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Review Article
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RECENT DEVELOPMENTS IN DRUG REPURPOSING: A MEDICINAL CHEMISTRY PERSPECTIVE

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Abstract
Drug repurposing, also known as drug repositioning, has emerged as an effective strategy for accelerating drug development by identifying new therapeutic uses for existing drugs. From a medicinal chemistry perspective, drug repurposing leverages known chemical scaffolds, established safety profiles, and well-characterized pharmacokinetic properties to reduce development time, cost, and risk. Recent advances in computational chemistry, high-throughput screening, and systems biology have significantly expanded the scope of repurposing approaches. This review discusses contemporary strategies in drug repurposing with emphasis on medicinal chemistry principles, including structure–activity relationships, target promiscuity, and chemical optimization. Key therapeutic applications, challenges, and future prospects are also highlighted, demonstrating the growing importance of repurposing in modern drug discovery.

Keywords: *Drug repurposing; Medicinal chemistry; Structure–activity relationship; Polypharmacology; Computational drug discovery; Therapeutic innovation.*

INTRODUCTION

The traditional drug discovery pipeline is associated with high attrition rates, long development timelines, and escalating costs. Drug repurposing offers an attractive alternative by exploring new indications for approved or investigational drugs whose pharmacological and toxicological profiles are already known [1]. This approach has gained renewed interest due to its success in addressing unmet medical needs and responding rapidly to emerging diseases.

From a medicinal chemistry standpoint, drug repurposing exploits the intrinsic chemical properties of drug molecules, including their ability to interact with multiple biological targets. Advances in chemical biology and computational tools have further strengthened the role of medicinal chemistry in systematic repurposing efforts [2].

MEDICINAL CHEMISTRY BASIS OF DRUG REPURPOSING

1. Structural and Chemical Considerations

Many small-molecule drugs exhibit structural features that enable binding to more than one biological target, a phenomenon known as polypharmacology [3]. Functional groups, heterocyclic scaffolds, and molecular flexibility play key roles in determining off-target interactions that may translate into new therapeutic applications.

2.Structure–Activity Relationship and Optimization

Understanding structure–activity relationships (SAR) is central to drug repurposing. Minor chemical modifications to an existing drug can improve potency, selectivity, or pharmacokinetic properties for a new indication while retaining a known safety profile [4]. Medicinal chemists often apply scaffold modification and bioisosteric replacement to optimize repurposed leads.

APPROACHES TO DRUG REPURPOSING

1. Computational and In Silico Methods

In silico methods such as molecular docking, pharmacophore modeling, and machine learning-based prediction have become essential tools in repurposing research [5]. These approaches allow rapid screening of approved drug libraries against new biological targets, significantly reducing experimental effort.

2. Phenotypic and Target-Based Screening

High-throughput phenotypic screening enables the identification of unexpected biological activities without prior knowledge of molecular targets [6]. Target-based screening, in contrast, focuses on testing known drugs

against specific disease-relevant targets, supported by medicinal chemistry-driven assay development.

3 Network Pharmacology and Systems Biology

Network-based approaches integrate chemical, biological, and clinical data to uncover drug–target–disease relationships [7]. These methods support rational repurposing by considering complex biological pathways rather than single-target interactions.

THERAPEUTIC APPLICATIONS

1. Oncology

Drug repurposing has led to the identification of several non-oncology drugs with anticancer activity. For example, certain anti-inflammatory and antiparasitic agents have demonstrated potential in cancer therapy through modulation of signaling pathways and tumor metabolism [8].

2. Infectious Diseases

Repurposing has proven particularly valuable in infectious diseases, where rapid therapeutic intervention is critical. Broad-spectrum antiviral and antibacterial activities have been identified for drugs originally developed for unrelated indications [9].

3. Neurological and Rare Diseases

Neurological and rare diseases often lack effective treatments due to limited commercial incentives. Drug repurposing offers a promising route by leveraging existing compounds with central nervous system penetration and known safety profiles [10].

CHALLENGES AND LIMITATIONS

Despite its advantages, drug repurposing faces several challenges, including intellectual property issues, dosage optimization for new indications, and incomplete understanding of mechanisms of action [11]. From a medicinal chemistry perspective, achieving target specificity without compromising safety remains a key hurdle.

FUTURE PERSPECTIVES

The future of drug repurposing lies in the integration of medicinal chemistry with artificial intelligence, real-world clinical data, and advanced experimental models. Rational chemical optimization of repurposed candidates and the development of hybrid analogs are expected to expand therapeutic potential. Collaborative frameworks involving academia, industry, and regulatory agencies will further enhance the success of repurposing strategies [12].

CONCLUSION

Recent developments in drug repurposing underscore its growing importance as a complementary approach to traditional drug discovery. Medicinal chemistry plays a pivotal role in understanding molecular mechanisms, optimizing chemical structures, and expanding therapeutic applications. Continued advancements in computational tools, screening technologies, and chemical optimization are expected to drive the next generation of repurposed drugs, addressing unmet medical needs efficiently and sustainably.

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