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Principles of Drug Design

Swetha Pandit*

Department of Pharmacy Practice, University of Calcutta, Kolkata, India

INTRODUCTION

Drug design is an integrated development field heralding the era of "tailored drugs". It involves studying the effects of bioactive compounds based on molecular interactions related to molecular structure or its associated physicochemical properties. Study the process by which drugs exert their effects, how they react with the cytoplasm to produce specific pharmacological effects or responses, how they are modified or detoxified, metabolized or eliminated from the body. Drugs are most commonly small organic molecules that activate or inhibit the function of biomolecules, such as proteins, to provide a therapeutic benefit to patients [1]. At its simplest, drug design involves designing small molecules that are complementary in shape and charge to the bio-molecular targets with which they interact and bind. Pharmaceutical design often, but not always, relies on computer modeling techniques [2]. This type of modeling is often referred to as computational drug design. Finally, drug discovery based on knowledge of the three-dimensional structure of bio-molecular targets is known as structure-based drug discovery.

DESCRIPTION

Lipinski's rule of 5 additionally called the Pfizer's rule of 5 or sincerely the Rule of 5 (RO5) is a rule of thumb to assess drug likeness or decide if a chemical compound with a sure pharmacological or organic pastime has homes that might make it a probable orally lively drug in humans. The rule turned into formulated with the aid of using Christopher A. Lipinski in 1997, primarily based totally at the remark that maximum remedy tablets are distinctly small and lipophilic molecules [3]. The rule describes molecular homes crucial for a drug's pharmacokinetics with inside the human body, inclusive of their absorption, distribution, metabolism, and excretion ("ADME"). However, the guideline of thumb does now no longer are expecting if a compound is pharmacologically lively. The modern fashion within side the drug layout is to expand new clinically powerful sellers thru the structural change of lead nucleus. The lead is a prototype compound that has the favored organic or pharmacological pastime however may also have many unwanted characteristics, like excessive toxicity, different organic pastime, insolubility or metabolism problems [4]. Such natural leads as soon as identified, are clean to exploit. This technique is alternatively straightforward. The actual take a look at is living with the identity of such lead actual take a look at is living with the identity of such lead bioactive positions at the fundamental skeleton of such leads [5]. Drug layout is the innovative procedure of locating new treatments primarily based totally at the understanding of an organic target.

CONCLUSION

Sometimes a drug candidate in the course of medical trials will show off a couple of pharmacological interest; that is, it is able to produce a facet effect. This compound, then, may be used as a lead (or, with luck, as a drug) for the secondary interest. This assessment discusses precept of drug layout, numerous methods of drug layout, lead discovery, lead change and numerous styles of drug discovery. Bioisosterism is a vital lead change method that has been proven to be beneficial to minimize toxicity or to regulate the interest of a lead, and might have a sizeable position within side the alteration of pharmacokinetics of a lead.

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CONFLICT OF INTEREST

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Corresponding author Swetha Pandit, Department of Pharmacy Practice, University of Calcutta, Kolkata, E-mail: swetha@hotmai.com

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