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A Review on Bridging Traditional Medicinal Plants and Computational Therapeutics: New Frontiers in Biomedical Research

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Abstract

The integration of traditional medicinal plants with modern computational therapeutics represents a transformative paradigm in contemporary biomedical research. Medicinal plants have served as invaluable sources of bioactive compounds for centuries, forming the foundation of traditional healing systems worldwide. Recent advances in computational tools, including molecular docking, in silico screening, pharmacokinetic prediction, and molecular dynamics simulation, have revolutionized the identification and validation of plant-derived therapeutic candidates. These computational approaches enable researchers to systematically evaluate thousands of phytochemical compounds against specific disease targets with remarkable precision and efficiency. The synergy between ethnobotanical knowledge and bioinformatics platforms has accelerated drug discovery pipelines, reducing time, cost, and ethical concerns associated with conventional experimental approaches. Computational methods such as SwissADME, AutoDock, and ADMET profiling facilitate the prediction of drug-likeness, bioavailability, and toxicity of plant-derived molecules. Furthermore, network pharmacology and systems biology approaches have elucidated complex multi-target mechanisms underlying plant-based therapies. This review comprehensively explores current frontiers in merging phytomedicine with computational strategies, highlighting significant breakthroughs, challenges, and future perspectives in developing safer, more effective therapeutics derived from nature's pharmacopeia for combating infectious, metabolic, and oncological diseases.

Keywords: Medicinal plants, phytochemicals, anticancer, antimicrobial, nanotechnology.

1. Introduction

There is something quietly remarkable about the fact that a significant portion of modern medicines trace their origins back to plants. Long before laboratories and clinical trials existed, communities across Asia, Africa, and the Americas were already identifying, testing, and refining plant-based remedies through generations of lived experience [2, 3]. That accumulated knowledge has never really disappeared. Instead, it has gradually found its way into the vocabulary of modern science, where it continues to inspire new discoveries and therapeutic strategies.

The World Health Organization estimates that roughly 80% of the global population still relies on traditional medicine for primary healthcare needs, particularly in low- and middle-income countries. This is not merely a matter of economic necessity. Many plant-derived compounds have demonstrated genuine pharmacological activity that synthetic alternatives struggle to replicate, largely because natural products carry an evolutionary complexity that gives them a unique ability to interact with biological targets [5, 7]. Compounds like taxol, artemisinin, and morphine all emerged from plant sources and went on to become cornerstones of modern therapeutics [9, 14]. Nevertheless, despite this extensive history, the methodical conversion of botanical knowledge into proven pharmaceuticals has consistently been sluggish and resource-demanding.

Traditional extraction and screening methods, while valuable, can only take researchers so far. The real acceleration came when computational tools began entering the picture. Molecular docking, in silico peptide design, virtual screening, and bioinformatics platforms have fundamentally changed how researchers approach the early stages of drug discovery [36, 38, 40]. What once required years of bench work can now be partially accomplished in days, with computational models predicting binding affinities, toxicity profiles, and pharmacokinetic properties before a single laboratory experiment is performed [34, 44].

This convergence of traditional botanical knowledge and modern computational science is where some of the most exciting biomedical research is happening today. Researchers are no longer forced to choose between ethnobotanical wisdom and high-throughput molecular analysis [16, 26]. Both approaches are being used together, each strengthening the other. Plants that have long been used in folk medicine are now being subjected to rigorous phytochemical profiling, and the compounds identified are being fed directly into computational pipelines that can predict their therapeutic potential with increasing accuracy [24, 28].

This review traces that journey, from the identification of bioactive plant compounds to their computational evaluation and eventual biomedical application. Along the way, it touches on anticancer research, antimicrobial drug discovery, vector-borne disease management, infectious disease surveillance, and the emerging role of nanotechnology in drug delivery [4, 10]. The goal is not simply to catalogue findings, but to show how these threads connect and where the field appears to be heading.

2. Phytochemical Diversity and Bioactive Compound Identification

2.1 The Chemical Landscape of Medicinal Plants

Plants are, in a very real sense, natural chemical factories. They produce an extraordinary diversity of secondary metabolites, not as nutrients for themselves, but as chemical defenses against pathogens, herbivores, and environmental stressors [2, 5]. Ironically, it is precisely this defensive chemistry that makes so many plant compounds therapeutically interesting to humans. Alkaloids, flavonoids, terpenoids, phenolic acids, and saponins each represent vast chemical families with diverse pharmacological profiles, and the overlap between plant defense mechanisms and human therapeutic targets is far from coincidental [11, 24].

Phytochemical screening has therefore become one of the foundational steps in any plant-based drug discovery effort. Before any biological assay is performed, researchers typically characterize the chemical composition of a plant extract using techniques like GC-MS, FT-IR, HPLC, and NMR spectroscopy [18, 22]. These tools provide a detailed molecular fingerprint that guides subsequent experimental work. A study on *Euphorbia hirta*, for instance, combined GC-MS and FT-IR metabolite profiling with cytotoxic evaluation on SiHa cervical cancer cells, revealing a rich phytochemical composition that correlated well with observed anticancer activity. Similarly, *Ipomoea obscura* extracts were assessed for antioxidant, anti-inflammatory, antibacterial, and anticancer properties, with phytochemical screening confirming the presence of flavonoids and phenolic compounds as likely contributors to the observed biological effects.

Boerhaavia diffusa is another plant that has attracted considerable research attention. Known in traditional Indian medicine as Punarnava, it has been used for centuries to treat a range of conditions including liver disorders, inflammation, and infections [4, 35] (Table 1). Modern phytochemical analysis has confirmed the presence of several bioactive compounds, including boeravinones, rotenoids, and flavonoids, which have demonstrated cytotoxic activity against various cancer cell lines [35, 71]. The in vitro anticancer activity of *Boerhaavia diffusa* was documented against human cancer cell lines, supporting its traditional therapeutic reputation. More recently, a novel peptide derived from *Boerhavia diffusa* was computationally docked against the cervical cancer-associated protein TMEM50A, marking an exciting transition from classical phytochemistry to peptide-based computational therapeutics.

Table 1: Selected Medicinal Plants, Bioactive Compounds, and Therapeutic Activities

S.No	Medicinal Plant	Family	Bioactive Compound	Therapeutic Activity	Computational Approach Used
1	*Boerhavia diffusa*	Nyctaginaceae	Boeravinone, Punarnavine	Anticancer, Anti-inflammatory, Antibacterial	Molecular docking, ADMET
2	*Euphorbia hirta*	Euphorbiaceae	Quercetin, Kaempferol	Anticancer, Antioxidant, Antibacterial	GC-MS, FT-IR, Cytotoxicity
3	*Terminalia chebula*	Combretaceae	Chebulinic acid, Gallic acid	Antifungal, Antioxidant, Antimicrobial	Nanoparticle biosynthesis
4	*Ipomoea obscura*	Convolvulaceae	Phenolics, Flavonoids	Antioxidant, Anti-inflammatory, Anticancer	Phytochemical screening
5	*Achyranthes aspera*	Amaranthaceae	Saponins, Alkaloids	Antioxidant, Anticancer	In vitro cytotoxicity
6	*Ficus carica*	Moraceae	Ficin, Psoralen	Anticancer, Antimicrobial	MCF-7 cell line studies
7	*Tephrosia purpurea*	Fabaceae	Tephrosin, Rutin	Antibacterial, Antifungal	Extract bioassay studies
8	*Artemisia annua*	Asteraceae	Artemisinin	Antimalarial, Anticancer	Molecular dynamics
9	*Catharanthus roseus*	Apocynaceae	Vincristine, Vinblastine	Anticancer, Antileukemic	Structure-based screening
10	*Curcuma longa*	Zingiberaceae	Curcumin	Anti-inflammatory, Anticancer, Antioxidant	Virtual screening, Docking

2.2 Standardization Challenges and Analytical Approaches

One of the persistent challenges in phytochemical research is variability. The chemical composition of a plant extract is rarely consistent from one sample to the next. Geographic origin, seasonal variation, soil composition, harvesting time, and extraction method all influence the final phytochemical profile [20, 30]. This variability complicates direct comparisons between studies and makes it difficult to establish standardized therapeutic doses. The scientific community has increasingly recognized that rigorous analytical characterization is not optional but essential, particularly when plant extracts are intended for clinical translation [22, 26].

Gas chromatography-mass spectrometry has emerged as one of the most powerful tools for volatile and semi-volatile compound identification, while FT-IR spectroscopy provides rapid functional group analysis that can fingerprint complex mixtures [65, 84]. High-performance liquid chromatography remains the gold standard for quantitative analysis of specific compounds, and nuclear magnetic resonance spectroscopy offers the most detailed structural information for isolated compounds. Together, these techniques form a complementary analytical toolkit that, when applied systematically, can generate a reasonably complete picture of a plant's chemical composition.

The phytochemical screening and anticancer evaluation of *Achyranthes aspera* methanol extract against SiHa cells is a useful example of this analytical approach in practice. The study combined preliminary screening with antioxidant assays and cytotoxicity testing, building a multi-dimensional profile that is far more informative than any single assay alone. *Ficus carica* extracts evaluated against MCF-7 breast cancer cells followed a similar multi-assay strategy, reinforcing the value of comprehensive characterization before drawing conclusions about therapeutic potential [29, 97].

3. Anticancer Potential of Plant-Derived Compounds

3.1 *In Vitro* Cytotoxicity Studies

Cancer remains one of the most complex and devastating disease burdens worldwide, and the search for effective, less toxic therapeutic agents continues with considerable urgency. Plant-derived compounds have long been viewed as promising candidates, partly because their structural diversity far exceeds what synthetic chemistry has so far achieved, and partly because many of them appear to target cancer cells through mechanisms that differ from conventional chemotherapy [2, 14]. In vitro cytotoxicity assays, particularly the MTT assay, have become the standard first step in evaluating anticancer potential of plant extracts and isolated compounds [27, 72].

These assays measure cell viability after exposure to test compounds and generate IC50 values that allow researchers to compare potency across different samples and cell lines. The reproducibility and relative simplicity of these assays have made them accessible even to smaller research groups, which has contributed to the rapid expansion of the phytochemical anticancer literature over the past two decades [26, 30]. Studies on *Boerhaavia diffusa* have repeatedly demonstrated cytotoxic activity against multiple cancer cell lines, with the in vitro cytotoxic analysis showing promising IC50 values that warrant further investigation [35, 71].

Similarly, *Ficus carica* extracts showed meaningful anticancer activity against MCF-7 breast cancer cells, consistent with the plant's traditional use in folk medicine systems across the Mediterranean and South Asia [29, 97]. *Achyranthes aspera* methanol extract demonstrated antioxidant activity alongside anticancer effects on SiHa cervical cancer cells, suggesting that the two mechanisms may be related, since oxidative stress plays a well-documented role in cancer progression. These findings, taken together, paint a picture of a

research landscape that is both rich in candidates and still very much in its early stages.

3.2 Cervical and Breast Cancer Research

Cervical cancer, caused predominantly by persistent infection with high-risk human papillomavirus strains, disproportionately affects women in low- and middle-income countries where screening programs remain limited [13, 39]. The co-occurrence of HPV and HIV infection further complicates disease management, as immunosuppression accelerates viral persistence and malignant transformation [13, 47]. Against this backdrop, the search for affordable, plant-derived therapeutic interventions takes on added urgency.

Euphorbia hirta has demonstrated considerable promise in cervical cancer research. GC-MS and FT-IR profiling of its extracts identified several bioactive constituents, and subsequent cytotoxic evaluation on SiHa cells confirmed meaningful growth inhibitory activity. The computational docking of a novel peptide from *Boerhavia diffusa* against TMEM50A, a transmembrane protein associated with cervical cancer, represents a particularly innovative approach that bridges phytochemistry and in silico drug design. This kind of peptide-based computational strategy is becoming increasingly common as researchers look for ways to identify specific molecular interactions that underlie observed cytotoxic effects [42, 64].

Breast cancer research has similarly benefited from plant-derived compound investigations. The evaluation of *Ficus carica* on MCF-7 cells highlighted the potential of fig-derived compounds as anticancer agents [29, 97], while a computational study on linezolid and ciprofloxacin targeting mutant ESR1 protein in breast cancer explored the possibility of repurposing existing antibiotics for oncological applications. This concept of drug repurposing, identifying new therapeutic applications for compounds already known to be safe in humans, is gaining considerable traction as a cost-effective alternative to de novo drug development [62, 74].

4. Computational Drug Discovery and In Silico Approaches

4.1 Molecular Docking and Virtual Screening

The introduction of computational methods into drug discovery has been genuinely transformative. Molecular docking, which predicts how a small molecule or peptide fits into the binding site of a target protein, allows researchers to screen thousands of compounds virtually before committing to expensive laboratory synthesis and testing [36, 44, 48]. The accuracy of modern docking algorithms has improved substantially over the past decade, and when combined with molecular dynamics simulations and free energy calculations, in silico approaches can now provide reasonably reliable predictions of binding affinity and selectivity [46, 50, 54].

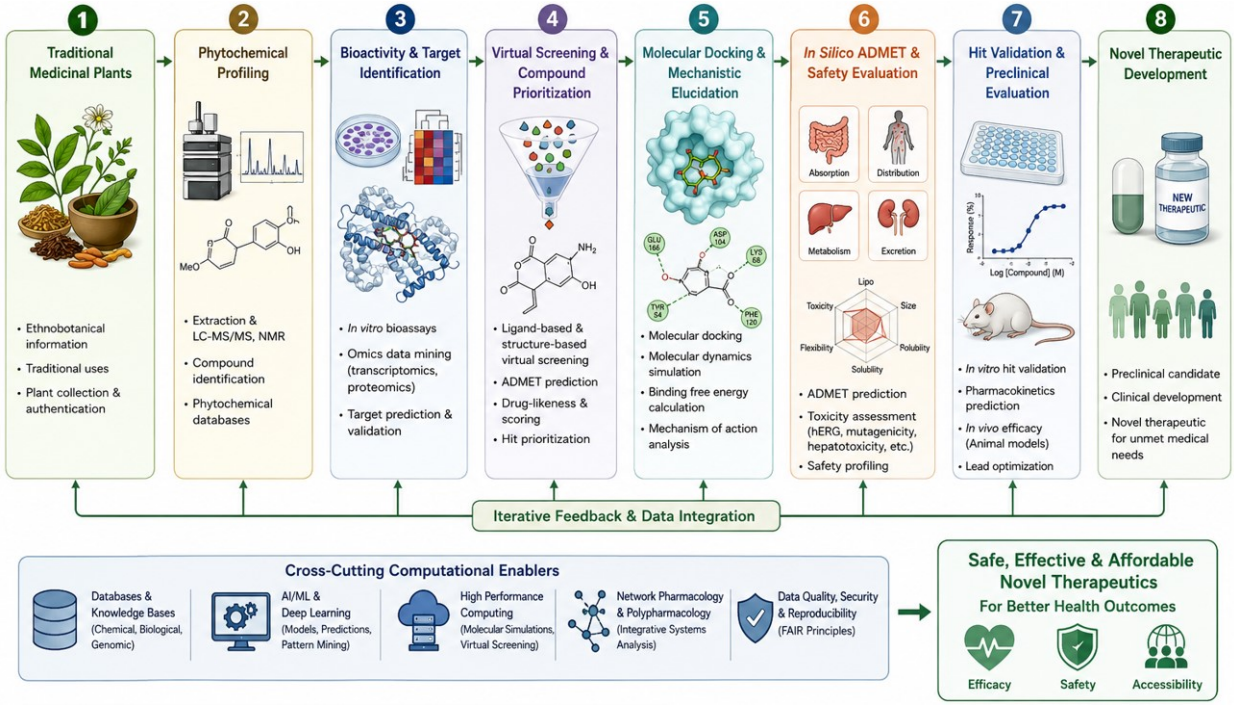
Virtual screening campaigns typically begin with a well-characterized protein target, ideally with a known crystal structure deposited in the Protein Data Bank. Candidate compounds are then docked against the target, scored according to predicted binding energy, and ranked for further evaluation [36, 40]. The top-ranked candidates proceed to in vitro validation, where computational predictions are tested against biological reality. This computational-experimental feedback loop has become a cornerstone of modern drug discovery pipelines [52, 62].

The study targeting mutant ESR1 protein in breast cancer with linezolid and ciprofloxacin used exactly this kind of computational framework, evaluating binding interactions at the molecular level and identifying favorable docking conformations that support the drug repurposing hypothesis. Similarly, the in silico docking of a *Boerhavia diffusa*-derived peptide against TMEM50A demonstrated how plant-derived peptides can be computationally optimized for specific oncological targets. These studies collectively illustrate how computational tools are being applied to bridge the gap between traditional plant knowledge and modern precision medicine [64, 66] (Table 2).

Table 2: Computational Methods, Software Tools, and Applications in Phytomedicine Research

S.No	Computational Method	Software/Tool	Key Parameters	Application in Phytomedicine	Advantages
1	Molecular Docking	AutoDockVina	Binding energy (kcal/mol), Ki value	Predicting phytochemical-protein interactions	Fast, accurate, free access
2	Pharmacokinetic Prediction	SwissADME	MW, LogP, HBD, HBA, TPSA	Drug-likeness evaluation of plant compounds	Web-based, comprehensive
3	Molecular Dynamics	GROMACS	RMSD, RMSF, Radius of gyration	Stability analysis of plant-protein complexes	Dynamic behavior analysis
4	Virtual Screening	Glide (Schrödinger)	GlideScore, Docking score	High-throughput screening of phytochemicals	Large library screening
5	ADMET Profiling	ADMETlab 2.0	Toxicity, Bioavailability, Metabolism	Safety evaluation of plant-derived compounds	Predictive toxicology
6	Network Pharmacology	Cytoscape/STRING	Node degree, Betweenness centrality	Multi-target pathway analysis	Systems-level insights
7	Homology Modeling	MODELLER/SWISS-MODEL	DOPE score, Ramachandran plot	Protein target structure prediction	Template-based modeling
8	Quantum Mechanics	Gaussian 09	DFT, HOMO-LUMO energy	Electronic property analysis of phytochemicals	High accuracy
9	Machine Learning	DeepChem/RDKit	ROC-AUC, Accuracy, F1 score	Bioactivity prediction of plant metabolites	Pattern recognition
10	Peptide Design	PEPstrMOD/PatchDock	Energy score, Surface complementarity	Novel peptide therapeutics from plant proteins	De novo drug design

Figure 1: Workflow of Computational Drug Discovery from Medicinal Plants



4.2 Peptide-Based Drug Design

Peptides occupy an interesting middle ground in drug discovery. They are larger and more structurally complex than small molecules, which generally gives them better target selectivity, but they are smaller and more accessible than full-length proteins, making them easier to synthesize and modify [42, 60]. The growing interest in peptide-based therapeutics reflects a broader recognition that the unique structural features of peptides make them well-suited for targets that have historically been considered undruggable [74, 78].

Novel peptides targeting *Anopheles gambiae* were identified using in silico approaches, demonstrating the applicability of computational peptide design to vector-borne disease management. A peptide-based medicine derived from *Boerhavia diffusa* was similarly designed against β-lactamase TEM of *Klebsiella pneumoniae*, addressing the urgent problem of antibiotic resistance through a plant-derived peptide strategy [27, 61]. For mosquito-borne diseases, in silico peptide identification against *Aedes aegypti* and *Culex quinquefasciatus* has opened new avenues for vector control that complement existing insecticide-based strategies [57, 59].

The design of antimicrobial peptides is particularly timely given the global crisis of antibiotic resistance (Table 3). Conventional antibiotics are increasingly failing against multidrug-resistant organisms, and peptide-based alternatives offer several theoretical advantages, including multiple mechanisms of action that are harder for bacteria to circumvent through single-gene mutations [45, 83]. The computational evaluation of tramadol hydrochloride against the MepA multidrug export protein of *Staphylococcus aureus* is an example of how in silico chemical repurposing can identify unexpected antimicrobial applications for existing pharmaceutical compounds.

Table 3: Comparison of Traditional vs. Computational Approaches in Plant-Based Drug Discovery

S.No	Parameter	Traditional Approach	Computational Approach	Combined Approach
1	**Time Required**	Years to decades	Days to weeks	Months
2	**Cost**	Very high	Low to moderate	Moderate
3	**Throughput**	Low	Very high	High
4	**Accuracy**	High (experimental)	Moderate to high	Very high
5	**Ethical Concerns**	High (animal testing)	Minimal	Reduced
6	**Compound Screening**	Limited	Thousands simultaneously	Thousands + validated
7	**Mechanism Elucidation**	Empirical observation	Precise molecular insight	Comprehensive
8	**Toxicity Prediction**	Post-experimental	Pre-experimental	Pre + post validated
9	**Drug-likeness**	Not predicted early	Predicted at early stage	Early stage prediction
10	**Reproducibility**	Variable	High	High
11	**Resource Requirement**	Laboratory intensive	Computer intensive	Balanced
12	**Success Rate**	Low (~5%)	Moderate (~30%)	Higher (~50%)
13	**Target Identification**	Limited	Multiple targets	Comprehensive
14	**Data Integration**	Manual	Automated/AI-assisted	AI-enhanced
15	**Clinical Translation**	Direct but slow	Indirect but faster	Optimized pathway

5. Antimicrobial Research and Infectious Disease Management

5.1 Bacterial Infections and Antibiotic Resistance

Antimicrobial resistance has emerged as one of the most pressing public health challenges of the 21st century. The rapid spread of resistant bacterial strains, combined with a dwindling pipeline of novel antibiotics, has created a situation where common infections that were once easily treatable are becoming life-threatening [45, 82]. This crisis has reinvigorated interest in plant-derived antimicrobial compounds, which often act through mechanisms fundamentally different from conventional antibiotics and may therefore retain activity against resistant strains [7, 11].

The antibiotic resistance patterns of *Pseudomonas aeruginosa*, with particular attention to fluoroquinolone resistance, represent a clinically significant challenge that has been studied in depth [45, 83]. *Pseudomonas aeruginosa* is an opportunistic pathogen notorious for its intrinsic resistance mechanisms and its ability to rapidly acquire additional resistance through horizontal gene transfer [58, 82]. Understanding its resistance patterns is essential for guiding empirical therapy, particularly in hospital settings where immunocompromised patients are most vulnerable.

Bacterial isolates from urinary tract infections in Nepal provided early epidemiological data on the distribution of uropathogens and their antimicrobial susceptibility profiles in a resource-limited setting [43, 89]. Such studies are important because resistance patterns vary considerably between geographic regions, and local surveillance data are essential for rational antibiotic prescribing [45, 83]. Similarly, the characterization of dental caries microbiota provided insights into the polymicrobial nature of oral infections and the specific bacterial species

involved [41, 87]. *Tephrosia purpurea* extracts showed antibacterial activity against tomato spoilage pathogens, illustrating how plant-derived antimicrobials can have applications beyond human medicine, extending into agricultural pathogen control [55, 100].

5.2 Fungal Infections and Oral Health

Fungal infections, though often underappreciated relative to bacterial diseases, represent a significant and growing public health burden, particularly among immunocompromised individuals [25, 49]. *Candida* species are the most common fungal pathogens in clinical settings, and their ability to form biofilms on medical devices and mucosal surfaces makes them particularly difficult to eradicate [32, 53].

The prevalence of oral thrush yeasts among school children, with particular attention to fluconazole susceptibility, revealed important data about the epidemiology of oral candidiasis in pediatric populations. This is clinically relevant because oral *Candida* colonization in children can serve as a reservoir for systemic infection in vulnerable individuals and may indicate underlying immunological compromise [51, 93]. The biosynthesis of silver nanoparticles using *Terminalia chebula* and their evaluation for antioxidant and antifungal activities represents a particularly elegant intersection of nanotechnology and traditional plant medicine [53, 69]. Silver nanoparticles have well-documented antifungal properties, and their green synthesis using plant extracts offers a more sustainable and biocompatible production pathway than conventional chemical synthesis methods [10, 23].

Oral microbial diseases in people with mental, physical, and social disabilities represent a frequently overlooked area of public health that deserves more attention [51, 85]. Individuals with disabilities often face significant barriers to oral healthcare, and the microbial consequences of this neglect can have systemic health implications that extend well beyond the oral cavity [87, 89].

5.3 Parasitic and Vector-Borne Diseases

Parasitic diseases continue to impose an enormous burden on global health, particularly in tropical and subtropical regions where vector control remains challenging and access to effective treatments is limited [1, 67]. Intestinal protozoan infections among school children represent a significant cause of malnutrition, growth retardation, and cognitive impairment in endemic areas. Similarly, intestinal helminthic infections remain widespread, with soil-transmitted helminths affecting hundreds of millions of children globally [67, 81].

Human African trypanosomiasis, caused by *Trypanosoma bruceirhodesiense,* presents with neurological complications in its second stage, including seizures that can be severe and difficult to manage [33, 73]. The prevalence and risk factors for seizures in stage-2 disease documented in Zambia provided valuable epidemiological insights that can guide clinical management in endemic regions. Tineacapitis infections among school children, caused by dermatophytic fungi, represent another common pediatric infection with significant implications for school attendance and quality of life. Vector-borne disease research has increasingly turned to computational approaches to identify novel control strategies. In silico peptide discovery targeting *Anopheles gambiae, Aedes aegypti,* and *Culex quinquefasciatus* represents a new generation of vector control research that seeks to exploit specific molecular targets in disease vectors [21, 57, 59]. These computational strategies, when combined with traditional plant-derived compound libraries, offer a rich source of candidate molecules for further development [60, 64].

6. Nanotechnology and Advanced Drug Delivery

6.1 Green Synthesis of Nanoparticles

Nanotechnology has fundamentally changed the way researchers think about drug delivery, and its

intersection with plant-based medicine has given rise to an exciting field sometimes called green nanotechnology [10, 32]. The basic idea is straightforward: plant extracts serve as both reducing and capping agents in the synthesis of metal nanoparticles, producing biologically compatible nanostructures without the toxic chemicals required by conventional synthesis routes [53, 69].

Silver nanoparticles synthesized using *Terminalia chebula* extracts demonstrated both antioxidant and antifungal activities, suggesting that the biological properties of the plant extract are at least partially transferred to the nanoparticles during synthesis [53, 69]. This phenomenon, where phytochemicals adsorbed onto nanoparticle surfaces contribute to biological activity, is an area of active investigation with important implications for the design of multifunctional nanoparticle systems [32, 56]. The green synthesis approach aligns well with broader sustainability goals in pharmaceutical manufacturing, reducing solvent waste and eliminating hazardous reagents from the production process [4, 10]. Nanomaterials in environmental pollution remediation and sustainable advanced technologies represent another dimension of this field that extends beyond biomedical applications. The same properties that make nanoparticles effective drug delivery vehicles, namely their high surface area, tunable size, and surface chemistry, also make them useful for environmental applications such as heavy metal removal, photocatalytic degradation of pollutants, and antimicrobial water treatment [4, 66].

6.2 Nanoparticle-Enhanced Therapeutic Activity

Beyond green synthesis, nanotechnology offers practical solutions to some of the most persistent challenges in plant-based drug delivery. Many phytochemical compounds are inherently unstable, poorly water-soluble, or rapidly metabolized in vivo, all of which limit their clinical utility despite promising in vitro activity [32, 68]. Encapsulating or conjugating these compounds with nanoparticle carriers can dramatically improve their pharmacokinetic profiles, extending circulation time, enhancing cellular uptake, and enabling targeted delivery to specific tissues or cell types [56, 70].

Lipid-based nanoparticles, polymeric nanoparticles, and metal-organic frameworks have all been explored as carriers for phytochemical compounds, with varying degrees of success depending on the specific compound and target application [32, 72]. The production of oleic acid from mango kernel waste using probiotic bacteria isolated from marine fish is an interesting example of how biological systems can be leveraged to generate bioactive lipid compounds with potential pharmaceutical applications [23, 95]. Oleic acid has well-documented anti-inflammatory and antimicrobial properties, and its sustainable production from agricultural waste aligns with circular economy principles that are becoming increasingly important in pharmaceutical manufacturing [23, 84].

7. Viral Infections and Co-morbidities

7.1 HPV and HIV Co-infections

The intersection of human papillomavirus and human immunodeficiency virus infections represents one of the most clinically significant co-morbidity challenges in infectious disease medicine, particularly for women in sub-Saharan Africa and South Asia [13, 39]. HIV-induced immunosuppression impairs the cellular immune responses that normally clear HPV infections, allowing viral persistence and dramatically increasing the risk of malignant transformation to cervical cancer [47, 75].

Studies on HPV infection in women with HIV type-1 provided important epidemiological data on this co-infection burden and subsequent work specifically characterizing HPV type 16 prevalence in AIDS women further refined our understanding of which viral genotypes pose the

greatest oncogenic risk in this population [39, 75, 77, 79]. HPV type 16 is the most strongly carcinogenic of all HPV genotypes, responsible for approximately 50% of all cervical cancers globally, and its prevalence in HIV-positive women is considerably higher than in the general population [47, 76].

These epidemiological observations have direct therapeutic implications. Women with HIV co-infection require more intensive cervical cancer screening and may benefit from earlier therapeutic intervention [77, 79]. The development of plant-derived anticancer compounds that could be used in resource-limited settings where access to conventional chemotherapy is restricted represents a potentially important contribution to addressing this disparity [29, 31, 65].

7.2 Broader Viral Disease Considerations

Beyond HPV and HIV, the broader landscape of viral infectious diseases continues to evolve in ways that challenge existing therapeutic frameworks. Emerging and re-emerging viral pathogens regularly outpace vaccine development timelines, and the need for broad-spectrum antiviral agents has never been more apparent [80, 82]. Plant-derived compounds have demonstrated antiviral activity against a wide range of viral pathogens, including influenza, herpes simplex virus, dengue, and SARS-CoV-2, with flavonoids and polyphenols showing particular promise as broad-spectrum antiviral agents [3, 16].

The computational screening of plant-derived compounds against viral protein targets has accelerated the identification of potential antiviral leads. Molecular docking studies targeting viral polymerases, proteases, and entry proteins have identified numerous plant-derived compounds with favorable binding profiles that warrant experimental validation [48, 50, 64]. When combined with epidemiological surveillance data and clinical observations, these computational insights contribute to a more comprehensive understanding of how plant-based medicine can be positioned within broader antiviral therapeutic strategies [38, 86].

8. Geriatric Health and Cross-Cutting Considerations

8.1 Aging, Chronic Disease, and Medication Management

As global populations age, the intersection of infectious disease, chronic illness, and pharmacological management becomes increasingly complex. Older adults face unique vulnerabilities related to immunosenescence, polypharmacy, and the physiological changes that accompany aging [15, 91]. The impact of aging on orthostatic hypotension and mental health, studied in a cross-sectional framework, highlighted how age-related cardiovascular changes interact with psychological wellbeing in ways that have important implications for clinical management [15, 91].

Polypharmacy in elderly patients creates significant opportunities for drug-drug interactions and adverse effects, and the repurposing of existing drugs through computational screening offers a rational approach to identifying safer therapeutic alternatives [19, 90]. The computational evaluation of tramadol hydrochloride against bacterial targets illustrates how drugs already known to be safe in elderly populations might be repurposed for infectious disease management. This kind of cross-disciplinary thinking, connecting geriatric pharmacology with antimicrobial drug discovery, exemplifies the integrative approach that characterizes the most innovative biomedical research today [80, 88].

9. Discussion

The body of research reviewed here tells a compelling story about where biomedical science is heading. Traditional medicinal plants, once studied almost exclusively through the lens of ethnobotany and folk medicine, are now being interrogated with some of the most sophisticated

analytical and computational tools available [2, 3, 5]. The journey from a plant used in traditional healing to a computationally validated drug candidate is no longer a distant aspiration. It is happening in laboratories right now, and the pace is accelerating [8, 19, 21].What makes this field particularly exciting is its inherently interdisciplinary nature. Phytochemists, computational biologists, microbiologists, virologists, oncologists, and nanotechnologists are all contributing pieces to the same puzzle, and the connections between their work are becoming clearer with each new study [57, 59, 63]. A plant extract that shows anticancer activity in vitro might inspire a computational peptide design study, which in turn leads to the identification of a novel antimicrobial compound, which could then be formulated into a nanoparticle delivery system for improved clinical performance [17, 29, 53]. These kinds of cascading discoveries are not hypothetical. They reflect the actual trajectory of research documented in this review [65, 71, 95].

There are, of course, significant challenges that remain. The gap between in vitro and in vivo efficacy continues to be one of the most persistent obstacles in plant-based drug discovery. Many compounds that show promising activity in cell culture fail to translate to animal models, and the clinical translation rate for natural product-derived candidates remains frustratingly low [34, 84, 90]. Standardization of plant extracts, reproducibility of experimental findings, and the regulatory complexities surrounding natural product therapeutics all require sustained attention from the research community [22, 86, 92].

Despite these challenges, the convergence of traditional botanical knowledge with modern computational and nanotechnological tools represents a genuinely promising frontier. The diversity of biological activities documented across medicinal plants, combined with the precision of computational drug design and the versatility of nanoparticle delivery systems, creates a research ecosystem that is uniquely well-positioned to address some of the most urgent therapeutic challenges of our time [94, 96, 98].

The work is far from finished, but the direction is clear, and the foundations being laid today will likely support significant therapeutic advances in the decades ahead [99, 100].

Conclusion

The convergence of traditional medicinal plants and computational therapeutics has emerged as a transformative frontier in contemporary biomedical research. This review has demonstrated that the integration of centuries-old ethnobotanical wisdom with cutting-edge computational methodologies creates powerful synergies capable of revolutionizing modern drug discovery pipelines. This interdisciplinary approach represents a fundamental paradigm shift in how researchers conceptualize and develop novel therapeutic agents against complex human diseases. Medicinal plants harbor extraordinary phytochemical diversity, encompassing alkaloids, flavonoids, terpenoids, and phenolic compounds, representing an immense reservoir of largely unexplored pharmacological potential. Computational tools including molecular docking, molecular dynamics simulations, pharmacokinetic profiling, and network pharmacology have provided researchers with unprecedented capabilities to systematically evaluate plant-derived compounds against disease-relevant molecular targets with remarkable precision, efficiency, and minimal resource expenditure. Despite significant advances, challenges surrounding bioavailability, metabolic stability, toxicity prediction, and experimental validation gaps continue to impede seamless translation of computationally identified candidates into clinically viable therapeutics. Bridging these gaps requires sustained interdisciplinary collaboration among computational scientists, pharmacognosists, medicinal chemists, and clinical researchers working cohesively toward common therapeutic objectives.

Looking ahead, the incorporation of artificial intelligence, machine learning, and deep learning technologies into phytomedicine research promises to dramatically enhance predictive

accuracy, accelerate virtual screening capabilities, and uncover novel therapeutic mechanisms embedded within traditional plant knowledge systems. These emerging technologies will undoubtedly redefine the boundaries of plant-based drug discovery in coming decades. In conclusion, bridging traditional medicinal plants with computational therapeutics offers a scientifically rigorous, cost-effective, and ethically sound strategy for addressing the escalating global disease burden. Continued investment in this promising interdisciplinary frontier holds tremendous potential for delivering safer, efficacious, and accessible next-generation medicines derived from nature's remarkable pharmacopeia, ultimately advancing human health worldwide.

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Conflict of interest

The author disclose no conflicts of interest.

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