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A Brief Note on Pro Drug Design

Tyler Grant*

Department of Chemical and Biomolecular Engineering, University of Tennessee Knoxville, Knoxville, TN, 37996, USA

Commentary

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***For Correspondence:**
Tyler Grant, Department of Chemical and Biomolecular Engineering, University of Tennessee Knoxville, Knoxville, TN, 37996, USA
E-mail: tayliergr567@edu.com

ABOUT THE STUDY

Many traditional herbal preparations contain glycosides (sugar derivatives) of the active ingredient, which are digested in the intestines to produce the active and more accessible aglycone. Salicin, for example, is a -D-glucopyranoside that esterase cleave to liberate salicylic acid. Aspirin, also known as acetylsalicylic acid, is a synthetic prodrug of salicylic acid that was initially developed by Felix Hoffmann at Bayer in 1897. Other drugs, such as codeine and morphine, are enzymatically activated to generate sugar derivatives (morphine-glucuronides) that are more active than the parent substance.

Arsphenamine, the first synthetic antimicrobial medicine developed in 1909 by Sahachiro Hata in Paul Ehrlich's laboratory, is not poisonous to bacteria until the body converts it to an active form. Similarly, in order to release the active chemical, sulfanilamide, prontosil, the first sulfa medication, must be cleaved in the body. Many more cases have been discovered since then.

Because of the minuscule possibility of a dangerous side effect, terfenadine, the first non-sedating antihistamine, had to be withdrawn from the market. Terfenadine, on the other hand, was determined to be a prodrug of the active molecule fexofenadine, which does not pose the same dangers as the parent chemical. As a result, fexofenadine could be approved for use as a safe substitute for the original medicine.

Loratadine is a non-sedating antihistamine that is the prodrug of desloratadine, which is largely responsible for the parent compound's antihistaminergic actions. However, because the parent molecule in this situation does not have the same adverse effects as terfenadine, loratadine and its active metabolite, desloratadine, are already on the market. The imaginative process of identifying novel pharmaceuticals based on knowledge of a biological target

is known as drug design, also known as rational drug design or simply rational design. The drug is usually an organic small molecule that activates or inhibits the action of a biomolecule such a protein, providing a therapeutic benefit to the patient.

Drug design, in its most basic form, is creating molecules that are complimentary in shape and charge to the biomolecular target with which they interact and hence bond to it. Computer modelling approaches are commonly used in drug development, but they are not always used. Computer-aided drug design is a term used to describe this type of modelling. Finally, structure-based drug design refers to drug development that is based on knowledge of the biomolecular target's three-dimensional structure. Biopharmaceuticals, which include peptides and, in particular, therapeutic antibodies, are becoming a more important class of medications, and computational approaches for boosting the affinity, selectivity, and stability of these protein-based treatments have been created. To some extent, the term "drug design" is a misnomer. Ligand design is a more accurate term. Although design strategies for predicting binding affinity are quite successful, many other qualities, such as bioavailability, metabolic half-life, side effects, and so on, must first be improved before a ligand can be made into a safe and effective medicine. With rational design methodologies, these other traits are typically impossible to predict.

Nonetheless, due to high attrition rates, particularly during the clinical phases of drug development, more emphasis is being placed early in the drug design process on selecting candidate drugs with physicochemical properties that are predicted to result in fewer development complications and, as a result, are more likely to lead to a drug that is approved and marketed. *In vitro* tests, in combination with computational methods, are increasingly being utilised in early drug development to choose molecules with better ADME (Absorption, Distribution, Metabolism, and Excretion) and toxicity profiles.