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Plant-Derived Bioactive Compounds: Phytochemistry, Pharmacological Mechanisms and Therapeutic Potential

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Abstract

Plants elaborate an extraordinary diversity of secondary (specialized) metabolites that have served as a principal source of therapeutic agents for millennia and continue to inspire modern drug discovery. These bioactive compounds-broadly grouped into polyphenols (including flavonoids, phenolic acids, curcuminoids and stilbenes), alkaloids, terpenoids, saponins, and sulfur- or nitrogen-containing metabolites-exert antioxidant, anti-inflammatory, antimicrobial, anticancer, antidiabetic and neuroprotective effects through the modulation of multiple molecular targets and signalling pathways. Representative molecules such as curcumin, resveratrol, quercetin, berberine, artemisinin, paclitaxel, ginsenosides, cucurbitacins, sulforaphane and epigallocatechin gallate exemplify the structural and mechanistic breadth of this chemical space, and several of them have become clinically established drugs. Nevertheless, the translation of most phytochemicals from preclinical evidence to clinical practice remains constrained by poor aqueous solubility, low oral bioavailability, rapid phase II metabolism, and the limited chemical standardization of plant extracts. This mini-review summarizes the principal classes of plant-derived bioactive compounds, their pharmacological activities and mechanisms of action, and the major bioavailability and translational challenges that must be addressed to advance these natural molecules towards clinical application.

Keywords: Phytochemicals; Polyphenols; Alkaloids; Terpenoids; Saponins; Drug Discovery

Introduction

Natural products have historically been one of the most productive sources of new medicines. A systematic survey of the origin of small-molecule drugs approved between 1981 and 2019 showed that natural products, their direct derivatives and compounds inspired by natural pharmacophores together account for a very large proportion of all approved agents, and that natural-product scaffolds remain highly represented among new chemical entities [1]. Plants, in particular, constitute a vast reservoir of chemically diverse metabolites that have been shaped by evolution primarily as chemical defences against herbivores, pathogens and abiotic stress [2,3]. Although industrial interest in natural-product screening declined during the 1990s, technological advances in genome mining, metabolomics, synthetic biology, high-throughput screening and computational target prediction have revitalized the exploration of plant chemical diversity and accelerated the discovery of new leads [1,4].

Ethnopharmacological knowledge-encompassing Ayurveda, Traditional Chinese Medicine, Unani medicine and other systems-continues to provide valuable guidance for the identification of pharmacologically active plants and their constituents, and many modern drugs can be traced to such traditional knowledge [3,5]. Beyond their role in defence, plant secondary metabolites also mediate interactions with pollinators and symbionts and can act as signalling molecules, blurring the traditional functional dichotomy between primary and secondary metabolism [2]. Environmental factors, including light, temperature, water availability and soil nutrition, strongly influence the accumulation of these metabolites in medicinal plants, with important implications for the quality and reproducibility of herbal raw materials [6]. Modern analytical platforms, particularly high-resolution mass spectrometry, nuclear magnetic resonance and multi-omics approaches, now enable the comprehensive

profiling ("phytochemical omics") of medicinal plants and the rapid dereplication of known and novel compounds [7]. The aim of this mini-review is to provide a concise, up-to-date overview of the major classes of plant-derived bioactive compounds, their pharmacological activities and mechanisms of action, and the principal challenges that limit their clinical translation.

Chemical Classification and Diversity of Plant Bioactive Compounds

The bioactive constituents of medicinal plants are conventionally grouped according to their biosynthetic origin and chemical structure. The four principal classes are the phenolic compounds (derived largely from the shikimate and phenylpropanoid pathways), the alkaloids (nitrogen-containing compounds derived mainly from amino acids), the terpenoids (built from isoprene units via the mevalonate and methylerythritol phosphate pathways), and a heterogeneous group of sulfur- and nitrogen-containing metabolites, including glucosinolates and their isothiocyanate derivatives [3,7]. Saponins, which are glycosylated triterpenoid or steroidal aglycones, form an important sub-group of the terpenoid family [8]. Each class encompasses hundreds to thousands of individual structures, and the same plant frequently accumulates a complex mixture of compounds that act in a synergistic or additive manner [3]. This structural diversity underpins the broad and often pleiotropic pharmacological profiles of plant extracts, which distinguishes them from single-target synthetic drugs. It also complicates their standardization and mechanistic study, because biological activity is typically the result of multiple constituents interacting with multiple targets [3,7]. The following sections review the principal classes and their most studied representatives.

Phenolic Compounds and Flavonoids

Phenolic compounds are the most abundant and widely distributed class of plant secondary metabolites. They range from simple phenolic acids, such as gallic acid and caffeic acid, to complex polymers such as tannins and lignins. Flavonoids-comprising flavonols, flavones, flavanones, flavan-3-ols, isoflavones and anthocyanidins-are the largest sub-group and share a common diphenylpropane (C6-C3-C6) skeleton [8]. Their biosynthesis proceeds through the phenylpropanoid pathway, and their structural variation (number and position of hydroxyl, methoxyl and glycosyl substituents) governs their biological properties [8,9].

The antioxidant activity of flavonoids derives principally from the ability of their phenolic hydroxyl groups to donate hydrogen atoms or electrons, to scavenge reactive oxygen and nitrogen species, and to chelate transition-metal ions; the classical structure-activity relationships established for flavonoids and phenolic acids remain a foundation of the field [9,10]. Beyond direct radical scavenging, flavonoids modulate endogenous antioxidant defences, inhibit pro-oxidant enzymes such as xanthine oxidase and lipoxygenase, and interfere with multiple kinase signalling cascades [9,10].

Quercetin, a ubiquitous flavonol, illustrates this multifunctional profile. It displays antioxidant, anti-inflammatory, antiviral, antihypertensive and anti-diabetic activities and has been examined in a wide range of age-related and chronic diseases [11]. Citrus fruits are especially rich in flavanones (hesperidin, naringenin) and other flavonoids, and their antioxidant properties and potential health benefits have been extensively reviewed [10]. However, the clinical exploitation of flavonoids is limited by their extensive phase II conjugation and generally low systemic bioavailability, an issue addressed later in this review [8,11].

Curcumin and Resveratrol: Representative Polyphenols

Two polyphenols-the curcuminoid curcumin and the stilbene resveratrol-have become the most intensively investigated plant-derived molecules and serve as instructive examples of both the promise and the limitations of phytochemical drug development. Curcumin, the yellow pigment of turmeric (Curcuma longa), exhibits potent anti-inflammatory, antioxidant and anticancer activities and has been shown to interfere with numerous molecular targets, including transcription factors (NF-κB, STAT3), kinases, growth-factor receptors and inflammatory cytokines [12,13]. In colorectal cancer, curcumin modulates multiple signalling pathways involved in proliferation, apoptosis, angiogenesis and metastasis, and it has been evaluated in several clinical trials as an adjunct to chemotherapy [13]. Nevertheless, the therapeutic potential of curcumin is severely constrained by its low aqueous solubility, poor intestinal absorption, rapid metabolism and rapid systemic elimination [14].

Resveratrol, a stilbene found in grapes, red wine and several berries, has attracted attention for its cardioprotective, anti-inflammatory, antioxidant and anticancer effects and for its ability to modulate the activity of sirtuins, AMP-activated protein kinase and other longevity-associated pathways [15]. In vivo evidence supports beneficial effects on cardiovascular and metabolic parameters, although the translation of these findings to human disease has been tempered by its low bioavailability and by the often supraphysiological concentrations required in vitro [15,16]. Recent comprehensive assessments have also highlighted the potential adverse effects and drug-interaction risks of resveratrol, underscoring the need for careful dose optimization [16]. Together, curcumin and resveratrol exemplify the recurring theme of this field: remarkable preclinical activity coupled with formidable pharmacokinetic barriers.

Alkaloids

Alkaloids are a structurally diverse group of nitrogen-containing compounds with pronounced pharmacological activity, and they include some of the oldest and most important plant medicines [17]. Their basic nitrogen atom readily forms hydrogen bonds and ionic interactions with biological targets,

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and many alkaloids act on central nervous system receptors, ion channels, enzymes and nucleic acids. Because of their potent activity, alkaloids have also been an important source of cytotoxic anticancer agents and antimalarials [17,18].

The isoquinoline alkaloid berberine, obtained from Berberis and Coptis species, provides a particularly well-studied example. Berberine improves glucose and lipid homeostasis and has demonstrated antidiabetic effects in randomized controlled trials; moreover, a large body of evidence indicates that many of its metabolic effects are mediated through modulation of the gut microbiota and its metabolites [19,20]. Berberine also exerts broad anti-inflammatory effects through the regulation of multiple signalling pathways, as revealed by network-pharmacology analyses [21]. Other medicinally important alkaloids include the protoberberine and aporphine alkaloids of Corydalis yanhusuo, whose composition, pharmacological effects and drug-delivery strategies have been comprehensively reviewed [18]. The alkaloids therefore illustrate how a single biosynthetic class can yield compounds with activities spanning the metabolic, inflammatory and central nervous systems.

Terpenoids

Terpenoids (isoprenoids) constitute the largest and most structurally diverse family of plant natural products, with more than 40,000 known structures. They are biosynthesized from the universal five-carbon precursors isopentenyl diphosphate and dimethylallyl diphosphate, and they perform essential functions in plants, including roles in photosynthesis (carotenoids, the phytol chain of chlorophyll), membrane architecture (sterols) and defence (volatile monoterpenes and sesquiterpenes, and bitter triterpenoids) [22]. The pharmaceutical importance of terpenoids is difficult to overstate, as they include widely used drugs and drug leads. Artemisinin, a sesquiterpene lactone isolated from Artemisia annua by Tu Youyou and her colleagues, is the paradigmatic example of a plant-derived terpenoid that transformed medicine. Its discovery, grounded in Traditional Chinese Medicine, earned the 2015 Nobel Prize in Physiology or Medicine and provided the basis for artemisinin-based combination therapies, the current first-line treatment for Plasmodium falciparum malaria [23]. To secure a stable supply of this compound, a semi-synthetic route based on engineered yeast that produces the precursor artemisinic acid at high titre was subsequently developed, representing a landmark achievement in synthetic biology [24]. The artemisinins are now also being repurposed for the treatment of cancer and other diseases [25].

Paclitaxel (Taxol), a complex diterpenoid originally isolated from the bark of the Pacific yew (Taxus brevifolia), stabilizes microtubules and thereby blocks mitotic cell division; it is one of the most important anticancer drugs in clinical use for breast, ovarian, lung and other solid tumours [26,27]. Its mechanism of action-suppression of microtubule dynamics leading to mitotic arrest and cell death-has been dissected in detail and continues to inform the development of new anti-mitotic agents [26]. Ginsenosides, the triterpenoid saponins of Panax ginseng and related species, display a wide spectrum of pharmacological activities. Ginsenoside Rg3 has been shown to inhibit tumour growth, angiogenesis and metastasis, and its mechanisms and delivery strategies have been comprehensively reviewed [28]. Ginsenoside Rh4 suppresses colorectal cancer through the modulation of gut-microbiota-mediated bile-acid metabolism [29], whereas ginsenoside Re has shown therapeutic promise in non-alcoholic fatty liver disease through integrated pharmacological and experimental studies [30]. These examples demonstrate the ability of individual terpenoid glycosides to engage metabolic, microbial and oncogenic pathways simultaneously.

Cucurbitacins, a family of highly oxygenated tetracyclic triterpenoids characteristic of the Cucurbitaceae family, are potent cytotoxic compounds with considerable anticancer potential. They inhibit the JAK/STAT, Wnt and other oncogenic pathways and induce apoptosis and cell-cycle arrest, and their potential as anticancer drugs and the structure-activity relationships of their derivatives have been reviewed [31,32]. The Cucurbitaceae family, which includes economically important vegetables such as wax gourd (Benincasa hispida), cucumber and melon, thus represents a promising but still underexplored source of bioactive terpenoids; the recent availability of a chromosome-level reference genome for wax gourd provides a valuable resource for the genomic dissection of such compounds [33].

Saponins

Saponins are glycosides in which one or more sugar moieties are attached to a triterpenoid or steroidal aglycone. They are widely distributed in plants and are characterized by surface-active (foaming) properties and by a broad range of biological activities, including immunomodulatory, hypocholesterolaemic, haemolytic, cytotoxic and anti-inflammatory effects [8]. Astragalus membranaceus, a cornerstone of Traditional Chinese Medicine, accumulates triterpene saponins (astragalosides) together with flavonoids and polysaccharides, and its biosynthesis and pharmacological activities have been comprehensively reviewed [8]. Synthetic and semi-synthetic saponins are being developed as vaccine adjuvants and immunostimulants, illustrating how the saponin scaffold can be optimized for defined pharmacological purposes [34]. Soybean-derived saponins have attracted interest for their immunomodulatory and cholesterol-lowering effects [35]. Because the biological activity of saponins depends critically on the nature and number of their sugar residues, they are particularly amenable to structural optimization.

Glucosinolate-Derived Isothiocyanates and Tea Catechins

Two further groups of plant bioactive compounds deserve mention because of their strong association with dietary chemoprevention. Glucosinolates are sulfur- and nitrogen-

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containing secondary metabolites found mainly in the Brassicaceae (cruciferous vegetables such as broccoli, cabbage and watercress). Upon tissue disruption they are hydrolysed by myrosinase to yield isothiocyanates, of which sulforaphane is the most studied [36]. Sulforaphane exerts chemopreventive and cytoprotective effects largely through activation of the Keap1-Nrf2-ARE pathway, induction of phase II detoxifying enzymes and inhibition of histone deacetylases, and it also displays anti-inflammatory and antimicrobial activities [36,37]. Its derivatives and synthetic analogues are being explored to improve stability and bioavailability.

Tea catechins, particularly epigallocatechin gallate (EGCG) from green tea (Camellia sinensis), are the most abundant flavonoids in tea and display antioxidant, anti-inflammatory, anti-angiogenic and anticancer activities [38]. EGCG targets multiple cancer hallmarks-including proliferation, apoptosis resistance, invasion and metastasis-through the modulation of diverse signalling pathways, and it has been evaluated extensively for cancer prevention [38,39]. Green tea consumption and EGCG supplementation have shown favourable, though not uniform, effects in cancer-prevention studies, and a recent systematic review and meta-analysis highlighted the need for well-designed trials to confirm clinical benefit [40]. The catechins also interact with the gut microbiota, which may contribute to their systemic effects [41].

Mechanisms of Action

Although plant bioactive compounds are structurally heterogeneous, a limited set of conserved mechanisms underlies much of their pharmacological activity. The most frequently cited are antioxidant and anti-inflammatory actions, often accompanied by modulation of cell-death, metabolic and microbiota-related pathways. Oxidative stress and chronic low-grade inflammation are mechanistically linked and contribute to the pathogenesis of cardiovascular disease, diabetes, cancer and neurodegeneration. Polyphenols counteract oxidative stress both by directly scavenging reactive species and by upregulating endogenous antioxidant systems, while simultaneously suppressing pro-inflammatory signalling cascades such as NF-κB and the NLRP3 inflammasome and reducing the production of cytokines, prostaglandins and nitric oxide [42,43]. Systematic reviews of plant-derived natural products confirm their broad anti-inflammatory potential across experimental and clinical settings [44].

In addition to these intracellular mechanisms, many phytochemicals exert effects through the gut microbiota. Polyphenols are extensively metabolized by intestinal bacteria into bioactive catabolites that can modulate microbial composition and host physiology, establishing a bidirectional interaction between these compounds and the microbiome [45]. This "polyphenol-microbiota" axis is increasingly recognized as an important mediator of the systemic effects of dietary phytochemicals, including their influence on metabolic and neurological health [45,46]. Berberine and ginsenoside Rh4 provide further examples of plant compounds whose therapeutic effects are at least partly microbiota-dependent [19,29]. The pleiotropic and often synergistic nature of these mechanisms helps to explain why plant extracts frequently produce effects that cannot be attributed to a single constituent or target.

Bioavailability and Challenges in Clinical Translation

Notwithstanding their striking preclinical activities, the clinical translation of most plant-derived compounds remains limited by unfavourable pharmacokinetics. Curcumin is the classic example: it is poorly soluble in water, poorly absorbed, and rapidly conjugated and eliminated, resulting in extremely low systemic exposure after oral administration [14]. Strategies to overcome this barrier include co-administration with absorption enhancers such as piperine-which markedly increases curcumin bioavailability in animal and human studies [47]-as well as lipid-based formulations, nanoparticle and micellar delivery systems, and targeted delivery approaches [48,49]. Similar bioavailability problems affect resveratrol, quercetin and most other polyphenols [15,50].

Flavonoids and other polyphenols undergo extensive phase II metabolism (glucuronidation, sulfation and methylation) in the intestine and liver, so that circulating concentrations of the parent compounds are typically far below the concentrations used in vitro [50]. Reliable assessment of bioavailability therefore requires the measurement of metabolites rather than parent aglycones, and the design of appropriate formulations and dosing regimens [50]. The chemical standardization of herbal materials introduces an additional layer of complexity: the content of bioactive constituents varies with plant genotype, geographical origin, harvest time and processing, demanding rigorous quality control to ensure reproducible efficacy and safety [6,51]. Addressing these obstacles requires an integrated strategy that combines improved formulation and delivery technologies [48,49], mechanistic and pharmacokinetic characterization of active metabolites [50], and rigorous, well-controlled clinical trials [52]. Encouragingly, several plant-derived compounds-among them artemisinin, paclitaxel, berberine and saponin-based adjuvants-have already achieved clinical use, demonstrating that these barriers can be surmounted when pharmacology, formulation science and clinical development are pursued systematically.

Conclusion

Plant secondary metabolites constitute an exceptionally rich and structurally diverse source of pharmacologically active compounds, and they continue to provide both essential medicines and valuable leads for drug discovery. The major classes-polyphenols and flavonoids, alkaloids, terpenoids, saponins, and sulfur-containing isothiocyanates-exhibit antioxidant, anti-inflammatory, anticancer, antidiabetic and immunomodulatory

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activities that are mediated through a limited set of conserved molecular mechanisms, including direct antioxidant and anti-inflammatory actions and the modulation of the gut microbiota. Compounds such as curcumin, resveratrol, quercetin, berberine, artemisinin, paclitaxel, ginsenosides and sulforaphane illustrate the breadth of this chemical space and the recurring challenge of poor bioavailability. Future progress will depend on the integration of advanced analytical and biosynthetic technologies, rational formulation and delivery strategies, and rigorous clinical evaluation, to convert the remarkable chemical diversity of plants into effective and reproducible therapies.

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