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AI, Novel Strategies Accelerate Drug Discover

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Introduction

This article offers a comprehensive overview of how artificial intelligence is transforming drug discovery and development, discussing its historical context, current applications in various stages of the process, and predicting its future impact. It highlights AI's role in accelerating lead identification, optimizing drug candidates, and improving preclinical and clinical outcomes, positioning it as a critical tool for future pharmaceutical innovation [1].

This paper explores the significant advancements in identifying and validating drug targets, tracing the evolution from genomic approaches to their application in clinical practice. It delves into how new technologies and methodologies are improving the precision and efficiency of discovering disease-modifying targets, thereby paving the way for more effective and personalized therapies [2].

This article discusses the current state of computational methods in small molecule drug discovery, highlighting both the significant challenges faced and the emerging opportunities. It covers various in silico techniques used for virtual screening, lead optimization, and ADMET prediction, underscoring their potential to streamline the drug discovery pipeline and reduce costs [3].

This review provides an in-depth look at targeted protein degradation (TPD), including the rapidly evolving field of PROTACs, as a transformative strategy in drug discovery. It details the mechanisms, recent advances in designing effective degraders, and explores future perspectives for leveraging TPD to tackle previously undruggable targets and address unmet medical needs [4].

This article explains the principles and applications of fragment-based drug design (FBDD), from the initial identification of small fragments that bind weakly to a target to their subsequent optimization into potent lead compounds. It highlights FBDD's ability to efficiently explore chemical space and its increasing role in discovering novel drug candidates across various therapeutic areas [5].

This paper discusses drug repurposing as a highly strategic and cost-effective approach to accelerate drug discovery by identifying new therapeutic uses for existing, approved, or investigational drugs. It explores various strategies, including computational and experimental methods, emphasizing its advantages in reducing development timelines and risks compared to de novo drug discovery [6].

This review focuses on the current applications and emerging trends of computational methods in drug discovery and development. It covers a broad spectrum of in silico techniques, from virtual screening and molecular docking to ADME/Tox prediction and de novo drug design, illustrating how these tools are becoming indispensable for efficient and rational drug development [7].

This article examines the contemporary strategies and future challenges in integrating phenotypic and target-based approaches for drug discovery. It discusses how combining these methods can provide a more holistic understanding of disease biology and drug action, leading to the identification of novel therapeutic mechanisms and more effective drug candidates [8].

This review highlights the recent progress in peptide-based drug discovery and development, underscoring the increasing interest in peptides as therapeutic agents due to their high specificity and low toxicity. It covers advancements in peptide design, synthesis, delivery, and their applications across various disease areas, pointing towards a promising future for peptide therapeutics [9].

This article reviews the significant advancements in antibody-based drug discovery and engineering, emphasizing their growing importance as therapeutics for a wide range of diseases. It covers innovative techniques in antibody generation, optimization, and conjugation, discussing how these developments are leading to more potent, specific, and safer antibody drugs [10].

Description

Artificial Intelligence (AI) is fundamentally transforming drug discovery and development [1]. This includes its historical context, current applications across various stages, and its predicted future impact, especially in accelerating lead identification, optimizing drug candidates, and improving preclinical and clinical outcomes [1]. AI stands as a critical tool for future pharmaceutical innovation [1]. Complementing this, computational methods are extensively applied in drug discovery and development, covering a broad spectrum of in silico techniques [7]. These range from virtual screening and molecular docking to ADME/Tox prediction and de novo drug design, proving indispensable for efficient and rational drug development [7]. Specifically for small molecule drug discovery, computational methods address significant challenges while presenting emerging opportunities, notably in virtual screening, lead optimization, and ADMET prediction, ultimately streamlining the drug discovery pipeline and reducing costs [3].

Significant advancements are continually being made in identifying and validating drug targets [2]. This evolution traces from genomic approaches right through to their application in clinical practice, improving the precision and efficiency of discovering disease-modifying targets and paving the way for more effective, personalized therapies [2]. A transformative strategy in this domain is Targeted Protein Degradation (TPD), particularly the rapidly evolving field of PROTACs [4]. TPD mechanisms, alongside recent advances in designing effective degraders, offer future perspectives for tackling previously undruggable targets and addressing unmet medical needs [4]. Moreover, Fragment-Based Drug Design (FBDD) leverages the initial identification of small fragments that bind weakly to a target, subsequently optimizing them into potent lead compounds [5]. FBDD is highly valued

for its ability to efficiently explore chemical space and its increasing role in discovering novel drug candidates across diverse therapeutic areas [5].

Drug repurposing stands out as a highly strategic and cost-effective approach to accelerate drug discovery [6]. It involves identifying new therapeutic uses for existing, approved, or investigational drugs, utilizing various computational and experimental methods [6]. The primary advantages lie in reducing development timelines and risks compared to de novo drug discovery [6]. Furthermore, contemporary strategies actively integrate phenotypic and target-based approaches for drug discovery [8]. Combining these methods offers a more holistic understanding of disease biology and drug action, which is essential for identifying novel therapeutic mechanisms and developing more effective drug candidates [8]. These integrations also highlight future challenges in maximizing their synergistic potential [8].

Peptide-based drug discovery and development have seen recent substantial progress [9]. There's growing interest in peptides as therapeutic agents due to their inherent high specificity and low toxicity [9]. Advancements span peptide design, synthesis, delivery, and their applications across various disease areas, indicating a promising future for peptide therapeutics [9]. Similarly, antibody-based drug discovery and engineering have made significant strides, emphasizing their increasing importance as therapeutics for a wide range of diseases [10]. Innovative techniques in antibody generation, optimization, and conjugation are leading to the development of more potent, specific, and safer antibody drugs [10].

Conclusion

The landscape of drug discovery and development is rapidly evolving through diverse and innovative strategies. Artificial Intelligence (AI) has become a pivotal force, accelerating lead identification, optimizing drug candidates, and enhancing outcomes across all stages of drug development. Simultaneously, significant advancements are being made in the precise identification and validation of drug targets, moving from genomic insights to practical clinical applications to create more effective and personalized therapies. Computational methods are indispensable, streamlining drug discovery pipelines by enabling virtual screening, lead optimization, and ADMET prediction for small molecule drugs. Beyond traditional small molecules, novel modalities such as Targeted Protein Degradation (TPD), including PROTACs, are emerging as powerful tools to address previously undruggable targets. Fragment-Based Drug Design (FBDD) offers an efficient way to explore chemical space, evolving weak binders into potent lead compounds. Drug repurposing provides a strategic and cost-effective path, identifying new therapeutic uses for existing drugs and significantly reducing development timelines and risks. The field is also seeing substantial progress in peptide-based and antibody-based therapeutics. Peptides are increasingly valued for their high specificity and low toxicity, benefiting from advances in design and delivery, while antibodies are becoming more potent, specific, and safer through innovative engineering techniques. Crucially, integrating phenotypic and target-based approaches offers a holistic understanding of disease biology and drug action, fostering the identification of novel therapeutic mechanisms and superior drug candidates. These combined efforts highlight a dynamic period of innovation aimed at developing more effective treatments.

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Conflict of Interest

None.

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