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Review Article

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Recent Advances in Infectious Diseases, Natural Product Therapeutics, Nanotechnology, and Computational Drug Discovery: A Review

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Abstract

The escalating global burden of infectious diseases, antimicrobial resistance, and cancer necessitates innovative therapeutic strategies that transcend conventional drug discovery frameworks. This integrated review examines recent advances across four synergistic domains: infectious disease management, natural product therapeutics, nanotechnology, and computational drug discovery. Infectious diseases, encompassing parasitic, fungal, bacterial, and viral pathogens, continue to impose substantial morbidity and mortality worldwide, particularly among vulnerable populations. Natural products derived from medicinal plants, including *Boerhaaviadiffusa, Euphorbia hirta, Terminaliachebula, Ipomoea obscura,* and*Ficuscarica*, have demonstrated significant pharmacological activities, including antioxidant, antibacterial, antifungal, anti-inflammatory, and anticancer properties, representing valuable sources for novel drug leads. Nanotechnology has further enhanced therapeutic efficacy through biosynthesis of silver nanoparticles and development of advanced nanomaterials, offering improved drug delivery, bioavailability, and

environmental sustainability. Simultaneously, computational drug discovery approaches, encompassing molecular docking, in silico peptide design, virtual screening, and chemical repurposing, have transformed the drug development pipeline by facilitating rapid, cost-effective identification of promising therapeutic candidates against diverse targets, including antimicrobial resistance proteins, cancer-associated proteins, and vector-borne disease targets. The convergence of these disciplines represents a transformative approach toward developing safe, effective, and accessible therapeutics, ultimately bridging the gap between traditional medicinal knowledge and modern biomedical innovation.

Keywords: Infectious Diseases, Natural Product Therapeutics, Nanotechnology, Computational Drug Discovery, Epidemiology.

1. Introduction

Infectious diseases have shaped human history in ways that few other forces have. From ancient plagues to modern pandemics, the story of humanity is, in many ways, a story of its struggle against microbial life [1, 2]. What has changed profoundly in recent decades is not the nature of that struggle but rather the sophistication of the tools we bring to it. Where once a physician could only observe and record, today's researcher can model a drug-target interaction on a computer, synthesize a nanoparticle from a plant extract, and test it against a cancer cell line before breakfast [3, 4].

Yet for all this sophistication, the basics still matter enormously. Understanding who gets infected, why, and under what conditions remains the indispensable starting point for any meaningful therapeutic or preventive strategy [5, 6]. Community-based epidemiological studies, sometimes dismissed as old-fashioned in an era of genomics and artificial intelligence, continue to generate insights that no algorithm can replace [7, 8]. The prevalence of intestinal parasites among school children, the distribution of fungal infections in tropical climates, and the pattern of antibiotic resistance in regional hospitals are all facts that must be known before solutions can be designed [9, 10].

This review takes the position that progress in medicine comes not from any single discipline but from the productive tension between them. Natural product research feeds computational chemistry. Epidemiology motivates nanotechnology. Clinical microbiology informs in silico drug repurposing. Each domain strengthens the others, and together they form an integrated research ecosystem capable of addressing some of the most pressing health challenges of our time [11, 12].

2. Infectious Disease Epidemiology: The Foundation of Therapeutic Strategy

Any serious engagement with infectious disease must begin with epidemiology. Before a drug can be designed, a pathogen must be identified and characterized within its human and environmental context [13, 14]. Studies examining the prevalence of intestinal helminthic infections among school-going children have consistently revealed that parasitic burden is strongly correlated with sanitation infrastructure, household income, and access to clean water [15, 16]. These are not merely academic observations. They have direct implications for where public health resources should be directed and what kinds of interventions are most likely to succeed [17].

Protozoan infections tell a similarly important story. The incidence of intestinal protozoa among school children in endemic regions reflects broader failures of water treatment and food hygiene [18, 19]. Children bearing these infections often show measurable deficits in cognitive performance and physical growth, making parasitic control not just a medical issue but an educational and developmental one as well [20]. Recognizing this broader context is what

separates effective public health strategy from purely clinical thinking.

Fungal infections add another layer of complexity to the epidemiological picture. Tineacapitis, caused by dermatophytic fungi, is remarkably common among school-aged children in tropical and subtropical regions [21]. The condition is often underdiagnosed and undertreated, partly because it is perceived as cosmetic rather than medical. But chronic scalp infections can lead to scarring, permanent hair loss, and significant psychological distress [22, 23]. Similarly, oral candidiasis or thrush, particularly in immunocompromised individuals and children, represents a persistent clinical challenge that demands both better diagnostics and more effective antifungal agents [24].

3. Viral Co-Infections and Their Clinical Consequences

The intersection of viral infections creates clinical scenarios of particular complexity and gravity. Among these, the co-occurrence of Human Immunodeficiency Virus and Human Papillomavirus stands out as both well-documented and deeply consequential [25, 26]. Women living with HIV face a substantially elevated risk of acquiring and maintaining persistent HPV infections, largely because the immunosuppression driven by HIV impairs the normal immune surveillance mechanisms that would otherwise clear the virus [27, 28].

HPV type 16, recognized as one of the most oncogenic of all HPV strains, has been detected at significantly elevated prevalence in HIV-positive and AIDS-affected women across multiple study populations [29, 30]. The progression from HPV infection to cervical intraepithelial neoplasia and ultimately invasive cervical cancer is accelerated in the context of HIV-mediated immunosuppression, making regular cervical screening in this population not just recommended but genuinely urgent [31, 32]. Integrated HIV and cervical cancer screening programs have shown promise in several low- and middle-income countries, though implementation gaps remain wide [33].

What makes this viral co-infection story particularly compelling from a research perspective is how it connects epidemiological observation to molecular biology to computational drug discovery. The oncoproteins encoded by HPV-16, particularly E6 and E7, are well-characterized molecular targets, and the availability of structural data on these proteins has made them attractive subjects for in silico drug design [34, 35]. A finding that begins in a community clinic, documenting HPV prevalence in HIV-positive women, can thus trace a direct line to a computational laboratory where novel peptide-based therapeutics are being designed and evaluated [36].

4. Antimicrobial Resistance: Mechanisms, Patterns, and Novel Solutions

Antimicrobial resistance has emerged as one of the defining public health crises of the twenty-first century. The scale of the problem is genuinely alarming. Bacteria that were once reliably controlled by first-line antibiotics are now surviving treatment in clinical settings worldwide, driving up mortality, extending hospital stays, and exhausting therapeutic options [37, 38]. Understanding resistance patterns at the local and regional level is therefore an essential first step toward managing this crisis intelligently.

Studies examining the antibiotic susceptibility profiles of *Pseudomonas aeruginosa* have documented particularly concerning levels of resistance to fluoroquinolone antibiotics, a group that had long been considered reliable for managing serious gram-negative infections [39]. The mechanisms underlying this resistance are multiple and overlapping, involving efflux pump up regulation, outer membrane porin mutations, and enzymatic drug inactivation [40, 41]. Each mechanism represents both a biological challenge and, viewed through a different lens, a potential therapeutic target.

Urinary tract infections caused by multidrug-resistant organisms present similar challenges in clinical settings across different geographic regions [42, 43]. Isolates from hospital and community settings alike have shown resistance profiles that leave clinicians with few effective options, particularly in resource-limited environments where newer antibiotics may not be available or affordable (Table 1) [44]. Dental microbiomes, too, harbor organisms with resistance determinants, and the oral cavity is increasingly recognized as a reservoir that can seed systemic infections in vulnerable patients [45, 46].

Table 1: Antimicrobial Resistance Profiles of Key Clinical Pathogens

Pathogen	Resistance Mechanism	Antibiotic Class Affected	Clinical Impact
P. aeruginosa	Efflux pumps, porin loss	Fluoroquinolones	High mortality in ICU
K. pneumoniae	β-Lactamase (TEM, SHV)	β-Lactams, Carbapenems	Nosocomial outbreaks
S. aureus	mecA gene (PBP2a)	Methicillin, β-Lactams	Surgical site infections
E. coli	ESBL production	Cephalosporins	UTI treatment failure
Candida spp.	ERG11 mutations	Azoles/Fluconazole	Oral/systemic candidiasis

Novel solutions to the resistance problem are emerging from several directions simultaneously. Peptide-based antibacterials derived from natural sources offer a particularly promising avenue, since their mechanisms of action often differ fundamentally from those of conventional antibiotics, making cross-resistance less likely [49, 50]. Computational approaches to identifying new peptide leads, particularly those targeting resistance-conferring proteins like β-lactamase TEM in *Klebsiella pneumoniae*, are demonstrating genuine predictive value [51].

5. Natural Products as Therapeutic Agents: A Renaissance in Progress

The idea that plants and other natural organisms harbor compounds with medicinal value is as old as medicine itself. What is new is the analytical precision with which we can now identify, characterize, and evaluate those compounds [52, 53]. Gas chromatography-mass spectrometry, Fourier transform infrared spectroscopy, high-performance liquid chromatography, and a battery of standardized bioassays have transformed natural product research from art to science [54]. *Boerhaavia diffusa* is a plant whose therapeutic potential has been explored across multiple research programs. Its extracts have demonstrated meaningful in vitro anticancer activity against established human cancer cell lines, and its phytochemical profile reveals a rich mixture of alkaloids, flavonoids, and phenolic acids that likely contribute to these effects [55, 56]. The plant's bioactive compounds have also been used as the basis for computational peptide design, demonstrating how traditional ethnobotanical knowledge can directly inspire cutting-edge molecular research (Table 2) [57].

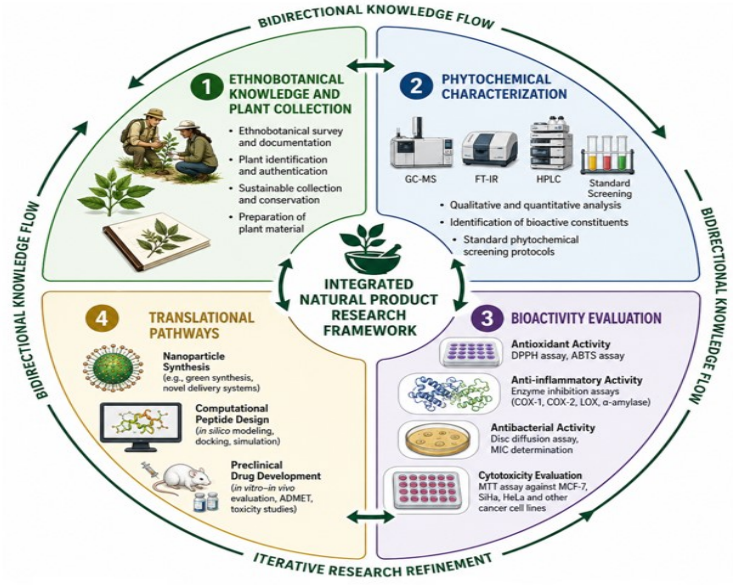
Ipomoea obscura presents another compelling case. Crude extracts from this plant have shown significant antioxidant, anti-inflammatory, antibacterial, and anticancer activities in systematic laboratory evaluations [58]. The antioxidant capacity alone is medically relevant, since oxidative stress underlies the pathophysiology of conditions ranging from cancer to cardiovascular disease to neurodegeneration [59, 60]. Plants like *Euphorbia hirta* and *Achyranthes aspera* have similarly yielded extracts with measurable cytotoxic effects on cervical and breast cancer cell lines, reinforcing the argument that natural product screening remains a productive strategy for therapeutic lead discovery [61, 62].

Table 2: Bioactive Plants and Their Documented Therapeutic Properties

Plant Species	Extract Type	Key Activities	Cancer Cell Line Tested
Boerhaavia diffusa	Methanol/aqueous	Anticancer, antioxidant	Various
Ipomoea obscura	Crude extract	Antioxidant, anti-inflammatory, antibacterial	General
Ficus carica	Methanol	Anticancer, phytochemical	MCF-7 (breast)
Achyranthes aspera	Methanol	Antioxidant, anticancer	SiHa (cervical)
Euphorbia hirta	Various	GC-MS profiling, cytotoxic	SiHa (cervical)
Terminalia chebula	Nanoparticle-mediated	Antifungal, antioxidant	General
Tephrosia purpurea	Aqueous/organic	Antibacterial	Tomato pathogens

Ficus carica extracts tested against MCF-7 human breast cancer cells have shown dose-dependent cytotoxic activity in preliminary screening studies [63]. *Terminalia chebula*, used as the biological substrate for silver nanoparticle synthesis, demonstrated antifungal activity that exceeded what the plant extract alone could achieve, suggesting a synergistic relationship between the phytochemical constituents and the nanoparticle scaffold [64]. This kind of finding sits precisely at the intersection of natural product research and nanotechnology, a productive boundary zone where some of the most interesting current work is happening (Figure 1).

Figure 1: Integrated Natural Product Research Framework



A circular integration diagram with four quadrants representing: (1) Ethnobotanical knowledge and plant collection; (2) Phytochemical characterization using GC-MS, FT-IR, HPLC, and standard screening protocols; (3) Bioactivity evaluation through antioxidant DPPH and ABTS assays, anti-inflammatory enzyme inhibition assays, antibacterial disc diffusion and MIC determination, and MTT cytotoxicity assays against MCF-7, SiHa, HeLa,

and other cancer cell lines; (4) Translational pathways toward nanoparticle synthesis, computational peptide design, and preclinical drug development. Arrows connecting all four quadrants indicate bidirectional knowledge flow and iterative research refinement.

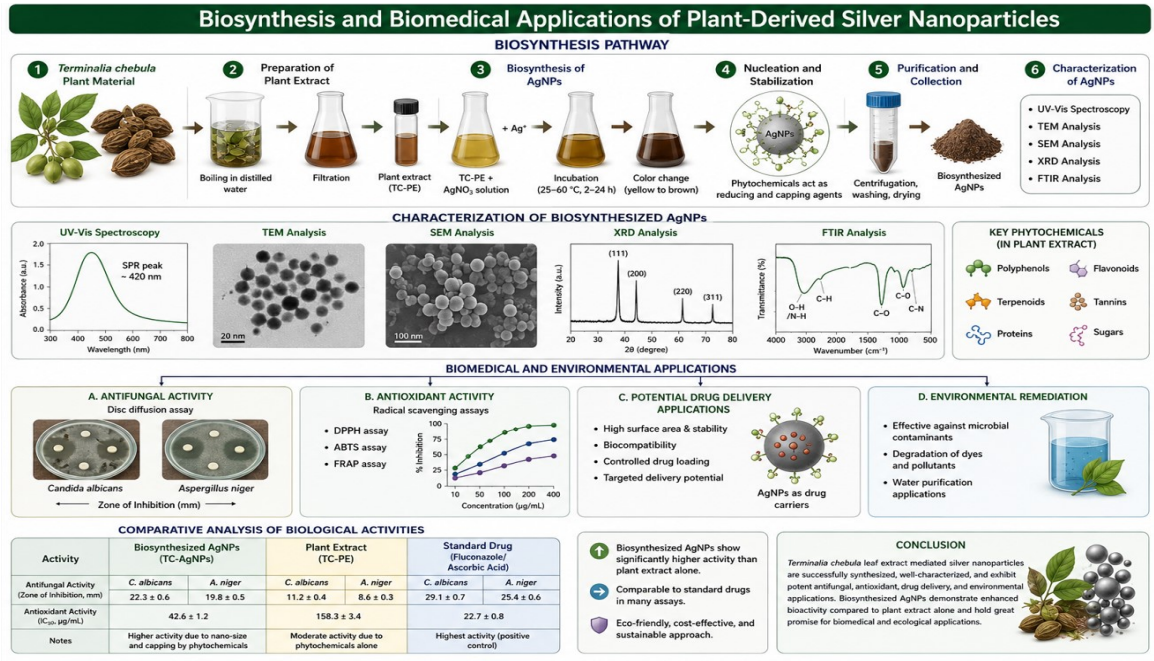
6. Nanotechnology in Medicine: From Synthesis to Application

Nanotechnology has moved rapidly from theoretical promise to practical application across multiple domains of medicine. The synthesis of metallic nanoparticles using biological methods, particularly using plant extracts as both reducing and stabilizing agents, has attracted enormous research interest because it combines the bioactivity of natural compounds with the unique physicochemical properties of nanoscale materials [66, 67]. Silver nanoparticles biosynthesized from *Terminaliachebula* extracts represent exactly this kind of synergistic system, combining the inherent antimicrobial properties of silver with the phytochemical richness of the plant source [64].

The antifungal applications of biosynthesized silver nanoparticles are particularly timely given the global rise of drug-resistant fungal infections. Conventional antifungals like fluconazole face increasing resistance from Candida and other pathogenic fungi, and silver nanoparticles offer a mechanistically distinct alternative that targets multiple cellular processes simultaneously [68, 69]. Their ability to disrupt cell membrane integrity, generate reactive oxygen species, and interfere with fungal enzymatic systems makes them genuinely difficult for fungi to develop resistance against through conventional mechanisms [70].

Beyond direct antimicrobial applications, nanomaterials are playing an increasingly important role in environmental health, which is itself a form of disease prevention (Figure 2). The relationship between environmental pollution and infectious disease burden is well established, and nanomaterial-based remediation strategies offer new tools for addressing contamination of water, soil, and air [71, 72]. The editorial perspective on nanomaterials in environmental pollution and sustainable technologies underscores the dual role these materials can play, both as therapeutic agents and as environmental management tools [73].

Figure 2: Biosynthesis and Biomedical Applications of Plant-Derived Silver Nanoparticles



A step-by-step schematic diagram showing the biosynthesis pathway from *Terminalia chebula* plant extract preparation through nanoparticle nucleation and stabilization, characterized by UV-Vis spectroscopy, TEM, SEM, XRD, and FTIR analysis. Application branches extend from the characterized nanoparticles toward antifungal activity testing with zone of inhibition measurements against *Candida albicans* and *Aspergillusniger*, antioxidant radical scavenging assays, potential drug delivery applications, and environmental remediation uses. A comparison panel shows activity differences between biosynthesized nanoparticles, plant extract alone, and standard drug controls.

7. Computational Drug Discovery: Modeling the Future of Medicine

Computational drug discovery has matured from a supplementary technique into a central pillar of modern pharmaceutical research. The ability to model three-dimensional protein structures, simulate ligand binding, predict pharmacokinetic properties, and screen vast virtual libraries of compounds has fundamentally changed the economics and efficiency of drug development [74, 75]. Where traditional drug discovery relied heavily on serendipity and empirical screening, computational approaches bring rational design to the process, allowing researchers to identify promising candidates before committing to expensive laboratory work [76].Molecular docking studies have proven particularly valuable in exploring the therapeutic potential of peptides derived from natural sources. The investigation of a novel peptide from *Boerhavia diffusa* docked against Transmembrane Protein 50A, a protein implicated in cervical cancer pathogenesis, produced docking scores and binding interaction profiles that justify further experimental investigation [57]. This study exemplifies how computational methods can bridge the gap between natural product chemistry and targeted cancer therapy, a connection that would have been difficult to establish through purely experimental means [77, 78].

Drug repurposing represents another domain where computational approaches are delivering genuine value (Table 3). The idea of finding new therapeutic applications for existing approved drugs is appealing for obvious reasons: safety profiles are already established, regulatory pathways are shorter, and development costs are dramatically lower [79, 80]. The computational evaluation of linezolid and ciprofloxacin as potential inhibitors of mutant ESR1 protein in breast cancer is a compelling example of this approach, revealing unexpected therapeutic possibilities for drugs originally developed for entirely different purposes [81].

Table 3: Computational Drug Discovery Studies and Key Outcomes

Study Focus	Compound/ Peptide	Molecular Target	Docking Score	Therapeutic Implication	Reference
Cervical cancer	*B. diffusa* peptide	TMEM50A	Favorable binding	Novel peptide therapy	[57]
Breast cancer	Linezolid, Ciprofloxacin	Mutant ESR1	Strong affinity	Drug repurposing	[81]
Malaria vector	Novel peptide	*A. gambiae* proteins	High specificity	Vector control	[82]
Filariasis vector	De novo peptide	*C. quinquefasciatus*	Active site binding	Mosquito control	[83]
AMR bacteria	*B. diffusa* peptide	β-Lactamase TEM	Competitive inhibition	Antibacterial strategy	[51]
S. aureus AMR	Tramadol HCl	MepA efflux pump	Inhibitory binding	Repurposing analgesic	[84]

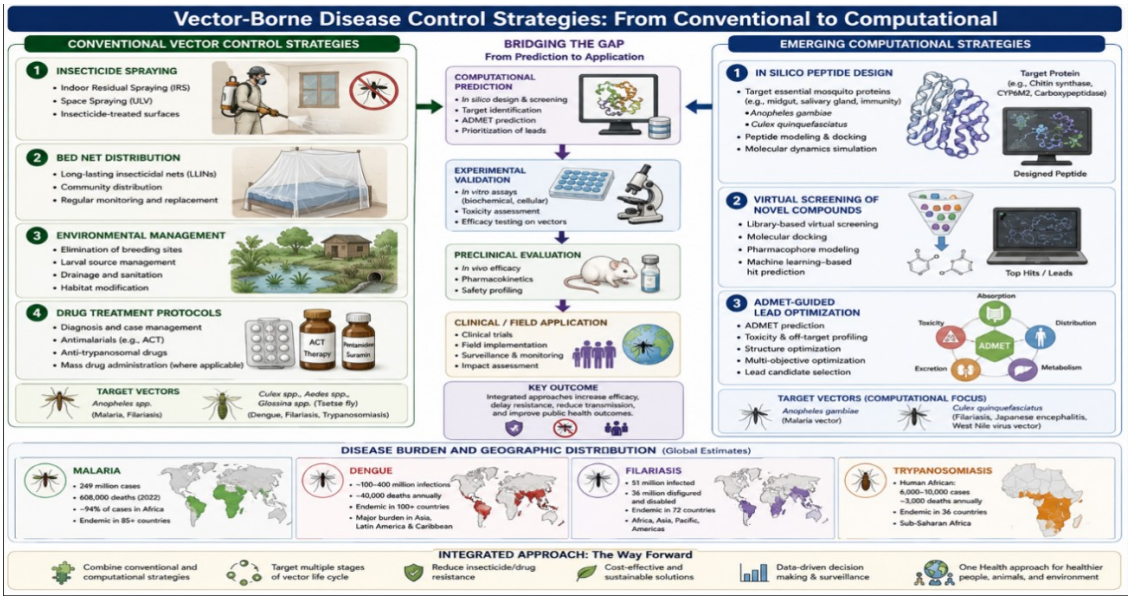
The application of in silico methods to vector-borne disease control is one of the more creative developments in this space. Identifying novel peptides that target essential proteins in mosquito species like *Anopheles gambiae* and *Culex quinquefasciatus* offers a highly specific alternative to broad-spectrum chemical insecticides [82, 83]. The specificity of peptide-target interactions means that non-target organisms, including beneficial insects and humans, are far less likely to be affected, addressing one of the most serious ecological criticisms of conventional vector control strategies [85, 86].

8. Vector-Borne and Neglected Tropical Diseases

Vector-borne diseases carry a disproportionate share of the global infectious disease burden, particularly in tropical and subtropical regions where poverty, inadequate healthcare infrastructure, and favorable environmental conditions for vector proliferation converge [87, 88]. Malaria, dengue, lymphatic filariasis, and human African trypanosomiasis are among the conditions that continue to exact enormous tolls in human lives and economic productivity, despite decades of control efforts [89].

Human African trypanosomiasis, caused by *Trypanosoma bruceirhodesiense* and transmitted by the tsetse fly, presents with particularly severe neurological manifestations in its second stage (Figure 3). The occurrence of seizures in stage-2 rhodesiense trypanosomiasis patients has been documented in clinical studies from Zambia, highlighting the neurological complexity of this disease and the inadequacy of current staging and treatment protocols [90]. These findings underscore the need for both better diagnostic tools that can reliably identify disease stage and more effective treatments that can address central nervous system involvement [91, 92].

Figure 3: Vector-Borne Disease Control Strategies: From Conventional to Computational



A comparative diagram organized in two parallel columns. The left column shows conventional vector control strategies including insecticide spraying, bed net distribution, environmental management, and drug treatment protocols for established diseases like malaria and trypanosomiasis. The right column shows emerging computational strategies including in silico peptide design targeting mosquito proteins in *Anopheles gambiae* and *Culex quinquefasciatus*, virtual screening of novel compounds, and ADMET-guided lead optimization. A central bridge section highlights the transition pathways from computational

prediction to experimental validation and ultimately clinical or field application. Disease burden statistics for malaria, dengue, filariasis, and trypanosomiasis are annotated alongside relevant geographic distributions.

9. Biotechnology, Oleic Acid, and Sustainable Pharmaceutical Production

The boundaries between biotechnology, environmental science, and pharmaceutical production are becoming increasingly permeable, and this permeability is generating genuinely useful innovations. The biological production of oleic acid from mango kernel waste using probiotic bacteria isolated from marine fish represents exactly the kind of creative, resource-efficient approach that sustainable medicine requires [93]. Oleic acid is a monounsaturated omega-9 fatty acid with well-documented anti-inflammatory properties, and its production from agricultural waste using marine-derived microorganisms represents a double environmental dividend [94, 95].

The probiotic bacteria responsible for this biotransformation are themselves interesting research subjects. Marine microorganisms have evolved in extreme and competitive environments, developing metabolic capabilities that terrestrial organisms often lack [96, 97]. Harnessing these capabilities for pharmaceutical production is a relatively young field, but one that is generating increasing interest as researchers recognize the extraordinary chemical diversity of marine microbial communities [98]. The connection between this kind of biotechnological innovation and disease prevention may not be immediately obvious, but it becomes clear when one considers that sustainable, affordable production of bioactive compounds is a prerequisite for their widespread therapeutic use.

10. Aging, Comorbidities, and the Broadening Scope of Infectious Disease Research

Infectious disease research cannot be conducted in isolation from the broader clinical context in which infections occur. The aging of populations worldwide is creating new vulnerabilities and new clinical challenges that intersect directly with infectious disease epidemiology [99, 100]. Older adults are more susceptible to certain infections, more likely to experience severe disease, and more likely to harbor comorbidities that complicate treatment.

Orthostatic hypotension, a condition characterized by a significant drop in blood pressure upon standing, becomes increasingly prevalent with age and is associated with elevated risk of falls, syncope, and cognitive decline. A cross-sectional investigation of the impact of aging on orthostatic hypotension and mental health outcomes found significant and clinically meaningful associations that deserve greater attention in geriatric medicine. While this condition is not itself infectious, its presence in older patients creates management complexity when infections requiring aggressive antibiotic therapy are also present, since many antibiotics affect cardiovascular parameters.

11. Oral Health, Disability, and Systemic Disease Connections

The oral cavity is both a gateway and a mirror for systemic health. Microbial communities resident in the mouth are capable of seeding infections throughout the body, particularly in patients with compromised immune function or cardiac structural abnormalities. Studies characterizing the microbial ecology of dental caries have revealed complex polymicrobial communities where acidogenic organisms interact synergistically to drive enamel destruction and pulpal infection. These communities harbor resistance determinants that may complicate the treatment of secondary systemic infections.

For people living with physical, mental, or social disabilities, maintaining adequate oral hygiene represents a particular challenge, and the consequences of neglect extend well beyond dental pain and tooth loss. Systemic conditions including endocarditis, aspiration pneumonia, and adverse pregnancy outcomes have all been linked to poor oral health, making dental care a genuinely important component of comprehensive disease prevention (Table 4). Community-based programs that bring dental care to disabled populations are cost-effective interventions with benefits that ripple outward into general health outcomes.

Table 4: Intersections between Oral Health, Systemic Disease, and Microbial Resistance

Oral Condition	Causative Organisms	Systemic Risk	Resistance Concern	Reference
Dental caries	*S. mutans*, mixed flora	Endocarditis, bacteremia	Broad-spectrum resistance	[45]
Oral candidiasis	*Candida albicans*	Systemic candidiasis	Fluconazole resistance	[24]
Periodontal disease	*P. gingivalis*, anaerobes	Cardiovascular disease	Metronidazole resistance	[107]
Dental abscess	Mixed anaerobes	Brain abscess, sepsis	Polymicrobial resistance	[106]
Disability-related neglect	Mixed community	Aspiration pneumonia	Multiple resistance	[108]

12. Discussion

What emerges from this integrated review is a picture of infectious disease research that is simultaneously more complex and more hopeful than it might have appeared a generation ago. The complexity comes from the recognition that diseases do not exist in isolation. They occur in social, environmental, and biological contexts that shape their epidemiology, their clinical presentation, and their response to treatment. The hope comes from the remarkable range of tools now available to researchers and clinicians, tools that span from community surveys to quantum mechanical calculation.

The integration of natural product research with computational drug discovery is perhaps the most intellectually exciting frontier in this landscape. When a traditional medicinal plant yields a bioactive compound that can be characterized by mass spectrometry, modeled by molecular dynamics simulation, and tested against a specific oncogenic or antimicrobial target, the entire chain of discovery becomes visible and tractable. This is not just scientifically satisfying. It is practically important because it dramatically increases the efficiency of the drug discovery process and opens doors to therapeutic leads that purely synthetic chemistry might never have found [116].

Nanotechnology adds yet another dimension to this integrated picture. Biosynthesized nanoparticles that combine the bioactivity of plant compounds with the physical properties of nanoscale materials represent genuinely novel therapeutic entities, distinct from both their organic and inorganic components. Their potential applications in antimicrobial therapy, cancer treatment, drug delivery, and environmental remediation make them one of the most versatile tools in the emerging biomedical toolkit. Translating this potential into clinical practice will require rigorous safety evaluation, standardized manufacturing protocols, and carefully designed clinical trials.

13. Conclusion

The fields reviewed here, infectious disease epidemiology, natural product therapeutics, nanotechnology, and computational drug discovery, are not separate endeavors. They are facets of a single, integrated scientific enterprise whose ultimate goal is the reduction of human suffering from disease. The research reviewed in this article demonstrates that progress is being made on all fronts, from counting parasites in school children to designing peptides that target cancer proteins, from characterizing plant extracts to synthesizing nanoparticles with tailored bioactivity. The challenge now is to accelerate the translation of these discoveries into clinical and public health practice, ensuring that the benefits of scientific innovation reach the populations who need them most. That will require not just scientific creativity but sustained investment, genuine interdisciplinary collaboration, and an unwavering commitment to health equity.

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Conflict of interest

The author disclose no conflicts of interest.

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