

FACULTY OF ENGINEERING AND TECHNOLOGY

Department of Biotechnology

Computer Aided drug design

abc

What is CADD



- Drug design is the inventive process of finding new medications based on the knowledge of a biological target.
- If the same process was done by using Computer/Software then it is referred as CADD

Why CADD...?

□ Drug Discovery today are facing a serious challenge because of the increased cost and enormous amount of time taken to discover a new drug, and also because of rigorous competition amongst different pharmaceutical companies.

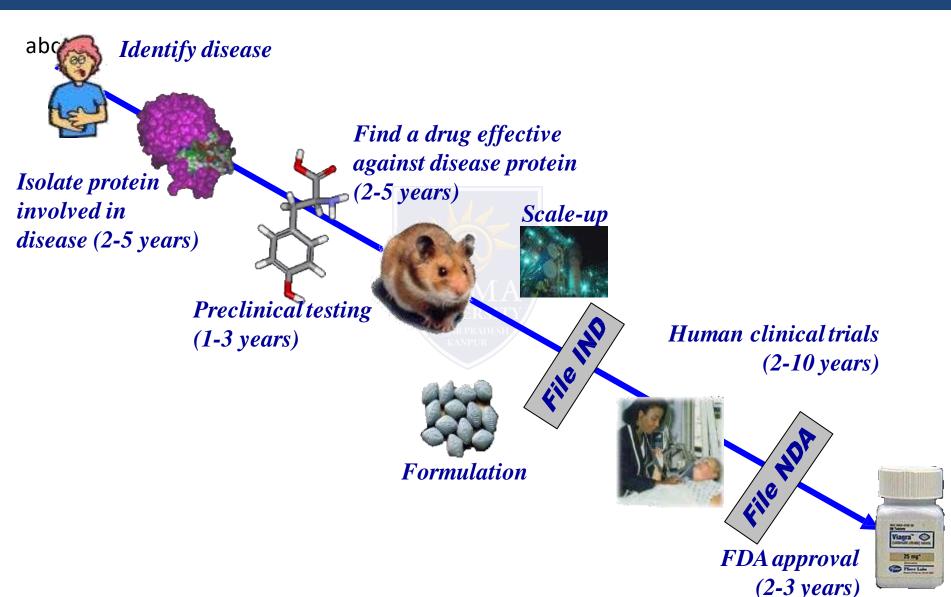
Some of the earliest examples of approved drugs that awe their discovery in large part to the tools of CADD include the following:

- ✓ Carbonic anhydrase inhibitor Dorzolamide used to treat glaucoma (Vijayakrishnan 2009)
- ✓ The angiotensin-converting enzyme (ACE) inhibitor, Captopril, an antihypertensive drug (Talele et al., 2010)
- ✓ Three therapeutics for the treatment of human immunodeficiency virus (HIV): Saquinavir, Ritonavir, and Indinavir (Van Drie 2007)
- ✓ Tirofiban, a fibrinogen antagonist (Hartman et al., 1992)

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Some of the earliest examples of approved drugs that owe their discovery in large part to the tools of CADD

DrugyDiscovery & Development



GENOMICS, PROTEOMICS & BIOPHARM.

Potentially producing many more targets and "personalized" targets

Identify disease

Identify disease Isolate protein

disease (2-5 years)

involved in

THROUGHPUT SCREENING

against diseasé prot**gin**eening up to 100,000 compounds a

VIRTUAL SCREENING

Using a computer to predict activity

Human clinical trials

(**2-10** years)

Find a drug effective HIGH

-5 years) day for activity against a target protein

Presdintequesting

(1-3 years)

COMBINATORIAL CHEMISTRY

Rapidly producing vast numbers of compounds

MOLECULAR MODELING

Formulation

Computer graphics & models help improve activity

SILICO ADME MODELS

Tissue and computer models begin to replace animal testing

Preclinic I testing FDA approval

(2-3 years)

09-Feb-2019















MCQs

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- 10. A

