

Bioprospecting Wild Plants for Novel Antimicrobial Compounds with Pharmaceutical and Agricultural Value

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Abstract

The growing crisis of antimicrobial resistance (AMR) in both human medicine and agriculture necessitates the urgent discovery of new antimicrobial agents. Plants represent one of the richest sources of bioactive compounds, many of which have yet to be fully characterized. Wild plants, in particular, exhibit a unique reservoir of phytochemicals shaped by evolutionary adaptation to diverse ecological pressures such as herbivory, microbial invasion, and abiotic stress. These compounds often exhibit potent antibacterial, antifungal, antiviral, and antiparasitic activities. Bioprospecting wild flora offers a dual opportunity: addressing the urgent need for new therapeutics in human and veterinary medicine, and providing natural alternatives to chemical pesticides in agriculture. This review synthesizes recent advances in the exploration of wild plants for antimicrobial discovery, highlights key classes of phytochemicals (alkaloids, flavonoids, terpenoids, phenolics, and peptides), discusses methodologies in bioprospecting, including ethnobotany, metabolomics, and molecular docking, and examines translational pathways from discovery to commercialization. Finally, it outlines challenges and future directions in ensuring sustainable, ethical, and innovative utilization of wild plant biodiversity for antimicrobial development.

Keywords: Bioprospecting, wild plants, antimicrobial resistance, phytochemicals, natural products, drug discovery, biopesticides.

1. Introduction

The global rise of antimicrobial resistance (AMR) represents one of the most urgent threats to human health, food security, and sustainable development. The overuse and misuse of antibiotics in human medicine, veterinary practice, and agriculture have accelerated the emergence of resistant pathogens, rendering many frontline therapies ineffective. According to the World Health Organization (WHO), AMR could cause as many as 10 million deaths annually by 2050, surpassing cancer and diabetes as a leading cause of mortality. This looming crisis demands the discovery and development of new antimicrobial compounds that can act against resistant strains while minimizing collateral environmental impacts [1]. At the same time, the agricultural sector faces growing pressure to reduce reliance on synthetic pesticides and antibiotics in livestock production, both to mitigate resistance and to align with consumer demand for safer, eco-friendly practices. Against this backdrop, natural products derived from plants, particularly those from wild species, are gaining renewed attention as a sustainable and promising source of novel antimicrobial agents. Plants have co-evolved with microbial pathogens and herbivores for millions of years, resulting in the development

of sophisticated defense mechanisms. Unlike animals, plants lack an adaptive immune system and instead rely heavily on chemical defenses, producing an extraordinary array of secondary metabolites to deter or neutralize pathogens and pests. These metabolites—such as alkaloids, terpenoids, phenolics, flavonoids, and peptides—are structurally diverse and biologically optimized by evolution [2]. Many of them exert antimicrobial activity by targeting multiple cellular pathways, reducing the likelihood of resistance development. Indeed, a significant proportion of modern pharmaceuticals trace their origins to plant-derived compounds, underscoring the relevance of natural products in drug discovery. Artemisinin, derived from *Artemisia annua*, remains a cornerstone of antimalarial therapy, while morphine, quinine, and paclitaxel are other examples of the enduring contribution of plants to human medicine.

Wild plants, in particular, present an underexplored yet immensely valuable reservoir of antimicrobial compounds. Unlike domesticated crops, which have undergone genetic narrowing through selective breeding, wild species often retain broader genetic diversity and are subject to stronger ecological pressures such as drought, salinity, herbivory, and pathogen attack.

These stressors drive the synthesis of unique secondary metabolites not typically found in cultivated plants. For example, plants growing in arid deserts often produce high levels of essential oils and terpenes with antimicrobial and insect-repelling functions, while those in tropical forests may develop potent alkaloids as defenses against fungi and bacteria in humid environments [3]. The ecological and evolutionary adaptations of wild flora therefore, make them especially rich targets for bioprospecting.

Ethnobotanical knowledge provides an additional layer of insight into the antimicrobial potential of wild plants. For centuries, indigenous communities across Asia, Africa, and the Americas have relied on herbal remedies for treating infections and preserving food. This traditional knowledge often serves as a valuable guide to identifying promising candidate species for scientific investigation. For instance, extracts of wild *Azadirachta indica* (neem) have long been used in South Asia for their antibacterial and antifungal properties, later validated by laboratory studies. However, modern scientific tools such as high-throughput screening, metabolomics, and molecular docking now allow researchers to move beyond ethnobotany, systematically exploring the vast chemical diversity of wild plants with unprecedented precision and efficiency [4].

The potential applications of wild plant-derived antimicrobials extend beyond human health into agriculture. Synthetic pesticides, while effective, pose environmental risks including soil degradation, water contamination, and harm to beneficial organisms. Additionally, pathogens such as *Fusarium*, *Aspergillus*, and *Phytophthora* are developing resistance to widely used agrochemicals. Natural antimicrobials derived from wild plants can serve as eco-friendly biopesticides, reducing crop losses while maintaining soil and ecosystem health. Similarly, antimicrobial peptides and essential oils from wild flora offer alternatives for post-harvest food preservation, helping reduce spoilage and extending shelf life without chemical additives [5]. The dual relevance of plant-based antimicrobials to both pharmaceuticals and agriculture amplifies their importance in addressing the intertwined crises of AMR, food security, and environmental sustainability.

In recent years, advances in omics technologies have revolutionized the way researchers approach bioprospecting. Genomics, transcriptomics, and metabolomics allow the identification of biosynthetic pathways responsible for antimicrobial metabolites. Computational approaches such as molecular docking and machine learning accelerate the screening process, predicting interactions between plant-derived compounds and microbial targets before laboratory validation. Furthermore, synthetic biology now offers the possibility of producing complex plant compounds in microbial hosts, overcoming challenges of limited supply and sustainability associated with wild harvesting. These technological innovations are transforming bioprospecting from a largely empirical practice into a rational, data-driven science. Overharvesting of wild plants can threaten biodiversity and ecological balance. Issues of biopiracy and inequitable benefit-sharing with indigenous communities have also raised ethical concerns, underscoring the need for international frameworks such as the Nagoya Protocol to guide bioprospecting activities. Additionally, the translation of plant-derived compounds into viable commercial products involves hurdles in standardization, toxicity testing, formulation, and large-scale production [6]. Addressing these barriers requires a multidisciplinary effort involving plant biologists, chemists, pharmacologists, agricultural scientists, policymakers, and local communities, to explore the potential of wild plants as sources of novel antimicrobial compounds with dual value in pharmaceuticals and agriculture. We discuss the diversity of phytochemicals involved, highlight recent advances in bioprospecting methodologies, and examine case studies where plant-derived antimicrobials have shown promise against resistant pathogens and agricultural pests. Furthermore, we consider the challenges associated with sustainability, ethics, and commercialization, and suggest future research directions to fully harness the potential of wild flora. By bridging the knowledge of traditional medicine with modern scientific tools, bioprospecting wild plants offers a powerful strategy for discovering next-generation antimicrobial agents that are both effective and sustainable.

Table 1. Representative antimicrobial phytochemicals from wild plants and their biological activities

Phytochemical Class	Representative Compounds	Wild Plant Sources	Target Pathogens	Applications
Alkaloids	Berberine, Lupine alkaloids	<i>Berberis spp.</i> , Wild lupine (<i>Lupinus spp.</i>)	<i>Staphylococcus aureus</i> , fungal pathogens	Antibacterial, antifungal, insecticidal
Flavonoids & Phenolics	Quercetin, Catechins, Tannic acid	<i>Eucalyptus spp.</i> , <i>Terminalia spp.</i>	Gram-positive/negative bacteria	Antioxidant, antibacterial, crop protection
Terpenoids	Thymol, Carvacrol	Wild thyme (<i>Thymus vulgaris</i>), Oregano (<i>Origanum vulgare</i>)	<i>Candida albicans</i> , <i>E. coli</i> , viruses	Food preservation, biopesticide, antiviral
Tannins & Saponins	Hydrolyzable tannins, Quillaja saponins	Wild legumes, <i>Quillaja saponaria</i>	Fungal pathogens, helminths	Antifungal, anthelmintic, and immune enhancer
Antimicrobial Peptides (AMPs)	Defensins, Thionins	Wild legumes, grasses	Bacteria, fungi	Alternative antibiotics, agricultural bio-control

Table 2. Bioprospecting approaches for identifying antimicrobial compounds from wild plants

Approach	Description	Advantages	Limitations
Ethnobotanical Surveys	Documentation of traditional uses of wild plants	Culturally informed, targeted discovery	Risk of biopiracy, knowledge erosion
Metabolomics & Chemical Profiling	LC-MS, GC-MS, NMR for metabolite identification	High-throughput, precise profiling	Requires advanced instrumentation
Molecular Docking & In silico Screening	Computational binding prediction of plant metabolites to microbial targets	Cost-effective, rapid pre-screening	Predictions need wet-lab validation
High-Throughput Screening	Robotic microplate assays of extracts	Rapid testing of many samples	Resource-intensive, requires libraries
Endophyte Exploration	Screening symbiotic microbes inside plants	Expands the diversity of bioactive metabolites	Requires specialized microbial culture techniques

Table 3. Applications of wild plant-derived antimicrobials in pharmaceuticals and agriculture

Application Area	Examples	Benefits
Human Pharmaceuticals	Berberine for MDR bacteria, Thymol for fungal infections, AMPs for viral inhibition	Alternative to synthetic antibiotics, combat AMR
Veterinary Medicine	Plant saponins for deworming, essential oils for livestock infections	Reduced antibiotic use in animals
Agriculture – Biopesticides	Terpenoids against <i>Fusarium</i> , alkaloids as natural insecticides	Eco-friendly pest management
Agriculture – Post-Harvest Preservation	Essential oils (clove, thyme, oregano) for the storage of grains and fruits	Reduces spoilage, extends shelf life

2. Phytochemicals with Antimicrobial Potential from Wild Plants

Wild plants synthesize a vast repertoire of phytochemicals that serve as defensive molecules against pathogens and herbivores. These secondary metabolites not only safeguard plant survival but also provide structurally diverse scaffolds with therapeutic and agricultural value. The major classes of antimicrobial phytochemicals include alkaloids, flavonoids, terpenoids, tannins, saponins, and antimicrobial peptides [7]. Their relevance lies not only in their broad-spectrum activity but also in their relatively low risk of inducing resistance, given their tendency to act on multiple microbial pathways simultaneously.

2.1. Alkaloids

Alkaloids are nitrogen-containing compounds widely distributed in wild plants, exhibiting antibacterial, antifungal, and insecticidal activities. For instance, berberine, isolated from *Berberis* species, has demonstrated significant inhibitory effects against *Staphylococcus aureus*, including multidrug-resistant strains. Berberine acts by disrupting bacterial cell wall integrity and inhibiting efflux pumps, thereby sensitizing pathogens to conventional antibiotics. Other wild species, such as lupines, produce quinolizidine alkaloids with insecticidal properties, highlighting their dual applications in both pharmaceuticals and agriculture [8]. The structural diversity of alkaloids—ranging from indole to isoquinoline derivatives—makes them particularly valuable in the search for novel antimicrobial scaffolds.

2.2. Flavonoids and Phenolic Compounds

Flavonoids and phenolic acids represent another crucial category of bioactive molecules in wild flora. Compounds such as quercetin, catechins, and gallic acid display strong antibacterial activity by destabilizing microbial membranes, inhibiting nucleic acid synthesis, and modulating microbial enzyme activity.

Wild *Eucalyptus* species are rich in phenolics, known for their broad-spectrum antimicrobial activity, particularly against respiratory pathogens. Similarly, *Terminalia* species produce ellagic and gallic acids, which inhibit both Gram-positive and Gram-negative bacteria [9]. In addition to their antimicrobial roles, flavonoids act as antioxidants, protecting host tissues from oxidative stress during infections.

2.3. Terpenoids

Terpenoids are the largest class of plant-derived metabolites, with more than 40,000 identified structures. Wild plants such as thyme (*Thymus vulgaris*) and oregano (*Origanum vulgare*) produce thymol and carvacrol, monoterpenoids with proven antibacterial and antifungal efficacy [10]. These compounds disrupt microbial membranes by altering lipid bilayer permeability, leading to rapid cell lysis. Beyond pharmaceuticals, terpenoids serve as natural pesticides and food preservatives, offering environmentally friendly alternatives to synthetic chemicals. Other notable examples include limonene from citrus peels and azadirachtin from wild neem (*Azadirachta indica*), both widely studied for agricultural pest management.

2.4. Tannins and Saponins

Tannins and saponins represent multifunctional phytochemicals with both antimicrobial and immunomodulatory properties. Hydrolyzable tannins, abundant in wild legumes, exert antifungal effects by binding to microbial proteins and enzymes, disrupting their function. Condensed tannins also inhibit bacterial growth by chelating essential minerals such as iron. Meanwhile, saponins derived from *Quillaja saponaria* display potent antifungal and antihelminthic activities. They act by forming complexes with sterols in microbial cell membranes, resulting in pore formation and cell death. Additionally, both tannins and saponins enhance immune responses, positioning them as potential pharmaceutical adjuvants in vaccine formulations [11].

2.5. Plant-derived Antimicrobial Peptides (AMPs)

In addition to small secondary metabolites, several wild plants produce antimicrobial peptides (AMPs) as part of their innate defense system. These peptides, typically rich in cationic and hydrophobic residues, target microbial membranes, causing rapid disruption. Unlike conventional antibiotics, AMPs exert broad-spectrum effects while minimizing resistance development. For example, defensins and thionins from wild species have been investigated for activity against fungi such as *Candida albicans* and bacteria such as *Escherichia coli* [12]. Their small size, high potency, and stability make them attractive candidates for both medical and agricultural applications.

3. Bioprospecting Approaches for Wild Plants

Bioprospecting for novel antimicrobials in wild plants requires a combination of traditional knowledge, modern analytical techniques, and innovative discovery platforms. This multidisciplinary approach ensures efficient identification, isolation, and characterization of bioactive compounds with pharmaceutical and agricultural potential [13].

3.1. Ethnobotanical Surveys

Ethnobotanical studies provide an invaluable starting point by documenting traditional uses of wild plants in local healthcare practices. Communities across Asia, Africa, and South America have long relied on herbal remedies to treat infections, and many such plants have later been scientifically validated. For instance, ethnobotanical research on wild *Azadirachta indica* guided investigations into azadirachtin, now widely used as a biopesticide. Integrating indigenous knowledge with modern screening accelerates the identification of promising species for antimicrobial discovery [14].

3.2. Metabolomics and Chemical Profiling

Recent advances in metabolomics enable comprehensive profiling of plant metabolites, offering insights into their chemical diversity. Techniques such as liquid chromatography–mass spectrometry (LC-MS), nuclear magnetic resonance (NMR), and gas chromatography–mass spectrometry (GC-MS) allow high-throughput identification of bioactive compounds [15]. These methods not only streamline the discovery of novel antimicrobials but also support comparative analyses between domesticated and wild species, revealing unique phytochemicals enriched in wild plants.

3.3. Molecular Docking and Computational Biology

Computational biology plays a transformative role in modern bioprospecting. Molecular docking predicts interactions between plant-derived compounds and microbial targets such as bacterial topoisomerases or fungal ergosterol synthesis enzymes. This in silico screening significantly reduces experimental costs by prioritizing the most

promising candidates for in vitro validation. Integration with machine learning further enhances predictive power, enabling the discovery of antimicrobial mechanisms and structure–activity relationships [16].

3.4. High-Throughput Screening

The use of robotics and microplate-based assays allows simultaneous testing of hundreds of plant extracts against multiple microbial pathogens. Such high-throughput screening platforms provide rapid assessments of antimicrobial activity, enabling researchers to identify compounds effective against multidrug-resistant bacteria, fungi, and viruses [17]. These approaches are critical in scaling up the search for plant-derived antimicrobials and accelerating their progression to preclinical development.

3.5. Endophyte Exploration

Endophytes—microorganisms that live symbiotically within plant tissues—represent an often-overlooked source of antimicrobial metabolites. Many endophytes share biosynthetic pathways with their host plants, producing similar or complementary compounds. For example, endophytic fungi isolated from wild medicinal plants have yielded antimicrobial metabolites effective against resistant bacterial strains [4]. Exploring the plant–endophyte holobiont therefore, broadens the chemical space available for discovery and reduces the pressure on wild plant harvesting.

4. Applications of Wild Plant Antimicrobials

The discovery and characterization of antimicrobial compounds from wild plants offer diverse applications across human health and agriculture. Their dual pharmaceutical and agricultural potential is particularly important in the era of rising antibiotic resistance and increasing demand for sustainable farming practices.

4.1. Pharmaceutical Applications

Wild plant-derived antimicrobials are emerging as critical alternatives to synthetic antibiotics in tackling multidrug-resistant (MDR) pathogens.

- **Treatment of multidrug-resistant infections:** Compounds such as berberine, eugenol, and flavonoid derivatives have demonstrated activity against *methicillin-resistant Staphylococcus aureus* (MRSA), *vancomycin-resistant Enterococci* (VRE), and *Mycobacterium tuberculosis* strains resistant to first-line drugs. These natural molecules often act through multiple mechanisms, reducing the likelihood of resistance development.
- **Antifungal therapies:** Opportunistic fungal infections, especially in immunocompromised patients (e.g., HIV/AIDS, organ transplant recipients), are increasingly problematic.

Plant-derived phenolics, terpenoids, and saponins have shown strong efficacy against *Candida albicans*, *Aspergillus fumigatus*, and dermatophytic fungi.

- **Antiviral potential:** Wild plants also serve as sources of antiviral agents. Extracts containing flavonoids, alkaloids, and essential oils have been reported to inhibit influenza virus replication, block HIV entry into host cells, and show promise against coronaviruses and emerging zoonotic viruses [7]. The structural novelty of these compounds provides unique scaffolds for drug development, especially as synthetic modifications can further optimize their bioactivity and pharmacokinetics.

4.2. Agricultural Applications

In agriculture, wild plant antimicrobials align with the global push for eco-friendly pest and disease management.

- **Biopesticides against crop pathogens:** Essential oils and phenolic compounds derived from wild plants have shown efficacy against common fungal pathogens such as *Fusarium oxysporum* and *Aspergillus flavus*. These natural biopesticides reduce reliance on chemical fungicides, thereby lowering environmental contamination and health risks.
- **Natural insecticides:** Alkaloids and terpenoids from wild species such as *Azadirachta indica* (neem) and wild lupines exhibit insecticidal and insect-deterrent properties. Unlike conventional pesticides, they degrade rapidly in the environment and pose minimal risk of bioaccumulation.
- **Post-harvest preservation:** Essential oils from wild thyme, oregano, and clove are effective against microbial spoilage of stored grains, fruits, and vegetables [8]. Their integration into packaging materials or coatings offers a sustainable strategy for extending shelf life and reducing food waste. Together, these applications illustrate the versatility of wild plant antimicrobials in addressing both public health challenges and food security concerns.

5. Challenges in Bioprospecting Wild Plants

Despite their promise, translating wild plant antimicrobials from discovery to practical application faces multiple challenges.

- **Biodiversity loss:** Rapid deforestation, urbanization, and climate change threaten wild habitats, reducing access to unique plant species that may harbor valuable metabolites. Many candidate species risk extinction before their potential is even explored.
- **Sustainability concerns:** Overharvesting wild plants for research or commercial extraction poses ecological risks.

Rare and slow-growing species may be particularly vulnerable, necessitating sustainable collection practices or ex situ cultivation.

- **Biopiracy and intellectual property issues:** Unequal access to traditional knowledge and unfair exploitation of indigenous practices remain significant ethical barriers. The lack of transparent benefit-sharing undermines trust between researchers and local communities.
- **Variability in phytochemical composition:** Environmental factors such as soil type, climate, seasonality, and geography influence phytochemical profiles, making it difficult to standardize extracts for consistent efficacy.
- **Barriers to translation:** Moving from laboratory discovery to clinical or field application requires extensive toxicological testing, large-scale production, and regulatory approval. This process is resource-intensive and often discourages investment in natural product research [9]. These challenges highlight the need for integrative strategies combining conservation, advanced screening methods, and ethical frameworks for sustainable and equitable bioprospecting.

6. Future Perspectives

The future of wild plant antimicrobial research lies at the intersection of traditional knowledge, cutting-edge technologies, and global cooperation. Several emerging directions stand out:

- **Artificial intelligence and predictive screening:** The integration of AI with phytochemical and ethnobotanical databases can accelerate the discovery pipeline by predicting bioactive structures and identifying underexplored plant families [6]. Machine learning-driven structure–activity relationship models may guide rational selection of plant candidates for antimicrobial screening.
- **Synthetic biology and metabolic engineering:** Advances in genetic engineering allow the biosynthesis of plant-derived antimicrobials in microbial or yeast hosts, ensuring large-scale production without overharvesting wild plants. This approach has already been successful in producing compounds like artemisinin (antimalarial) and can be extended to antimicrobial alkaloids, flavonoids, and peptides [4].
- **Development of multi-target antimicrobials:** Single-target drugs are prone to resistance, whereas plant-derived compounds often act on multiple microbial pathways. Future research should focus on harnessing and optimizing these multi-target effects, particularly in drug-resistant pathogens.

- **Strengthening global policies:** Frameworks such as the Nagoya Protocol on Access and Benefit-Sharing should be reinforced to ensure equitable sharing of benefits between researchers, industries, and indigenous communities. International collaboration is essential to balance conservation with innovation [3].
- **Community-based conservation and cultivation:** Promoting the cultivation of wild medicinal plants in community-based programs not only conserves biodiversity but also provides economic opportunities for local populations, creating a sustainable supply chain for antimicrobial research [12].

7. Conclusion

Bioprospecting wild plants represents a frontier in the search for novel antimicrobial agents at the interface of human health, agriculture, and biodiversity conservation. Unlike domesticated or widely cultivated species, wild plants have evolved under diverse ecological pressures, leading to unique structural and functional adaptations in their secondary metabolites. These compounds—ranging from alkaloids and flavonoids to terpenoids and antimicrobial peptides—demonstrate potent activities against bacteria, fungi, viruses, and agricultural pests. Their dual applicability in pharmaceuticals and sustainable agriculture positions them as valuable tools to combat two of the most pressing global challenges: antimicrobial resistance (AMR) and food security. Unlocking this potential requires navigating a complex set of challenges. Biodiversity loss and habitat degradation threaten the very reservoirs of chemical diversity we aim to study. Overharvesting, if unmanaged, can compromise ecosystem stability and push rare species toward extinction. Ethical dilemmas, including biopiracy and inequitable use of traditional knowledge, further complicate research and development pathways. Variability in phytochemical composition across geographical and seasonal scales also makes standardization and commercialization difficult; recent advances offer pathways forward. Metabolomics and high-throughput chemical profiling now enable systematic exploration of plant metabolomes with unprecedented depth. Computational tools, including artificial intelligence and molecular docking, accelerate the identification of lead compounds, while synthetic biology provides scalable production platforms that reduce dependency on wild harvests. At the same time, global frameworks such as the Nagoya Protocol emphasize the importance of equitable access and benefit-sharing, ensuring that conservation and community rights remain central to innovation, a multidisciplinary, ethically guided, and sustainability-focused approach is critical. Integrating traditional knowledge with modern science, fostering collaboration between pharmacology, agriculture, and ecology, and promoting conservation alongside commercialization can transform wild plants into reliable sources of next-generation antimicrobials.

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