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Review Article

Bioactive Compounds of Medicinal Plants: Structure, Function, and Bioactivity

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Abstract: Medicinal plants harbour a diverse array of bioactive compounds that contribute to their therapeutic potential and pharmacological diversity. These compounds include phenolics, alkaloids, terpenoids, flavonoids, tannins, steroids, glycosides, and lignans, which demonstrate various biological activities such as antioxidant, antimicrobial, anti-inflammatory, anticancer, and neuroprotective properties. This review provides a comprehensive overview of the main classes of phytochemicals, highlighting their structural characteristics, dual function, and therapeutic significance. Recent studies offer valuable insights into how these molecules interact with cellular pathways, paving the way for new opportunities in drug discovery and biomedical research.

Keywords: Bioactive compounds, medicinal plants, natural products chemistry, structure–function relationship, therapeutic applications

Introduction

Medicinal plants have been a vital part of human healthcare since ancient civilizations, serving as the primary source of therapeutic agents for both traditional and modern medicine. Their curative potential comes from a diverse range of secondary metabolites, which function as defensive and signalling molecules in plants and serve as bioactive compounds with pharmacological significance for humans. These compounds include phenolics, alkaloids, terpenoids, flavonoids, steroids, and glycosides, all of which exhibit diverse biological activities such as antioxidant, anti-inflammatory, antimicrobial, anticancer, and neuroprotective effects. Recent advances in analytical chemistry, molecular biology, and metabolomics have enhanced our understanding of their structure-function relationships, bioavailability, and mechanisms of action (Rahman et al., 2021; Costa et al., 2022). Despite remarkable progress in synthetic drug discovery, modern therapeutics face major challenges, including drug resistance, adverse side effects, and limited efficacy against complex, multifactorial diseases. The study of plant-derived bioactive compounds has recently gained significant scientific attention due to their multitarget actions, enhanced biocompatibility, and reduced toxic effects compared to synthetic alternatives. Additionally, investigating phytochemicals creates an opportunity to bridge traditional medicinal wisdom with modern pharmacology, facilitating the discovery of novel compounds for emerging health challenges. India, with one of the richest floral biodiversity in the world, possesses an extensive range of medicinal plants traditionally used in Ayurveda, Siddha, Unani, and folk healing systems. Notable Indian species such as *Curcuma longa* (turmeric), *Azadirachta indica* (Figure 1A), *Ocimum sanctum*, and *Phyllanthus emblica* (Figure 1B), *Withania somnifera* (Figure 1C), *Rauvolfia serpentina* (Figure 1D) are recognized for their potent bioactive compounds and proven therapeutic efficacy. These plants not only enhance the country's ethnomedicinal heritage but also serve as a valuable resource for global pharmaceutical research aimed at developing safe and effective natural drugs. Given this context, the present study aims to document and analyze the bioactive compounds of these medicinal plants, their chemical diversity, structure and function relationships, as well as their biological significance, based on comprehensive literature reviews (Kumar, 2025). The research is important as it consolidates scattered information into a structured overview, highlighting key plant-derived compounds and their pharmacological roles. Such documentation will assist in identifying potential lead molecules for drug discovery, promote the sustainable use of India's medicinal plant wealth, and guide future research in natural product chemistry and pharmacognosy.

Classification and functional diversity of bioactive compounds

Bioactive molecules found in medicinal plants are structurally diverse and functionally dynamic. Table 1 provides a summary of the main groups of phytochemicals, their pharmacological potentials, and relevant literature.

Phenolic compounds: Phenolic compounds represent a broad category of plant metabolites known for their antioxidant and anti-inflammatory properties. They play a role in scavenging reactive oxygen species, regulating enzymatic systems, and modulating inflammatory signalling (Rahman et al., 2021).

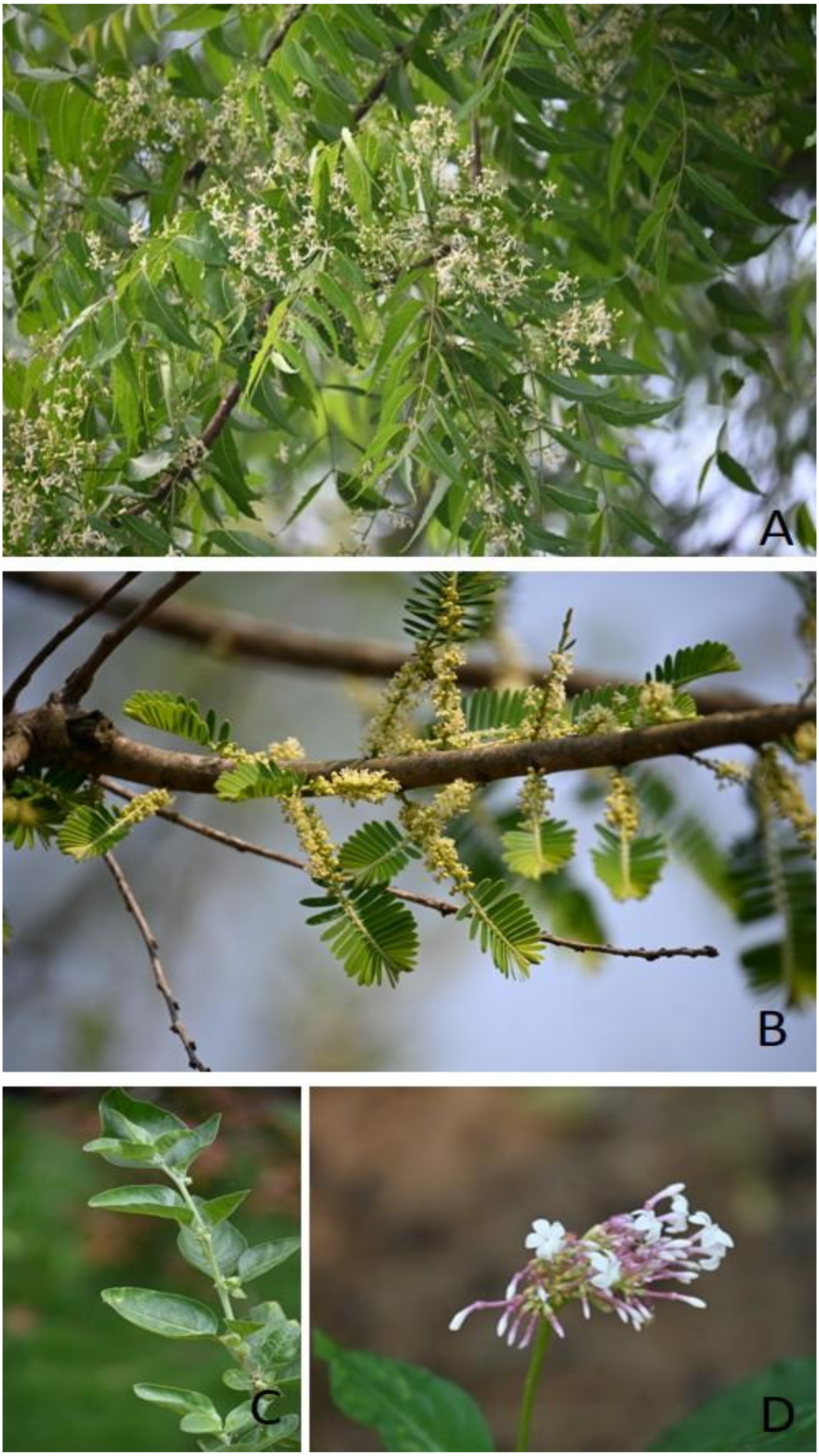

Figure 1: Habit of A) *Azadirachta indica*, B) *Phyllanthus emblica*, C) *Withania somnifera* and D) *Rauvolfia serpentina*

Their therapeutic applications include the management of neurodegenerative disorders, cancer, cardiovascular diseases, and skin conditions. Table 2 lists notable phenolic compounds such as caffeic acid, curcumin, ferulic acid, and resveratrol, highlighting their unique mechanisms in disease prevention.

Tannins: Tannins have been shown to possess antimutagenic, antioxidative, and anticarcinogenic properties (Chung et al., 1998). Their ability to bind proteins and metals contributes to their protective effects against metabolic and cardiovascular disorders. Additionally, tannins show potential in weight management and anti-nociceptive functions (Cosme et al., 2025).

Saponins: Saponins are glycosidic compounds with amphiphilic structures, which give them their surface-active properties. These compounds demonstrate various beneficial effects, including antimicrobial, antiparasitic, antiviral, and cholesterol-lowering activities (Timilsena et al., 2023). Their ability to inhibit tumour proliferation and angiogenesis suggests potential applications in cancer therapy.

Terpenoids: Terpenoids form the largest group of natural products and are synthesised through the mevalonate and methylerythritol phosphate (MEP) pathways. They serve various functions, including antimicrobial, anti-tumour, and wound-healing properties, while also playing ecological roles as attractants or repellents (Masyita et al., 2022). As shown in Table 3, compounds such as andrographolide, β-elemene, and linalool demonstrate significant pharmacological effects, including cell cycle regulation and induction of apoptosis.

Steroids: Plant steroids, also known as phytosterols, exhibit anti-inflammatory, neuroprotective, and immunomodulatory properties (Costa et al., 2022). Their derivatives are actively being researched for anticancer and antidiabetic drug development, primarily due to their structural similarity to endogenous hormones (Hajdaś et al., 2025).

Alkaloids: Alkaloids are nitrogen-containing compounds recognized for their significant neurological, cardiovascular, and antimicrobial effects. They interact with various physiological pathways, affecting enzyme activity and receptor function (Heinrich et al., 2021). Table 4 lists pharmacologically important alkaloids, including morphine (an analgesic), quinine (an antimalarial), and galantamine (used in the treatment of Alzheimer’s disease). Their wide therapeutic range, which extends from pain relief to neuroprotection, makes them invaluable in modern pharmacology (Aryal et al., 2022).

Flavonoids and lignans: Flavonoids serve as powerful antioxidants, promoting cardiovascular and hepatic protection (Kumar and Pandey, 2013). Their antiviral properties against herpes and rabies viruses indicate their potential in medicine. Similarly, lignans exhibit immunosuppressive, antioxidant, and anticancer effects (Osmakov et al., 2022).

Carotenoids, glycosides, and reducing sugars: Carotenoids improve skin health, vision, and immune response by acting as powerful antioxidants (Bas, 2024). Glycosides possess analgesic and antioxidant properties, often serving as precursors to other active molecules (Johnson et al., 2021).

Though primarily metabolic intermediates, reducing sugars also play regulatory roles in plant stress responses and signalling (Khatri & Chhetri, 2020).

Structure-function relationship

The biological function of these compounds is closely related to their molecular structures. For instance, the hydroxyl groups in phenolics provide radical scavenging capabilities, while the nitrogen heterocycles in alkaloids interact with neural receptors. Terpenoids, characterised by their isoprene-based structures, demonstrate membrane-permeable properties, enabling a range of pharmacological interactions. Understanding these structural details is crucial for designing drugs and making synthetic modifications that enhance efficacy and bioavailability.

Mechanisms of bioactivity

Bioactive compounds exert therapeutic effects through several mechanisms:

1. Antioxidant defence: They neutralise reactive oxygen species (ROS) and inhibit lipid peroxidation.
2. Anti-inflammatory action: They downregulate cytokines such as tumour necrosis factor-alpha (TNF-α) and interleukin-6 (IL-6), and inhibit nuclear factor kappa-light-chain-enhancer of activated B cells (NF-κB) pathways.
3. Antimicrobial effects: They disrupt microbial membranes and interfere with enzyme systems.
4. Neuroprotection: They modulate neurotransmitter systems and reduce neuronal apoptosis.
5. Anticancer potential: They induce apoptosis, inhibit angiogenesis, and interfere with cell cycle progression.

These mechanisms highlight their role as multi-target natural therapeutics that can address complex diseases.

Pharmacological and clinical significance

The pharmacological spectrum of plant bioactive compounds includes their effectiveness against infectious diseases, metabolic syndromes, and neurodegenerative disorders. Compounds such as curcumin, quercetin, resveratrol, and andrographolide have transitioned from laboratory research to clinical trials, thanks to their low toxicity and high efficacy. Additionally, the synergistic effects of multiple phytochemicals found in plant extracts can enhance therapeutic outcomes, a benefit often overlooked in single-compound synthetic drugs.

Table 1: Bioactive compounds obtained from medicinal plants and their therapeutic effects

Bioactive compound(s)	Potential	Sources
Phenolic compounds	Anti-inflammatory drugs	Rahman et al., (2021)
	Hypertension	Rahman et al., (2021)

	Metabolic problems	Rahman et al., (2021)
	Incendiary infections	Rahman et al., (2021)
	Neurodegenerative diseases	Rahman et al., (2021)
	Alzheimer's disease	Rahman et al., (2021)
	Skin diseases	Rahman et al., (2021)
	Rheumatoid arthritis	Rahman et al., (2021)
	Inflammatory bowel disease	Rahman et al., (2021)
	Anticancer	Rahman et al., (2021)
	Anti-aging	Rahman et al., (2021)
	Antibacterial	Rahman et al., (2021)
	Antiviral activities	Rahman et al., (2021)
	Allergy-related diseases	Rahman et al., (2021)
Tannin	Anticarcinogenic	Chung et al., (1998)
	Antimutagenic	Chung et al., (1998)
	Antioxidative	Chung et al., (1998)
	Antimicrobial	Chung et al., (1998)
	Cardiovascular disease	Cosme et al., (2025)
	Diabetes	Cosme et al., (2025)
	Weight management	Cosme et al., (2025)
	Anti-nociceptive	Fraga-Corral et al., (2021)
Saponin	Anti-inflammatory	Timilsena et al., (2023)
	Antimicrobial	Timilsena et al., (2023)
	Antiviral	Timilsena et al., (2023)
	Antiparasitic	Timilsena et al., (2023)
	Inhibit tumour cell proliferation	Timilsena et al., (2023)
	Suppress angiogenesis	Timilsena et al., (2023)
	Reduction in blood cholesterol levels	Timilsena et al., (2023)
	Antimicrobial	Timilsena et al., (2023)
	Antiprotozoal effects	Timilsena et al., (2023)
Terpenoids	Anti-malarial	Masyita et al., (2022)
	Anxiolytic	Masyita et al., (2022)
	Anaesthetic	Masyita et al., (2022)
	Anti-tumor	Masyita et al., (2022)
	Anti-inflammatory	Masyita et al., (2022)
	Antimicrobial	Masyita et al., (2022)
	Antiallergic	Masyita et al., (2022)
	Anticancer activity	Masyita et al., (2022)
	Wound healing	Masyita et al., (2022)

	Asthma	Masyita et al., (2022)
	Gastric ulcer	Masyita et al., (2022)
Steroids	Anti-inflammatory	Costa et al., (2022)
	Neuroprotective activity	Costa et al., (2022)
	Antidiabetic	Hajdaś et al., (2025)
	Immunomodulatory properties	Hajdaś et al., (2025)
	Anticancer activity	Gomes et al., (2023)
Alkaloids	Antibacterial activity	Adamski et al., (2020)
	Antiviral	Thawabteh et al., (2019)
	Antimutagenic	Thawabteh et al., (2019
	Anticarcinogenic	Thawabteh et al., (2019
	Antimicrobial agents	Thawabteh et al., (2019
	Anticonvulsant	Thawabteh et al., (2019
	Analgesic	Thawabteh et al., (2019
	Antifungal	Thawabteh et al., (2019
	Anthelmintic	Thawabteh et al., (2019
	Anti-inflammatory	Thawabteh et al., (2019
	Anti-bacterial and cardiotonic	Thawabteh et al., (2019
	Reduce fever	Heinrich et al., (2021)
	Peptic ulcers	Heinrich et al., (2021)
	Relieves intestinal colic	Heinrich et al., (2021)
	Decongestant	Heinrich et al., (2021)
	Angina treatment	Heinrich et al., (2021)
	Uterine contraction agents	Heinrich et al., (2021)
	Altitude sickness treatment	Heinrich et al., (2021)
	Antirheumatic	Heinrich et al., (2021)
	Parkinson's disease treatment	Heinrich et al., (2021)
	Myasthenia gravis treatment	Heinrich et al., (2021)
	Treatment of traumatic injuries to the nervous system	Heinrich et al., (2021)
	Treatment for depression	Heinrich et al., (2021)
	Hypertension	Heinrich et al., (2021)
Flavonoids	Coronary heart disease prevention	Kumar and Pandey, (2013)
	Hepatoprotective	Kumar and Pandey, (2013)
	Anti-inflammatory	Kumar and Pandey, (2013)
	Anticancer activities	Kumar and Pandey, (2013)
	Antiviral activities	Kumar and Pandey, (2013)
	Parkinson's disease	Kumar and Pandey, (2013)
	Treatment of hypertension	Kumar and Pandey, (2013)

	Flavonoids protect lipids against oxidative damage	Kumar and Pandey, (2013)
	Antioxidant activity	Kumar and Pandey, (2013)
	Hapato-protective activities	Kumar and Pandey, (2013)
	Antibacterial Activity	Kumar and Pandey, (2013)
	Herpes simplex virus	Kumar and Pandey, (2013)
	Rabies virus	Kumar and Pandey, (2013)
Lignans	Anti-inflammatory	Osmakov et al., (2022)
	Antioxidant effects	Osmakov et al., (2022)
	Antimicrobial	Saleem et al., (2005)
	Immunosuppressive activities	Saleem et al., (2005)
	Anticancer	Saleem et al., (2005)
Carotenoids	Skin health	Bas, (2024)
	Improving defense against ultraviolet (UV) radiation	Bas, (2024)
	Diabetes	Bas, (2024)
	Cancer	Bas, (2024)
	Inflammation	Bas, (2024)
	Quality of vision	Bas, (2024)
	Antioxidant	Bas, (2024)
	Immune function	Bas, (2024)
	Promoting cardiovascular wellness	Bas, (2024)
Glycosides	Antioxidant activity	Johnson et al., (2021)
	Reserve pool of precursors of more bioactive compounds	Johnson et al., (2021)
	Analgesic potential	Khan et al., (2020)
Reducing Sugars	Triggers oxidative modification and apoptosis in pancreatic beta-cells by provoking oxidative stress	Kaneto et al., (1996)
	Pivotal role in plants as both nutrients and central signalling or regulatory molecules that modulate gene expression related to plant growth, development, metabolism, stress response, and disease resistance.	Khatri and Chhetri, (2020)

Table 1 provides a comprehensive overview of the diversity, multifunctionality, and therapeutic spectrum of bioactive compounds derived from medicinal plants. These phytoconstituents include phenolics, tannins, saponins, terpenoids, steroids, alkaloids, flavonoids, lignans, carotenoids, glycosides, and reducing sugars, all of which form the biochemical basis of traditional and modern plant-based medicine. Their varied structures contribute to a wide pharmacological versatility, which allows them to target many different physiological and pathological processes.

Table 2: Phenolic compounds reported from medicinal plants and their therapeutic activities

Compound(s)	Plant or Group Source	Functions	Source(s)
Caffeic Acid	*Symphytum officinale*	Anti-inflammatory activity	Sun and Shahrajabian, (2023)
Coumarins	*Angelica dahurica*	Anticancer agent	Sun and Shahrajabian, (2023)
Curcumin (Figure 2)	*Curcuma zedoaria*	Anti-inflammatory actions for drug repurposing in traumatic brain injury	Sun and Shahrajabian, (2023)
Curcuminoids	*Curcuma longa*	Alzheimer's disease	Sun and Shahrajabian, (2023)
Esculetin	*Artemisia scoparia*	Neurological disorders	Sun and Shahrajabian, (2023)
Ferulic acid	*Angelica sinensis*	Anti-apoptosis	Sun and Shahrajabian, (2023)
Gallic acid	*Emblica officinalis*	Antidiabetic potential	Sun and Shahrajabian, (2023)
Hydroxycinnamic acid	Cereals	Antioxidant	Sun and Shahrajabian, (2023)
Piceatannol	*Passiflora edulis*	Treatment of Leukaemia	Sun and Shahrajabian, (2023)
Proanthocyanidins	*Pinus thunbergii*	Diabetes, asthma, neuropathologies, cardiovascular ailments, obesity, and cancer	Sun and Shahrajabian, (2023)
Protocatechuic acid	*Hibiscus sabdariffa*	Neuroprotective activities	Sun and Shahrajabian, (2023)
Pterostilbene	*Vitis vinifera*	Anticancer	Sun and Shahrajabian, (2023)
Quercetin	*Allium cepa*	Anticancer Properties	Veiga et al., (2022)
Resveratrol	*Rheun rhapontiicum*	Cardiovascular diseases	Sun and Shahrajabian, (2023)

Scopoletin	*Convolvulus prostrates*	Antioxidative properties	Sun and Shahrajabian, (2023)
Stilbenes	Dipterocarpaceae	Antiviral	Sun and Shahrajabian, (2023)
Umbelliferone	*Artemesia tridentata*	Anti-inflammatory	Sun and Shahrajabian, (2023)

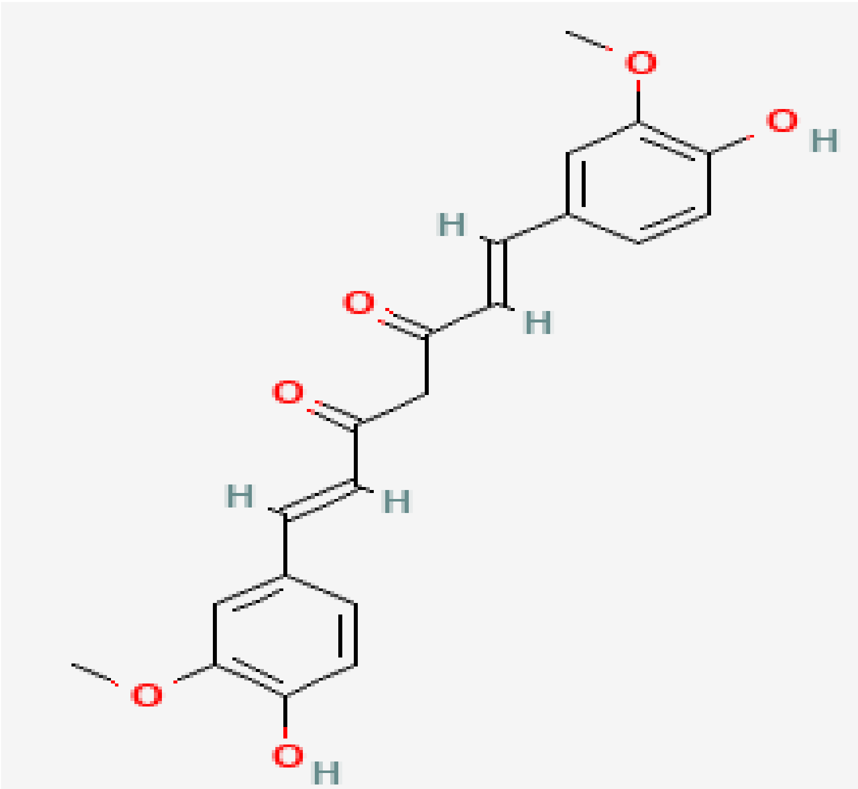

Figure 2: Structure of Curcumin (Source: PubChem)

The data presented in Table 2 indicate that phenolic compounds derived from medicinal plants exhibit a wide range of therapeutic activities, with a primary focus on antioxidant, anti-inflammatory, and anticancer properties. Compounds such as caffeic acid, curcumin, gallic acid, and scopoletin exhibit strong antioxidative and anti-inflammatory effects, which are crucial for reducing oxidative stress, a central factor in chronic and degenerative diseases. These compounds function through various mechanisms, including the inhibition of inflammatory mediators, enhancement of cellular antioxidant defence systems, and modulation of important signalling pathways such as NF-κB and Nrf2. Their structural characteristics, particularly hydroxyl and methoxy substitutions, allow them to neutralize reactive oxygen species and stabilise free radicals, thereby maintaining cellular homeostasis. Additionally, a notable trend in the table is the diverse pharmacological spectrum of phenolic compounds, which encompasses applications in metabolic, neurological, and oncological applications.

Curcuminoids and protocatechuic acid, for example, exhibit neuroprotective potential against Alzheimer’s and other neurological disorders. Similarly, coumarins, quercetin, and pterostilbene are recognized as potent anticancer agents, acting through mechanisms such as apoptosis induction and cell-cycle arrest. Additionally, compounds like gallic acid and proanthocyanidins display antidiabetic and cardioprotective effects by regulating glucose metabolism and enhancing vascular function. The repeated presence of compounds like resveratrol and quercetin across various disease models highlights their pleiotropic nature, allowing them to affect interconnected biological systems, including inflammation, oxidative stress, and cell signalling. Overall, the findings highlight that phenolic compounds constitute the biochemical foundation of plant-based pharmacology, offering multi-target therapeutic benefits with relatively low toxicity. Their wide presence in medicinal and dietary plants such as *Curcuma longa*, *Emblica officinalis*, *Allium cepa*, and *Vitis vinifera* suggests immense potential for the development of nutraceuticals and pharmaceuticals. However, challenges such as poor bioavailability and stability hinder their clinical translation. Therefore, future research should concentrate on improving delivery systems, exploring the synergistic effects among phenolic compounds, and validating their efficacy through mechanistic and clinical studies to establish their role as reliable natural therapeutics in modern medicine.

Table 3: Terpenoids reported from medicinal plants and their activities

Compound	Plant Source	Potential	Source(s)
Andrographolide	*Andrographis paniculata*	Cell cycle arrest and apoptosis	Câmara et al., (2024)
A-pinene	*Eucalyptus grandis*	Attractant to pests	Câmara et al., (2024)
Eugenol (Figure 3)	*Syzygium aromaticum*	Toxic and repellent effects	Câmara et al., (2024)
Linalool	*Ficus hispida*	Signalling pollinators	Câmara et al., (2024)
Triterpenoid	*Saccharomyces cerevisiae*	Antifungal agent	Câmara et al., (2024)
α-Thujone	*Thuja occidentalis*	Induction of cell death, reduced proliferation and invasiveness	Câmara et al., (2024)
β-elemene	*Curcuma wenyujin*	β-elemene-derived antitumor drug	Câmara et al., (2024)
B-ocimene	*Solanum lycopersicum*	Attractant to parasitoids and defense against pests	Câmara et al., (2024)

The results presented in Table 3 highlight the significant structural and functional diversity of terpenoids derived from medicinal plants, emphasizing their ecological and pharmacological importance. Compounds such as andrographolide, α-thujone, and β-elemene demonstrate potent anticancer and cytotoxic properties through mechanisms such as cell cycle arrest, induction of apoptosis, and inhibition of tumour invasiveness, indicating their potential in cancer therapy. On the other hand, terpenoids such as α-pinene, linalool, and β-ocimene serve important ecological functions. These compounds act as semiochemicals that facilitate plant–insect interactions by attracting pollinators, deterring pests, or recruiting parasitoids, thereby contributing to natural pest management.

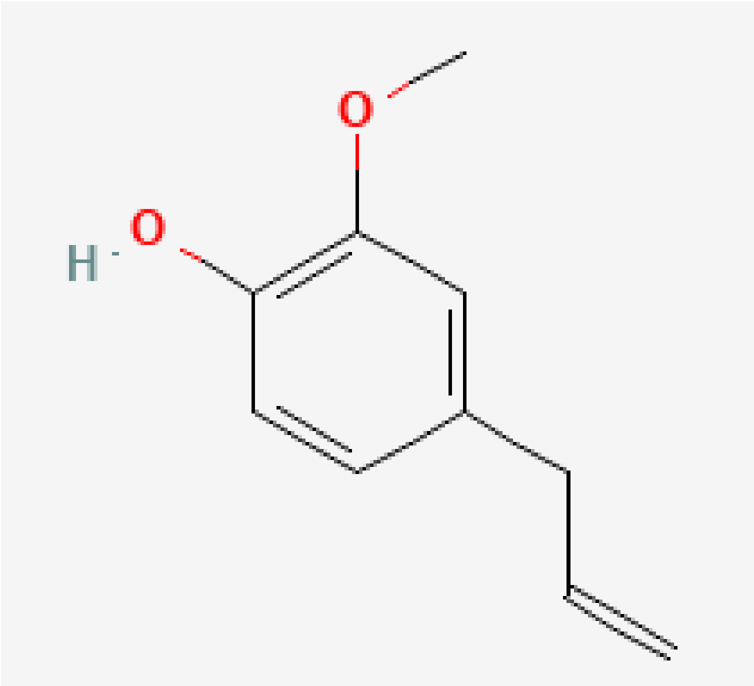

Figure 3: Structure of Eugenol (Source: PubChem)

Table 4: Alkaloids reported from medicinal plants and their activity

Compound	Plant Source	Pharmacological Effect	Source
Aconitine	*Aconitum napellus*	Rheumatism	Heinrich et al., (2021)
Ajmaline	*Rauvolfia serpentina* (Figure 1D)	Hypertension	Heinrich et al., (2021)
Aloperine	*Sophora alopecuroides*	Neurodegenerative diseases	Aryal et al., (2022)
Atropine (Figure 4)	*Atropa bella-donna*	Antispasmodic	Heinrich et al., (2021)

Berberine	*Berberis vulgaris*	Eye irritations; Immunomodulatory effects	Heinrich et al., (2021); Aryal et al., (2022)
Boldine	*Lindera aggregata*	Constipation	Heinrich et al., (2021)
Caffeine	*Theobroma cacao*	Hypertension treatment	Heinrich et al., (2021)
Cathine	*Catha edulis*	Psychostimulatory effects	Heinrich et al., (2021)
Cinchonidine	*Cinchona tucujensis*	Malaria treatment	Heinrich et al., (2021)
Cocaine	*Erythroxylum coca*	Altitude sickness treatment	Heinrich et al., (2021)
Diethanolamine	*Schinopsis balansae*	Used in dermatological products	Heinrich et al., (2021)
Ergometrine	*Claviceps purpurea* var. *purpurea*	Migraine treatment	Heinrich et al., (2021)
Galantamine	*Galanthus woronowii*	Alzheimer's disease	Aryal et al., (2022)
Harmine	*Peganum harmala*	Treating inflammation	Aryal et al., (2022)
Morphine	*Papaver somniferum*	Pain relief	Heinrich et al., (2021)
Oxymatrine	*Sophora flavescentis*	Cardiovascular protective properties	Aryal et al., (2022)
Quinine	*Cinchona officinalis*	Myotonic disorders	Heinrich et al., (2021)
Sinomenine	*Sinomenium acutum*	Rheumatoid arthritis	Aryal et al., (2022)
Vinblastine	*Catharanthus roseus*	Hypoglycaemic agent	Heinrich et al., (2021)
Vincamine	*Vinca minor*	Arteriosclerosis	Heinrich et al., (2021)

Eugenol and triterpenoids demonstrate significant antimicrobial and antifungal potential, highlighting the broad-spectrum bioactivity of this class of compounds. Overall, the table emphasizes that terpenoids, due to their isoprenoid structure and lipophilic nature, are essential for plant defence and ecological adaptation. They also have important therapeutic applications as anticancer, antimicrobial, and anti-inflammatory agents, making them valuable candidates for both pharmaceutical and agrochemical applications. The data presented in Table 4 illustrates the extensive pharmacological versatility of alkaloids derived from medicinal plants, underlining their crucial role in both traditional and modern medicine. These nitrogen-containing compounds exhibit activities related to the neurological, cardiovascular, anti-inflammatory, and antimicrobial activities, with several serving as precursors or active ingredients in clinically used medications. For example, morphine derived from *Papaver somniferum* remains a cornerstone analgesic for pain management. Quinine and ajmaline, which are extracted from *Cinchona* and *Rauvolfia* species, respectively, are essential in treating malaria and hypertension. Neuroactive alkaloids such as galantamine and aloperine show significant promise in managing neurodegenerative problems like Alzheimer's diseases due to their effects on neurotransmission and neuroprotection. Similarly, berberine and sinomenine possess potent immunomodulatory and anti-inflammatory properties, while oxymatrine and vinblastine demonstrate cardioprotective and antitumor effects. Additionally, the presence of compounds like cocaine and cathine underscores the psychostimulatory and anaesthetic characteristics of this chemical group.

Collectively, alkaloids, with their structural diversity and high receptor affinity, represent one of the most pharmacologically significant classes of natural products. They offer therapeutic potential for a wide range of diseases, although they often require careful dosage control because of their potent bioactivity and narrow therapeutic index.

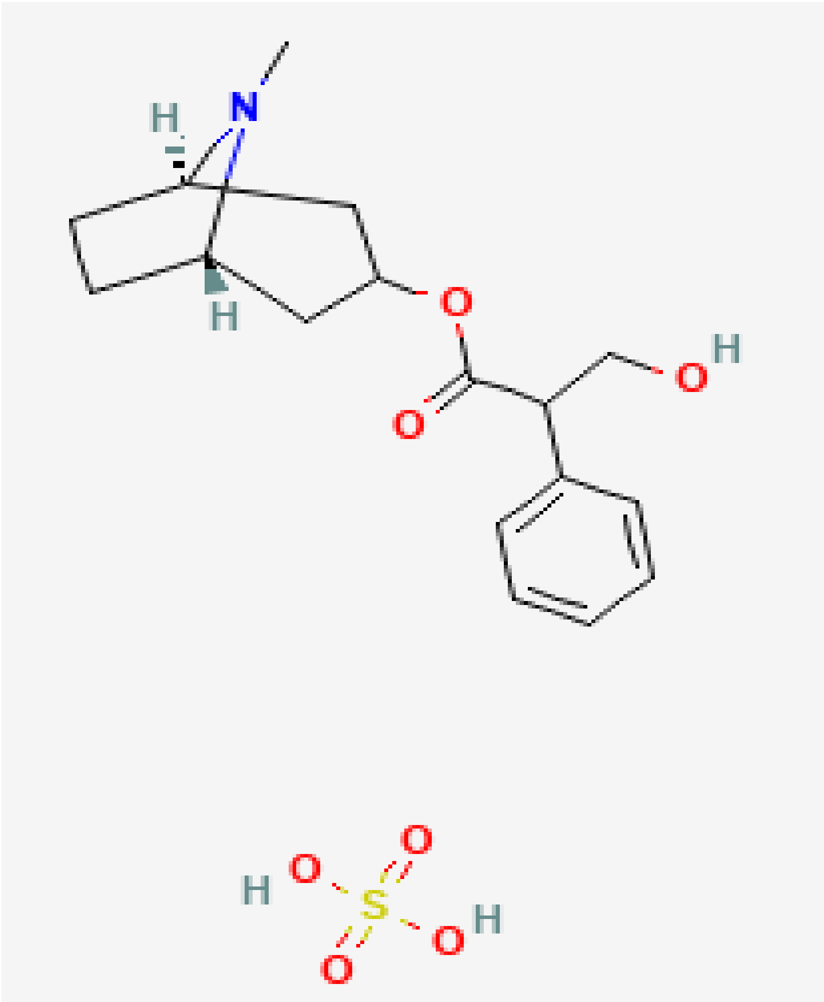

Figure 4: Structure of Atropine sulfate (Source: PubChem)

The heat map shows that phenolic compounds, alkaloids, and flavonoids have the broadest pharmacological spectrum, displaying activity across nearly all therapeutic categories. This versatility is due to their structural flexibility, ability to interact with multiple molecular targets, and their essential central role in plant defence and human health. Other groups, such as terpenoids, steroids, and tannins, show strong associations with anticancer, antimicrobial, and anti-inflammatory activities, suggesting these could serve as promising lead compounds for pharmaceutical development. In contrast, classes such as glycosides and reducing sugars display more specialised roles, primarily related to antioxidant properties and metabolic regulation (Figure 5).

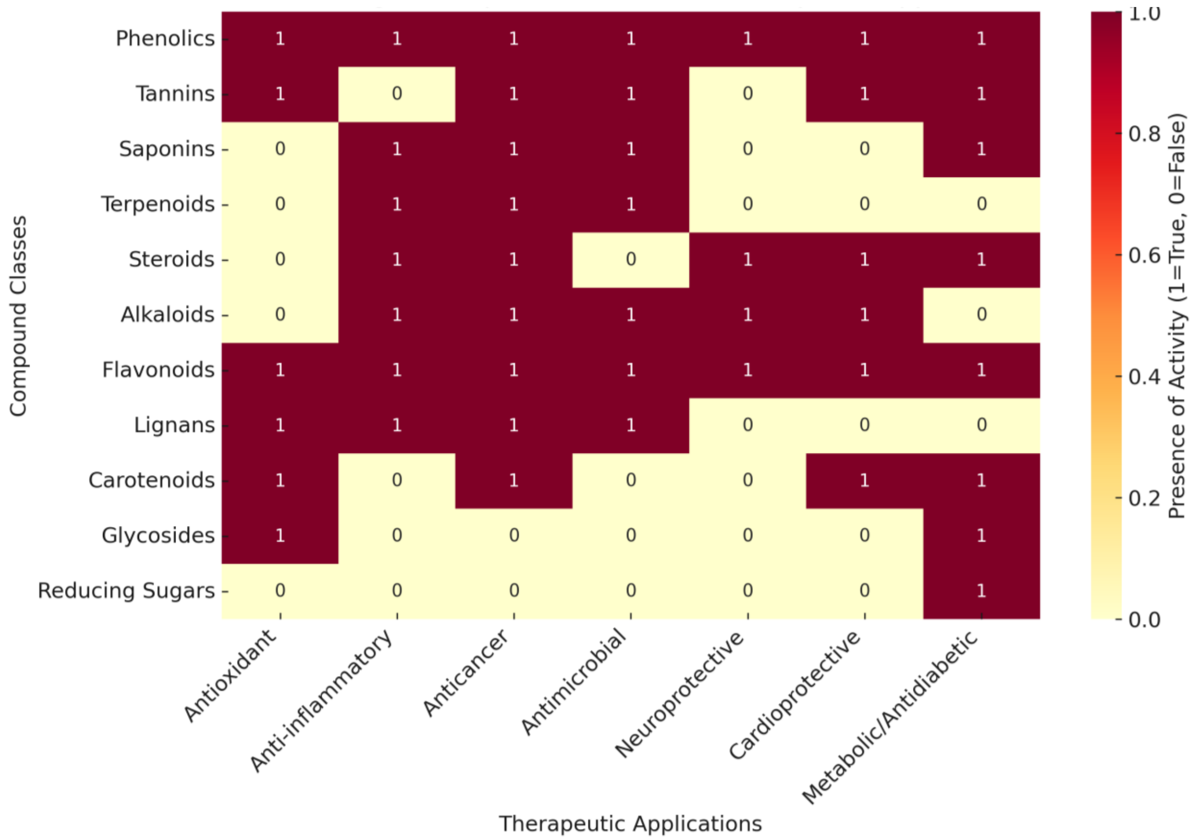

Figure 5: Inter-connection of compound classes and their therapeutic applications.

Conclusion

The collective analysis of the data presented in this review highlights the vast chemical and pharmacological diversity of bioactive compounds found in medicinal plants. These compounds include major classes such as phenolics, terpenoids, alkaloids, flavonoids, tannins, saponins, steroids, lignans, carotenoids, glycosides, and reducing sugars. These compounds exhibit a wide spectrum of biological activities, including antioxidant, anti-inflammatory, antimicrobial, anticancer, antidiabetic, neuroprotective, and cardioprotective properties. Phenolic compounds and flavonoids are particularly prominent for their antioxidant and anti-inflammatory functions, which play a role in the prevention of chronic disorders such as cancer, diabetes, and Alzheimer’s disease. Likewise, terpenoids and steroids demonstrate a variety of pharmacological actions, from antimicrobial and wound-healing properties to antitumor and immunomodulatory effects. Alkaloids, on the other hand, are among the most potent and therapeutically valuable classes, showing strong effects on the nervous and cardiovascular systems. These phytochemicals exhibit multi-target therapeutic potential, supporting their historical use in traditional medicine and highlighting their relevance in modern biomedicine. The multifunctional nature of these compounds offers advantages over synthetic drugs by targeting multiple physiological pathways with fewer side effects. However, challenges such as low bioavailability, poor solubility, and variability in phytochemical composition must be addressed through advanced extraction, standardization, and formulation strategies. Future research should aim to elucidate mechanistic pathways, synergistic interactions, and pharmacokinetics of these compounds to optimize their therapeutic effectiveness. Integrating traditional ethnobotanical knowledge with contemporary molecular and analytical techniques will be crucial in unlocking the full pharmaceutical potential of plant-derived bioactive compounds.

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