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Opinion Article

The Evolution in Pro-Drug Design for Enhanced Therapeutic Outcomes

Amphansap Garner*

Department of Pharmacy, University of Warwick, England, UK

ABOUT THE STUDY

The concept of pro-drug design has emerged as a promising strategy to improve drug delivery and efficacy while mitigating potential side effects. Pro-drugs are inactive compounds that undergo enzymatic or chemical transformation *in vivo* to release the active drug at the desired site of action. This approach offers several advantages, including improved bioavailability, enhanced targeting, and reduced toxicity. Recent advancements in pro-drug design have paved the way for the development of novel therapeutics with improved clinical outcomes.

One of the key challenges in drug development is achieving optimal bioavailability, which refers to the fraction of the administered dose that reaches the systemic circulation unchanged and is available to exert its therapeutic effects. Pro-drug design addresses this challenge by modifying the physicochemical properties of the parent drug to enhance its solubility, stability, and membrane permeability. By masking functional groups or introducing specific chemical moieties, pro-drugs can bypass biological barriers more effectively, leading to improved absorption and distribution.

Protein-ligand interactions are essential to the functioning of cells and are crucial to the development of new drugs. For ligand identification, deep learning techniques have the potential to be more affordable than high-throughput experimental techniques. Here, Ligand-Transformer, a deep-learning algorithm relying on the AlphaFold2 architecture, to predict the affinity for binding between proteins and small ligands. We used Ligand-Transformer to find low nanomolar potency molecules by screening inhibitors against the mutant EGFRLTC kinase. Next, the method used to the prediction of conformational population alterations caused by inhibitors of ABL kinase. In order to demonstrate the usefulness of Ligand-Transformer for disorganized proteins, the investigation of interaction between small molecules and the Alzheimer's disease Aβ peptide, detecting substances that postponed the peptide's agglomeration. Overall, Ligand-Transformer demonstrates how transformers may be used to precisely anticipate how tiny compounds would interact with both organised and random proteins, thereby elucidating molecular mechanisms and expediting the first stages of drug discovery.

Furthermore, pro-drug strategies offer precise control over drug release kinetics, allowing for sustained or targeted delivery to the site of action. This is particularly advantageous for drugs with a narrow therapeutic window or those requiring localized treatment. For example, pro-drugs can be designed to selectively accumulate in diseased tissues or cells, minimizing systemic exposure and off-target effects. Such targeted delivery systems hold great promise for the treatment of cancer, inflammatory diseases, and neurological disorders. Moreover, pro-drug design facilitates the conversion of poorly soluble or unstable drugs into more pharmacologically active forms. By conjugating the parent drug with biocompatible carriers or pro-moieties, pro-drugs can overcome formulation challenges and improve pharmaceutical properties. This approach has been successfully employed to develop oral formulations of hydrophobic drugs, thereby enhancing patient compliance and convenience.

Recent advances in pro-drug design have also focused on improving drug safety and reducing adverse effects. Through molecular modifications, pro-drugs can be engineered to undergo selective activation in response to specific physiological cues or enzymatic pathways. This enables precise control over drug release and metabolism, minimizing the risk of toxicity and enhancing therapeutic efficacy. Additionally, pro-drugs can be designed to enhance drug stability in biological fluids, thereby reducing degradation and potential side effects associated with rapid metabolism. Furthermore, pro-drug strategies offer opportunities for drug repurposing and combination therapy, leveraging existing drugs for new indications or enhancing their therapeutic effects through synergistic interactions. By modulating the pharmacokinetic and pharmacodynamic properties of drugs, pro-drug design enables the development of innovative treatment regimens with improved efficacy and reduced resistance.

CONCLUSION

Pro-drug design represents a paradigm shift in drug development, offering tailored solutions to overcome challenges

Correspondence to: Amphansap Garner, Department of Pharmacy, University of Warwick, England, UK, E-mail: garner@amp.uni.uk

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associated with conventional therapeutics. By harnessing the principles of medicinal chemistry and molecular pharmacology, researchers can design pro-drugs with enhanced pharmacological properties and therapeutic benefits. With continued advancements in pro-drug design, the future holds great promise for the development of safer, more efficacious, and targeted therapies across a wide range of medical conditions.