CHAPTER 05

Terpenoids and Terpenes: Diverse Bioactivities and Therapeutic Potential

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ABSTRACT: Terpenoids and terpenes constitute one of the most structurally heterogeneous and biologically multifaceted classes of plant metabolites, being a pillar of plant-derived therapeutics. Due to their intricate chemical frameworks and broad-spectrum bioactivities, these compounds have an extensive pharmacological potential, including antioxidants, anti-inflammatory, antimicrobial, anticancer, antiviral, and neuroprotective activities. The effects of terpenoids and terpenes acting through various molecular and cellular mechanisms modulate oxidative stress, inflammation, apoptosis, and transduction signals that are pivotal to many diseases. The recent development of metabolic engineering, synthetic biology, and nanotechnology has improved their pharmacokinetics significantly, stability, and targeted delivery, leading to their translation from conventional medicine to contemporary clinical practice. However, standardization, mass production and extensive clinical verification related issues remain problematic. This chapter critically explains the chemical diversity, mechanistic insights, and therapeutic importance of terpenes and terpenoids, highlighting their crucial role as molecular templates for new generation drug discovery and development.

Natural products exist as substances that humans obtain from plants as well as animals and microbes (Ahmed et al., 2025). The term secondary metabolites describe these compounds because they form through enzymatic reactions that start with primary metabolites including sugars, vitamins, and amino acids. The largest group of secondary metabolites exists as terpenes which consist of five-carbon isoprene units arranged in different patterns to form simple hydrocarbon structures. The process of modifying terpenes leads to the creation of terpenoids through changes that include oxidizing methyl groups and shifting or removing different functional groups. Depending on how many isoprene units are connected, terpenes and terpenoids can be categorized as into different classes are described in Table 1.

These compounds are abundantly present in all biological kingdoms from terrestrial to marine ecosystems. Forest trees are sources of wide range of biogenic volatile organic compounds (BVOCs) that comprise a huge and diverse class of plant secondary metabolites, majority of which are terpenes and terpenoids. Here they play a critical role in plant protection from pathogenic microorganisms and herbivores via exhibiting direct toxicity, by attracting enemies of herbivores and repelling herbivores. These compounds are characterized with approximately 55,000 different structures representing one of the largest group of plant secondary metabolites (Kim et al., 2020).

Terpenes and terpenoids are highly valuable compounds due to their remarkable diversity, natural structures and different chemical and physical properties. They have long been a center of interest for both traditional and modern applications

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Table 1. Natural sources of Terpenes and Terpenoids and their class

Class	Plants	Fungi	Marine	Microorganisms	References
Monoterpenes	Peppermints (Menthone/menthol)	*Tricholoma vaccinum* (Limonene)	*Portieria hornemanni* (β-myrcene)	*Streptomyces clavuligerus* (Cineole/Linalool)	Tani et al., 2025
Sesquiterpenes	*Lactuca virosa* (Lactucopicrin)	*Tricholoma vaccinum* (β-barbatene)	*Laurencia viridis* (Viridiane)	*Myxococcus xynthus* (Geosmin)	Abdulsalam et al., 2021
Diterpenes	*Andrographis paniculate* (Andrographolide)	*Penicillium cyclopium* (Conidiogenone)	*Sphaerococcus coronopifolius* (Corotrienone)	*Streptomyces melanosporofaciens* (Cyclooctatin)	Zhang et al., 2025
Triterpenes	*Centella asiatica* (Asiaticoside)	*Ganoderma lucidum* (Ganoderic acid)	*Asterias rollestoni* (Rollentosides)	*Piptoporus betulinus* (betulinic acid)	Malyarenko et al., 2021
Tetraterpenes	*Citrullus lanatus* (Lycopene)	*Penicilium sclerotiorum* (Red γ-carotene)	*Dunaliella salina* (B-carotene)	*Botryococcus braunii* (Lycopadiene)	Gonzalez-Hernandez et al., 2024

in agriculture, biomaterials, fragrance and flavor industries, cosmetics, medicines, food ingredients or dietary supplements. Moreover, they are also used as coatings, industrial resins, and most recently as biofuels (Mosquera et al., 2021).

Terpenes and terpenoids exhibit remarkable medicinal properties (Fig. 1). The majority of the structurally varied terpenoids are active biologically and used in the treatment of many diseases worldwide such as used as anticancer drugs for inhibiting cancer cell (Taxol and its derivatives) along with significant roles in cosmetics, food, drugs, hormones, and vitamins. Terpenes and its derivatives are used as antimalarial drugs (Artemisinin) and many nice fragrances and flavorings for its nice aroma (Mabou & Yossa, 2021). This chapter provides a detailed and comprehensive insight into the biologically active terpenes and terpenoids.

CHEMISTRY AND BIOSYNTHESIS OF TERPENES AND TERPENOIDS

Chemistry

Terpenes are further classified into many types on the basis of their structure (Table 2).

Monoterpenes: $C_{10}H_{16}$ consists of two isoprene units (C_5H_8) which form a hydrocarbon structure that scientists call monoterpenoids when they contain oxygen-based functional groups. The production of various compounds results from stereoisomers and structural isomers (including

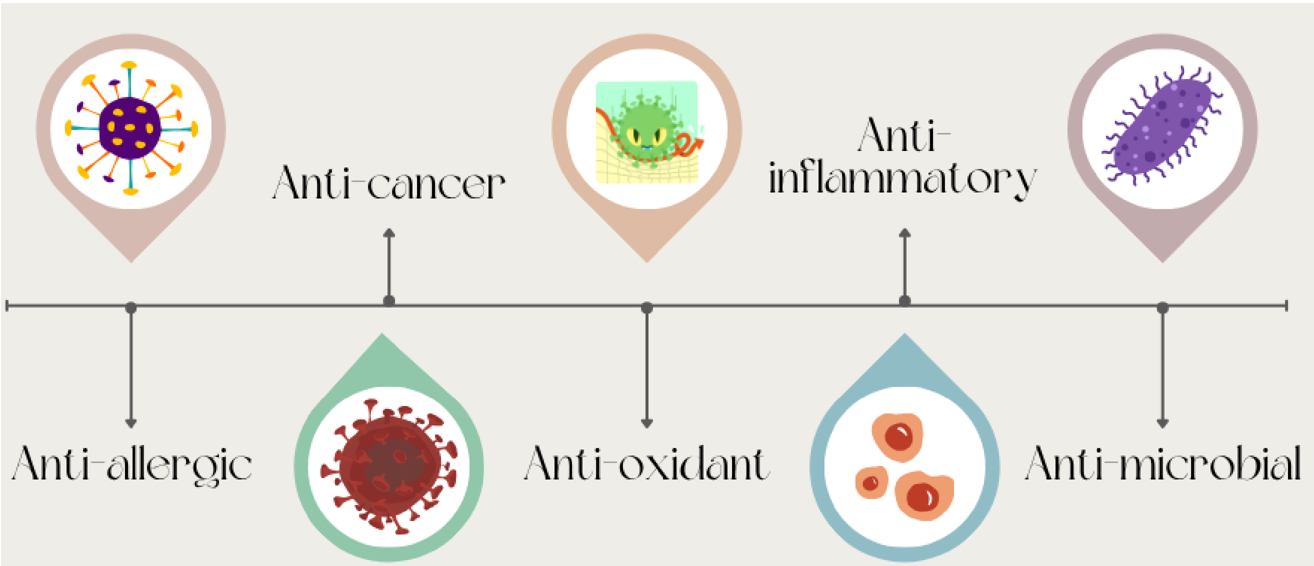

Fig 1. Medicinal properties of terpenes and terpenoids

Table 2. Major compounds of terpenes and terpenoids and their activities			
Class	**Representative compounds**	**Activities**	**References**
Hemiterpenes	Isoprene	• Signaling molecule affecting gene networks involved in stress responses • Plant defense mechanism, antioxidant, Synthetic rubber as major component in vehicle tires, Flavors and fragrances etc.	Srikanth et al., 2024
	Prenol	• Used as bio-fuel or fuel additive due to high heating value and octane rating • Precursor to chlorophyll, fragrances, protect plants from abiotic stresses	Al Mawla et al., 2025
Monoterpenes	Limonene	• Used as Pesticide, have citrus scent, perfumes, flavors, bio-solvent • antioxidant, anti-inflammatory, anticancer, neuroprotective, antimicrobial activities, gastroprotective effects	Gupta et al., 2021
	Linalool	• Antimicrobial, anticancer, anti-depressant, anxiolytic, neuroprotective, hepato and renal-protective, lung protective activities • Cleaner, food additive, cosmetic & fragrance industry, precursor to vitamin E	Herman et al., 2016
Sesquiterpenes	Farnesene	• Thermoplastic elastomer alternate, crop protection, pollination, as alarm pheromone in insects, bio-fuel, skin whitening agent, vitamin E synthesis, flavorant in e-cigarettes • Antiseptic, antioxidant, anticancer, neuroprotective	Rautela et al., 2024
	Farnesol	• Bio-pesticide, anti-cancer drug precursor, fragrance and flavor industries, jet-fuel substitute, antimicrobial activities, anti-inflammatory activities, antioxidant, depressant • To treat allergic asthma, edema, diabetes, atherosclerosis, hyperlipidemia, obesity	George et al., 2015
Diterpenes	Phytane	• Geochemical marker	Ignea et al., 2015
	Taxol	• Chemotherapeutic agent, anticancer activity, prevent microtubule depolymerization, apoptosis	Gallego-Jara et al., 2020
Triterpenes	Squalene	• Antioxidant, cardio protector, anti-cancer, antifungal, antibacterial, detoxifying properties, precursor of cholesterol and phytosterols	Micera et al., 2020
	Lanosterol	• Precursor of animal and fungal steroids, cataract prevention	Sun et al., 2025
Tetraterpenes	B-carotene	• Anticancer, antioxidant, coloring agent, vitamin A precursor, prevent age-related muscular degradation, enhancing immune system activity	Bogacz-Radomska & Harasym, 2018
	Astaxanthin	• Anti-lipid peroxidation activity, anti-diabetic, antioxidant, anticancer activities, enhance antibody production, prevent cardiovascular diseases	Stachowiak & Szulc, 2021

acyclic and mono and bicyclic monoterpenes) and different substitution patterns as described by Marmulla & Harder (2014). Ninety percent of essential oils are made up of monoterpenes and monoterpenoids, which serve as aroma and flavoring ingredients. The substances exist in both natural and synthetic forms which exhibit multiple biological activities including antibacterial, antifungal, local anesthetic, anti-inflammatory, anticancer, antioxidant, anti-aggregating and anti-diabetic properties. These compounds serve dual functions in plants because they work as insect deterrents and simultaneously attract cats and dogs and regulate heat, water loss as well as plant development (Roba, 2020).

Sesquiterpenes: ($C_{15}H_{24}$) containing three isoprene units are widely distributed in various angiosperms, gymnosperms and bryophytes predominantly in the Asteraceae family as well as in fungi and invertebrates. In plants, it is associated with defense mechanisms having antifungal, antibacterial and antiviral activities along with many other health promoting activities against metabolic diseases i.e. hyperlipidemia, hyperglycemia, diabetes, cancer, anti-HIV, neural and cardiovascular disorders (Dhyani et al., 2022)

Diterpenes: ($C_{20}H_{32}$) having four isoprene units joined in head to tail fashion occur in plants, animals, fungi, corals, and algae. They are used as preservatives, food additives, cosmetics, and flavoring. They exhibit insecticidal, anti-carcinogenic, anti-viral, anti-microbial, and anti-inflammatory activities (Zhang et al., 2025).

Triterpenes: ($C_{30}H_{48}$) consisting of six isoprene units are extensively distributed in plant kingdom and are present in roots, leaves, fruits and stem barks (especially pentacyclic ones) (Nazaruk & Borzym-Kluczyk, 2015). Based on the structure, they can be linear (squalene derivatives), bicyclic, tricyclic, tetra and pentacyclic triterpenes. They induce cell proliferation, migration, collagen deposition, and accelerate tissue repair by modulating ROS production in wound microenvironment (Agra et al., 2015).

Tetraterpenes: ($C_{40}H_{64}$) consisting of 8 isoprene units are found in different types of plants, fungi and bacteria. They are responsible for imparting orange, red, or yellow fat-soluble plant and animal pigments.

Biosynthesis

Isoprene units (C_5) are the fundamental building blocks for the biosynthesis of terpenes, acting as key precursors in their construction. In the cell, these units exist largely either as isopentenyl pyrophosphate (IPP) and its allylic isomer, dimethylallyl pyrophosphate (DMAPP). Terpenes of different chain lengths are biosynthesized by specific condensation patterns, such as head-to-tail (1,4 linkage), head-to-head (1,1 linkage), or tail-to-tail (4,4 linkage). Further modifications in structure, including methyl group rearrangement or incorporation of oxygen, produce a wide array of chemical and biological variants known as terpenoids. Two pathways are involved in biosynthesis of terpenes and terpenoids i.e. Mevalonate acid (MVA) pathway, mainly occuring in the cytoplasm leading to formation of high-terpene compounds (di, tri, and polyterpenes), and Methylerythritol phosphate (MEP) pathway, occuring mainly in plastids resulting in low-terpene compounds (mono and sesquiterpenes) formation (Xie et al., 2024)

ANTIMICROBIAL ACTIVITY OF TERPENES AND TERPENOIDS

Terpenes and terpenoids represent promising antimicrobial agents that are active against a wide range of pathogenic microorganisms, including bacteria and fungi that threaten human health worldwide. Due to their bioactive nature, these compounds are widely used in various industrial fields, such as food preservation, cosmetics, and healthcare formulation in toothpaste, soaps, and body lotions. In general, they act through several mechanisms, such as disruption of microbial cell membranes, inhibition of essential enzymatic processes, and modulation of efflux pump activity. Although some terpenes have only partial intrinsic antimicrobial activity, their usage in combination with conventional antibiotics enhances the efficacy of the latter against resistant microbial strains (Huang et al., 2022). Comparative studies also indicated that most terpenoids generally show better antimicrobial activities compared to their parent terpenes (Rao et al., 2019).

Membrane Disruption Mechanism

Generally, terpenes and terpenoids manifest their antimicrobial activity mainly by disrupting microbial cell membranes, which are critical for maintaining cellular integrity and viability. Due to their lipophilic nature, most terpenes (hydrocarbon-based) and terpenoids interact rather easily with the membrane lipid components. Hydroxyl groups in some terpenoids, also responsible for their antioxidant properties, further facilitate permeation and integration into the phospholipid bilayer. Such an interaction increases membrane fluidity and permeability, jeopardizing membrane stability and subsequently leading to cellular dysfunction and death.This results in the loss of intracellular components (organelles, proteins, ions, ATP etc.) disrupting the normal physiological functions needed for cellular integrity leading to the shrinkage and death of cell, finally achieving antimicrobial effect (Huang et al., 2022).

Enzyme Inhibition Mechanism

Another mechanism through which terpenes and terpenoids achieve their antimicrobial activity is through inhibiting the enzymes involved in essential pathways required for normal microbial functions. These antimicrobial agents inhibit the enzymes either by chelating (removing) metal ions (enzyme cofactors) in the active site inducing allosteric effect or binding to enzymes in different orientation based on their structure. This inhibition is based on the presence of functional groups (-OH, -COO, C=C etc.) involved in interaction with active site of enzymes. Some terpenes and terpenoids (citral, limonene, carvone, eugenol) disrupt the mitochondrial function by inhibiting key enzymes involved in Krebs cycle thereby interfering with cell's energy production eventually leading to death (Silva-Beltran et al., 2023).

Efflux Pump Modulation

Efflux pump modulation serves as an important mechanism used by terpenes and terpenoids to accomplish their antimicrobial activity. Efflux pumps are specialized protein channels located on the microbial cell membrane functioning to transport toxic metabolites and antimicrobial agents actively out of the cell before they reach their intracellular concentrations. Overexpression of these efflux pumps induces antimicrobial resistance by lowering the intracellular concentration of antibiotics thus, modification of efflux pumps prevents the extrusion of antibiotics decreasing microbial resistance to drugs. The above two mechanisms play role in the inhibition of energy dependent function of efflux pumps as terpenes and terpenoids disrupts the microbial cell membrane, collapsing the proton gradient or ATP levels hence increasing the retention of antibiotics to effective concentrations within the cell. Moreover, some terpenes and terpenoids (camphor, thymol and eucalyptol) negatively impact the genes encoding efflux pumps (Yang et al., 2021).

Synergistic Effect with Antibiotics and Resistance Modulating Potential

Resistance to antibiotics probably arises due to continuous exposure of microbes to antibiotics and mutations that lead to the accumulation of antibiotic-resistant genes with ultimate evolution of multidrug-resistant microbes posing difficulty in their control through traditionally effective antibiotics. Many terpenes and terpenoids have been shown to exhibit synergistic effect with antibiotics lowering their Minimum Inhibitory Concentrations (MIC) and effective doses required to inhibit the microbial growth thus having resistance modulating potential (Gan et al., 2023). Thymol with Ampicillin acts synergistically against *E coli* by disrupting the cell membrane increasing its susceptibility and sensitivity to Ampicillin. The -OH group in thymol disrupts membrane integrity, increasing ion leakage , permeability, and loss of membrane potential. Subsequently, Ampicillin binds to Penicillin-binding proteins inhibiting the production of peptidoglycans of bacterial cell wall by inhibiting transpeptidases finally destroying bacterial cell wall. Tetracycline can enter the *E. coli* cells due to thymol's ability to form pores in cell membranes, also inhibiting the action of the tetA (tetracycline resistance gene class A) efflux pumps that remove antibiotics from the cytoplasm. Thymol can inhibit the action of efflux pumps directly too. Similarly, thymol degrades *E. coli* membrane to expose the lipopolysaccharide portion that Colistin finally acts upon, exerting antibiotic action via lipid A modification (protection of the membrane from Colistin) (Shirmohammadpour & Mirzaei, 2024).

ANTI-INFLAMMATORY AND IMMUNOMODULATORY ACTIVITIES

When the body tissues are damaged by different things like wounds, infections, bacteria, or other dangerous chemicals, it goes through a complex process called inflammation. The body tries to eliminate these dangerous substances and guard against illness. The body uses this process to protect itself and heal (Chong et al., 2019). A protein known as NF-κB is activated in the inflammation pathway by specific signals known as pro-inflammatory cytokines, such as TNF-α and IL-1. This protein enters the nucleus of the cell and triggers the production of genes that induce inflammation. Terpenes have been shown in numerous trials to reduce the levels of these pro-inflammatory

cytokines. TNF-α, IL-1, and IL-6 in macrophage cells can be decreased by some terpenes, such as D-limonene, α-phenelandrene, terpinolene, borneol, linalool, and triterpene glycosides (Li et al., 2019).
In vivo experiments have shown that terpenes and terpenoids exhibit significant anti-inflammatory outcomes (Gonçalves et al., 2020). Terpenes are used as a potential treatment for conditions like arthritis, asthma, inflammation of the skin, and inflammation of the brain. A typical symptom of conditions like Parkinson's and Alzheimer's is inflammation. Immunomodulators are chemicals that alter the immune system's function, either via strengthening or regulating it. Few plants have been demonstrated to possess this capacity, and research on using plants as a source of immunomodulators is still ongoing (Renda et al., 2022).

ANTICANCER PROPERTIES

Terpenes influence signaling pathways that regulate different cellular processes through their interaction with biological targets which include enzymes, receptors and ion channels. The scientific community has shown growing interest in studying the anticancer effects of terpenes throughout recent years (Kamran et al., 2022). The research evidence from multiple preclinical studies shows that terpenes exhibit anticancer properties when tested against melanoma and other cancer types. The ability of terpenes to enhance cancer cell response to chemotherapy and decrease treatment side effects makes them suitable for use as supplementary treatment in melanoma cases (Woo et al., 2011).
Melanoma is a malignant neoplasm that originates from melanocytes, the pigment-producing cells in the basal layer of the epidermis. It is one of the most aggressive types of skin cancer, with a poor prognosis and a high metastatic capacity if not found and treated early (Ferlay et al., 2021). Through their anticancer effects, terpenes regulate different molecular signaling pathways which control blood vessel formation, cell growth and cell death processes. The DNA of cancer cells undergoes oxidative damage because of terpenes which activates the internal programmed cell death mechanisms that fight against tumor growth (Jiang et al., 2020).
Lupeol exists as a natural pentacyclic triterpenoid which appears in different edible and therapeutic plants such as grapes, cabbages and olives. Research has shown that this substance can fight cancerous cells because it controls various biological signal pathways. The research conducted by Pitchai et al. (2014) reveals that lupeol induces cell death in MCF-7 breast cancer cells through mitochondrial mechanisms which suppress anti-apoptotic protein expression. Babu (2019) documented that lupeol inhibits the proliferation of A549 lung carcinoma cells by downregulating mRNA expression of anti-apoptotic genes. Research indicates that lupeol blocks cell growth in PC3 prostatic cancer and GBC-SD gallbladder cancer cells through its effects on PI3K and EGFR/MMP-9 signaling pathways. Lupeol effectively stops melanoma cell growth through its strong blocking effect on the Wnt/β-catenin signaling pathway (Tarapore et al., 2010).

MEDICINAL SIGNIFICANCE OF ESSENTIAL OILS

Monoterpenes are the simplest class of terpenes, with a molecular formula of $C_{10}H_{16}$. These naturally occurring compounds are synthesized in various plant organs, including flowers, fruits, and leaves, and constitute the major constituents of essential oils, fragrances, and related derivatives (Dehsheikh et al., 2020). They represent a major reason for the typical odour of many plants, such as α-pinene in pine species, and limonene from citrus plants. The aromatic substances in plants produce their distinctive scents because of α-pinene and limonene which occur naturally in pine trees and citrus fruits (Cox et al., 2020). Monoterpenes generate plant aromas which operate as pollinator attractants while simultaneously serving as protective mechanisms against herbivores and pathogens in their ecological functions (Tetali, 2019).
Monoterpenes are abundantly present in essential oils. Essential oils exist as highly concentrated hydrophobic volatile liquids which obtain their form through the process of distilling various parts of the plants. The distinct physicochemical characteristics of each compound determine their biological actions and medical usefulness. Scientists conduct extensive research on these substances because of their wide-ranging medical effects and multiple uses. The substance demonstrates antibacterial and antiviral properties together with antiparasitic and

antiulcer effects as well as strong anti-inflammatory and antioxidant activities. The insecticidal effectiveness of these substances depends on their ability to either disrupt or eliminate insect larvae during their developmental stage. The multiple biological effects of essential oils make them important for medical and pharmaceutical applications as well as pest management and various scientific fields (Dhifi et al., 2016).

FUTURE PROSPECTS AND CHALLENGES

Terpenes and terpenoids are used in pharmaceutical products, agricultural operations, cosmetic products and sustainable industrial sectors. The industrial and therapeutic potential of these compounds remains limited because multiple interconnected elements create obstacles to their full utilization. The field of metabolic engineering and synthetic biology now provides researchers with innovative methods to boost both production rates and product variety through recent scientific developments. The engineering of MVA and MEP biosynthetic pathways enables scientists to create microbial cell factories which generate increased quantities of terpene flavor and fragrance precursors through sustainable production methods (Khanam et al., 2025).

Extensive research on terpenes is required before their usage for commercial and clinical applications. The main obstacle stems from their physicochemical characteristics because terpenoids possess low water solubility, high volatility and unstable structures which makes them vulnerable to heat, light and oxidative damage that reduces their bioavailability and therapeutic effectiveness (Atriya et al., 2023). Synthetic biology has made impressive strides, yet technical obstacles remain because enzyme activities continue to perform below expectations and precursor availability is restricted. In addition, metabolic flux remains out of balance and microorganisms demonstrate limited ability to handle high terpene concentrations which together hinder their production performance (Kaspute et al., 2025).

Third, there is a scarcity of full translational and clinical data; many promising benefits are only seen in cell cultures, with fewer rigorous animal studies or human trials to establish safety, dose, pharmacodynamics, and long-term effects. The production of natural products faces major difficulties because of regulatory requirements, standardization processes and economic constraints. The production of natural products requires overcoming multiple obstacles which include maintaining consistent quality standards for plant and microbial sources and creating scalable purification methods that are affordable and compliant with safety regulations as well as legal requirements for natural products.

CONCLUSION

Terpenoids and terpenes constitute one of the most diverse and biologically important groups of natural compounds with significant therapeutic potential against a broad spectrum of diseases and disorders. Their antioxidant, anti-inflammatory, antimicrobial, anticancer, hepatoprotective, neuroprotective, and cardioprotective effects are due to the interaction with several molecular targets and pathways. Ongoing improvements in analytical chemistry and molecular biology have increased our knowledge about their structure, the mode of biosynthesis, and pharmacological actions. Recent methods like metabolomics, genomics, and computational modeling have made the process of discovering new derivatives with enhanced activity even faster. Their clinical translation is still hampered by their pharmacological usefulness, low bioavailability and structural complexity, as well as sustainable production. New developments in nanotechnology, metabolic engineering and synthetic biology are opening new paths by which these limitations might be overcome, and their therapeutic usefulness may be increased. Taken together, terpenoids and terpenes are a key bridge for connecting natural product chemistry, and modern pharmacotherapy. Long-term interdisciplinary studies will be essential in reengineering their various bioactivities into effective, safe and sustainable therapeutic agents to improve human health.

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