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Drug Repurposing Strategies for Emerging Infectious Diseases: A Review

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ABSTRACT

Emerging andre-emerging contagious conditions pose a patient global health challenge, boosted by rapid-fire pathogen elaboration, antimicrobial resistance, and the lengthy timelines of conventional medicine discovery. medicine repurposing, which involves relating new remedial suggestions for being or preliminarily approved medicines, has surfaced as a promising and cost-effective strategy to address these challenges. This review provides a comprehensive overview of medicine repurposing strategies for arising contagious conditions, encompassing classical, target- grounded, phenotypic, and computational approaches. crucial methodological tools and coffers, including network- grounded analyses, transcriptomic profiling, and curated databases similar as DrugBank, DisGeNET, and the Connectivity Map, are bandied for their part in accelerating seeker identification. substantiation from viral outbreaks, including Ebola, SARS, MERS, and COVID- 19, highlights the successful operation of repurposed medicines in preclinical and clinical settings. The review further examines critical aspects of efficacity evaluation, clinical restatement, and nonsupervisory considerations. Despite its advantages, medicine repurposing faces limitations related to pharmacokinetics, intellectual property, clinical trial design, and target particularity. Arising inventions similar as artificial intelligence, machine literacy, and systems biology are transubstantiating repurposing channels and perfecting prophetic delicacy. Overall, medicine repurposing represents a vital, adaptable strategy for rapid-fire remedial response to arising contagious pitfalls and will remain central to unborn epidemic preparedness.

Keywords : Medicine repurposing; Drug displacing; Arising contagious conditions; Computational medicine discovery; Network pharmacology; COVID- 19; Artificial intelligence; Clinical restatement; Antiviral remedy; Systems biology

1.INTRODUCTION

Emerging infectious diseases (EIDs) pose a persistent and escalating global health threat due to factors such as globalization, climate change, urbanization, zoonotic spillover, and antimicrobial resistance. Traditional de novo drug discovery is a lengthy, expensive, and high-risk process, often requiring 10–15 years and substantial financial investment before regulatory approval. In the context of rapidly spreading outbreaks—such as Ebola, Zika, Severe Acute Respiratory Syndrome(SARS), Middle East Respiratory Syndrome Coronavirus (MERS), and COVID-19—this timeline is impractical. Drug repurposing, also referred to as drug repositioning, has therefore emerged as a strategically critical approach for the rapid identification of therapeutic options against EIDs.(1,2,3,28,29).

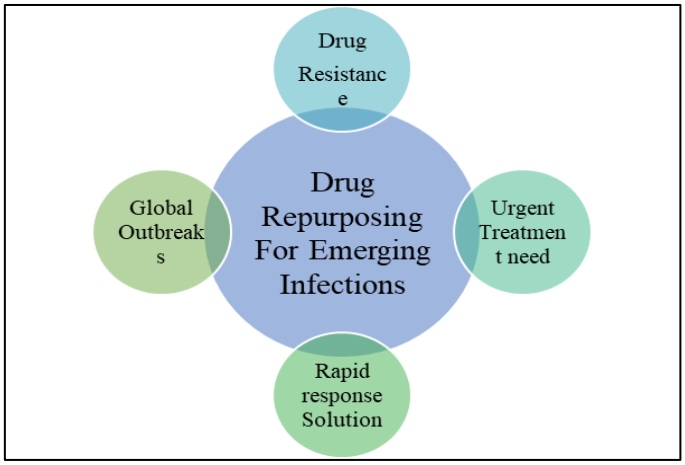

Fig 1 : Drug Repurposing For Emergency Infections.

Drug repurposing involves identifying new therapeutic indications for existing drugs, including approved, investigational, or discontinued compounds. As highlighted in the seminal work by Ashburn and Thor, repurposed drugs benefit from established pharmacokinetic, pharmacodynamic, toxicity, and manufacturing profiles, which substantially reduces development time, cost, and risk. This approach is particularly valuable for infectious diseases, where urgent clinical need often outweighs commercial incentives for traditional drug development.(1,14,15,30)

The relevance of drug repurposing has been strongly reinforced during recent pandemics. During the COVID-19 crisis, multiple existing drugs—such as remdesivir, dexamethasone, and baricitinib—were rapidly evaluated and deployed based on prior knowledge, preclinical evidence, and early data. Repurposing not only accelerates therapeutic availability but also enables parallel evaluation of multiple candidates, increasing the probability of success under emergency conditions.

From a mechanistic perspective, repurposed drugs may act through diverse pathways, including direct antiviral activity, inhibition of host cell entry or replication machinery, modulation of host immune responses, or mitigation of inflammatory and pathological sequelae. Network medicine and systems biology approaches have further expanded the conceptual framework by revealing shared molecular pathway between seemingly unrelated diseases, thereby uncovering non-obvious therapeutic opportunities.

Importantly, drug repurposing is not limited to viral infections. It has shown promise across bacterial, parasitic, and fungal diseases, particularly in addressing antimicrobial resistance and neglected tropical diseases. Broad-spectrum antivirals and host-targeted agents can be strategically repositioned to counter multiple viral families, enhancing pandemic preparedness. Despite its advantages, drug repurposing is not without limitations. Challenges include suboptimal dosing for new indications, intellectual property constraints, regulatory complexities, and variable clinical efficacy. The balance of speed, safety, and feasibility makes drug repurposing an indispensable pillar of modern infectious disease therapeutics.

In summary, drug repurposing represents a pragmatic, scientifically grounded, and clinically impactful strategy to address the urgent therapeutic needs posed by emerging infectious diseases. Its integration with computational tools,high-throughput screening, and clinical translation frameworks continues to redefine how global health systems respond to infectious threats.(1,2,28,29).

2. CLASSIFICATION OF DRUG REPURPOSING STRATEGIES

Drug repurposing strategies can be broadly classified based on the underlying rationale, methodological approach, and stage of evidence generation. A clear classification framework is essential for systematic review writing and for guiding future research efforts in emerging infectious diseases.(4,5,6)

One of the most widely accepted classifications divides drug repurposing into disease-centric, drug-centric,and target-centric approaches. Disease-centri repurposing involves applying drugs already approved for one infectious disease to another disease with similar clinical or pathological features. For example, broad-spectrum antivirals initially developed for influenza or hepatitis have been evaluated for Ebola and coronaviruses due to shared viral replication mechanisms.

Drug-centric repurposing focuses on the known pharmacological properties of a drug, independent of disease similarity. In this approach, drugs are screened for unexpected antiviral or immunomodulatory effects. High-throughput phenotypic screening assays,have been instrumental in identifying such candidates against high-risk pathogens.(4,5)

Target-centric repurposing is based on identifying common molecular targets shared across diseases. This strategy leverages advances in genomics, proteomics, and structural biology to map pathogen or host targets to existing drugs. Network-based analyses, enable identification of host proteins exploited by multiple pathogens, allowing repositioning of drugs that modulate these targets(4,5,23).

Another important classification distinguishes computational (in silico) and experimental (in vitro/in vivo) repurposing approaches. Computational methods include molecular docking, machine learning, network pharmacology, and transcriptomic signature matching. These methods allow rapid prioritization of candidates from large chemical libraries. Experimental approaches involve cell-based assays, animal models, and mechanistic validation, providing biological relevance and translational confidence.

Repurposing strategies can also be classified based on the stage of drug development. Approved drugs offer the fastest clinical translation due to existing safety data, while investigational drugs may provide higher efficacy but require additional evaluation. Discontinued drugs, though abandoned for reasons unrelated to safety, represent a valuable but underexplored resource.

From a regulatory perspective, repurposing can be categorized into on-label, off-label, and re-labeling pathways. Off-label use is common during outbreaks but lacks formal regulatory endorsement, whereas re-labeling involves systematic clinical trials and regulatory approval for the new indication.

In the context of emerging infectious diseases, hybrid classification approach is often adopted, integrating disease urgency, mechanistic plausibility, and translational feasibility. The COVID-19 pandemic exemplified the need for adaptive classification frameworks that allow rapid movement from computational prediction to clinical evaluation.

Overall, methodical bracket of medicine repurposing strategies provides abstract clarity, enhances reproducibility, and supports rational decision - timber in outbreak settings. similar structured approaches are essential for maximizing the impact of repurposed rectifiers against current and unborn contagious pitfalls.(5,6,20)

3. KEY METHODOLOGICAL TOOLS & DATABASES

Relating new remedial uses for being composites has surfaced as a rapid-fire, cost-effective volition to de novo medicine discovery, especially in the environment of arising contagious conditions similar as COVID- 19. At its core, repurposing exploration depends on the capability to integrate and dissectmulti-scale biomedical data, from gene expression autographs and complaint genetics to medicine- target relations and protein – protein networks. Several methodological fabrics and curated databases have come keystones in this trouble, enabling methodical vaticination, prioritization, and natural interpretation of repurposing campaigners. Then we bandy five vital coffers and approaches network- grounded repurposing fabrics, DrugBank, DisGeNET, gene expression-grounded displacing.(8)

3.1 Network- Grounded medicine Repurposing Frameworks :

The Case of COVID- 19 Network drug conceptualizes natural systems as complex, connected networks of genes, proteins, and pathways, rather than insulated molecular realities. Under this paradigm, both conditions and medicines are counterplotted into high- dimensional interactome geographies, and their connections are inferred through network topology and propinquity measures.

In this frame, the mortal protein – protein commerce(PPI) network serves as the foundational backbone. Given host proteins that interact with viral factors are integrated into this interactome, and medicine – target information is overlaid to produce a complaint – medicine network. The abecedarian thesis is that medicines whose targets are " proximal " to complaint- associated proteins within this interactome are more likely to ply remedial goods. A network propinquity score is reckoned grounded on shortest- path distances between medicine targets and complaint- associated proteins; medicines with significantly small propinquity distances are also prioritized for farther disquisition.

Applied this methodology to identify 16 seeker medicines and several medicine combinations potentially effective against SARS-CoV- 2, integrating transcriptomic data to support mechanistic applicability. This network- centric strategy exemplifies how high-dimensional interactome data can be converted into practicable repurposing suppositions, offering a scalable volition to trial- and-error pharmacology.

Strengths and Challenges:

Strengths: Network approaches prisoner systems- position connections that single- gene analyses miss, allowing the identification of medicines acting on pathways rather than just single targets.

Challenges : Results depend on the absoluteness and quality of PPI data, the delicacy of complaint gene lists, and represent suppositions that bear experimental confirmation.(8)

3.2 DrugBank 5.0:

A Comprehensive medicine – Target Knowledgebase DrugBank stands as one of the most comprehensive, curated public coffers for medicine data. Firstly developed as an intertwined depository of chemical, pharmacological, and pharmaceutical information, DrugBank combines detailed medicine biographies with annotated medicine targets, medium- of- action data, pharmacokinetics, and more. The DrugBank 5.0 release represented a major expansion of this knowledgebase, mainly adding entries and data depth. In interpretation 5.0, the database contains information on thousands of medicines — including FDA- approved small motes, biotech medicines, nutraceuticals, and experimental composites — alongside their known and prognosticated targets.

Crucial features applicable to repurposing exploration include:

✧ **Medicine – Target relations(DTIs):** Curated links between medicines and their molecular targets are pivotal for constructing medicine – target networks, as used in network- grounded prioritization.

✧ **Medium and suggestion reflections:** These allow experimenters to snappily assess being remedial surrounds and infer implicit off- marker uses.

✧ **Pharmacogenomics and clinical reflections:** Inheritable variation impact and clinical trial data can inform perfection repurposing sweats.

DrugBank is extensively used as a primary source of medicine biographies in computational channels, serving as the backbone of numerous repurposing algorithms that bear dependable DTI data. Its integration into network- centric and machine literacy fabrics underscores its foundational part in data- driven medicine discovery(8).

3.3 DisGeNET Mapping the inheritable Base of Disease

DisGeNET is a rich gene – complaint association database that summations genotype phenotype connections from expert- curated sources, Genome-wide association studies(GWAS), and literature- booby-trapped data. It stands out as one of the most comprehensive depositories for complaint- related gene information. Disease gene data is critical for repurposing because it defines the molecular " hand " of a complaint state — the set of genes whose anxiety through inheritable variation, expression change, or mutation contributes to complaint pathogenesis. An accurate complaint hand allows repurposing algorithms to: Anchor network-grounded propinquity computations(e.g., situating complaint modules within global interactomes). Inform pathway analyses linking medicines to complaint mechanisms. high- dimensional interactome data can be converted into practicable repurposing suppositions, offering a scalable volition to trial- and- error pharmacology. Strengths and Challenges Strengths Network approaches prisoner systems- position connections that single- gene analyses miss, allowing the identification of medicines acting on pathways rather than just single targets. Provide scoring and prioritization criteria for candidate drugs based on overlap with disease gene sets. DisGeNET's integration with visualization tools and programmatic access mechanisms also facilitates interactive exploration of disease gene networks, enabling researchers to identify key hubs and modules that might constitute effective intervention points (9).

3.4 Gene Expression-Based Repurposing:

A complementary methodological axis in repurposing leverages gene expression profiles rather than solely network topology or curated Drug-target interactions(DTIs) Sirota and colleagues pioneered an influential gene expression-focused strategy, proposing that if a drug induces gene expression changes that are inverse to those observed in a disease state, then that drug may counteract the disease's molecular phenotype.

This method requires two foundational datasets: a disease's differential expression signature (derived from patient tissue or experimental models) and a compendium of drug-induced expression signatures. By comparing these profiles using pattern matching algorithms, the method identifies drugs whose transcriptional effects potentially reverse the disease phenotype(10).

Advantages of expression-based approaches include:

◆ Mechanism-agnostic hypothesis generation: Unlike target-centric methods, this strategy doesn't require prior knowledge of drug targets or mechanisms, enabling discovery in poorly understood diseases.

◆ Functional insights: Expression profiles reflect downstream functional consequences, offering a proxy for biological impact.

◆ Nevertheless, challenges include variability in expression data across platforms, tissue specificity, and the complexity of translating in vitro signatures to in Vivo efficacy.

3.5 The Next-Generation Connectivity Map

The Connectivity Map (CMap) concept, originally introduced by Lamb and colleagues, establishes a large reference compendium of gene expression profiles induced by chemical and genetic perturbations. Expanded this into a next-generation platform based on the L1000 profiling method, generating more than a million transcriptomic profiles.

Unlike early microarray-based collections, the L1000 platform uses areduced representation transcriptomics approach that enables high throughput at lower cost, making comprehensive profiling of gene expression responses to thousands of drugs feasible. This expanded CMap now acts as a massive signature database, where disease signatures can be systematically compared to drug-induced signatures to identify compounds with reversal or mimicking potential. CMap's role in repurposing research includes:

Signature matching: Ranking drugs based on similarity to disease expression signatures.

Mechanism discovery: Revealing unexpected mechanistic connections between compounds and pathways. Drug clustering and annotation: Identifying drug classes with shared functional impact.

The synergy between CMap and network-based methods (e.g., integrating CMap signatures into interactome contexts) further amplifies repurposing potential, bringing together transcriptomic and systems biology insights.

Integrating Tools in Practice: A Unified Workflow

A typical drug repurposing workflow might integrate these tools as follows:

Define Disease Signature: Curate disease-associated genes using DisGeNET and gene expression datasets

Construct Biological Networks: Build PPI networks anchored on disease genes.

Incorporate Drug Data: Use DrugBank to map drug targets onto networks. **Compare Expression Signatures:** Use CMap/L1000 and expression-based scoring algorithms to prioritize drugs whose transcriptional impact reverses disease signatures.

Prioritize Candidates: Combine proximity scores with expression signature reversal and clinical annotations for candidate ranking. This integrated strategy capitalizes on the complementary strengths of network and expression-based methods, enabling hypothesis-driven repurposing research.(11)

3.6 Concluding Thoughts

The landscape of drug repurposing is increasingly defined by integrative, data-driven methodologies. Resources such as DrugBank, DisGeNET, the Connectivity Map, and network-based frameworks together form a powerful toolkit for identifying and prioritizing repurposing candidates across disease contexts. While each approach carries inherent limitations — from data incompleteness to context specificity — their combined use enhances robustness and biological relevance. Continued development and integration of these databases and analytical platforms will be essential for rapid responses to future emerging infectious diseases and other complex medical challenges.(11)

4. CASE STUDIES: SUCCESSFUL REPURPOSING IN EMERGING INFECTIOUS DISEASES

Host Responses and Therapeutic Innovation in Emerging infectious diseases- from Ebola to COVID-19 and beyond — remain among the most pressing challenges in global health. With high mortality rates, unpredictable spread, and limited treatment options, these diseases strain healthcare systems and highlight gaps in our ability to respond swiftly and effectively. Over the past decade,

research efforts have increasingly focused not only on targeting pathogens directly but also on leveraging our understanding of host biology, repurposing existing drugs, and designing next generation antivirals to prepare for future outbreaks. This synthesis reviews four major strands of research: Host-directed therapies (HDTs), drug repurposing for viral infections, repurposing clinically developed drugs for Ebola virus disease, and the development of novel nucleoside analogues for emerging viruses.(14)

4.1 Host-Directed Therapies (HDTs):

Rethinking the Target Traditional antimicrobial strategies have focused on killing or inhibiting pathogens directly. While effective in many cases, this pathogen-centric approach faces limitations including drug resistance, narrow antiviral spectra, and the inability to mitigate pathogen-induced host damage. Interventions that modulate host immune responses, bolster innate defenses, or dampen pathological inflammation — as adjuncts or alternatives to conventional antimicrobial treatment.

Why Focus on the Host?

Infectious diseases cause significant morbidity and mortality not just through direct pathogen effects, but through the host's response to infection. In diseases like tuberculosis, HIV, influenza, and emerging viral infections, collateral tissue damage, immune dysregulation, and inflammatory cascades often drive pathology. HDTs aim to:

✓ Enhance protective host immune mechanisms.

✓ Suppress excessive inflammatory responses.

✓ Improve clinical outcomes even when pathogen-directed therapy is limited.

For example, in tuberculosis — a bacterial infection long challenged by multidrug resistance — HDTs seek to augment phagocyte antimicrobial activity, improve autophagy, and modulate granuloma formation. In viral infections, therapies that prevent or reduce cytokine storms (hyperinflammatory responses) could reduce disease severity, as observed in severe influenza or SARS-CoV-2 cases.

Types and Examples of Host Directed Therapies(HDTs)

HDTs classified into several categories:

Immunomodulatory agents: drugs that modify immune cell activity.

Biologics: monoclonal antibodies or cytokine therapies that target specific inflammatory pathways.

Repurposed non-infectious disease drugs: compounds used in non-communicable diseases that have immunomodulatory or host-enhancing effects. Cellular therapies and nutritional support.

Because these therapies target host responses rather than pathogen components, they may retain effectiveness even when pathogens mutate to evade direct-acting drugs. However, identifying which host pathways to target without inducing immunosuppression or harming necessary defense mechanisms remains a central Challenge(14).

4.2 Drug Repurposing:

Speeding the Search for Antivirals

Developing new drugs from scratch typically takes a decade or more. In the face of rapidly escalating outbreaks, drug repurposing — identifying new therapeutic uses for existing drugs — presents a faster, cost-effective alternative. Rationale and Advantages. Repurposing benefits from existing safety and pharmacokinetic data, which accelerates the transition to clinical evaluation. Repurposed antivirals can be: Direct-acting (targeting viral proteins like polymerases or proteases). Host-targeting (modulating cellular pathways exploited by virus In the 2013–2016 Ebola epidemic, urgent repurposing screens tested hundreds of approved drugs to find compounds with antiviral activity. Many drugs originally designed for other viruses or non-infectious conditions demonstrated unexpected antiviral functions, suggesting broad potential if appropriately validated(15,30).

4.3 Key Outcomes and Challenges

Identification of drug classes with antiviral promise, including nucleoside analogues, antimalarials, and antipsychotics.

Integration of repurposing with animal models to validate efficacy.

The need for innovative validation strategies to predict clinical usefulness more reliably than traditional in vitro modelsThe primary challenge remains translating in vitro and animal findings into meaningful clinical efficacy. Many promisin candidates fail due to insufficient potency, toxicity at effective doses, or lack of benefit in real disease contexts. Even so, repurposing remains vital for rapid epidemic response.

Repurposing Clinically Developed Drugs for Ebola Virus Disease The Ebola virus epidemic highlighted both the urgency and difficulty of treating acutal viral infections with no approved therapeutics. Some conducted one of the earlier systematic analyses of repurposing clinically developed drugs for Ebola virus disease (EVD). Their work underscores the potential and limitations of this strateg Screening and Findings. Developed drugs for antiviral activity against coronaviruses like MERS-CoV and SARS-CoV as stand-ins for filoviruses like Ebola.

27 compounds active against both Middle East Respiratory Syndrome(MERS) and Severe acute respiratory syndrome(SARS). Many compounds originated from cancer chemotherapy, antipsychotics, or cardiovascular drugs — highlighting that non-antiviral drugs can have unexpected antiviral effects. Supporting evidence from broader Ebola repurposing reviews suggests similar patterns: drugs with known safety profiles but unrelated original targets showed some efficacy in vitro or in early preclinical models. However, high risk of bias and heterogeneity across studies meant that none could be definitively recommended without further research. (16)

Clinical and Research Implications

Repurposing can generate hypotheses rapidly, but clinical translation remains challenging. Ebola and other acute viral infections demand rapid-onset, potent antivirals, which many repurposed drugs fail to deliver at safe doses. Drug combinations targeting multiple stages of the viral life cycle or host pathways may offer synergistic benefits and deserve deeper investigation.

Nucleoside Analogues: A Cornerstone of Antiviral Innovation De Clercq (2020) and related literature emphasize the enduring importance of nucleoside and nucleotide analogues as antiviral agents. These compounds mimic natural building blocks of nucleic acids, becoming incorporated into viral genomes or inhibiting viral polymerases, thus halting replication.

Mechanisms of Action

Nucleoside analogues exploit a fundamental similarity between their structures and natural nucleotides. When incorporated into viral DNA or RNA:

They can cause chain termination, preventing elongation.

They can introduce mutations that render genomes nonviable (a concept utilized by drugs like molnupiravir).

Because viral polymerases often lack the proofreading capabilities of host enzymes, these compounds preferentially disrupt viral replication.(17)

Examples and Clinical Impact

Some of the most successful antivirals are nucleoside analogues:

Remdesivir, originally developed for hepatitis C and studied for Ebola, demonstrated broad antiviral activity in vitro against filoviruses and coronaviruses, leading to emergency use for COVID-19.

Molnupiravir is a prodrug that induces replication errors in SARS-CoV-2, Showcasing the potential for broad-spectrum antiviral action even decades after initial development Integrated Perspectives and Future Directions.

4.4 Complementarity of Approaches

HDTs address the host's role in disease progression and may mitigate damage even when pathogen clearance is incomplete.

Drug repurposing accelerates therapeutic deployment and informs which biological pathways may be clinically exploitable.

Repurposing clinically developed drugs, particularly in outbreak settings, remains a pragmatic interim strategy while targeted antivirals are developed.

Nucleoside analogues exemplify a class of drugs with demonstrated efficacy across multiple viral families and continued relevance in future outbreaks.

Challenges to Overcome

Key hurdles include:

✧ Ensuring safety and tolerability in diverse populations.

✧ Avoiding the development of resistance.

✧ Translating in vitro potency into clinical benefit.

✧ Understanding the complex interplay between host immune responses and pathogen biology.(17)

5. EVALUATION OF EFFICACY AND CLINICAL

RESTATEMENT

The global outbreak of COVID- 19, caused by the new severe acute respiratory pattern coronavirus 2(SARS- CoV- 2), created a major public health extremity beginning in late 2019. Unlike former coronavirus outbreaks similar as SARS- CoV in 2003 and MERS- CoV in 2012, the SARS- CoV- 2 epidemic spread fleetly across mainlands, with high transmissibility and significant morbidity and mortality worldwide. In this environment, there was an critical need for effective rectifiers, especially in the early stages before vaccines were extensively available. Traditional medicine discovery and development timelines frequently a decade or further were inharmonious with the immediate demand for treatments. As a result, experimenters fleetly turned to medicine repurposing(also known as medicine displacing) as a doable strategy to identify being medicines with implicit exertion against COVID- 19.

Explanation for Repurposing in COVID- 19

Drug repurposing leverages the given safety biographies and pharmacokinetic data of approved or investigational medicines to explore new remedial suggestions. This approach dramatically shortens development timelines and reduces cost and threat compared with de novo medicine development. In the environment of a epidemic, medicine repurposing can accelerate the identification of implicit treatments that may alleviate complaint inflexibility or reduce viral replication During the early months of the COVID- 19 epidemic, repurposing sweats were motivated by several factors:

The absence of approved antiviral treatments specifically targeting SARS- CoV- 2 Vacuity of structural and functional information about viral proteins soon later the genomic sequence was published. A large force of approved medicines with known mechanisms of action and mortal safety biographies. wide access to computational and experimental platforms to screen being composites. Repurposed medicine campaigners for COVID- 19 Antiviral Agents Several medicines firstly developed for other viral infections were estimated for exertion against SARS- CoV- 2.

Remdesivir — originally developed for Ebola contagion complaint, this broad- diapason antiviral that targets RNA-dependent RNA polymerase was among the foremost repurposed agents to show exertion against SARS- CoV- 2. It entered exigency use authorization in numerous countries and remains one of the first antivirals recommended for rehabilitated cases taking supplemental oxygen.

Lopinavir/ Ritonavir — Antiretroviral agents used in HIV treatment were snappily tested due to their known protease- inhibiting exertion. Beforehand in vitro findings suggested possible Exertion, but posterior clinical data showed limited benefit in treating COVID- 19 cases.

Ribavirin, Favipiravir — Nucleoside analogues with exertion against other RNA contagions were also delved through repurposing defenses. Some were taken into clinical trials, though harmonious clinical efficacity remained unproven. Anti-Inflammatory and Immune Modulators Beyond antivirals, medicines that modulate host vulnerable responses gained attention in managing the hyperinflammatory state seen in severe COVID- 19.

Dexamethasone — A corticosteroid that showed mortality benefit in severe complaint by dampening inordinate inflammation. Its repurposed use came part of standard care for cases taking oxygen.

Baricitinib — An immunomodulatory agent originally approved for rheumatoid arthritis, baricitinib showed salutary goods in combination with remdesivir by reducing recovery time, particularly in rehabilitated cases.

Other medicine Classes Explored

Anticoagulants — Dabigatran and analogous medicines were delved due to the thrombotic complications associated with COVID-19 infections. Azithromycin and other antibiotics — While primarily antibacterial, these agents were estimated foranti-inflammatory and immunomodulatory parcels in COVID- 19 Antimalarials(Chloroquine/ Hydroxychloroquine) — These medicines originally showed in vitro goods against SARS- CoV- 2 but were eventually not recommended due to lack of clinical efficacity and cardiac safety enterprises.(18,19)

5.1 Computational Approaches to Drug Repurposing

Given the vast number of approved medicines available for webbing, computational styles came inestimable in prioritizing campaigners during COVID- 19.a comprehensive view of these strategies, demonstrating how in silico tools accelerate repurposing exploration.

Crucial Computational styles:

Molecular Docking and Virtual Webbing — These ways prognosticate how medicines bind to viral or host protein targets. For SARS- CoV- 2, common targets included:

- Main protease(Mpro) responsible for viral polyprotein processing.
- RNA-dependent RNA polymerase(RdRp) essential for viral replication.
- Shaft protein and host receptor relations(e.g., ACE2 list).

Network- grounded Approaches — These styles model relations between viral proteins, mortal proteins, and medicine targets. Network drug fabrics can identify medicine campaigners by assaying how being medicines undo host- pathogen commerce networks.

Machine literacy and AI — Arising machine literacy ways enablevaticination of medicine – target relations grounded on large datasets. These approaches can fleetly screen thousands of molecules and prioritize candidates based on predicted efficacy.

Examples of In Silico Findings

Many repurposing screens identified drug candidates beyond antivirals, including anti-inflammatory agents and cardiovascular drugs that may mitigate COVID-related pathology.

Graph neural network and AI models enabled integrative analysis of biological data, revealing drug combinations that could synergize against COVID-19.

5.21 Clinical Translation and Outcomes

Although computational and early experimental evidence generated hundreds of repurposed drug candidates, clinical translation has been mixed:

Remdesivir achieved widespread use based on clinical trial data supporting shortened recovery time in some patient groups.

Dexamethasone significantly reduced mortality among patients with severe disease. Many other candidates — including lopinavir/ritonavir and hydroxychloroquine — did not show consistent clinical benefit and are no longer recommended. Several drugs identified via computational repurposing continue to be evaluated in clinical trials (e.g., baricitinib, inhaled corticosteroids, other antivirals), underscoring that repurposing remains an evolving therapeutic strategy. (20,7)

5.2 Challenges and Limitations

Despite its promise, drug repurposing for COVID-19 faces several challenges: Predictive Limitations — Computational predictions require experimental validation, and many in silico hits fail in clinical contexts.

Clinical Evidence Gaps — Early repurposing efforts were sometimes based on limited or low-quality clinical data.

Disease Complexity — COVID-19 pathogenesis involves viral replication, immune dysregulation, and host co-morbidities; a single drug may not address all disease mechanisms efficiently.

5.3 Efficacy: From Preclinical Signals to Clinical Outcomes

A central challenge in repurposing is validating that a drug's activity in preclinical models translates into meaningful clinical benefit. Many repurposing initiatives begin with in vitro assays, computational predictions, or mechanistic hypotheses that suggest a drug may affect a new target or pathway. While these approaches can generate promising leads, they often fail to capture the biological complexity of human disease. preclinical efficacy data must be robust and reproducible before advancing to human trials. Many repurposed candidates demonstrate activity in simplified cellular systems, but their effect sizes decrease or disappear in vivo due to pharmacokinetic differences, tissue distribution issues, or off-target interactions that originally indication did not reveal. This distinction between early signals and clinical efficacity contributes to waste in repurposing channels.

Clinical substantiation from the COVID- 19 epidemic illustrates this well multitudinous medicines showed in vitro antiviral exertion but eventually failed to demonstrate efficacity in patient issues. Agents like hydroxychloroquine and certain antivirals generated violent early interest, but latterly controlled trials revealed limited or no benefit, pressing the peril ofoverinterpreting primary results without mechanistic confirmation and rigorous clinical testing.(21,22)

5.4 Clinical Trial Design & substantiation norms

A alternate translational challenge concerns the design and interpretation of clinical trials for repurposed medicines. Traditional medicine development benefits from precisely controlled studies that precipitously escalate through Phase I(safety), Phase II (efficacity), and Phase III(evidence). In repurposing, investigators occasionally attempt to compress this process, counting on being safety data to streamline trials for new suggestions. still, this can undermine assessment of efficacy.However, its optimal cure, authority, if a medicine's safety profile is well known.window in a new suggestion may differ mainly from those established for the original use. Trials must thus be designed to explore these parameters strictly, yet backing and nonsupervisory pressures frequently push investigators toward lower or lower rigorous studies that warrant power to descry true clinical goods.

Also, biomarkers and endpoints suitable in the original complaint may be inapplicable or unhappy in the repurposed environment. Without validated surrogate endpoints or prophetic biomarkers, trials threat failing not because the medicine is ineffective, but because the study was n't sufficiently aligned to capture its true impact. Regulatory & Commercial walls Impacting Translation Nonsupervisory and marketable surroundings significantly impact whether repurposed medicines reach the clinic. On the nonsupervisory side, agencies like the FDA and EMA bear data demonstrating both safety and efficacity in the new suggestion, frequently with analogous norms to entirely new medicines. This effectively requires conducting Phase II and III trials, which are time- consuming and precious.

Commercially, lack of intellectual property protection for repurposed uses reduces impulses for pharmaceutical companies to invest in late- stage trials. Patents on the original medicine may have expired, and system- of- use patents for a new suggestion are weaker

and harder to apply. This disincentivizes investment despite potentially high public health value. Without strong marketable backing, numerous repurposing campaigners stall at Phase II or fail to attract backing for confirmational trials.

5.5 Integrating efficacity with Real- World substantiation

To bridge gaps between controlled trial results and real- world effectiveness, arising strategies emphasize the integration of Real-world substantiation(RWE) from electronic health records, insurance claims, and patient registries. This approach can help validate efficacity signals linked in trials and upgrade understanding of patient groups most likely to profit. still, developing fabrics that strictly combine RWE with clinical trial data remains grueling and requires new statistical and nonsupervisory norms.(21,22)

5.6 Systemic results & unborn Direction.

Both reviews stress that improving clinical translation of repurposed drugs will require systemic changes:

Collaborative networks that bring together academia, industry, and regulators to share data early and coordinate development plans. Innovative funding models that subsidize Phase II/III trials for repurposed candidates, especially for rare or neglected indications where commercial interest is low but unmet need is high. Adaptive regulatory pathways that allow conditional approvals based on strong surrogate endpoints with ongoing post-marketing confirmation.(21,22).

6. CHALLENGES AND LIMITATIONS OF DRUG REPURPOSING

Drug repurposing—discovering new therapeutic uses for existing or shelved drugs—has gained momentum as an alternative or complement to traditional de novo drug discovery, promising reduced development time, known safety profiles, and lower early-stage costs. However, this strategy also faces significant challenges that can limit its impact and commercial viability. (1,5,23).

One central scientific limitation relates to efficacy and target relevance. Many repurposed candidates have pharmacological activities optimized for their original indication, meaning that their potency toward new targets is often lower or mechanistically ambiguous. Drugs initially developed for one target may not interact strongly enough with a new disease pathway, complicating the establishment of clinical effectiveness and increasing the likelihood of costly late-stage failures. Moreover, many computational and high-throughput repurposing predictions generate long lists of candidate drugs, but poor specificity and mechanistic validation often hinder prioritization and follow-through into robust clinical evaluating Intellectual property (IP) and commercial barriers also pose major obstacles. Because repurposed drugs are often already marketed or well-described in the literature, securing new patents or effective market exclusivity can be difficult. Prior publication of repurposing hypotheses may constitute “prior art” that blocks new IP claims, discouraging investment by companies that cannot reliably recoup development costs without exclusivity. In many cases, generic competitors can limit profit margins even after a new indication is approved.

Additional limitations include regulatory and clinical development hurdles: although safety profiles are known, regulators still require evidence of efficacy for the new indication, sometimes necessitating extensive trials. Reformulation, different dosing, or altered routes of administration may trigger additional early-phase studies. Furthermore, access to historic clinical data on shelved compounds is often limited by confidentiality, reducing the ability of researchers to evaluate repurposing potential fully.

Lastly, resource constraints and industry incentives influence repurposing efforts. Academic groups may generate innovative hypotheses, but lack funding or infrastructure to advance them through expensive later-stage trials. Pharmaceutical firms may deprioritize repurposing when strategic business priorities favor novel, high-profit targets. Together, these scientific, regulatory, economic, and IP challenges illustrate that while drug repurposing offers real advantages, its full potential requires targeted efforts to address these key limitations.(21,22,24)

7. EMERGING INNOVATIONS IN DRUG REPURPOSING

In the last decade, traditional drug development has increasingly incorporated artificial intelligence (AI), machine learning (ML), deep learning (DL), and systems biology approaches to enhance drug repurposing strategies—identifying new therapeutic uses for existing drugs more quickly and cost-effectively than conventional discovery pathways. At the core of this transformation is AI’s ability to process massive, complex biomedical datasets—ranging from genomic and proteomic profiles to real-world clinical and chemical data—to uncover hidden drug-disease relationships that would otherwise be difficult or impossible to detect. These computational methods can sift through billions of data points to recognize patterns predictive of drug efficacy toxicity, or novel target engagement, forming the basis for repurposing hypotheses.

Machine Learning & Deep Learning in Repurposing Pipelines

Machine learning methods—such as neural networks, random forests, and support vector machines—have become standard tools for evaluating drug-target interactions, predicting bioactivity, and screening vast libraries of compounds. Deep learning, a subset of ML characterized by multi-layer neural architectures, excels at modeling highly nonlinear relationships inherent in biological systems without manual feature engineering, making it especially suited for big data integration in repurposing tasks For example, deep learning-assisted virtual screening accelerates the identification of drug candidates by evaluating how well existing molecules might bind to new targets, thereby highlighting promising repurposing candidates for further experimental validation. Generative models, including deep neural networks and graph convolutional networks, enable prediction of drug-disease associations and inform repurposing opportunities across therapeutic areas.(26)

7.1 Case Study: AI-Discovered Antibiotics

A landmark demonstration of AI's potential came from the work by Stokes and colleagues, where a deep learning model screened millions of chemical structures and identified halicin—a molecule with antibiotic properties distinct from known classes—which showed broad-spectrum activity, including against drug-resistant pathogens. This breakthrough illustrated how AI can uncover repurposing opportunities that traditional chemical intuition might miss, especially for urgent needs like antimicrobial resistance(25,27).

7.2 Systems Biology and Integrative Approaches

Systems biology complements AI and ML by providing a holistic view of biological networks. By representing drugs, targets, pathways, and diseases as interconnected networks—often in the form of knowledge graphs—researchers can apply graph based learning models to detect non-obvious relationships across multi-omics layers. These approaches have been particularly impactful in contexts like COVID-19, where rapid repurposing was essential, as graph neural networks integrated heterogeneous data sources to suggest plausible candidates for experimental validation. Integrating systems biology with ML also improves mechanistic interpretability: rather than treating the prediction task as a "black box," sophisticated models can trace pathways linking drugs to disease phenotypes, which supports biological plausibility and strengthens confidence in repurposing hypotheses.

Translational Impact & Future Directions

AI-driven repurposing has already shown promise in oncology, infectious diseases, and rare disorders by linking existing drugs to novel targets more rapidly than traditional methods. However, achieving clinical translation still requires rigorous experimental validation and regulatory navigation, and the integration of systems biology is expected to further enhance both predictive accuracy and Looking forward, innovations such as explainable AI, multi-modal data integration, and AI-augmented laboratory automation are poised to make repurposing even more efficient, transparent, and biologically grounded—potentially reshaping how we respond to emerging diseases and unmet medical needs. Looking forward, innovations such as explainable AI, multi-modal data integration, and AI-augmented laboratory automation are poised to make repurposing even more efficient, transparent, and biologically grounded—potentially reshaping how we respond to emerging diseases and unmet medical needs.(6,7)

8. FUTURE DIRECTIONS & POLICY IN DRUGREPURPOSING

Drug repositioning—finding new therapeutic uses for existing drugs—continues to grow as an essential strategy for accelerating drug discovery, reducing costs, and addressing unmet medical needs. Early articulations of the repositioning concept highlighted its promise: the high time and cost demands of de novo drug development and the consistent failure rates in late-stage clinical trials created a compelling rationale for "new uses for old drugs." Chong & Sullivan (2007) argued that systematically screening existing compounds could help overcome the traditional challenges of drug discovery while expanding therapeutic options. A core pillar shaping future directions is the integration of repositioning into mainstream pharmaceutical strategy. Emphasized that drug repositioning should not be viewed as a niche or last-ditch effort but as a primary strategy embedded in the portfolios of research-intensive pharmaceutical companies. Drugs with established safety and pharmacokinetic profiles can potentially reach patients faster and at lower development costs, enhancing pipeline productivity and reducing dependence on entirely new molecular entities. This is especially compelling given that repurposed drugs often bypass early safety testing phases and shorten development timelines relative to new drugs.(28,29).

Looking ahead, infectious diseases represent a critical frontier in repositioning research. Repositioning has already been explored for infectious disease threats such as HIV, malaria, and most recently COVID-19, where existing antivirals an immunomodulators were evaluated for efficacy against SARS-CoV-2. The urgency of pandemic response illustrated how repositioning could rapidly generate clinical candidates during public health crises—far faster than typical de novo pipelines. Although repositioning is not

exclusively confined to infectious diseases, its potential to deliver therapies where none exist or where resistance has emerged remains a high priority. Studies related to repositioning in infectious disease contexts underscore the need for coordinated policy and funding frameworks that support rapid clinical evaluation, data sharing, and regulatory flexibility during outbreaks.

A key future direction is the integration of personalized and precision medicine with repositioning approaches. Li & Jones (2012) articulated how genomic insights and individualized disease mechanisms can guide the selection of repositioned therapies Acclimatized to specific patient groups. By linking molecular autographs with medicine action biographies, experimenters can move beyond one- size- fits- all models and identify precise matches between patient pathophysiology and remedial agents formerly on the request. This paradigm aligns with broader healthcare pretensions of adding efficacity and minimizing adverse goods while making medicine development more effective.

From a policy perspective, several strategic themes are arising.

- **Regulatory Adaptation:**

Traditional nonsupervisory pathways were designed for new chemical realities. To completely influence displacing, agencies can consider adaptive pathways, accelerated blessings, and real- world substantiation fabrics that fete previous safety data without compromising rigor. Regulatory wisdom must evolve in resemblant with scientific invention to insure safe but effective transitions from laboratory to clinic.

- **Incitement Structures:**

Intellectual property(IP) and request impulses presently disincentivize investment in displacing, particularly for medicines that have lost exclusivity. Innovative policy mechanisms — similar as * extended exclusivity for new suggestions, duty impulses for displacing exploration, and public-private hookups * could stimulate investment by balancing affordable access with reasonable returns.

- **Collaborative Data Ecosystems:**

Open data architectures and participated knowledge platforms can accelerate identification of displacing openings. By pooling clinical data, molecular biographies, and medicine action databases, experimenters and policymakers can reduce duplication, enhance translucency, and foster invention.

- **Global Health Prioritization:**

Drug displacing holds special applicability for neglected conditions and low- resource settings where request impulses alone fail to deliver necessary treatments. Policy fabrics that encourage cooperative R&D for these areas can help close critical gaps in global health equity.(21,30)

9. CONCLUSION

Medicine repurposing — also known as medicine displacing has surfaced as a vital strategy in combating contagious conditions, offering a compelling volition to conventional medicine discovery that's long, expensive, and fraught with high waste rates. Rather than beginning from scrape, repurposing identifies new remedial uses for medicines formerly approved for other suggestions, using being safety and pharmacological data to accelerate clinical restatement.

The traditional medicine discovery and development channel can take 10 – 15 times or more, with high costs and high failure rates profoundly limiting the pace at which new curatives reach cases. medicine repurposing addresses these challenges by shortening development timelines and reducing threat medicines preliminarily approved by agencies similar as the FDA or EMA formerly have established safety biographies, allowing experimenters to bypass early phases of toxicology testing and focus directly on efficacy in the new indication.

A key theme in this literature is the dual nature of repurposing approaches: Serendipitous discoveries, where unexpected clinical observations lead to new uses, and Systematic, hypothesis-driven strategies, where data mining and mechanistic insight guide the search for candidates.

Advantages of repurposing for infectious diseases include:

◆ Rapid response capabilities, critical during epidemics or pandemics, where time is of the essence.

◆ Reduced development risk and cost, since early toxicity and safety data already exist.

◆ Broad applicability across diverse pathogens, including viruses, bacteria, and parasites.

◆ Overall, the integrative literature affirms that drug repurposing holds immense promise for infectious disease control—especially when integrated with modern computational tools and cross-disciplinary research efforts that link mechanistic biology with clinical insights(1,15).

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