Phytochemicals Unveiled: The Science behind Plant-Based Medicines

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Abstract

Compounds or phytochemicals present in medicinally relevant plants may be used to cure illnesses or make medications. Plants' leaves, stems, bark, and roots naturally contain these compounds. Like primary metabolites, they are created for the plant's defense rather than for development, which is why they are named secondary metabolites. Fortunately, the majority of these secondary metabolites have therapeutic properties that aid in the treatment of a variety of diseases and health problems. Since many illnesses are growing resistant to conventional antimicrobials, antibiotic resistance is a serious worldwide health concern. Research labs are concentrating on creating novel antimicrobials because no medicine can reverse this resistance. Chemical compounds derived from plants have the potential to be potent anticancer medications without adverse effects. Bioactive phytochemicals are preferred because they have distinct effects on cancer cells while having no effect on healthy cells. This study covers the utility of medicinal plants and secondary metabolites of plants as drug sources, the process of developing novel medications, the safety and efficacy of phytochemicals, current applications, and developments in screening technology, challenges, and future directions.

Keywords: Phytochemicals, Antibiotic Susceptibility Testing, Metabolites, Novel Medications

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Introduction

People have been using plants as cures for a variety of ailments since ancient times. Ayurveda, Traditional Indian Medicine (TIM), and Traditional Chinese Medicine (TCM) are the oldest medical traditions still in use today, having been practiced since 4500 BC. In the past, people were aware of the right way to choose plants, when to harvest them, and how to make medications for specific uses. From one generation to the next, this knowledge is passed down orally. The folklore system has all of the information about the medications and how they are specifically used to cure different illnesses. These medications were prepared as decoctions, poultices, teas, tinctures, powders, and other forms (Ogbonna, Kenechukwu, Attama, & Chime, 2012).

Because of the broad spectrum of knowledge and expertise needed, the identification of chemicals originating from plants has altered during the past 200 years. A plant is initially identified by a botanist, ethnobotanist, ethno pharmacologist, or plant ecologist. Before separating the active ingredient, a phytochemist looks for potential therapeutic efficacy using biological screening assays and plant extracts. Molecular biology research is ultimately required to determine the mechanism of action and relevant molecular targets. The mixing of several sciences determines the interdisciplinary approach of pharmacognosy. The phrase "natural products," sometimes referred to as "phytochemicals," only describes compounds present in living organisms and can be referred to as secondary metabolites. Phytochemicals are bioactive compounds that plants produce to protect themselves (Anand, Jacobo-Herrera, Altemimi, & Lakhssassi, 2019).

They can be found in whole grains, fruits, vegetables, nuts, and herbs, among other meals. Carotenoids, polyphenols, and saponins are among the more than a thousand phytochemicals with antioxidant, antiviral, and antibacterial qualities. Phytochemicals present a viable substitute or addition to antibiotics in the fight against diseases, given the growing concerns regarding antimicrobial resistance (AMR). Their significance in tackling global health issues is shown by their capacity to treat cancer and microbiological illnesses. Chemically produced medications have not substantially increased survival rates, despite improvements in our understanding of cancer pathways. We need new chemo-preventive measures. Alkaloids, such as vincristine and vinblastine, are examples of phytochemicals derived from plants that provide valuable resources for the treatment of cancer and the creation of new drugs. The process of finding new drugs is expensive and time-consuming; it frequently takes more than ten years (Kumar et al., 2023).

Medicinal plants are a significant source of new therapeutic chemicals and are found in a variety of environments around the world. More than 197 different plant species have been mentioned in Ayurveda, together with details about their distribution and use. Therapeutic plants are among the 34 global "Biodiversity Hotspots" that have been identified based on a set of criteria. This article focuses on biodiversity hotspots and discusses the habitat and distribution of medicinal plants. The socioeconomic importance of traditional medicinal plant applications is also covered, as are techniques for distribution study based on geographic information systems and remote sensing. Medicines of natural origin offer an endless supply of different components to help create pharmacologically relevant medicines that operate at the molecular level.

It is well recognized that medicinal herbs can help with fundamental human requirements like food, shelter, clothes, and health. Because of their desire for longevity, perpetual health, and a way to alleviate pain, humans have created a wide range of healthcare systems. Traditional medicines were employed to heal ailments in ancient societies. In the quest for novel medications to treat severe conditions like cancer, malaria, diabetes, and heart problems, natural products have grown in importance. Many plant-based anticancer medications, such as vincristine, paclitaxel, docetaxel, topotecan, irinotecan, and vinblastine, have recently drawn interest. Plants naturally create a wide range of compounds with various chemical properties in order to grow and develop. The resources needed for respiration, translocation, and photosynthesis are supplied by primary metabolites (Ogwu, Ogwu, & Kosoe, 2024).

Primary metabolites are the source of secondary metabolites, which have no direct connection to growth and development. Primary metabolites typically result in secondary metabolites, which are created through biosynthetic modifications such as hydroxylation, glycosylation, and methylation. It is undeniable that secondary metabolites contain more intricate structural elements and side chains than primary metabolites. There are now several obstacles to the use of natural goods and the acknowledgement of their positive health effects, including the inability to establish standard operating procedures and the challenge of separating pure chemical compounds or constituents.

Uncertainty about the biological process and the inconsistent completion of clinical investigations that are supposed to be controlled and documented by "standards." As said earlier, historical scientific evidence demonstrates the efficacy of natural substances as medicines, which helped to establish several well-known conventional drugs. The complexity of the chemical combinations present in natural goods might occasionally make the hunt for new therapeutic options more difficult. Plant extracts typically offer therapeutic advantages due to the simultaneous and synergistic actions of many compounds (Dhyani et al., 2022).

Using Phytochemicals to Find New Drugs

New medication innovation is facing major challenges due to a decrease in new drug approvals and an increase in expenses. Natural products are the source of many new pharmaceutical drugs and active ingredients. A fuller understanding of the predominance of specific Ayurvedic attributes may be obtained by examining the frequency of substances in the ancient documented recipes and their Ayurvedic characteristics. It will therefore be simpler to select appropriate candidate plants for bioactivity-based fractionation. Phytochemicals obtained from different plant sources are used in drug discovery and lead compound development processes. Following pharmacological research, biochemical characterization, phytochemical identification, separation, and purification from the selected plant species, preclinical and clinical studies are carried out. Modern analytical techniques such as gas chromatography, high-performance liquid chromatography, and mass spectrometry are also required for structural elucidation in drug discovery. Sometimes, in order to increase the biological activity and stability of phytochemicals, their native structure must be changed (Dhyani et al., 2022).

The development of novel medications is essential to the fight against antibiotic resistance and other illnesses. Single molecules are frequently the focus of modern drug development, while complete plant extracts, where several metabolites cooperate, may have more powerful therapeutic effects. Whole plant extracts should be given priority in research, with an emphasis on examining their synergistic effects and their impacts on genes and proteins using "-omics" platforms. In natural product pharmacology, a systems biology approach can help biological systems regain equilibrium and provide a more comprehensive solution. Innovative drug design offers promising therapeutic potential. It is fueled by systems biology and contemporary technology, such as computational tools, transcriptomics, proteomics, metabolomics, genomics, and bioinformatics. This integrative approach stresses the synergistic effects of compounds rather than a reductionist focus on individual active components.

The Value of Bioactive Compounds from Medicinal Plants in Drug Discovery

Plants have played a significant role in medicine, serving as the foundation for conventional therapeutic approaches. Given the enormous potential offered by the extensive chemical variety found in natural products, ethnomedical research is still essential for developing new drugs. The market for herbal remedies has grown due to the rising desire for green medicines. Comprehensive biochemical profiling is still scarce, and drug development initiatives employing LC-MS and GC-MS are neglected mainly in Pakistan, despite evidence of potent antibacterial, anticancer, antiviral, and antioxidant qualities in Pakistani medicinal plants (Arnason et al., 2022).

1. Plants' Function in Drug Discovery

All societies have utilized medicinal plants as a source of medicine since prehistoric times. In the beginning, people used plants to meet their nutritional demands. The natural flora has proven to be a very beneficial source for enhancing health and treating a variety of ailments across various human populations. In Asia, South America, and Africa, numerous plant species are still utilized as remedies for various ailments. 60% of people worldwide utilize traditional medications, which have advantages over synthetic ones, such as greater compatibility, cultural acceptance, and less adverse effects. Considering that 25% of medications are made from plant chemicals, ethnobotany has made a substantial contribution to modern medicine. Plants have been used to extract substances like quinine and morphine since the 19th century. Ethnobotany is expanding in Pakistan, where 400–600 of the 5700 species of therapeutic plants have been examined biochemically (Berger-Gonzalez et al., 2022).

2. **Biochemical Characterization and Associated Methods**

The metabolome, which reflects variations in metabolite fluxes influenced by gene expression, comprises all of an organism's small molecules and is essential to postgenomic analysis. Gene function and enzyme activity can be revealed through metabolomics, which is aided by transcriptomics and proteomics. Natural product research has been transformed by contemporary methods like LC-MS and GC-MS, which allow for the sensitive and accurate examination of intricate biological materials. Due to its higher sensitivity for identifying secondary metabolites at low concentrations, LC/MS has supplanted previous techniques such as immunological and fluorometric tests (Asim, Hussien, Poveda, Arnason, & Durst, 2010).

3. **Bioactive Substances Derived from Therapeutic Plants**

Numerous medicinal plant extracts work well against microbial and parasite illnesses. For instance, antifungal proteins like chitinase and glucanase found in plant seeds shield developing embryos from harm. Antifungal and anticancer drugs produced from plants are currently used in clinical settings. Studies indicate that plant-based diets may lower cancer incidence, and plants are a substantial source of anticancer chemicals. With plants like Terminalia arjuna used to treat cardiovascular disease and Andrographis lineate used to cure snake bites, South Asian medicinal herbs are becoming more well-known for their antibacterial qualities (Pandohee, Kyereh, Kulshrestha, Xu, & Mahomoodally, 2023).

4. **Today's Herbal Remedies**

Drug development uses various methods, including synthetic chemistry, combinatorial chemistry, bioinformatics, and plant-based extractions. Simple plant medicines like syrups, tinctures, and herbal teas were used before the 19th century. Because native plants are frequently offered in marketplaces in developing nations, researchers look at their names, applications, and preparations.

In order to achieve effective health in poor countries, the WHO acknowledges the importance of using indigenous herbal treatments. Patients with chronic illnesses are increasingly using herbal medicines in wealthy nations because they are more affordable, effective, and have less adverse effects than synthetic pharmaceuticals. Researchers throughout the world are looking into medicinal plants in quest of novel phytochemicals and possible cures (Chihomvu, Ganesan, Gibbons, Woollard, & Hayes, 2024).

Experimental General Methods

1. **Methods of Chromatographic**

Reagents and Solvents

Methanol, n-hexane, ethyl acetate, n-butanol, pure ethanol (99.99%), and isopropyl alcohol are examples of analytical grade solvents. Every reagent is of analytical quality, including acetic acid (≥97%), sulfuric acid (≥95%), potassium hydrogen phosphate (≥98%), sodium hydrogen phosphate (≥95%), sodium hydroxide (≥98%), sodium carbonate (99%), dimethyl sulfoxide (DMSO) (≥95%), and hydrochloric acid (HCL) (≥95%). The solvents employed in HPLC, methanol (MeOH) and acetonitrile, were of HPLC quality. Water for HPLC is dispensed using a Milli-Q system, while RiOS water is produced via reverse osmosis. One of the solvents used in GC-MS is pyridine (dry, 99.8%) (Seccosolv). Reference materials include acarbose (≥95%), methylglyoxal (MGO) (≥99%), bovine serum albumin (BSA) (≥98%), aminoguanidine (≥99%), quercetin (≥98%), glucose (≥99%), and linoleic acid (99%) (Aggarwal, Sharma, Singh, & Sharma, 2024). Scheme for general extraction

2. **The Thin-Layer Chromatography Technique**

In thin layer chromatography (TLC), silica gel plates (20 x 20 cm) for the normal phase are utilized as analytical plates. The spraying reagent employed is P-anisaldehyde. Dragondorff's reagent is made by mixing solutions A and B. Solution A was made by mixing 100 mL of water and acetic acid with 1.7 g of bismuth subnitrate. Solution B was made by dissolving 40 g of potassium iodide in 100 mL of water. When solutions A and B are combined, the following is produced: 5 mL of A, 5 mL of B, 20 mL of acetic acid, and 70 mL of water. To make the cerium sulphate reagent, first 4 mL of 15% H_2SO_4 was combined with 1g $CeSO_4$ and 10g of trichloroacetic acid (TCA). This was thoroughly mixed to form a slurry.

3. Chromatography by Flash

A Grace Reveleris iES machine is used to perform flash column chromatography using the Reveleris® Navigator TM software. The system includes a binary pump with four solvent selections, a fraction collector, and an ultraviolet (UV) and evaporating light scattering detector (ELSD). The used column is an 80 g prepackaged Flash Grace Reveleris silica cartridge with a 40 µm particle size. The ELSD carrier solvent is isopropyl alcohol (Halder & Jha, 2023).

4 Liquid Chromatography with High Performance

HPLC analysis is performed using an Agilent® 1200 series equipment that includes a quaternary pump, automated injection, a thermostatic column compartment, a degasser, and a diode array detector (DAD). A silica-based Gracesmart C18 column (250 x 4.6 mm, 5 µm) and a Phenomenex luna C18 column (250 x 4.6 mm, 5 µm) are used in combination with a suitable precolumn to increase the lifespan of columns.

5. **High-Performance Liquid Chromatography that is Semi-preparative**

A Luna 5µm (C18) 100A 250 X 10.0 mm column is used to separate compounds in a semi-preparative HPLC-DAD-MS system. A diode array detector (DAD), make-up pump, HPLC pump 515, system fluid organizer (SFO), triple quadrupole mass spectrometer (TQD-MS), and an automated fraction collector for chemical isolation are all included in the system (Ogbuagu et al., 2022).

6. Methods of Spectroscopy

With a Bruker DRX-400 apparatus, which runs at 400 MHz for 1H and 100 MHz for 13C, nuclear magnetic resonance spectroscopy (NMR) spectra are recorded using either a 3-mm broadband inverse (BBI) probe or a 5-mm dual 1H/13C probe using standard Bruker pulse sequences. The chemical shifts are reported in ppm, while the coupling constants (J) are expressed in Hz. The 13C-NMR database NMR Predict version 4.8.57 facilitates the understanding of structure. Deuterated solvents that are used include $CDCl_3$ (99.8% D), DMSO-d6 (99.9% D), and CD_3OD (99.8% D).

7. Mass Spectrometry

To generate high-resolution mass spectra, an AgilentTM 6530 quadrupole-time-of-flight mass spectrometer (QTOF-MS) equipped with an AgilentTM Jetstream source is utilized with the following parameters: The gas temperature was 325 °C, and the sheath gas flow was 11 L/min. 750 V was the OCT 1RF Vpp, while 3500 V, 150 V, and 65 V were the capillary, fragmentary, and skimmer voltages, respectively. Both the positive and negative ion modes of the mass spectrometer were operated at 20,000 resolutions (Zakaria, El-Sayed, & Ali, 2025).

8. Analysis with GC-MS

For GC research, Thermo Scientific's TRACE® 2000 Ultra GC is utilized with a column AT-5MS (Grace) that has the following dimensions: 30m in length, 0.25mm in diameter, and 0.25 µm in film thickness. In order to derivatize dried materials, 20 µL of BSTFA + TMCS, 99: 1 (Supelco, USA) in pyridine (dry) (Seccosolv) in a molar ratio 2-1 is heated for one hour at 70°C.

9. Rotation of Optics

A Jasco P-2000 polarimeter is used to measure the exact optical rotation. While the samples were dissolved in methanol, optical rotation was measured at 589 nm along a 50 mm path. UV-Vis (ultraviolet-visible light) absorption is measured using a Genesys-10UV (Thermoscientific) spectrophotometer. To measure fluorescence, a Tecan™ Infinite M200 spectrofluorometric is utilized (Marchev et al., 2021).

10. Pytochemicals Screening

For every fraction, a phytochemical screening for various chemicals was carried out.

1. Chemical Test for Alkaloids

0.2 g of the extract was added to 2 mL of 2% H_2SO_4, and the mixture was then heated on a water bath for two to three minutes. It was applied in four to five drops of Dragondorff's reagent. An orange-red precipitate identified alkaloids.

2. Tannins can be Detected Chemically

On a water bath, a test tube with around 0.2 g of extract and 10 mL of distilled water was brought to a boil. Four or five drops of 0.1% ferric chloride ($FeCl_3$) were added. The color of tannins was described as dark green or blue-green (ASIF, 2024).

3. Chemical Saponin Test

0.2 g of the extract was shaken with 5 mL of distilled water, and then it was brought to a boil. The sight of foam indicated the presence of saponins.

4. Test for Flavonoids Chemically

About 0.2 grams of extract were dissolved in two milliliters of 10% NaOH. Flavonoids were present because the solution changed from yellow to colorless when 0.5 mL of HCl was added.

5. Steroid Chemical Test

0.2 grams of the extract were mixed with 2 milliliters of acetic anhydride. 1 mL of H_2SO_4 conc. was added. The color shifts from violet to blue or green indicated the presence of steroids (Wani et al., 2023).

6. Chemical Test for Terpenoids (Salkowski Test)

0.2 g of extract and 2 mL of chloroform were combined with 3 mL of H_2SO_4 conc. A reddish-brown hue was used to identify terpenoids.

Plant Drug Discovery and New Phytochemical Studies of Traditional Plant Medicine

At the beginning of the new century, US drug development money financed large research institutions in North and South America that worked on traditional indigenous treatments. These efforts brought together researchers, pharmaceutical companies, and Indigenous people to find new single entity medications for development from traditional cures. The Nagoya Protocol, an addition to the Convention on Biological Diversity that Canada cochaired, was born as a result of the development of international ethical norms. It provided a framework for biodiversity access and benefit sharing for Indigenous people (Mosoh, 2025).

Fortunately, efforts to re-establish ties with Indigenous people are underway, and research voices and leadership from First Nations are being heard. Healing practitioners prioritize patient care while appreciating scientific studies to support conventional treatments. They think that in order to be recognized by regulators, traditional knowledge must be translated scientifically. Finding active principles and evaluating their efficacy and safety are crucial. Benefit sharing with Indigenous populations is emphasized by international agreements such as the Nagoya Protocol. New, standardized treatments may result from research into traditional plant remedies. For instance, mountain ash bark is used by Cree healers to treat diabetes; its extract demonstrated actions akin to those of metformin, which led to the development of a novel triterpenoid called 23, 28-dihydroxylupan-20-ene-3β-caffeate, which promotes the uptake of glucose in muscle cells (Sharma et al., 2024).

Both active ingredients and synergistic factors are frequently responsible for the effects of medicinal plants. The discovery of bioactive substances is streamlined by contemporary techniques such as biochemometric analysis, which integrates metabolomics, bioassays, and statistics without evaluating every fraction. Nowadays, it is typical practice to compare known compound data to prevent redundancy by metabolomics-guided fractionation and dereplication. There is encouraging potential for finding new phytochemicals by focusing on understudied plant families (Fig 1).

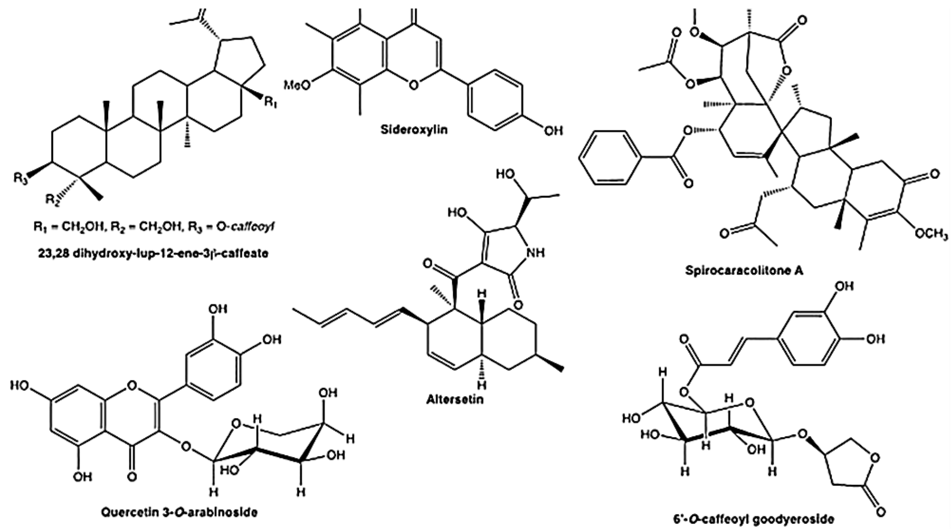

Fig. 1: New Bioactive Compounds from Plants and Fungi

Secondary Plant Metabolites with Medicinal Properties

The existence of so-called secondary plant metabolites is often credited with the pharmacological and therapeutic qualities of medicinal plants. A small number of plant species exhibit secondary metabolites with therapeutic qualities, in contrast to the universal macromolecules of primary metabolism (such as proteins, lipids, amino acids, polysaccharides, monosaccharides, and polysaccharides) that are present in all plants (Kaur, Sharma, Kabila, & Sidhu, 2025).

- **Polysaccharides**

Alkaloids, glycosides, terpenoids, phenolics (both simple and flavonoids), waxes, fatty acids, and their derivatives are examples of secondary metabolites from plants that have been demonstrated to have medicinal properties. A brief overview of some of these plants' secondary metabolites is provided below:

- **Carbohydrates and Associated Substances**

Fiber, cellulose and its derivatives, dextrin, fructans, pectin, starch and its derivatives, mucillages (polymers containing uronic acid), and gums are examples of carbohydrates and associated compounds that come from plants (Kaur et al., 2025).

Alkaloids

Alkaloids are chemical molecules that contain nitrogen and have potent pharmacological effects. They can be categorized based on their structure (e.g., indole, isoquinoline), effect (e.g., stimulant, analgesic), or plant source (e.g., opium, cinchona). Because alkaloids are poisonous and bitter, they act as defense mechanisms in plants shown in figure 2.

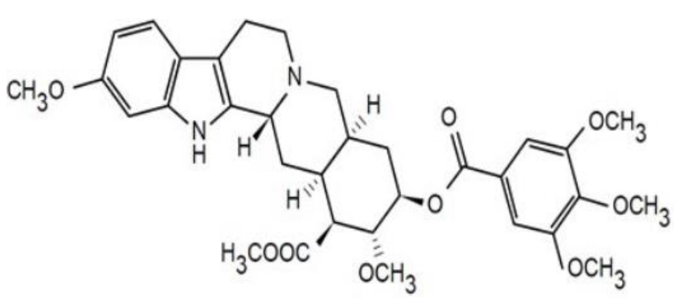

Fig. 2: Structure of Reserpine (An Alkaloid)

Phenolics

Secondary metabolites of plants that include one or more hydroxyl groups joined to an aromatic ring are called phenols. Many plant colors are caused by these chemicals, which are primarily divided into flavonoid and non-flavonoid categories. Flavonoids are known for their health benefits and feature a three-ring structure. For instance, flavonoids found in garlic can help lower cholesterol, atherosclerosis, and other dangerous diseases (fig 3).

Simple phenols, C6-C3 phenyl propanoids and their derivatives, C6-C1 benzoic acid, coumarins, hydrozable tannis, lignans, and other similar chemicals are examples of non-flavonoid phenolic compounds.

Terpenoids

Based on their isoprene units (C10 to C40), terpenoids, also known as isoprenoids, are the biggest class of secondary metabolites found in plants. In addition to contributing to fruit and floral aroma, they are essential for plant defense, wound healing, thermotolerance, and pollination. Plants such as *Salvia stenophylla* and *Plinia cerrocampanensis* contain the sesquiterpene (C15) bisabolol, which has antibacterial, antifungal, antimalarial, and molluscicidal properties shown in fig 4.

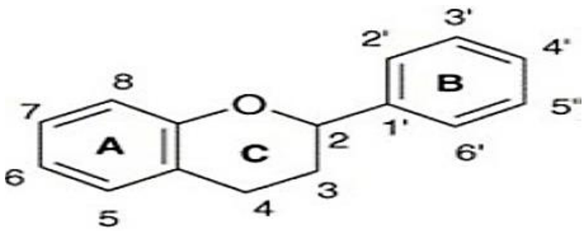

Fig. 3: Basic Structure of Flavonoids

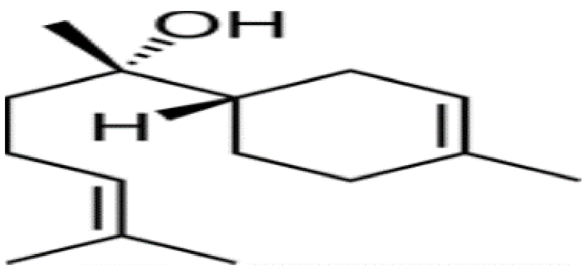

Fig. 4: Structure of Bisabolol

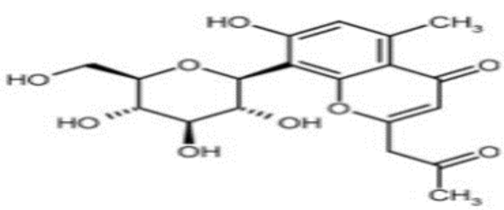

Fig. 5: Structure of aloesin (a glycoside)

Glycosides

Plant secondary metabolites known as glycosides are composed of two components: a glycone (a carbohydrate) and an aglycone (a non-carbohydrate). Anthraquinone, cardiac glycosides, and coumarin are examples of medical glycosides (Sakhale, Giri, & Borse, 2023). An antioxidant, free radical scavenger, and anti-inflammatory, aloesin is a glycoside found in aloe vera (Figure 5).

Bioactive Compounds and Defense Mechanisms in Plants

Bioactive compounds are diverse plant-derived molecules produced in response to microbial infections and insect attacks. These substances, which are widely utilized in food, medicine, and cosmetics, aid plants in fending against infections through biochemical and genetic reactions. Signaling networks involving hydrogen peroxide, ethylene, salicylic acid, and jasmonic acid trigger genes relevant to defense. Additionally, plants produce pathogenesis-related (PR) proteins that are essential for immunity, such as lipid transfer proteins, defensins, and thionins. Both biotic and abiotic elicitors, such as salicylic acid, DL-β-amino-n-butyric acid (BABA), and benzo (1,2,3) thiadiazole-7-carbothioic S-methyl ester (BTH), can activate these proteins (Hurkul, Cetinkaya, Yayla, & OZKAN, 2024).

AMPs, or Antimicrobial Peptides

Antimicrobial peptides (AMPs), which are produced by agricultural plants, aid in the defense against microbial infections. These peptides have potent antibacterial properties and are present in a variety of plant tissues. AMPs are classified according to their structure and function, including thionins and plant defensins. Protease inhibitors, chitin-binding proteins, and knottin-type peptides are other AMPs that have been found in medicinal plants.

Anticancer Substances

The development of cancer medicines has been greatly aided by plant secondary metabolites. For instance, extracts from *Pavetta crassipes*, which include alkaloids such hydroxyl-elaeocarpidin, may have anticancer properties. Additionally, for more than 40 years, vinca alkaloids which are derived from *Catharanthus roseus* and *Vinca rosea*have been used to treat cancer by interfering with mitosis. In contemporary medicine, these substances and their derivatives remain essential.

Current Techniques for Drug Discovery

Drug development has been transformed by the combination of molecular biology, biochemistry, and structural biology, which makes it possible to create tailored treatments. Although assay difficulties restrict the effectiveness of high-throughput screening (HTS), it improves the identification of active molecules. Prioritizing drugs prior to testing is aided by computational techniques such as docking and molecular modeling. While modern analytics help isolate and characterize possible therapeutic molecules, methods such as network pharmacology, virtual screening, and QSAR modeling speed up the identification and enhancement of natural compounds against drug-resistant targets (Maikhuri et al., 2024).

Computational Methods for Finding Possible Phytochemical Medicines

Computational techniques can now be used to efficiently identify and optimize phytochemical treatments. For instance, machine learning, virtual screening, molecular docking, and molecular dynamics simulations have all been employed in the past to identify and modify the biological activity of phytochemicals. Virtual screening is a popular computational technique in drug discovery that rapidly evaluates and selects compounds for experimental testing against a specific target or disease model.

Virtual screening approaches can scan large databases containing known phytochemicals or libraries created in silico that mimic natural substances. This efficient technique may manage large datasets and reduce the number of compounds evaluated in biological experiments.

Docking of Molecular Structures

Phytochemical drug research has been transformed by molecular docking, a computer technique that predicts a phytochemical's mechanism of binding to its target protein. Many computational tools and algorithms have been developed and are currently available.

Examples of often used technologies are AutoDock Vina, AutoDock GOLD, Discovery Studio, FRED, Glide, ICM, Surflex, MCDock, MOE-Dock, FlexX, DOCK, LeDock, rDock, Cdcker, LigandFit, and UCSF Doc. Molecular docking has become crucial for identifying the molecular targets of nutraceuticals used to treat a variety of ailments (Wali et al., 2025).

During the COVID-19 pandemic, for instance, molecular docking was crucial in assessing and confirming the ability of phytochemical ligands to interact with druggable targets for SARS-CoV-2 replication and pathogenesis. The main protease, often referred to as 3C-like protease (3CLpro), stood out among the anticipated SARS-CoV-2 targets as a significant druggable target due to its high conservation and the deadly impact that a mutation would have on the virus. Additionally, the ADME investigation demonstrated that all phytochemicals possess properties similar to those of drugs.

Dynamics of Molecular Structure

Molecular dynamics (MD) may also be particularly important in enhancing docking or virtual screening results since biomolecules in the human body are dynamic, unlike the static conformations used in traditional structure-based drug discovery approaches. Molecular dynamics (MD), which predicts molecular and structural alterations in biomolecules brought on by intramolecular and intermolecular interactions, is a key component of drug development research. There are several software tools available for MD simulation; for example, because of their powerful computational techniques and ability to handle complex and large molecular systems, computational scientists frequently employ GROMACS 2024.2, AMBER 2024, and NAMD 3.0. Several research have used MD simulations to examine the connection between flavonoids and G-quadruplex DNA. MD simulations are necessary to determine the degree to which flavonoids would bind to quadruplex DNA, which is important for cancer treatment (Auezov et al., 2024).

Both Artificial Intelligence and Machine Learning

Artificial intelligence (AI) and machine learning (ML) hold enormous promise for advancing phytochemistry and its therapeutic applications. They aid in understanding phytochemicals' mechanisms of action (MoA) and the prediction of therapeutic targets. Drug development and patient-specific therapy predictions are aided by machine learning techniques such as deep learning and network-based approaches, which provide insights on the bioactivities and molecular characteristics of phytochemicals.

Limitations of Phytochemistry

The use of phytochemicals in medication development has advantages, yet there are still drawbacks. Environmental considerations make it challenging to standardize the complex and varied phytochemical compositions of plants. Research can be hampered by the time-consuming and low-yield nature of extraction and purification. While some phytochemicals are difficult to optimize due to their complicated structures, others have low levels of stability, solubility, and bioavailability. Concerns of toxicity and safety must also be addressed. Nevertheless, these challenges are being progressively overcome by further study and developments, increasing the potential of phytochemicals in drug discovery (Onukwuli, Izuchukwu, & Paul-Chima, 2024).

Conclusion

A better knowledge of how phytochemicals might impact upstream endogenous cellular defense systems has led to an increase in research into their potential use in disease prevention and therapy. While nutraceutical medicine aims to preserve the bioactive qualities of plants as closely as possible to their natural state, pharmaceutical medicine has long strived to identify the building blocks for new drugs. The molecular structure of phytochemicals determines their bioavailability. A new strategy is required since drug discovery has a poor success rate. The first step in creating novel treatments for infectious and non-communicable diseases is to take inspiration from natural items. We can now better understand these intricate natural chemicals thanks to technological breakthroughs, which has resulted in the creation of novel drugs. Numerous well-known medications have natural origins. Because of this, creating new therapeutic medications using natural ingredients is a very effective tactic in this period of rapidly developing science and technology.

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