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Medicinal Plants as Sources of Multi-Target Therapeutics: Advances in Phytochemistry and Computational Biology

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ABSTRACT: Medicinal plants represent a valuable source of structurally diverse bioactive compounds with significant potential for the development of multi-target therapeutics against complex diseases. Unlike conventional single-target drugs, phytochemicals can simultaneously modulate multiple molecular pathways, offering improved therapeutic efficacy and reduced susceptibility to drug resistance. Recent advances in phytochemistry have facilitated the isolation and characterization of a wide range of secondary metabolites, while computational biology has transformed natural product research through molecular docking, molecular dynamics simulations, network pharmacology, artificial intelligence, and multi-omics approaches. The integration of these technologies enables efficient target identification, virtual screening, pharmacokinetic prediction, and lead optimization, thereby accelerating phytopharmaceutical discovery. This review highlights recent progress in medicinal plant-derived multi-target therapeutics, emphasizing the complementary roles of phytochemical diversity and computational biology in modern drug discovery. Furthermore, it discusses current challenges, emerging opportunities, and future perspectives for translating plant-based bioactive compounds into safe, effective, and evidence-based therapeutic agents.

1. INTRODUCTION

Medicinal plants have been a source of therapeutic agents for thousands of years and still remain a vital source of drugs today due to the wide range of their phytochemical diversity and pharmacologic activities (1,2). Natural products have been the source of 25% of the currently approved drugs, either directly or as a natural product scaffold, further underscoring the relevance of medicinal plants in drug development. Bioactive secondary metabolites like alkaloids, flavonoids, terpenoids, phenolics, glycosides, and saponins have various biological activities that have seen them be used in the prevention and treatment of various diseases in humans such as cancer, diabetes mellitus, cardiovascular disease, neurodegenerative diseases, inflammatory diseases, and microbial infections (3). The amazing structure diversity of the compounds also creates a wide range of new chemical entities that could interact with multiple biological targets, and medicinal plants are now considered as interesting candidates to develop future therapeutics (4). Traditional drug discovery has been mainly based on the "one drug–one target–one disease" concept. This approach has worked for diseases with single molecular abnormalities, but in most cases works poorly for multifactorial diseases with multiple genetic, protein, signaling pathway and environmental interactions (5). Chronic diseases like cancer, Alzheimer's disease, metabolic syndrome, and autoimmune diseases are not caused by a single molecular defect, but rather by dys- or loss-regulation of networks of interconnected biological processes. Thus, therapeutic approaches that could target multiple molecules in one shot have become of great interest. This is called the concept of polypharmacology or multi-target therapeutics (6) to increase clinical efficacy and reduce drug resistance and side effects of highly selective drugs. The natural composition of medicinal plant products is well-suited for multi-target therapy, as they often consist of complex mixtures of phytochemicals with synergistic or complementary pharmacological effects. Plant metabolites show broad therapeutic effects compared to synthetic single-target drugs, as they tend to target multiple signaling pathways involved in oxidative stress, inflammation, apoptosis, angiogenesis, immune function and cellular metabolism (7). The identification and characterization of thousands of plant metabolites have been greatly facilitated by recent advances in phytochemistry, together with the use of sophisticated analytical platforms such as high-performance liquid chromatography (HPLC), liquid chromatography–mass spectrometry (LC–MS), gas chromatography–mass spectrometry (GC–MS), and nuclear magnetic resonance (NMR) spectroscopy (2). At the same time, the field of computational biology has transformed the landscape of phytopharmaceutical research by introducing a series of advanced methodologies, such as molecular docking, molecular dynamics simulations, network pharmacology, systems biology, artificial intelligence (AI), and machine learning, into the drug discovery process. These computational methods can be used to identify targets, perform virtual screening, analyze interaction networks, predict pharmacokinetics and optimize leads, and can save a lot of time and money in the traditional experimental screening process (8). Thus, with the combination of phytochemistry and computational biology, a well-worked out roadmap has been created to identify evidence-based multi-target therapeutics from medicinal plants. In view of this, this review brings together the latest advancement in medicines derived from medicinal plants, which have multi-target activities, and combines the progress achieved in plant chemistry and computational biology. The phytochemical diversity, mechanisms of multi-target pharmacology, computational approaches in natural product drug discovery and future prospects for the development of medicinal plant-derived bioactive compounds as clinically viable therapeutic agents are discussed.

2. DIVERSITY OF PHYTOCHEMICALS AND THEIR MULTI-TARGET THERAPEUTIC POTENTIAL.

This medicinal value of medicinal plants is mainly due to its unique phytochemical diversity consisting of thousands of structurally different secondary metabolites with different biological activity. Phytochemicals can naturally target multiple proteins, signaling pathways and metabolic networks, and are, therefore, good candidates for multi-target therapeutics (9,10). This polypharmacological profile has been of great interest for the treatment of diseases that involve a complex set of biological pathways, including multifactorial diseases such as cancer, diabetes mellitus, cardiovascular diseases, neurodegenerative diseases, chronic inflammatory diseases, and microbial infections, where the regulation of multiple pathways is necessary for the best therapeutic efficacy (9,11). Phytochemicals are generally divided into alkaloids, flavonoids, terpenoids, phenolic acids, tannins, glycosides, lignans, coumarins and saponins. They are produced as secondary metabolites to resist environmental stress, oxidative damage, microbial pathogens, and herbivores, but also have significant pharmacological activity in humans (10,12). Alkaloids like berberine have antimicrobial, antidiabetic, anticancer effects through modulation of AMP-activated protein kinase (AMPK), nuclear factor-kappa B (NF-$\varkappa$B), and mitogen-activated protein kinase (MAPK) pathways. Quercetin and kaempferol are flavonoids with strong antioxidant and anti-inflammatory effects by modulating the activity of reactive oxygen species (ROS), phosphoinositide 3-kinase/protein kinase B (PI3K/Akt) and nuclear factor erythroid 2-related factor 2 (Nrf2) signaling pathways. Likewise, terpenoids like artemisinin and withanolides have been found to modulate apoptosis, angiogenesis and

immune responses, while phenolic compounds, such as curcumin and resveratrol have been shown to have a wide spectrum of activity, affecting multiple molecular targets related to inflammation, oxidative stress and carcinogenesis (11–13). Medicinal plants have multiple therapeutic applications, which are mainly attributed to synergism interactions between their phytochemical constituents. A collection of compounds in a plant extract often have synergistic or additive effects, by affecting different molecular pathways. These interactions have been shown to lead to greater therapeutic efficacy, lower effective doses, and lower rates and severity of side effects relative to individual drugs (9,13). Emerging evidence indicates that phytochemical combinations may simultaneously regulate inflammatory mediators, cytokines, transcription factors, metabolic enzymes and apoptotic proteins, thereby providing comprehensive disease management strategies that are hard to achieve by single-target drugs alone (14). The development of analytical technologies such as high-performance liquid chromatography (HPLC), liquid chromatography–mass spectrometry (LC–MS), gas chromatography–mass spectrometry (GC–MS), nuclear magnetic resonance (NMR) spectroscopy, and metabolomics-based profiling has greatly accelerated modern phytochemical research. These platforms will allow for high-resolution identification, structural characterization, and quantitative analysis of plant metabolites, which will help to discover new bioactive compounds and make herbal medicines more standardized (10,15). Additionally, curated phytochemical databases have helped to combine chemical data with biological targets, disease associations, and pharmacokinetic properties, and have helped to link traditional medicinal knowledge with computational drug discovery (16). Figure 1 illustrates how diverse phytochemical classes collectively regulate multiple molecular targets and signaling pathways to produce therapeutic effects in complex diseases.

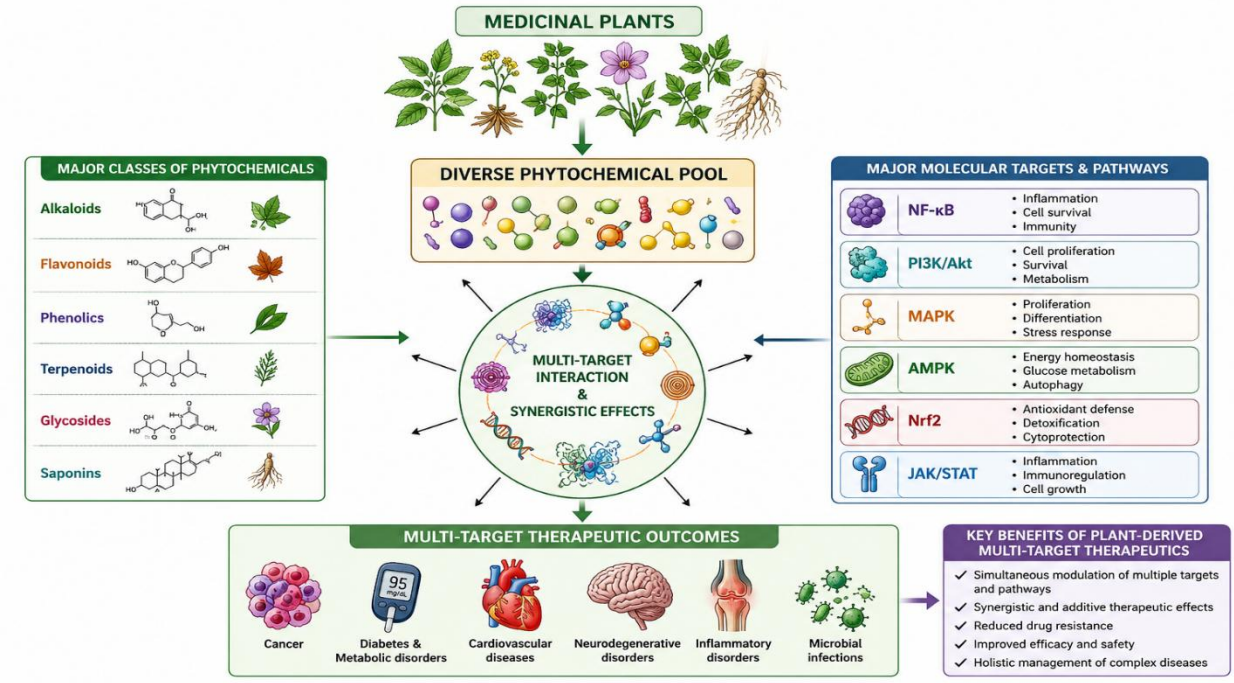

Figure 1. Phytochemical diversity, molecular targets, and multi-target therapeutic potential of medicinal plants.

Multi-target therapeutics has a wide range of applicability as illustrated by representative medicinal plants and their principle phytochemicals with applicability across various conditions of diseases. Curcuma longa (curcumin) modulates inflammatory and apoptotic pathways involved in cancer and inflammatory diseases and Withania somnifera (withanolides) has been found to have neuroprotective, immune modulating and anticancer properties. Berberis species contain berberine that is effective against glucose metabolism and inflammation, and microbial infections, while Camellia sinensis contains epigallocatechin gallate with antioxidant and cardioprotective properties. Likewise, resveratrol, a metabolite extracted from Vitis vinifera, affects oxidative stress, mitochondrial activity and inflammatory signaling, positioning it as a compound with a wide range of therapeutic applications using plant metabolites (12-18).

Table 1. Representative medicinal plants, major phytochemicals, molecular targets, and therapeutic applications.

Medicinal Plant	Major Phytochemical	Major Molecular Target(s)	Therapeutic Applications
Curcuma longa	Curcumin	NF-κB, COX-2, STAT3	Cancer, inflammation
Withania somnifera	Withanolides	PI3K/Akt, p53, HSP90	Neurodegenerative disorders, cancer
Berberis vulgaris	Berberine	AMPK, MAPK, NF-κB	Diabetes, obesity, microbial infections
Camellia sinensis	Epigallocatechin gallate (EGCG)	Nrf2, VEGF, MAPK	Cardiovascular diseases, cancer
Vitis vinifera	Resveratrol	SIRT1, AMPK, NF-κB	Aging-related disorders, metabolic diseases
Glycyrrhiza glabra	Glycyrrhizin	HMGB1, TLR4	Viral infections, inflammation
Andrographis paniculata	Andrographolide	JAK/STAT, NF-κB	Respiratory diseases, inflammatory disorders

Overall, the remarkable chemical diversity of medicinal plants provides an extensive repository of bioactive molecules capable of modulating complex biological networks. When combined with advanced phytochemical profiling and systems-level biological investigations, these natural products offer a promising foundation for the development of safe, effective, and evidence-based multi-target therapeutics capable of addressing the growing burden of chronic and multifactorial diseases (10,17,18).

3. COMPUTATIONAL BIOLOGY IN MEDICINAL PLANT-BASED DRUG DISCOVERY

The increasing complexity of chronic diseases has accelerated the adoption of computational biology as an indispensable component of medicinal plant-based drug discovery. Conventional phytopharmaceutical research largely depends on bioassay-guided fractionation and experimental validation, which are often labor-intensive, time-consuming, and expensive. Computational approaches overcome these limitations by enabling rapid identification of bioactive compounds, prediction of molecular targets, assessment of pharmacokinetic properties, and prioritization of promising lead molecules before experimental investigation (19,20). Consequently, the integration of phytochemistry with computational biology has significantly enhanced the efficiency and success rate of natural product research. Among the available computational techniques, molecular docking remains one of the most widely employed methods for evaluating the interaction between phytochemicals and disease-associated proteins. Docking algorithms predict the binding orientation, affinity, and intermolecular interactions of ligands within the active site of target proteins, thereby facilitating virtual screening of hundreds to thousands of plant-derived compounds (19,21). Numerous phytochemicals, including curcumin, berberine, quercetin, resveratrol, andrographolide, and withaferin A, have demonstrated favorable docking scores against molecular targets involved in inflammation, cancer progression, diabetes, and neurodegeneration, providing valuable insights into their potential mechanisms of action (20–22). Although docking provides an initial estimate of ligand–protein interactions, it represents a static model that cannot fully describe the dynamic behavior of biomolecular complexes. Molecular dynamics (MD) simulation addresses this limitation by evaluating the structural stability, conformational flexibility, hydrogen bonding patterns, and binding free energy of ligand–receptor complexes under physiologically relevant conditions (23). MD simulations therefore complement docking studies by confirming the stability of predicted interactions and identifying conformational changes that influence biological activity. The combined application of molecular docking and molecular dynamics has become a standard strategy for validating phytochemicals before in vitro and in vivo investigations (23,24). Network pharmacology has emerged as another powerful computational strategy for understanding the multi-target mechanisms of medicinal plants. Unlike conventional pharmacology, which focuses on individual targets, network pharmacology investigates complex interactions among phytochemicals, proteins, genes, signaling pathways, and diseases. Compound–target networks, protein–protein interaction (PPI) networks, Gene Ontology (GO) enrichment, and Kyoto Encyclopedia of Genes and Genomes (KEGG) pathway analyses collectively provide

a systems-level understanding of therapeutic mechanisms (25,26). This holistic approach is particularly suitable for herbal medicines because plant extracts usually contain numerous bioactive constituents that regulate interconnected biological pathways rather than single molecular targets (26).

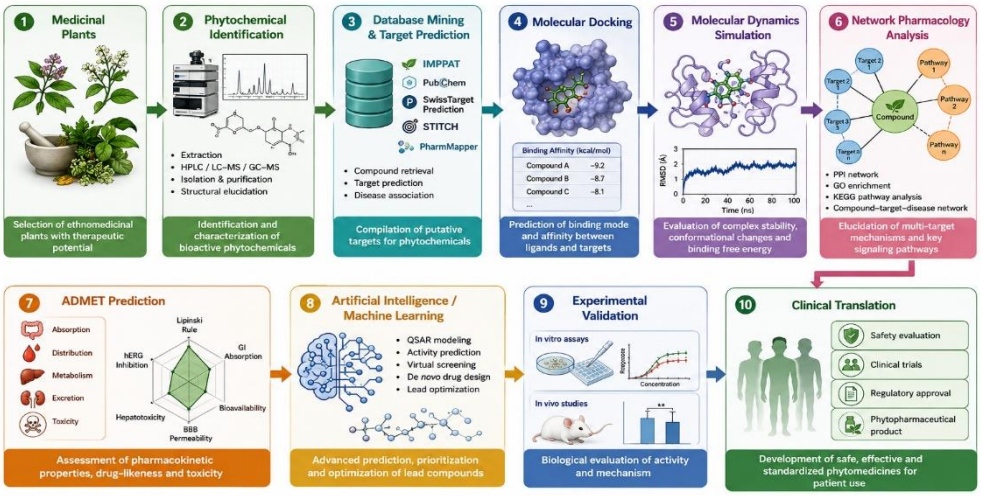

Figure 2. Computational biology workflow for medicinal plant-based multi-target drug discovery

Artificial intelligence (AI) and machine learning (ML) have further transformed natural product drug discovery by enabling the analysis of large and complex biological datasets. Machine learning algorithms can identify hidden relationships between chemical structures and biological activities, predict drug–target interactions, estimate toxicity, and optimize lead compounds with remarkable accuracy (27,28). Deep learning models have also demonstrated considerable promise in de novo drug design, compound prioritization, and prediction of pharmacological properties from high-dimensional datasets. These approaches substantially reduce the cost and time associated with conventional screening while improving the likelihood of identifying clinically relevant phytochemicals (28). In parallel, multi-omics technologies, including genomics, transcriptomics, proteomics, metabolomics, and lipidomics, have expanded the scope of computational phytopharmacology. Integration of omics datasets enables comprehensive characterization of disease-associated molecular networks and facilitates identification of biomarkers responsive to phytochemical intervention (29). When combined with network pharmacology, multi-omics analyses provide a deeper understanding of the mechanisms underlying the therapeutic efficacy of medicinal plants and support the development of personalized phytomedicine. Another critical aspect of computational biology is the prediction of pharmacokinetic and toxicological properties through ADMET (absorption, distribution, metabolism, excretion, and toxicity) analysis. Early assessment of ADMET characteristics allows researchers to eliminate compounds with poor bioavailability or unacceptable toxicity before costly experimental studies are initiated (30). Computational prediction tools have therefore become an integral component of modern phytopharmaceutical research by improving lead optimization and increasing the probability of clinical success. Several publicly available databases have substantially accelerated computational medicinal plant research by providing curated information on phytochemicals, protein structures, biological pathways, and drug-like properties. Resources such as IMPPAT, PubChem, ChEMBL, DrugBank, Protein Data Bank (PDB), BindingDB, STRING, STITCH, KEGG, and SwissADME enable efficient integration of chemical, biological, and pharmacological information, thereby supporting comprehensive in silico investigations (31,32). The interoperability of these resources has facilitated systems-level analyses that bridge traditional medicinal knowledge with evidence-based drug discovery. Collectively, computational biology has transformed medicinal plant research from empirical screening toward a rational, data-driven approach. The integration of molecular modeling, network pharmacology, artificial intelligence, multi-omics technologies, and predictive pharmacokinetic analyses has significantly accelerated the identification of multi-target phytochemicals with therapeutic potential. Continued advances in computational methodologies are expected to further strengthen the translation of medicinal plant-derived bioactive compounds into clinically effective and evidence-based therapeutics for complex human diseases (19–32).

Table 2. Common computational biology tools and databases used in medicinal plant-based multi-target drug discovery.

Tool/Database	Category	Primary Application	Typical Output
PubChem	Chemical database	Retrieval of phytochemical structures and physicochemical information	Chemical structures, molecular descriptors, and compound properties
Protein Data Bank (PDB)	Structural database	Retrieval of experimentally determined three-dimensional protein structures	3D structures of target proteins
AutoDock Vina	Molecular docking	Prediction of ligand–protein binding interactions	Binding affinity scores and binding poses
GROMACS	Molecular dynamics	Simulation of ligand–protein complex stability and dynamics	RMSD, RMSF, hydrogen bonds, and trajectory analysis
STRING	Protein interaction database	Construction of protein–protein interaction (PPI) networks	Functional interaction networks
KEGG	Pathway database	Functional annotation and pathway enrichment analysis	Biological pathways and signaling networks
SwissADME	ADMET prediction	Evaluation of drug-likeness and pharmacokinetic properties	ADME profile, Lipinski's rule, bioavailability, and physicochemical parameters
ChEMBL	Bioactivity database	Retrieval of compound–target bioactivity data	Bioactivity values (IC_{50}, EC_{50}, Ki, Kd) and target information
DrugBank	Drug database	Drug–target interaction and pharmacological information	Drug mechanisms, molecular targets, and pharmacological profiles
Cytoscape	Network visualization software	Visualization and analysis of compound–target and pathway networks	Biological interaction networks and topological analysis

4. CHALLENGES, FUTURE PERSPECTIVES, AND CLINICAL TRANSLATION

Despite remarkable progress in medicinal plant research, several scientific and translational challenges continue to limit the successful development of plant-derived multi-target therapeutics. One of the primary obstacles is the intrinsic complexity of medicinal plants, as a single extract may contain hundreds of phytochemicals with varying concentrations depending on geographical origin, cultivation conditions, harvesting season, and extraction methods (33). Such variability complicates the standardization of herbal preparations, often resulting in inconsistent pharmacological efficacy and reproducibility across experimental studies. Consequently, establishing standardized quality control protocols remains an essential prerequisite for the clinical acceptance of phytopharmaceuticals (33). Another major challenge involves the limited bioavailability of many bioactive phytochemicals. Although compounds such as curcumin, resveratrol, quercetin, and epigallocatechin gallate exhibit promising pharmacological activities, their poor aqueous solubility, rapid metabolism, and limited systemic absorption substantially reduce their therapeutic potential in vivo (34). Advances in nanotechnology, lipid-based delivery systems, phytosomes, polymeric nanoparticles, and targeted drug delivery platforms have demonstrated considerable promise in improving the pharmacokinetic behavior of these compounds. Nevertheless, further preclinical and clinical investigations are required to confirm their long-term safety, efficacy, and scalability for routine clinical application (34). The translation of computational predictions into experimental and clinical evidence also remains a significant challenge. Molecular docking, molecular dynamics simulations, network pharmacology, and artificial intelligence provide valuable insights into compound–target interactions; however, computational predictions alone cannot fully replicate the complexity of biological systems (35). Experimental validation through in vitro assays, animal studies, pharmacokinetic investigations, and well-designed clinical trials is therefore essential to confirm computational findings and establish reliable therapeutic efficacy. Strengthening the integration of computational and

experimental approaches will significantly improve confidence in medicinal plant-based drug discovery (35). Regulatory approval represents another important barrier to the widespread clinical use of phytopharmaceuticals. Compared with conventional synthetic drugs, herbal medicines frequently encounter difficulties related to quality assurance, batch-to-batch consistency, safety evaluation, and regulatory harmonization across different countries (36). The implementation of Good Agricultural and Collection Practices (GACP), Good Manufacturing Practices (GMP), standardized extraction procedures, and evidence-based regulatory frameworks will be critical for ensuring product quality, patient safety, and international acceptance of medicinal plant-derived therapeutics (36). Recent developments in artificial intelligence, systems pharmacology, and multi-omics technologies are expected to reshape the future of phytopharmaceutical research. Integration of genomics, transcriptomics, proteomics, metabolomics, and metabolite profiling with machine learning algorithms enables comprehensive characterization of disease-associated molecular networks and facilitates the identification of highly specific phytochemical combinations for precision medicine (37). These technologies provide opportunities to discover novel biomarkers, predict therapeutic responses, optimize drug combinations, and accelerate personalized phytotherapy. Figure 3 should illustrate the future roadmap beginning with medicinal plant resources, followed by phytochemical profiling, multi-omics integration, artificial intelligence and machine learning, network pharmacology, precision medicine, experimental validation, regulatory standardization, and ultimately clinical translation of evidence-based phytopharmaceuticals. Future research should also emphasize sustainable utilization of medicinal plant resources through conservation strategies, cultivation programs, and environmentally responsible harvesting practices. Combining traditional ethnopharmacological knowledge with advanced computational biology, high-throughput analytical technologies, and precision medicine approaches will accelerate the discovery of safer, more effective, and scientifically validated phytotherapeutics. Such multidisciplinary integration has the potential to transform medicinal plant research into a modern evidence-based discipline capable of addressing the growing global burden of complex chronic diseases (38).

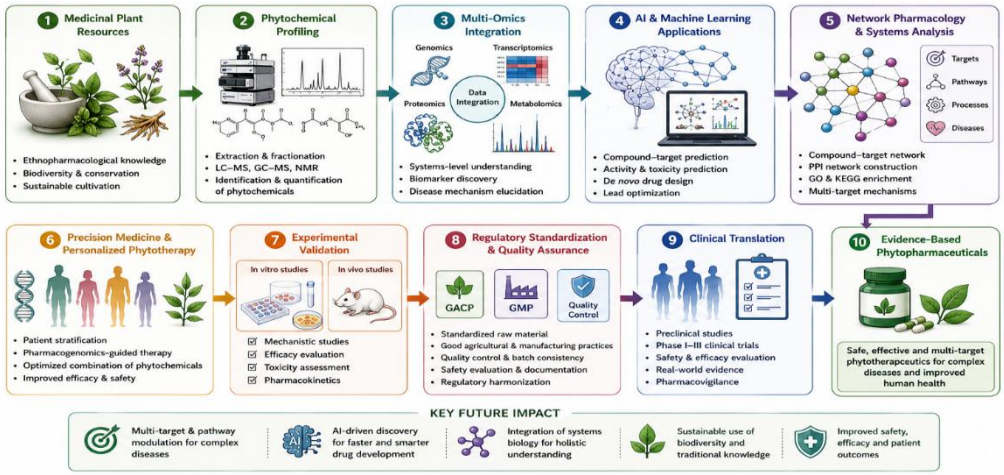

Figure 3. Future perspectives for AI-driven and systems biology-enabled medicinal plant-based multi-target drug discovery.

5. CONCLUSION

Medicinal plants remain an invaluable source of structurally diverse bioactive compounds with tremendous potential to be used in the development of multi-target therapeutics for complex human diseases. The major advantage of phytochemicals over the conventional single-target drugs is that they can act simultaneously on multiple targets and interconnected signaling pathways, providing a comprehensive therapeutic approach to diseases with multifactorial pathogenesis, such as cancer, diabetes mellitus, cardiovascular disorders, neurodegenerative diseases, inflammatory conditions, and infectious diseases. With the development of phytochemical profiling techniques in recent years, the knowledge of natural products has been significantly advanced through discovery of numerous phytochemicals from plants, and computational biology has been greatly revolutionized by molecular docking, molecular dynamics simulation, network pharmacology, artificial intelligence, and multi-omics integration in natural products research. In sum, these technologies have been instrumental in speeding up target identification, lead optimization, prediction of pharmacokinetics, and mechanistic research, in addition to cutting the time and expense of traditional drug discovery. Although these advances have been made, there are still issues of phytochemical standardization,

bioavailability, experimental validation, regulatory harmonization, and clinical translation that will be crucial to the broad use of medicinal plant-based compounds for therapeutic purposes. Multidisciplinary research efforts, involving phytochemistry, computational biology, pharmacology and nanotechnology, as well as clinical studies, will be necessary to overcome these challenges and bring some of these phytochemicals to fruition as evidence-based medicines. The future of integration of artificial intelligence, systems pharmacology, precision medicine and sustainable use of medicinal plant resources will further drive the discovery of safer and more effective multi-target therapeutics with clinical validation. In summary, the integration of phytochemistry and computational biology is a powerful and rational approach for the development of medicinal plant-based drug discovery and presents exciting opportunities to tackle the increasing global burden of complex diseases with novel, effective and sustainable therapeutic interventions.

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