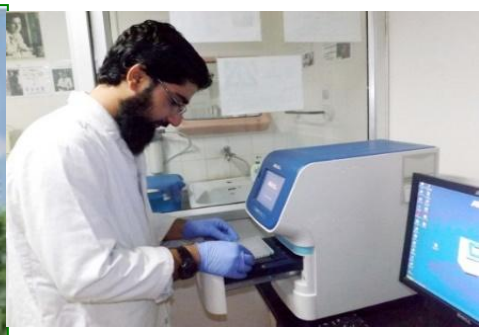
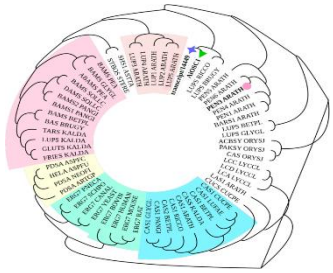
Neem Research Newsletter

Volume 6, Issue 6, 2026





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WORLD NEEM ORGANISATION (WNO)

From

The Editor's Desk……

In this Issue of the Newsletter, we see several novel research insights on neem. A study from Ethiopia concluded that the implementation of non-chemical pest control practices including use of neem extract was shaped by socioeconomic and farmland-level factors as well as farmland ownership. Insect growth regulators such as azadirachtin were reported to profoundly disrupt the development of two-spot cotton leafhopper, Amrasca biguttula, an emerging threat to cotton, vegetable, and ornamental crops supporting their use as selective and sustainable tools in integrated pest management programs.

A mixed insulation for transformer applications using mineral oil-neem oil ester was developed and characterised. The optimal ratio of 70:30 mineral oil: neem oil ester showed a notable level of durability after ageing, which helped to explain its high resistance and low conductivity. Neem biodiesel blended with Zinc oxide nanoparticles exhibited strong potential as a sustainable fuel for enhanced overall engine performance and cleaner emissions.

A narrative review of the ethnopharmacological landscape of neem provided a comprehensive coverage of its phytochemical diversity mapping over 140 bioactive compounds to specific molecular pathways underscoring the clinical potential of neem. Copper oxide nanoparticles prepared through a green synthetic strategy employing aqueous extracts of Azadirachta indica and Aloe vera as natural reducing and capping agents exhibited promising anti-inflammatory, antimicrobial, and antioxidant potential. A systematic review that summarized the effectiveness of mosquito repellents for humans indicated that plant-based repellents such as neem may serve as safer alternatives for short-term or adjunctive use. Despite the availability of conventional drugs, the use of medicinal plants such as neem for typhoid and malaria was found to be widespread in rural and urban Nsukka, Nigeria. The molecular mechanisms underlying the antiviral reprogramming induced by neem against Dengue virus was delineated. The efficacy of neem leaf extract against multidrug resistant bacteria that cause skin infections was demonstrated. Neem extract was shown as a biocompatible alternative irrigant for effective post-operative pain reduction following root canal treatment.

A transparent nanocomposite film fabricated using keratin from human hair waste and incorporated with neem-mediated silver nanoparticles, carboxymethyl cellulose, and aloe vera provided a multifunctional platform for wound healing by preserving moisture, reducing inflammation and infection, and promoting the regeneration of tissue. Investigations on the potential inhibitory activity of phytochemicals from Neem against tuberculosis revealed that quercetin may serve as a promising inhibitor candidate but requires further studies to better ascertain its efficacy as an anti-tubercular agent. In another study, the neem limonoid nimbolide was found to protect against osteoporosis. Quercetin derivatives from A. indica leaf represent promising lead compounds for targeted threonine tyrosine kinase inhibitors in lung and pancreatic cancers, highlighting their potential for further experimental validation.

S. Nagini

Core Founding Member &
Chief Scientific Advisor

Neem in Agriculture

Utilization of non-chemical pest control practices among agro-pastoralist farmers in Gambella region, Ethiopia.

Bor C.J Ethnobiol Ethnomed. 2026 Jun 7. doi: 10.1186/s13002-026-00913-5. Online ahead of print.PMID: 42252462

Background: Agricultural production continues to face critical problems, including persistent pest invasion, a lack of modern farm inputs, and climate change. Non-chemical pest control practices are vital, as they signify both cultural and practically embedded assets for sustainable agricultural practices in resource-limited environments. Therefore, this study aimed to assess the utilization of non-chemical pest control practices among agro-pastoralist farmers in the Gambella region of Ethiopia.

Methods: A mixed research design was used to assess the utilization of non-chemical pest control practices among farmers from a total sample size (n = 274). The purposive sampling technique was used to select kebelles, and the systematic random sampling technique was used to select the target households. Primary data were collected from the sample respondents using structured questionnaires, key informant interviews, focus group discussions, and direct observations. Secondary data were collected from the documented sources. Frequency, percentage, chi-square, H-test, and ordinal logit model were used for quantitative data analysis, while thematic analysis was employed for qualitative data.

Results: The common non-chemical pest control practices used by farmers were the application of ash (49.6%), crop rotation and intercropping (16.4%), use of neem extract (13.5%), physical removal of pests (10.2%), timing of planting based on the pest cycle (6.6%), and the use of chili or tobacco spray (3.7%). The ordinal logit model showed that farmers level of education negatively and significantly influenced the utilization of such practices ($p < 0.01$), and farmland ownership was positively and statistically associated with farmers non-chemical pest management systems ($p < 0.01$). The crops cultivated also showed a positive and statistically significant association with farmers' utilization of the practices ($p < 0.05$).

Conclusions: This study concludes that the implementation of non-chemical pest control practices is shaped by socioeconomic and farmland-level factors rather than being regularly practiced across all households. Therefore, improving the application of locally available pest management systems with appropriate agricultural support should strengthen sustainable pest control and enhance farmland resilience in the Gambella region.

Comparative impact of insect growth regulators on mortality and development of Amrasca biguttula (Hemiptera: Cicadellidae).

Attia S, Joseph SV.PLoS One. 2026 Jun 5;21(6):e0350736. doi: 10.1371/journal.pone.0350736. eCollection 2026.PMID: 42247431

The two-spot cotton leafhopper, Amrasca biguttula (Ishida) (Hemiptera: Cicadellidae), recently detected in the United States, represents an emerging threat to cotton, vegetable,

and ornamental crops. Insect growth regulators (IGRs) are considered reduced-risk insecticides. Despite their availability to growers and effectiveness on several piercing and sucking insects, the lethal effects of IGRs on the development of A. biguttula remain poorly understood. Thus, the objective of this study was to determine the effects of common IGRs on various stages of A. biguttula. We evaluated four IGRs: pyriproxyfen, novaluron, azadirachtin, and buprofezin applied at field-recommended rates, alone or combined with nonionic and organosilicone adjuvants, on survival, molting disruption (exuviae production), and longevity of early (1st-2nd), intermediate (3rd-4th), and late (5th) nymphal instars, as well as adults using leaf dip and adaxial leaf smear bioassays. All IGRs induced significant, stage-dependent lethal effects. Mortality of 1st-2nd instars reached over 90% with buprofezin and novaluron, and molting inhibition reached up to 55%, indicating strong effects of the tested insecticides. The chitin biosynthesis inhibitors buprofezin and novaluron caused rapid mortality, strong molting inhibition, and reduced longevity, particularly in early and intermediate instars. Pyriproxyfen and azadirachtin elicited weaker, delayed responses, with limited effects on late instars and adults. Although adding adjuvants slightly enhanced efficacy, their overall impact was marginal. These findings demonstrate that IGRs can profoundly disrupt A. biguttula population development through interference with insect growth and metamorphosis, supporting their use as selective and sustainable tools in integrated pest management programs targeting this invasive leafhopper.

Neem For Sustainable Energy & Industrial Applications

Integrated experimental and machine learning investigation of green-synthesized ZnO nanoparticle-dispersed **neem** biodiesel: effects on diesel engine performance, combustion, and emissions.

Srinivasarao M, Rao SC, Babu PR, Ramana AV, Venkatesh JD, Dasharath SM, Barik D, Dennison MS, Shanmugapriya D, Gnanasekaran L.Sci Rep. 2026 Jun 12. doi: 10.1038/s41598-026-57550-x. Online ahead of print. PMID: 42286173

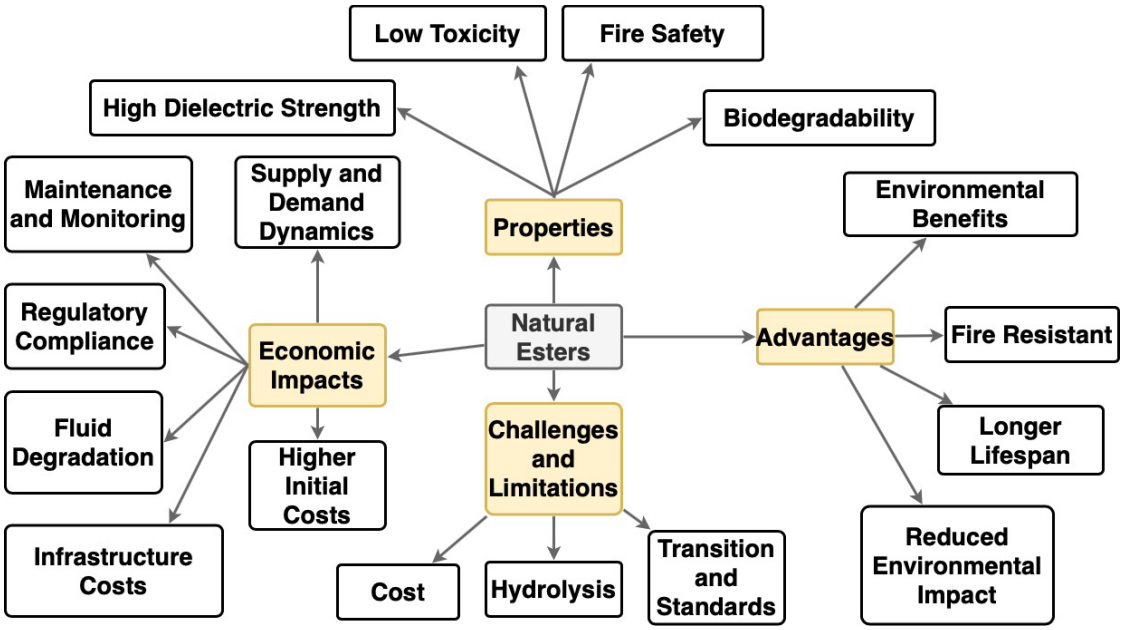
This study explores the performance, combustion, and emission parameters of a neem biodiesel enhanced with zinc oxide (ZnO) Nanoparticles (NPs) synthesized through a green method in a compression ignition (CI) engine. Neem oil was transesterified to produce biodiesel, while ZnO NPs were synthesized using neem leaf extract and dispersed at concentrations of 50 ppm and 100 ppm, denoted as NB25Zn50 and NB25Zn100, respectively. The outcomes showed that the addition of ZnO NPs significantly enhanced combustion efficiency, resulting in Brake Thermal Efficiency (BTE) increases of 1.51% for NB25Zn50 and 3.64% for NB25Zn100, along with Specific Fuel Consumption (SFC) decreases of 2.54% and 5.28%, respectively. Combustion analysis revealed a higher peak cylinder pressure (CP), increased Heat Release Rate (HRR), and quicker Mass Fraction Burning (MFB) progression for fuels blended with NPs, indicating a shorter Ignition Delay (ID) and more complete combustion. Emission analysis showed considerable reductions in Carbon monoxide (CO), Hydrocarbons (HC), and smoke opacity, whereas the optimal ZnO concentration (100 ppm) effectively controlled Nitrogen

Oxides (NO_x) emissions. Additionally, machine learning models such as K-Nearest Neighbors (KNN), Rrandom Forest (RF), Ssupport Vector Regression (SVR), and Extreme Gradient Boosting (XGB) were used to predict engine performance, emissions, and energy parameters. Among these, extreme gradient boosting demonstrated superior predictive accuracy with high correlation coefficients (R ≈ 0.99) and minimal error. Overall, neem biodiesel blended with ZnO NPs, especially at 100 ppm, exhibited strong potential as a sustainable fuel for enhanced overall engine performance and cleaner emissions.

Development and characterization of mineral oil-**neem** oil ester mixed insulation for transformer applications.

Pitchaimani SP, Raj RA, Muthusamy S, Sonawane C, Chan CK, Kamalrudin M.Sci Rep. 2026 Jun 12. doi: 10.1038/s41598-026-55461-5. Online ahead of print.PMID: 42286038

This study aims to establish an optimal ratio of Mineral Oil (MO) and Neem Oil After Esterification (NOAE) to develop a Mixed Insulation (MXI) that effectively replaces the MO for oil-filled transformers and other oil-filled electrical equipments. The effective use of two-stage esterification technique using Neem Oil (NO) as a base oil and concentrated sulfuric acid (H_2SO_4) and potassium hydroxide (KOH) as acid and base catalysts had been adopted to transform NO into NOAE. Further, the FAME formation is confirmed using the ^{1}H-NMR. By lowering the impact of MO in oil-cooled transformers, the proposed MXI's dielectric properties are critically analysed using its AC breakdown voltage (BDV) in sphere-sphere and point-plane, kinematic viscosity (KVIS), corona inception voltage (CIV) and interfacial tension (IFT), and other dielectric properties. The MXI proportions are subject to accelerated thermal ageing in the presence of a pressboard and copper plate. The changes in their dielectric properties are reported along with the information about the material characteristics using an FTIR. Further, the validation of the samples is verified using Weibull distribution and Kurtosis and Skewness values. The current study on MXI is given credence by the discovery that sample X30, or the optimal MO: NOAE blending ratio, is 70:30. The X30's dielectric properties showed a notable level of durability after ageing, which helped to explain its high resistance and low conductivity.



Ethnopharmacological landscape of Azadirachta indica (**Neem**): Phytochemical diversity bridging traditional heritage and modern medicine.

Sharma A, Raut SS, Shukla A, Parul N, Singh A, Mishra A.J Ethnopharmacol. 2026 Jun 19;371:122088. doi: 10.1016/j.jep.2026.122088. Online ahead of print.PMID: 42320775

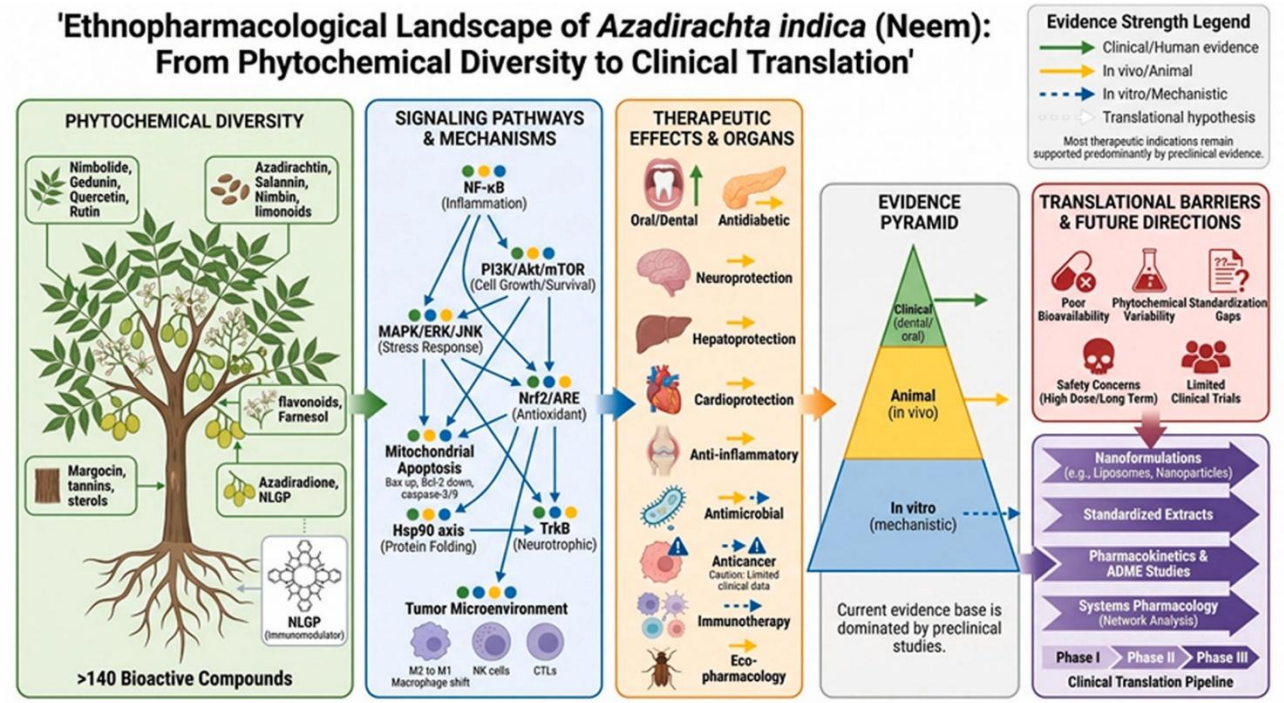
Ethnopharmacological relevance: Azadirachta indica A. Juss. (neem) is a cornerstone of traditional medicine across tropical regions, recognized for its broad-spectrum therapeutic applications. However, the translation of its extensive ethnopharmacological legacy into evidence-based therapy is hindered by fragmented reports and a lack of systematic integration.

Aim of the review: This narrative review aims to provide a quantitative and mechanistic synthesis of neem's phytochemical diversity and pharmacological landscape, explicitly distinguishing itself from prior work by mapping over 140 bioactive compounds to specific molecular pathways and clinical potential, while critically evaluating translational barriers.

Methods: A literature search of Web of Science, PubMed, and Scopus was conducted for peer-reviewed articles published between January 2001 and November 2025, using keywords related to Azadirachta indica, neem phytochemistry, pharmacology, and toxicology.

Results: Phytochemical investigations have identified over 140 distinct compounds, including limonoids (e.g., azadirachtin, nimbolide, gedunin), flavonoids, and phenolic acids, distributed across all plant parts. These compounds modulate core signaling hubs-NF-κB, PI3K/Akt/mTOR, Nrf2, and MAPK-underpinning a broad pharmacological spectrum. Preclinical studies suggest that neem-derived compounds exhibit antiproliferative activity against breast, cervical, colon, and prostate cancer cell lines, although in vitro IC_{50} values alone are not predictive of clinical efficacy. Neem extracts and phytochemicals have also demonstrated neuroprotective effects in experimental models of Alzheimer's and Parkinson's diseases and antidiabetic activity in streptozotocin-induced diabetic rodents; however, the translational relevance of these findings to human disease remains to be established through rigorous clinical investigation. Beyond human health, neem's insecticidal and antifeedant properties support eco-friendly agricultural applications. However, clinical validation remains strikingly limited: only fifteen interventional trials are registered, most for oro-dental conditions, with no published phase II/III results for systemic diseases. Toxicological reports confirm dose- and route-dependent risks, including pediatric encephalopathy from neem oil ingestion and embryotoxicity, necessitating explicit safety guidelines.

Conclusions: Neem possesses validated, multi-target therapeutic potential, yet its clinical translation is currently impeded by poor bioavailability, extract standardization gaps, and a paucity of rigorous human trials. Future research must prioritize pharmacokinetic optimization (e.g., nanoformulations), establishment of certified reference materials, and well-designed phase trials in oncology and metabolic disease, rather than further preclinical cataloging.



[Phytochemical-mediated green synthesis, mechanistic insights integrated with biological evaluation, density functional theory calculations and molecular docking studies of copper oxide nanoparticles.]

Devi A, Madhu, Chaudhary A.Sci Rep. 2026 Jun 19. doi: 10.1038/s41598-026-58053-5. Online ahead of print.PMID: 42321323

Copper oxide nanoparticles have attracted considerable attention due to their notable roles in catalysis, sensing technologies, and biomedical research. In the present work, copper oxide nanoparticles (CuONPs) were prepared through a green synthetic strategy employing aqueous extracts of Azadirachta indica and Aloe vera as natural reducing and capping agents. This plant-assisted approach offers an eco-friendly, economical, and sustainable substitute for traditional chemical synthesis routes that often involve hazardous reagents. Comprehensive characterization techniques were used to confirm nanoparticle formation and evaluate their properties. FTIR analysis showed a distinct Cu-O stretching band near 542 cm^{-1}, verifying the formation of copper oxide. XRD patterns confirmed the crystalline nature of the particles, with an average crystallite size of about 26.3 nm. Microscopic studies (SEM and TEM) revealed nanoscale particles mainly distributed between 20 and 50 nm with an average particle size of approximately 34 nm. Elemental analysis by EDX verified copper and oxygen as the dominant elements, with weight percentages of 77.51% and 22.49%, respectively, confirming the successful formation of CuONPs, while Zeta potential measurements revealed a zeta potential value of 4.93 mV with a polydispersity index (PDI) of 0.454, indicating moderate colloidal stability and a relatively broad particle size distribution of the synthesized CuONPs. Biological investigations demonstrated strong activity, with over 70% inhibition observed in antioxidant and anti-inflammatory assays at higher concentrations. Additionally, CuONPs exhibited highest antimicrobial activity against B. subtilis with zone of inhibition 23 ± 0.6 mm. Theoretical studies using density functional theory and molecular docking supported

the experimental findings. Collectively, the study highlights the promising biomedical potential of green-synthesized CuONPs.

Effectiveness of mosquito repellents for human: A systematic review of human-based studies.
Faridah L, Nurhakim RA, Astuti RRUNW, Melanie, Rohmawati E, Rachmawati Y, Carvajal T.Acta Trop. 2026 Jun 12;280:108182. doi: 10.1016/j.actatropica.2026.108182. PMID: 42285396

Mosquito repellents are personal protection tools against mosquito-borne diseases, but their effectiveness varies across active ingredients, formulations, and mosquito species. This systematic review followed PRISMA 2020 guidance to summarize human studies published between 2015 and 2025 that evaluated mosquito repellents delivered as topical application, wearable devices, spatial products, or treated clothing. Searches in Scopus and PubMed identified 1287 records, of which 19 met eligibility criteria. Data on complete protection time (CPT), repellency rate, safety, formulation type, and target species were synthesized descriptively because of methodological heterogeneity. Synthetic repellents, particularly DEET-based products in lotions or ointments, consistently provided the longest CPT, often five to nine hours, with repellency frequently approaching or exceeding 80-100% and no reports of adverse skin reactions. Natural repellents based on essential oils such as citronella, lemon eucalyptus, neem, and lemongrass usually achieve shorter CPT, commonly two to four hours. However, technologies such as microencapsulation and nanoemulsions improved performance in some formulations. Wearable products such as insecticide-treated clothing and spatial repellents demonstrated value as complementary measures in high-transmission settings. Synthetic topical repellents remain the most reliable option for prolonged protection, while optimized plant-based products may serve as safer alternatives for short-term or adjunctive use.

Family traditions, accessibility and cost shape the continued reliance on Cajanus cajan and Azadirachta indica for malaria and typhoid despite prescription medicines in urban and rural Nsukka, Nigeria.
Osayi EE, Urama DC, Amujiri AN, Agyo RA, Afyare AAA, Andong FA.BMC Complement Med Ther. 2026 Jun 4. doi: 10.1186/s12906-026-05426-y. PMID: 42237302

Despite the availability of conventional drugs, the use of medicinal plants for typhoid and malaria remains widespread in Nigeria. This study investigated the indigenous use of Cajanus cajan (pigeon pea) and Azadirachta indica (neem) in rural and urban Nsukka. We assessed: (i) socio-demographic factors influencing knowledge and use; (ii) the association between treatment practices and perceived efficacy; and (iii) socio-economic drivers of continued reliance on these herbal remedies. A cross-sectional survey of 400 respondents selected via stratified random sampling (200 urban, 200 rural) was conducted using structured questionnaires, where the primary outcome of this study was current herbal use, while knowledge was treated as a secondary outcome. Data were analyzed using generalized linear models (GLMs) and multinomial logistic regression (MLR) in R Statistical Software (version 4.3.0). Results indicated that rural residents relied more on

herbal remedies due to accessibility, affordability, and family traditions, while urban respondents, despite higher education levels, also used herbal extracts and often alternated them with prescription drugs. Residence, occupation, and age were significant predictors of knowledge and use ($P < 0.05$), whereas education was not. Nonetheless, perceived efficacy and high prescription costs further sustained herbal use. While these findings highlight socio-cultural and economic factors sustaining herbal medicine use, they also support the need for public health education and integration of evidence-based traditional practices into primary healthcare to ensure safer use. However, the cross-sectional design limits causal inference. Future studies should combine questionnaire-based surveys with laboratory-based assessments.

Transcriptome signature for host directed antiviral reprogramming by Nimba & Triphala in macrophage Dengue virus infection models.

Chakraborty D, Namitha R, Roy R, Devi KL.Sci Rep. 2026 Jun 5. doi: 10.1038/s41598-026-53729-4. Online ahead of print.PMID: 42243164

Dengue virus (DENV) is responsible for hundreds of millions of infections per year, but no clinically approved antiviral therapy exists, and direct-acting candidates are limited by toxicity and viral genetic diversity. Traditional medicinal preparations such as Nimba/Neem (Azadirachta indica) and polyherbal Ayurvedic preparation Triphala (a combination of Terminalia chebula, Terminalia bellirica and Phyllanthus emblica) contain multiple metabolites with antiviral and antioxidant properties but their mechanisms of action are not fully characterised. Here, we combined cell-based antiviral assays with transcriptome profiling to compare how Nimba and Triphala shape host responses during DENV infection in RAW264.7 macrophages, a key innate immune target. Nimba and Triphala demonstrated low cytotoxicity in the concentrations of our assays, which supports a favourable therapeutic window. The RNA-seq analysis showed that Nimba induced broader transcriptional reprogramming in DENV-infected macrophages than Triphala, with 4,182 differentially expressed genes in the NB + DV versus DV comparison, indicating a stronger host transcriptional impact during infection. It increased interferon-stimulated gene (Isg15) programs and attenuated inflammatory signalling (e.g., Cxcl10), oxidative stress (Txnip, Aox4, Phlda3), and endoplasmic reticulum stress pathways (Trib3) upon infection. Triphala, in contrast, caused relatively restrained baseline transcriptional reprogramming and a more selective infection-context response. Docking analysis suggested that Triphala-associated metabolites may engage multiple DENV proteins. In line with this, molecular docking of nine proteins of DENV indicated multi-target binding of Triphala metabolites, with corilagin showing favorable predicted binding affinities (ΔG -13.9 kcal/mol), in certain proteins, superior to that of reference compounds (Remdesivir and NITD008). Together, these data support broader host-response modulation by Nimba and a more selective host response with a possible virus-directed contribution for Triphala during DENV infection and lay the foundational research for synthesis of anti-viral herbal formulations using Nimba and Triphala ingredients.

Integrated in silico and in vitro assessment of Azadirachta indica leaf extract against multi-drug resistant Citrobacter koseri and Staphylococcus saprophyticus.
Shuvo MN, Arian TA, Hossain MM, Sil SK, Islam S, Shahadat MN, Rahman MH, Alam N, Shil A.Sci Rep. 2026 Jun 11. doi: 10.1038/s41598-026-51906-z. PMID: 42277134

Azadirachta indica (Neem) is well-known for its therapeutic potential against bacteria, while Staphylococcus saprophyticus and Citrobacter koseri are significant public health threats due to their potential to cause skin infections. This study aims to identify phytocompounds from the methanolic extract of A. indica leaves and evaluate their efficacy to inhibit those bacteria through in vitro and computational approaches. The bacteria were isolated from boil-derived pus, and the extract's growth-inhibitory effect was examined by the disc diffusion method. Additionally, GC-MS identified phytochemicals remaining in the extract. The pharmacokinetic and ADMET properties of those phytochemicals were assessed via PKCSM and SwissADME servers. Screened phytocompounds were docked with functional proteins using AutoDock Vina and GLIDE. Following that, molecular dynamics simulation in GROMACS, post-simulation, and DFT analysis were conducted. Five of the sixteen phytocompounds with favorable pharmacokinetics and toxicity profiles were docked with Peptidoglycan D, D-transpeptidase MrdA of Citrobacter koseri, and D-alanine--D-alanine ligase of Staphylococcus saprophyticus. Among them, 2-(Acetoxymethyl)-3-(methoxycarbonyl)biphenylene, and Cyclopropane-1-carboxamide,2-butyl-N-(5,6,7,8-tetrahydro-7,7-dimethyl-5-oxoquinazolin-2-yl)- demonstrated higher binding affinity, greater stability, and smaller energy gap in docking, simulation, and DFT analysis, respectively. This study highlights the two compounds as promising lead phytocompounds to inhibit those bacteria. Further in vivo investigations are essential to validate their therapeutic effectiveness.
Post-operative pain in molar teeth with symptomatic apical periodontitis using cryotreated **neem** extract and cryotreated 2.5% sodium hypochlorite: A randomised double-blinded clinical trial.
Vashisht R, Kumar U, Kakkar AK, Katare OP, Patil UK, Brar PK.Bioinformation. 2026 Apr 30;22(4):2701-2705. doi: 10.6026/973206300222701. eCollection 2026.PMID: 42282414

Post-operative pain following root canal treatment remains a significant clinical concern. Therefore, it is of interest to evaluate the effect of cryotherapy using sodium hypochlorite and neem extract on post-endodontic pain in 108 patients with symptomatic apical periodontitis undergoing single-visit treatment. Participants were divided into four groups: room temperature sodium hypochlorite, cryotreated sodium hypochlorite, room temperature neem extract and cryotreated neem extract and pain were assessed using the Visual Analogue Scale at 24 hours, 48 hours and 7 days. Cryotreated irrigants showed significantly lower pain scores at 24 and 48 hours compared to room temperature groups and neem extract demonstrated comparable efficacy to cryotreated sodium hypochlorite. Thus, the potential of cryotreated neem extract is shown as a biocompatible alternative irrigant for effective post-operative pain reduction.

Transparent keratin nanocomposite films incorporating silver nanoparticles and aloe vera for wound management.
Anitha S, Shivakumar S.3 Biotech. 2026 Jul;16(7):286. doi: 10.1007/s13205-026-04908-7. Epub 2026 Jun 27.PMID: 42368314

Keratin was extracted from human hair waste and incorporated with neem-mediated silver nanoparticles (AgNPs), carboxymethyl cellulose, and aloe vera to fabricate a transparent nanocomposite film. The extracted keratin exhibited a characteristic protein peak and porous morphology, while AgNPs demonstrated a surface plasmon resonance at 430-460 nm with spherical shape (< 100 nm). The fabricated film demonstrated high transparency (75.67 ± 0.57%), moderate porosity (63.38 ± 0.61%), and a high swelling ratio (818.36%), supporting moisture retention; its surface pH (5-6) and water vapor transmission rate (1799 ± 43 g/m²/day) favouring a moist healing environment, with 36.23% biodegradation over 28 days. The film showed potent bactericidal and antibiofilm properties towards *S. pyogenes*, *E. coli*, *S. aureus*, and *P. aeruginosa*, antioxidant activity (TPC 24.22 mg GAE/g, DPPH 71.31%, ABTS 63.55%), and anti-inflammatory effects (BSA 68.69%, egg albumin 92.91%, RBC 66.69%). Cytocompatibility on HaCaT and L929 cells (IC_{50} = 155 and 251 µg/mL) confirmed the film's safety and regenerative potential. Overall, the fabricated biodegradable, bioactive, and cytocompatible composite film provides a multifunctional platform for wound healing by preserving moisture, reducing inflammation and infection, and promoting the regeneration of tissue. Future studies focusing on in vivo validation and long-term biocompatibility are important to confirm the film's scalability, sustainability, and clinical applicability.

In-silico evaluation of Azadirachta indica (**neem**) against DprE1 of Mycobacterium tuberculosis with functional characterisation.
Rumide TS, Ojo AE, Golagha RO, Alake A, Suleiman ZA, Nwagbara LO, Alu OV, Olayiwola AE, Alkasim M, Sunmola A, Agbi M, Shehu AL, Okoroma B, Dabo MM, Ajayi OM, Asinmi MR.In Silico Pharmacol. 2026 Jun 20;14(2):162. doi: 10.1007/s40203-026-00666-9. eCollection 2026.PMID: 42333234

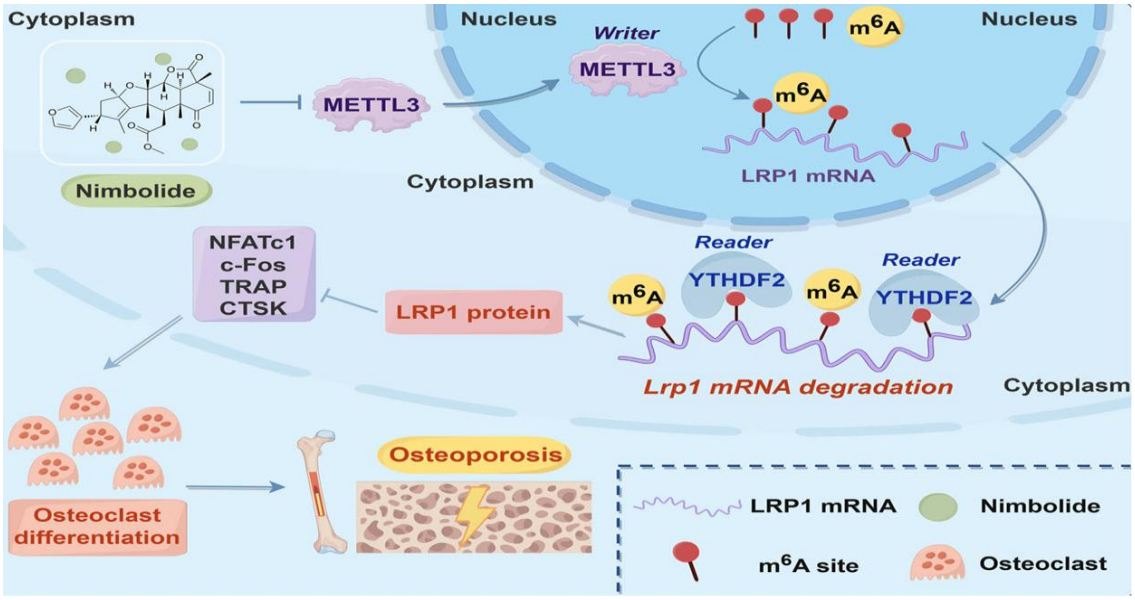
Tuberculosis remains a global health challenge, necessitating the discovery of novel inhibitors against *Mycobacterium tuberculosis*. This study investigates the potential inhibitory activity of phytochemicals from *Azadirachta indica* (Neem) against Decaprenylphosphoryl-β-D-ribose 2'-epimerase (DprE1), a validated target involved in cell wall biosynthesis. The DprE1 structure (PDB: 4FDP) and a total of 25 selected ligands of A. indica were retrieved and prepared using the Schrodinger Maestro suite. Functional enrichment and network analysis were conducted using STRING and Cytoscape. Molecular docking (Glide XP) was performed, followed by 100 ns molecular dynamics (MD) simulations using Desmond to evaluate the stability of the protein-ligand complexes. Pharmacokinetic and toxicity profiles were predicted using the pkCSM server. Network analysis supported the role of DprE1 as a key node in mycobacterial cell wall organization. Molecular docking identified Quercetin as the top-ranked candidate with a binding affinity of - 7.9 kcal/mol, comparable to the reference inhibitor BTZ043. MD simulations indicated that the DprE1-Quercetin complex maintained stable interactions, with a calculated binding

free energy (ΔG_bind) of - 51.52 kcal/mol compared to - 39.75 kcal/mol for BTZ043. Quercetin formed consistent hydrogen bond interactions with ASP318 and TYR314. ADMET predictions suggested that while BTZ043 exhibited higher intestinal absorption, Quercetin demonstrated a more favorable predicted safe compound, including the absence of AMES toxicity. Findings suggest that quercetin may serve as a promising inhibitor candidate, compared to the control inhibitor BTZ043, but requires further studies to better ascertain its efficacy as an anti-tubercular agent.

A novel METTL3 inhibitor **nimbolide** ameliorates osteoporosis via orchestrating osteoclastogenesis in an m6A-dependent manner.

Cai C, Zhang Z, Zhao X, Yang C, Huang X, Tang C, Qiu H, Yang S, Zhang Y, Hu X, Zuo R, Zhang C, Chen Y, Chu T.Phytomedicine. 2026 Jun;155:158048. doi: 10.1016/j.phymed.2026.158048. Epub 2026 Mar 7. PMID: 41865687

Osteoporosis (OP) is a prevalent chronic metabolic bone disease linked to estrogen deficiency and lacks effective therapies with minimal side effects. While N6-methyladenosine (m^6A) methylation plays a crucial role in OP progression, its critical effect on osteoclastogenesis during OP remains unclear. In this study, we demonstrate that METTL3 promotes osteoclast differentiation and bone erosion in OP, and its expression positively correlated with bone loss. METTL3 silencing abolished osteoclast formation, while its overexpression exacerbated bone resorption. Through molecular docking, dynamics simulation, cellular thermal shift assay and surface plasmon resonance assay, we identify the natural compound Nimbolide (Nim) as a direct METTL3 inhibitor that disrupts its methyltransferase activity. Nim treatment suppressed RANKL-induced osteoclastogenesis and attenuated ovariectomy-induced OP in mice. Mechanistically, multi-omics integration (RNA-seq/MeRIP-seq/RIP-seq) combined with in vitro molecular validation revealed that METTL3 installs m^6A on Lrp1 mRNA, recruiting the reader YTHDF2 to degrade transcripts and decrease the anti-osteoclastogenic protein LRP1. Nim restored LRP1 by blocking METTL3-mediated m^6A methylation, thereby inhibiting osteoclast hyperactivity. Critically, AAV9-driven METTL3 overexpression reversed Nim's efficacy in OVX mice. Our work identifies Nim as a novel METTL3 inhibitor that protects



against OP via the METTL3-m^{6}A-YTHDF2-LRP1 axis, providing novel insights into targeting METTL3-dependent m6A signaling as a promising therapeutic strategy for OP.

Computational exploration of quercetin derivatives from **Azadirachta indica** leaf as threonine tyrosine kinase inhibitors for potential lung and pancreatic cancer treatment.
Al Imran AQM, Sarker S, Priya SN, Hossain MR, Al Ashik SA.Comput Biol Chem. 2026 Jun 4;124(Pt 1):109159. doi: 10.1016/j.compbiolchem.2026.109159. PMID: 42247986

Lung and pancreatic adenocarcinomas account for substantial cancer-related mortality worldwide, with current therapeutic efficacy severely limited by the development of high drug resistance. Threonine tyrosine kinase (TTK) has emerged as both a therapeutic target and a critical prognostic marker in these malignancies, with elevated expression correlating strongly with poor clinical outcomes. Therefore, this study aimed to investigate natural quercetin derivatives from Azadirachta indica leaf as novel TTK inhibitors through comprehensive computational approaches. From initial TTK expression and survival analyses to subsequent Molecular docking, machine learning models predicted bioactivity estimation, quantum chemical calculations, molecular dynamics (MD) simulations, post-dynamics MM-PBSA calculations, and in silico toxicity profiling were performed to identify TTK inhibitors. TTK overexpression significantly correlated with diminished survival in both cancer types (hazard ratios: 1.5-2.0). Quercetin-3-rhamnoside, quercetin-3-glucoside, quercetin-3-O-galactoside, and quercetin-3-rutinoside demonstrated superior binding affinities (-9.5 to -11.089 kcal/mol) compared to control drug Luvixasertib (-8.869 kcal/mol), with enhanced electronic properties (electrophilicity index: 3.53-4.67 compared to control 2.70). Furthermore, Machine learning predictions demonstrated promising bioactivity (pIC_{50}: 6.915-7.835), while 200 ns MD simulations confirmed structural stability with optimal RMSD (1.419-2.035 Å). Subsequently, MM-PBSA calculations revealed markedly favorable binding free energies for quercetin-3-rhamnoside and quercetin-3-glucoside (-33.104 and -32.676 kcal/mol) compared to control (-28.430 kcal/mol). Additionally, toxicity profiling revealed favorable safety profiles with no hepatotoxic, carcinogenic, or mutagenic potential for most derivatives. Therefore, Quercetin derivatives from A. indica leaf represent promising lead compounds for targeted TTK inhibitors in lung and pancreatic adenocarcinomas, highlighting their potential for further experimental validation against TTK.