OPEN ACCESS Freely available online

Pharmaceutica Analytica Acta

Commentry

Description of Drug Design and its Types

Ozer Joseaf*

Department of Analytical Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece

DESCRIPTION

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.

Drug design can be divided into two categories. The first is known as ligand-based drug design, while the second is known as structure-based drug design

Ligand-based: The knowledge of other compounds that bind to the biological target of interest is used in ligand-based drug design. These additional compounds can be utilised to create a pharmacophore model, which specifies the structural features that a molecule must have in order to bind to a target. In other words, based on knowledge of what binds to the biological target, a model of the target may be developed, and this model can then be used to design new molecular entities that interact with the target.

Structure-based: The information of the three-dimensional structure of the biological target obtained through technologies like as x-ray crystallography or NMR spectroscopy is used in structure-based drug design. If a target's experimental structure isn't accessible, a homology model of the target based on the experimental structure of a comparable protein might be conceivable. Candidate medications that are projected to bind with high affinity and selectivity to the biological target can be generated utilising interactive graphics and the intuition of a medicinal chemist based on the structure of the target. Alternatively, new medication candidates could be suggested using a variety of automated computational processes.

Current structure-based drug design strategies can be loosely classified into three types. The first method involves exploring vast databases of 3D structures of tiny molecules for those that suit the receptor's binding pocket using quick approximation docking tools to find new ligands for a given receptor. Virtual screening is the name given to this procedure. De novo design of novel ligands is a second category. By building small parts in a sequential manner, ligand molecules are formed up within the confines of the binding pocket. Individual atoms or molecular fragments can be used as these parts. The main benefit of this strategy is that it can suggest novel structures that aren't found in any database. The optimization of existing ligands by evaluating putative analogues within the binding cavity is a third strategy.

Correspondence to: Ozer Joseaf, Department of Analytical Chemistry, Aristotle University of Thessaloniki, Thessaloniki, Greece, E-mail: tzapara167@gmail.com

Received: September 3, 2021; **Accepted:** September 22, 2021; **Published:** September 27, 2021

Citation: Joseaf O (2021) Description of Drug Design and its Types. Pharm Anal Acta. 12: 648