

# COMPUTER AIDED DRUG DESIGN

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## Introduction

Computers are an essential tool in medicinal chemistry. They offer a cheaper, easier, and faster way to build complex correlations, predict drug activity, ADMET properties, inspect 3D structures of proteins and ligands, search between millions of compounds about potential drugs and many many more. These all contributed to the modern rational drug design and discovery and are responsible for many available, safe, effective, and potent drugs.

## Structure Based Drug Design

As thousands of 3D protein structures are available in online databases for free, medicinal chemists can now work directly on the protein to design potent and selective ligands that provide desired potency.

## Ligand Based Drug Design

A study of the relationship between the ligand's properties and their activities on the receptor can provide us with key features required for ligands to bind the active site. These techniques facilitate the rational drug design of novel drugs especially when the target structure is not known.

### 1. Docking

A method for analyses of the ligand's conformations into the binding site of the target<sup>[1]</sup>. Different conformations of the ligand are generated, and a scoring algorithm is used to rank the possible binding conformations of the ligand to the target according to their estimated affinity. Docking can be used for virtual screening where thousands of molecules are tested for binding to the binding site<sup>[2]</sup>.



### 2. Molecular Dynamics

It is the simulation of proteins and ligands surrounded by solvent molecules in a virtual environment. It uses molecular or quantum mechanics to calculate applied forces between bonding and non-bonding atoms and move atoms according to it. It's used to study protein ligand interaction, discover the binding site of the ligand with the protein and guide leads optimization<sup>[3]</sup>.



### 3. De novo drug design

Ligands can be designed from de novo to bind in the active site with the maximum number of possible intermolecular interactions manually or programmatically where an algorithm can generate numerous ligands that could bind to the active site<sup>[4]</sup>.



## Artificial Intelligence

AI found many applications in drug design and discovery today as it can analyze the complicated data of drug structure and properties and link it to useful variables (e.g.: activity, ADMET, etc.). AI played different roles in many techniques of CADD<sup>[5]</sup>.

- Scoring function in docking.
- De novo generation of drug like molecules and prediction of their activities.
- Prediction of compounds activity based on QSAR analysis.
- Prediction of ADMET properties.
- Prediction of protein folding from sequence (e.g.: Alpha Fold 2).



### 1. QSAR

After identification of the leads medicinal chemists need to optimize them to have the highest potency<sup>[6]</sup>. This can be done rationally by constructing quantitative correlations between descriptors of the modified leads and their activity. This correlations can be used for ligand optimization or for virtual screening where we can predict compounds activities in silico<sup>[7]</sup>.

### 2. 3D QSAR

Like QSAR but the 3D structure of the compound is taken into account. This is done by studying the interaction between a probe atom (e.g.: CH<sup>+</sup>, H<sup>+</sup>, H<sub>2</sub>O, etc.) and the ligand where the probe is placed at different locations around the ligand<sup>[8]</sup>. By studying different ligands, a correlation between the energy of the interaction at each location of the probe and the activity of the ligand is built. This model can predict the activity of novel molecules and guide us to important properties that should be present in the ligand to be active which can be plotted as contour lines.



### 3. Pharmacophore

It is a simple representation of the relative positions of important binding groups fixed in a 3D space with disregard of the skeleton that connect them<sup>[9]</sup>. This representation facilitates virtual screening for other possibly active compounds in chemical databases.



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