

CADD:- Computer aided drug design.

it uses computational methods
to simulate drug interactions.

it employs several methodologies eg
computational genomics, molecular
modelling, 2D and 3D Quantitative structure
activity relationship (QSAR).

It is also k/a CDD - Computational Drug Discovery
it design compounds with "ADMET" properties.

Steps :- Hit Identification

↓
Pre-clinical studies

↓
Manufacturing

↓
Clinical trial stage

↓
Regulatory evaluation stage

↓
Marketing stage.

Structural Bioinformatics in Drug Discovery

Bioinformatics tools are capable of converting a sequence into structure in case of a protein. With these solved protein structures the drug designing has become convenient. The branch dealing with this aspect is called

Structural Bioinformatics or SBI

It is useful for $\left\{ \begin{array}{l} \text{Drug targets} \\ \text{Ligand binding.} \end{array} \right.$

On the basis of making drug Human genome can be divided into -

- ① Polysaccharide
 - ② Lipids
 - ③ Nucleic Acids
 - ④ Proteins.
- } Omitted for drug designing.

Steps of drug designing -

(Receptor binding)

→ Docking b/w drug & receptor

(molecular dynamics)

↓
energy of protein (" mechanics)

↓
heat of product (semi-empirical method)

↓
charge of ligand (DFT).

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Suggested readings:

<https://link.springer.com/article/10.1007/s13721-013-0039-5>

Review and research articles related to content is already sent.