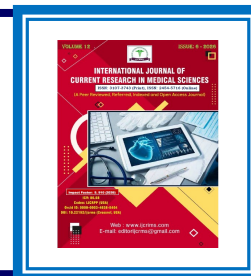




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A Multidisciplinary Review on Natural Products, Peptide Therapeutics, and Nanomedicine in Human Health and Disease: Current Perspectives

Venkatajothi Ramarao

Department of Microbiology, Saveetha Medical College and Hospital, Saveetha Institute of Medical and Technical Sciences (SIMATS), Saveetha University, Thandalam, Chennai - 602105, Tamil Nadu, India.

Correspondence author: Dr. Venkatajothi Ramarao

Address for correspondence: Department of Microbiology, Saveetha Medical College and Hospital, Saveetha Institute of Medical and Technical Sciences (SIMATS), Saveetha University, Thandalam, Chennai - 602105, Tamil Nadu, India.

Email id: drvjothi10@gmail.com; venkatajothir.smc@saveetha.com

Abstract

Natural products, peptide therapeutics, and nanomedicine represent three transformative pillars of modern biomedical research, collectively offering unprecedented opportunities for addressing complex human diseases. This review presents current perspectives on the therapeutic potential and pharmacological significance of these interconnected domains in human health and disease management. Natural products derived from medicinal plants, including *Boerhaaviadiffusa*, *Euphorbia hirta*, *Achyranthesaspera*, *Ficuscarica*, *Ipomoea obscura*, and *Terminaliachebula*, have demonstrated remarkable biological activities encompassing antioxidant, antibacterial, antifungal, anti-inflammatory, and anticancer properties, validating their ethnopharmacological applications and providing scientific foundations for novel drug development. Peptide therapeutics, designed through advanced computational approaches including molecular docking, in silico peptide design, and virtual screening, have emerged as highly selective, efficacious therapeutic candidates targeting cancer-associated proteins, antimicrobial resistance mechanisms, and vector-borne disease pathogens. Nanomedicine, particularly biosynthesized silver nanoparticles and advanced nanomaterials derived from plant extracts, has significantly enhanced drug delivery efficiency, bioavailability, and therapeutic outcomes against microbial infections and cancer. The convergence of these three disciplines, supported by computational methodologies and ethnopharmacological knowledge, represents a powerful integrated framework for

accelerating drug discovery and development. This review highlights current advances, challenges, and future perspectives, emphasizing the translational potential of natural products, peptide therapeutics, and nanomedicine in addressing global health burdens.

Keywords: Peptide therapeutics, silver nanoparticles, antimicrobial activities, Natural products, Computational drug discovery.

1. Introduction

Medicine has always drawn heavily from nature. Long before synthetic chemistry existed, healers relied on roots, bark, leaves, and seeds to treat illness, and many of those early observations have since been validated by rigorous science. Today, natural products remain one of the richest sources of pharmacologically active compounds, contributing directly or indirectly to a significant portion of approved drugs worldwide [1, 2]. What has changed, however, is the sophistication with which we now explore them. Modern analytical techniques, computational modeling, and nanotechnology have collectively transformed how researchers identify, isolate, and deliver bioactive molecules derived from plants and other natural sources [3, 4].

Alongside natural products, peptide-based therapeutics have emerged as a compelling class of medicines. Peptides occupy an interesting space between small molecules and large biologics, combining reasonable specificity with relative ease of synthesis [5, 6]. Researchers have increasingly turned to *in silico* methods to discover novel peptides capable of targeting specific disease-related proteins, from cancer receptors to bacterial enzymes [7, 8]. This computational-first approach has dramatically reduced the time and cost associated with early-stage drug discovery, making it particularly attractive for neglected tropical diseases and drug-resistant infections [9, 10].

Nanomedicine adds yet another dimension to this landscape. The ability to engineer nanoparticles that carry therapeutic payloads, protect them from degradation, and deliver them precisely to target tissues has opened new doors in cancer therapy, antimicrobial treatment, and beyond [11, 12]. Silver nanoparticles biosynthesized from

medicinal plants, for instance, have shown remarkable antifungal and antioxidant properties, combining the benefits of both natural products and nanotechnology in a single system [13, 14]. This convergence is not accidental. It reflects a broader recognition that no single approach is sufficient on its own, and that the most durable solutions will likely emerge from their thoughtful integration.

This review aims to synthesize current knowledge across these three domains, natural products, peptide therapeutics, and nanomedicine, and to explore how they intersect in addressing cancer, infectious diseases, and antimicrobial resistance. By drawing on recent experimental and computational studies, we hope to offer a coherent and accessible overview of where the field stands and where it might be headed.

2. Natural Products in Disease Management

2.1 Phytochemicals and Their Therapeutic Relevance

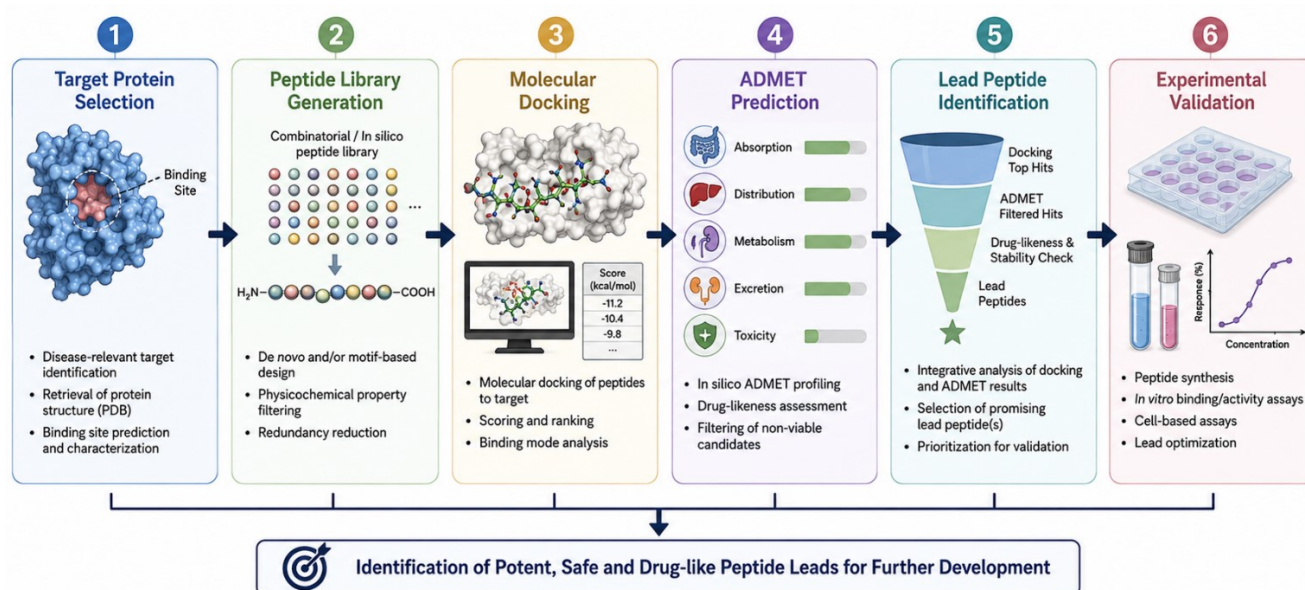
Plants produce an astonishing diversity of secondary metabolites, and many of these compounds have proven to be therapeutically significant. Alkaloids, flavonoids, terpenoids, tannins, and phenolic acids are among the most studied classes, each with distinct mechanisms of action that range from antioxidant scavenging to direct cytotoxicity against cancer cells [15, 16]. What makes phytochemicals particularly appealing is their multi-target nature. Unlike most synthetic drugs designed to hit a single molecular target, plant-derived compounds often interact with multiple pathways simultaneously, which can be both a strength and a complexity [17, 18].

Boerhaavia diffusa, a widely distributed medicinal herb, has attracted considerable attention for its anticancer and cytotoxic properties. Studies have demonstrated its activity against various cancer cell lines, suggesting the presence of potent bioactive constituents that warrant further characterization [2, 24]. Similarly, *Euphorbia hirta* has been evaluated using phytochemical screening, GC-MS, and FT-IR profiling, revealing metabolites with significant cytotoxic effects on SiHa cervical cancer cells. These findings illustrate how traditional plants, often used empirically for centuries, are now being examined through the lens of modern molecular biology.

Ficus carica and *Achyranthes aspera* represent two more examples of medicinal plants with documented anticancer potential. Preliminary studies on *Ficus carica* extracts have shown

encouraging cytotoxicity against MCF-7 breast cancer cells, while methanol extracts of *Achyranthes aspera* have exhibited antioxidant activity alongside anticancer effects in SiHa cells [20, 21]. The consistency of these findings across different plant species and cancer models strengthens the argument that phytochemicals deserve serious consideration as scaffolds for drug development. *I pomoea obscura* is another plant that has been assessed for multiple biological activities. Crude extracts from this species have demonstrated antioxidant, anti-inflammatory, antibacterial, and anticancer properties, suggesting a broad pharmacological profile that could be relevant across several disease contexts. Such multi-activity profiles are common among medicinal plants and reflect the complex mixture of compounds present in whole plant extracts (Figure 1).

Figure1: *In Silico* Peptide Drug Discovery Workflow



2.2 Antioxidant and Anti-inflammatory Properties

Oxidative stress and chronic inflammation are now recognized as central drivers of a wide range of diseases, including cancer, cardiovascular disorders, neurodegenerative conditions, and metabolic syndrome [19, 20]. It is therefore not

surprising that antioxidant and anti-inflammatory activities are among the most frequently evaluated properties of natural products. Many plant extracts show strong free radical scavenging activity in standardized assays such as DPPH and ABTS, and some have demonstrated comparable or superior potency to synthetic antioxidants [21, 22].

The anti-inflammatory potential of natural compounds is equally well-documented. Flavonoids, in particular, have been shown to inhibit key inflammatory mediators including cyclooxygenase enzymes, interleukins, and tumor necrosis factor-alpha [23, 24]. Some researchers have taken this further by exploring computational repurposing strategies, using existing anti-inflammatory drugs as starting points for new applications. For example, tramadol hydrochloride, primarily known as a pain reliever, was computationally evaluated against MepA, the multidrug export protein of *Staphylococcus aureus*, revealing potential antibacterial activity through molecular docking. This kind of cross-disciplinary thinking is becoming increasingly common and productive.

2.3 Oleic Acid and Microbial Biotransformation

An interesting development in natural product research involves the use of probiotic bacteria to produce valuable fatty acids from agricultural waste. Oleic acid, a monounsaturated omega-9 fatty acid with known anti-inflammatory and cardioprotective properties, has been successfully produced from mango kernel waste using probiotic bacteria isolated from marine fish. This approach not only adds value to waste biomass but also offers a sustainable and environmentally friendly route to bioactive lipids. It connects naturally to broader discussions about green chemistry and circular bioeconomy, themes that are gaining traction in pharmaceutical research [25, 26].

Table 1: Selected Medicinal Plants, Their Bioactive Compounds, and Documented Biological Activities

Plant Species	Key Bioactive Compounds	Biological Activities	Cancer/Disease Model
<i>Boerhaavia diffusa</i>	Punarnavine, flavonoids	Anticancer, cytotoxic	Cervical cancer
<i>Euphorbia hirta</i>	Terpenoids, phenolics	Cytotoxic, antioxidant	SiHa cells
<i>Ficus carica</i>	Tannins, flavonoids	Anticancer, antioxidant	MCF-7 cells
<i>Achyranthes aspera</i>	Saponins, alkaloids	Antioxidant, anticancer	SiHa cells
<i>Ipomoea obscura</i>	Phenolics, terpenoids	Anti-inflammatory, antibacterial	Multiple models
<i>Tephrosia purpurea</i>	Flavonoids, rotenoids	Antibacterial	Tomato pathogens

3. Peptide Therapeutics and In Silico Drug Discovery

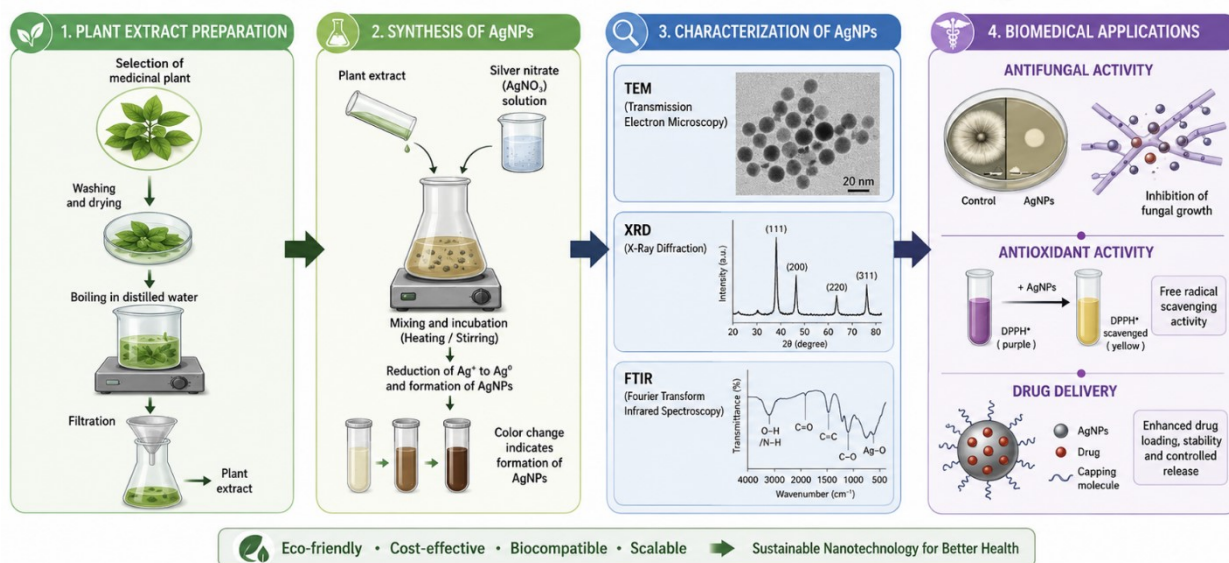
3.1 Rise of Peptide-Based Medicines

Peptides have grown from being biochemical curiosities to serious therapeutic candidates over the past two decades. Their ability to mimic protein-protein interactions, bind with high specificity to target receptors, and be engineered for stability and bioavailability makes them attractive alternatives to both small molecules and large biologics [27, 28]. The global peptide therapeutics market has expanded significantly, driven by advances in solid-phase synthesis, computational design, and a growing

understanding of disease-related protein structures [29, 30].

One of the most exciting developments has been the use of plant-derived peptides as starting points for drug design. Novel peptides derived from *Boerhavia diffusa* have been evaluated through molecular docking against TM50A, a transmembrane protein associated with cervical cancer, showing promising binding affinities that suggest potential therapeutic relevance. This kind of peptide-protein docking study, combining natural product knowledge with computational structural biology, exemplifies the convergent approach that characterizes much of modern drug discovery (Figure 2).

Figure 2: Green Synthesis of Silver Nanoparticles and Their Biomedical Applications



3.2 Computational Approaches in Peptide Discovery

In silico methods have become indispensable in modern drug discovery, particularly for peptide-based therapeutics. Molecular docking, molecular dynamics simulations, pharmacophore modeling, and ADMET prediction tools allow researchers to screen thousands of candidate molecules before committing to expensive wet laboratory experiments [31, 32]. This computational-first approach has proven especially valuable for resource-limited settings and for diseases where experimental infrastructure may be scarce.

Anopheles gambiae, the primary vector of malaria, has been targeted using novel peptides discovered through *in silico* approaches. Computational screening identified peptide candidates with strong predicted binding to key mosquito proteins, offering a potentially new avenue for vector control that could complement existing insecticide strategies. Similarly, novel peptides have been designed against *Aedes aegypti* and *Culex quinquefasciatus* using computational protocols, targeting specific proteins involved in mosquito survival and

reproduction [17, 18]. These studies collectively suggest that peptide-based vector control strategies deserve serious experimental follow-up.

Beyond vector control, *in silico* repurposing has been applied to bacterial targets. A novel peptide derived from *Boerhavia diffusa* was evaluated against β -lactamase TEM of *Klebsiella pneumoniae*, a clinically significant enzyme responsible for antibiotic resistance. The results showed favorable docking scores, suggesting that plant-derived peptides could serve as inhibitors of resistance enzymes, potentially restoring the efficacy of existing antibiotics. This is a particularly promising direction given the global crisis of antimicrobial resistance.

Computational evaluation has also been extended to cancer targets. Linezolid and ciprofloxacin, both established antibiotics, were computationally assessed for their potential to target mutant ESR1 protein in breast cancer, highlighting the possibility of repurposing existing drugs for oncological applications. Such studies underscore the versatility of *in silico* tools in exploring the therapeutic space beyond conventional indications.

Table 2: Summary of *In Silico* Peptide and Drug Discovery Studies

Target Organism/Protein	Peptide/Drug Source	Method Used	Key Finding
TM50A (Cervical cancer)	Boerhaviadiffusa peptide	3D docking	Strong binding affinity
<i>Anopheles gambiae</i> proteins	Novel peptides	In silico screening	Potential vector control
<i>Aedesaegypti</i> proteins	Novel peptides	Computational protocols	Anti-mosquito activity
<i>Culexquinquefasciatus</i>	De novo peptides	Computational protocols	Anti-mosquito activity
β -lactamase TEM (<i>K. pneumoniae</i>)	Boerhaviadiffusa peptide	Molecular docking	Resistance enzyme inhibition
Mutant ESR1 (Breast cancer)	Linezolid, Ciprofloxacin	Computational evaluation	Drug repurposing potential
MepA (<i>S. aureus</i>)	Tramadol hydrochloride	In silico docking	Antibacterial repurposing

4. Nanomedicine and Nanoparticle-Based Therapeutics

4.1 Green Synthesis and Biomedical Applications

Nanomedicine has fundamentally changed how we think about drug delivery and therapeutic design. At the nanoscale, materials acquire unique physical and chemical properties that differ markedly from their bulk counterparts, and these properties can be harnessed for targeted drug delivery, imaging, and therapy [33, 34]. Among the various types of nanoparticles explored for biomedical use, silver nanoparticles have received particularly widespread attention due to their broad-spectrum antimicrobial activity and relative ease of synthesis [35, 36].

Green synthesis, which uses plant extracts or microbial agents as reducing and capping agents, has emerged as a preferred approach for producing silver nanoparticles because it avoids harsh chemicals and aligns with principles of sustainable chemistry [37, 38]. Silver nanoparticles biosynthesized from *Terminaliachebula* extracts have demonstrated significant antifungal and antioxidant activities, combining the inherent bioactivity of the plant with the enhanced properties conferred by the

nanoscale format [12, 22]. This dual functionality is one of the most appealing aspects of green-synthesized nanoparticles in biomedical research.

4.2 Nanomaterials in Environmental and Health Contexts

The relevance of nanomaterials extends beyond direct therapeutic applications. Environmental pollution represents a major global health challenge, and nanomaterials are increasingly being explored as tools for pollution remediation and environmental monitoring. Advanced nanomaterial-based technologies offer promising solutions for detecting and removing heavy metals, organic pollutants, and microbial contaminants from environmental matrices [39, 40].

However, the widespread use of nanomaterials also raises legitimate concerns about their own environmental and health impacts. Nanotoxicology is a rapidly evolving field, and researchers are working to establish clearer guidelines for the safe design and disposal of engineered nanomaterials [41, 42]. The balance between therapeutic promise and potential risk is a recurring theme in nanomedicine, and it underscores the importance of rigorous safety evaluation alongside efficacy studies.

Table 3: Nanoparticle Types, Synthesis Methods, and Biomedical Applications

Nanoparticle Type	Synthesis Method	Plant/Agent Used	Key Activity
Silver nanoparticles	Green synthesis	<i>Terminalia chebula</i>	Antifungal, antioxidant
Silver nanoparticles	Chemical synthesis	N/A	Antimicrobial
Gold nanoparticles	Green synthesis	Various plants	Drug delivery
Zinc oxide NPs	Green synthesis	Medicinal plants	Anticancer, antibacterial
Lipid nanoparticles	Chemical synthesis	N/A	Cancer drug delivery
Polymeric nanoparticles	Emulsion method	N/A	Controlled release

5. Infectious Diseases: Microbial Threats and Natural Solutions

5.1 Parasitic and Fungal Infections

Infectious diseases, particularly those caused by parasites and fungi, continue to impose a heavy burden on human health, especially in low- and middle-income countries. Intestinal protozoan infections remain a significant public health problem among school-aged children, with poor sanitation and overcrowding being key risk factors [1, 47]. Helminthic infections similarly affect millions of children globally, contributing to malnutrition, stunted growth, and impaired cognitive development [13, 48].

Fungal infections, though often underappreciated, are also a considerable concern. Tinea capitis, a fungal infection of the scalp, is particularly prevalent among school children in tropical regions. Oral thrush caused by *Candida* species represents another frequently encountered fungal condition, especially among immunocompromised individuals [31, 49]. The emergence of fluconazole resistance among *Candida* strains has added urgency to the search for novel antifungal agents, and plant-derived compounds and biosynthesized nanoparticles have both shown promise in this regard [12, 50].

5.2 Bacterial Infections and Antimicrobial Resistance

Bacterial infections remain a leading cause of morbidity and mortality worldwide, and the growing problem of antimicrobial resistance threatens to undermine decades of progress in infectious disease management [51, 52].

Pseudomonas aeruginosa, a particularly troublesome opportunistic pathogen, has shown increasing resistance to fluoroquinolone antibiotics, a trend that was documented in clinical isolates from southern India. Understanding antibiotic resistance patterns at the local level is essential for guiding empirical therapy and stewardship programs. Urinary tract infections caused by multidrug-resistant organisms represent another persistent clinical challenge. Studies of bacterial isolates from UTI patients have highlighted the diversity of causative organisms and the variability in resistance profiles across geographic regions [28, 53]. Dental caries, though not typically considered an infectious disease in the classic sense, also involves a complex microbial community, and characterization of these organisms has both diagnostic and therapeutic implications [27, 54].

5.3 HPV, HIV, and Co-Infections

The intersection of human papillomavirus (HPV) and HIV infection presents a particularly challenging clinical and public health scenario. Women living with HIV are at significantly elevated risk of HPV infection, particularly high-risk types such as HPV-16, which is strongly associated with cervical cancer [5, 25]. Studies conducted in India have documented the prevalence of HPV-16 in HIV-positive women and AIDS patients, reinforcing the need for integrated screening and prevention programs [26, 30]. Human African trypanosomiasis, or sleeping sickness, represents yet another infectious disease with devastating neurological consequences. A cross-sectional study conducted in Zambia documented the prevalence of seizures among patients in stage-2 rhodesiense trypanosomiasis,

shedding light on the neurological burden of this neglected tropical disease. These kinds of epidemiological studies are essential for building the evidence base needed to guide clinical management in endemic regions.

Table 4: Infectious Disease Categories, Causative Agents, and Key Findings

Disease Category	Causative Agent	Population Studied	Key Finding
Intestinal protozoa	Multiple protozoa	School children	High prevalence in low-income settings
Helminthic infection	Intestinal helminths	School children	Nutritional impact documented
Tineacapitis	Dermatophytes	School children	Common in tropical regions
Oral thrush	<i>Candida</i> species	School children	Fluconazole resistance noted
UTI	Mixed bacteria	Hospital patients	Geographic resistance variation
HPV-16 & HIV	HPV-16, HIV-1	HIV-positive women	Elevated co-infection risk
Trypanosomiasis	<i>T. b. rhodesiense</i>	Zambian patients	Seizure prevalence in stage-2

6. Cross-Cutting Themes and Future Directions

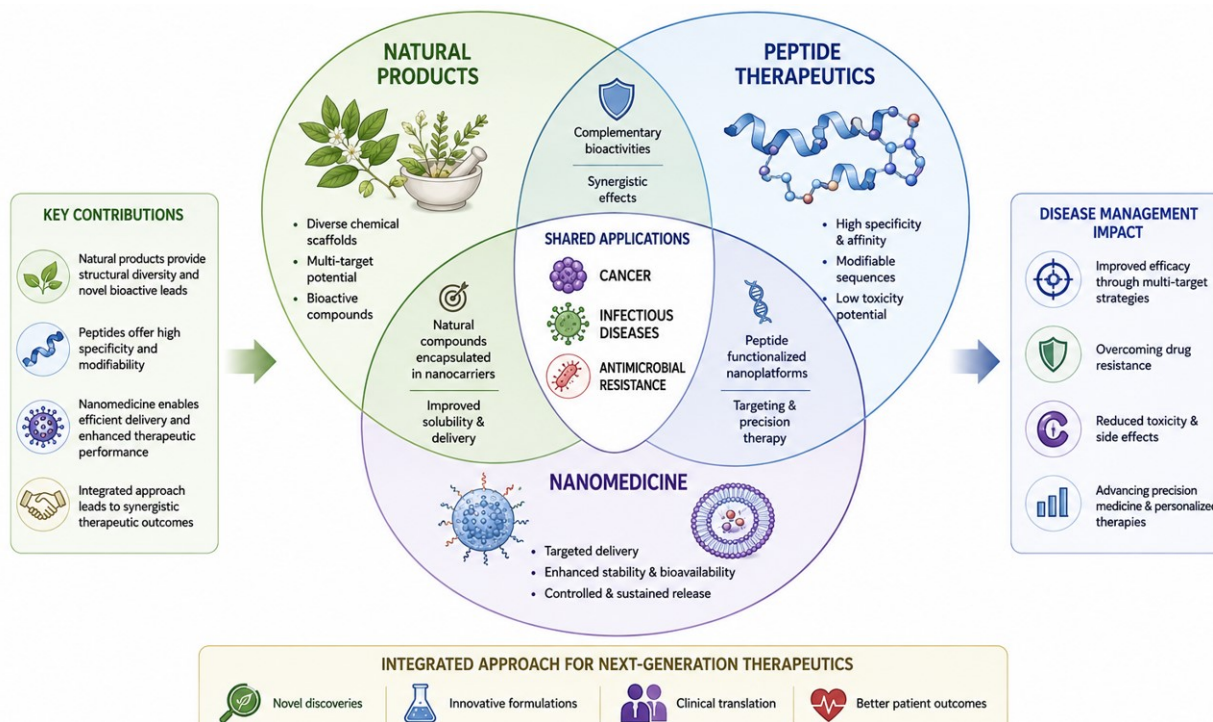
6.1 Integration of Traditional Knowledge and Modern Science

One of the most productive developments in contemporary biomedical research has been the renewed appreciation for traditional medicinal knowledge. Ethnobotanical surveys and traditional medicine systems have consistently pointed researchers toward plants and practices with genuine therapeutic merit, and modern analytical tools have allowed these leads to be systematically validated [55, 56]. The plants reviewed in this article, from *Boerhaavia diffusa* to *Ficus carica* to *Terminalia chebula*, all have roots in traditional medicine systems across Asia and Africa, and their scientific validation has strengthened the case for continued exploration of this knowledge base [2, 20, 12]. At the same time, it is important to acknowledge the limitations of traditional knowledge as a guide to drug development. Not all traditional remedies are safe or effective, and the complexity of whole plant extracts can make it difficult to identify and standardize the active constituents [57, 58]. A rigorous, evidence-based approach that respects traditional knowledge without uncritically accepting it is perhaps the most sensible path forward.

6.2 One Health and Interdisciplinary Approaches

The concept of One Health, which recognizes the interconnection between human health, animal health, and environmental health, provides a valuable framework for thinking about the topics covered in this review [59, 60]. Vector-borne diseases like malaria and dengue, antimicrobial resistance driven partly by agricultural antibiotic use, and environmental pollution from nanomaterials and pharmaceutical waste all sit at this human-animal-environment interface. Addressing them effectively requires interdisciplinary collaboration across medicine, veterinary science, ecology, chemistry, and computational biology [61, 62].

The ageing population presents its own set of challenges within this framework. Orthostatic hypotension and its relationship to mental health in elderly populations, for example, has been explored in cross-sectional studies that highlight the complex interplay between cardiovascular, neurological, and psychological factors in ageing. As populations age globally, the demand for safe, effective, and accessible therapeutics will only increase, making the development of natural product-based and peptide-based medicines all the more pressing [63, 64].

Figure 3: Interconnections Between Natural Products, Peptide Therapeutics, and Nanomedicine in Disease Management

6.3 Challenges and Opportunities

Despite the tremendous promise of natural products, peptide therapeutics, and nanomedicine, significant challenges remain. Bioavailability is a persistent issue for many phytochemicals, which may show excellent activity *in vitro* but poor absorption and distribution *in vivo* [65, 66]. Peptides face similar challenges, including rapid proteolytic degradation and limited membrane permeability, though these can often be addressed through chemical modifications or nanoparticle-based delivery [67, 68]. Regulatory pathways for plant-derived drugs and nanomedicines are still evolving, and the lack of harmonized international standards creates uncertainty for developers and regulators alike [69, 70]. Intellectual property issues around traditional knowledge add another layer of complexity, particularly when natural products from developing countries are commercialized by pharmaceutical companies in the developed world [71, 72]. These systemic challenges will need to be addressed through policy as much as through science.

7. Conclusion

This review has traced the current state of research across three deeply interconnected domains: natural products, peptide therapeutics, and nanomedicine. What emerges from this survey is not just a collection of findings but a coherent narrative about how the field is evolving. Researchers are moving away from isolated, single-target approaches toward integrated strategies that combine the richness of natural chemistry with the precision of computational design and the versatility of nanotechnology. The studies reviewed here, spanning medicinal plant evaluation, *in silico* peptide discovery, nanoparticle synthesis, and infectious disease epidemiology, all contribute to this larger picture.

The road ahead is demanding, but the tools available today are more powerful than ever. From molecular docking software that can screen thousands of peptide candidates *in silico* to green synthesis protocols that convert plant waste into therapeutic nanoparticles, the methodological toolkit available to researchers is both broad and deep. What is needed now is sustained investment

in translational research, stronger bridges between computational predictions and experimental validation, and policy frameworks that support equitable access to the resulting medicines. With those foundations in place, the convergence of natural products, peptide science, and nanomedicine holds genuine promise for addressing some of the most pressing health challenges of our time.

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Conflict of interest

The author disclose no conflicts of interest.

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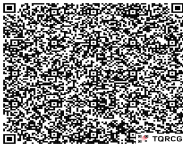
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