocompatible treatments.

[In-silico identification of COX-2 inhibitory phytochemicals from traditional medicinal plants: molecular docking, dynamics, and safety predictions.](#)

Abdollahi F, Hadizadeh F, Farhadian S, Assaran-Darban R, Shakour N. *In Silico Pharmacol*. 2025 Sep 16;13(3):133. doi: 10.1007/s40203-025-00407-4. PMID: 40969544

Inflammation is an essential biological response that facilitates tissue repair and immune defense; however, chronic inflammation is associated with numerous pathological conditions, including cardiovascular diseases, autoimmune disorders, and cancer. Cyclooxygenase-2 (COX-2) is a key enzyme in this process, catalyzing the synthesis of pro-inflammatory prostaglandins, thus representing a critical target for anti-inflammatory therapies. Conventional COX-2 inhibitors, particularly non-steroidal anti-inflammatory drugs (NSAIDs), often have significant side effects, creating an urgent need for safer alternatives. This *in-silico* study evaluates the binding affinities of bioactive compounds from *Gmelina arborea*, *Coriandrum sativum*, *Glycyrrhiza glabra*, *Terminalia chebula*, *Solanum nigrum*, *Vernonia cinerea*, *Portulaca oleracea*, *Azadirachta indica*, and *Thespesia populnea* to the COX-2 receptor. Molecular docking and dynamics simulations identified solasonine, solamargine, rutin, and glycyrrhizin as having binding affinities ranging from  $-9.40$  to  $-8.50 \text{ kcal/mol}$ , exceeding that of the standard NSAID diclofenac ( $-5.68 \text{ kcal/mol}$ ). While these docking results provide valuable insights, further *in-vitro* validation is necessary. Stability analysis of ligand-receptor complexes showed minimal structural fluctuations. Moreover, cardiotoxicity predictions indicated that

solamargine, rutin, and glycyrrhizin present a lower risk compared to diclofenac. ADMET profiling highlighted favorable pharmacokinetic properties for rutin, suggesting its potential as a promising COX-2 inhibitor with a beneficial safety profile. Subsequent MM-GBSA calculations revealed binding free energy values of - 11.316 kcal/mol for rutin and - 35.190 kcal/mol for diclofenac, indicating strong binding interactions. Overall, this study underscores the potential of these natural compounds as safer alternatives in anti-inflammatory therapy, paving the way for future experimental validation and clinical application.

#### [Hepatoprotective effects of albiziasaponin-A, ellagitannin and azadirachtin in iron-intoxicated animal model.](#)

Anwar T, Hayat S, Ali I, Malik A, Ullah Khan MI. *Pak J Pharm Sci.* 2025 Sep-Oct;38(5):1593-1604. doi: 10.36721/PJPS.2025.38.5.REG.14207.1.PMID: 40996175

Prolonged exposure to iron can result in severe hepatic complications such as chronic liver damage, jaundice, cirrhosis, and hepatocellular carcinoma. Current treatment options for metal-induced hepatotoxicity are limited and often associated with undesirable side effects. This study investigates the hepatoprotective and anti-inflammatory properties of three phytochemicals, albiziasaponin-A, ellagitannin and azadirachtin, against iron-induced liver toxicity. Both *in silico* and *in vivo* approaches were employed to assess their binding affinity as well as the therapeutic effects of selected phytochemicals against the target protein, cyclooxygenase-2, a marker of liver damage. Molecular docking revealed strong binding affinities of all compounds with COX-2, indicating promising anti-inflammatory potential. Hepatic injury was assessed through biomarkers including ALT, 4HNE, 8-OHdG, TNF- $\alpha$ , IsoP-2 $\alpha$ , MDA, and COX-2 levels. The rat group exposed to iron overdose exhibited significantly elevated biomarker levels compared to controls, confirming hepatotoxicity. However, combination therapy with the selected phytochemicals led to a significant reduction in these biomarkers, suggesting effective hepatoprotection. These findings indicate that albiziasaponin-A, ellagitannin and azadirachtin possess potent therapeutic properties that may be beneficial in mitigating iron-induced liver damage. Further investigation is needed to establish their potential for inclusion in novel drug formulations targeting inflammatory liver diseases.

#### [Hypertremia Caused by Saltwater Emesis in a Case of Neem Powder Poisoning.](#)

Alla KR, Pulluri R. *Cureus.* 2025 Aug 9;17(8):e89685. doi: 10.7759/cureus.89685. eCollection 2025 Aug. PMID: 40932984

Table salt is widely available and, in some cases, inappropriately used as an emetic in poisoning incidents, both in clinical and domestic settings. However, saltwater-induced emesis can lead to severe hypertremia, which, although rare, carries a high risk of morbidity and mortality. Early recognition, prompt diagnosis, and urgent management are essential to prevent irreversible neurological injury or death. We report a case of severe hypertremia (serum sodium 187 mmol/L) following saltwater-induced emesis in a young woman with suspected neem powder poisoning, in whom timely intervention led to complete recovery. Clinical features, management strategies, and the urgent need to eliminate this dangerous practice are discussed.