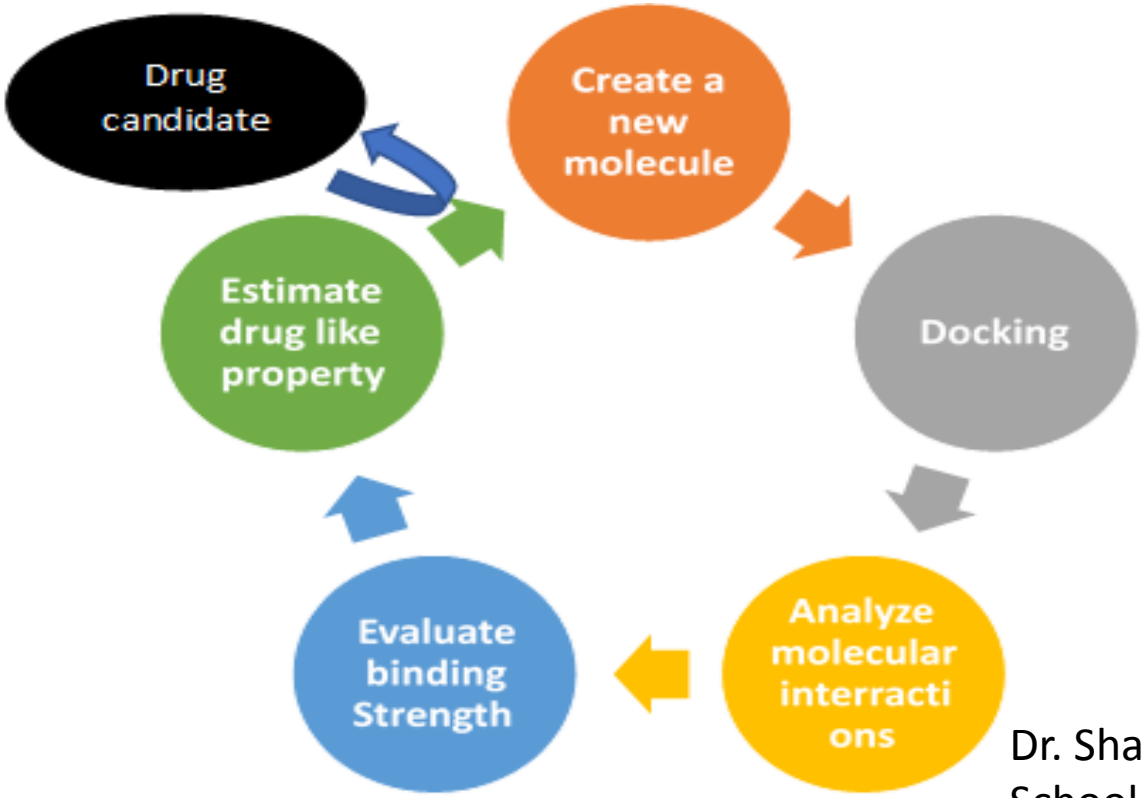
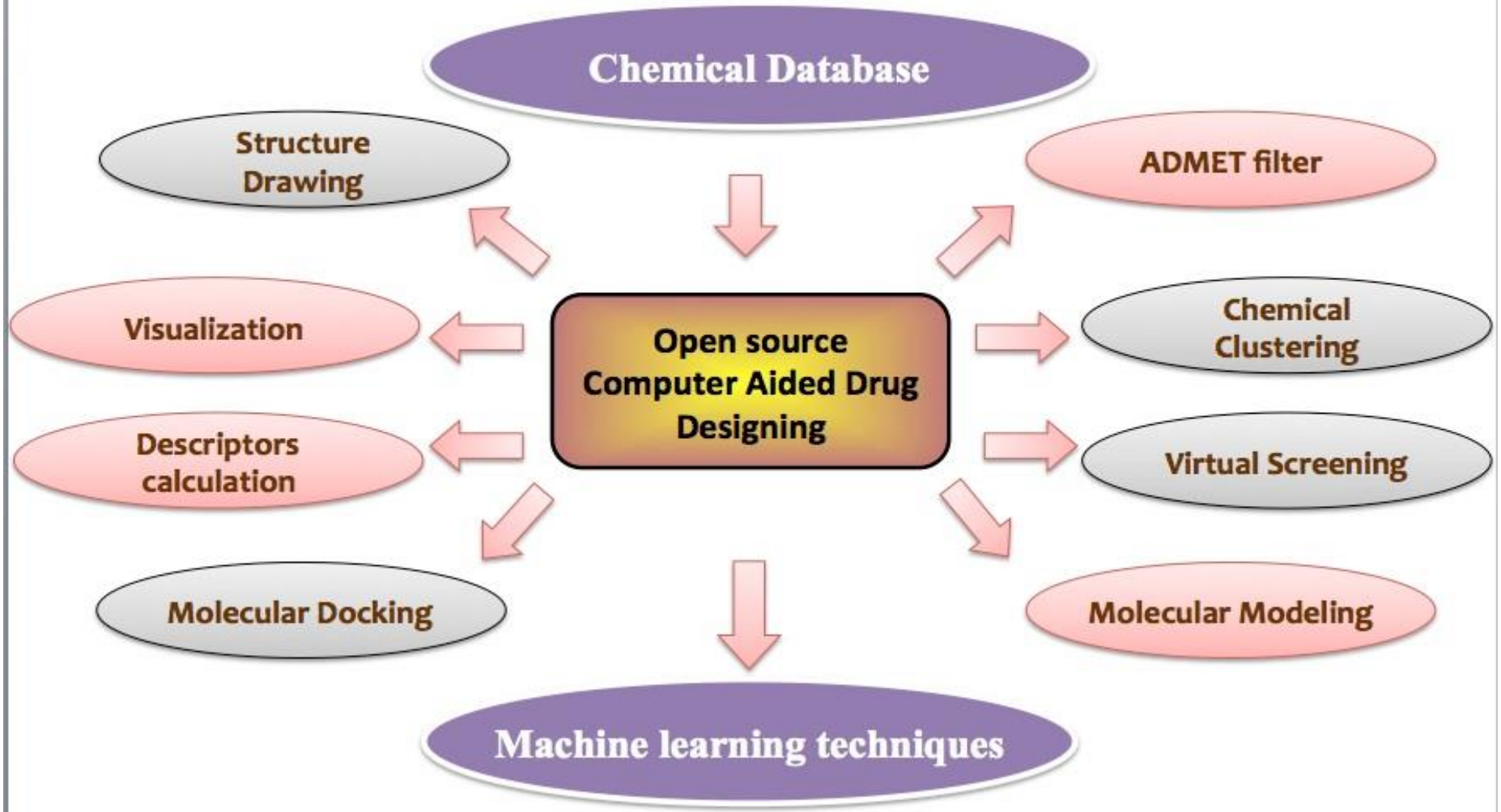
Unit 1

History of computer in pharmaceutical sciences



Dr. Shashi Kiran Misra
School Of Pharmaceutical Science

Computer aided drug delivery system



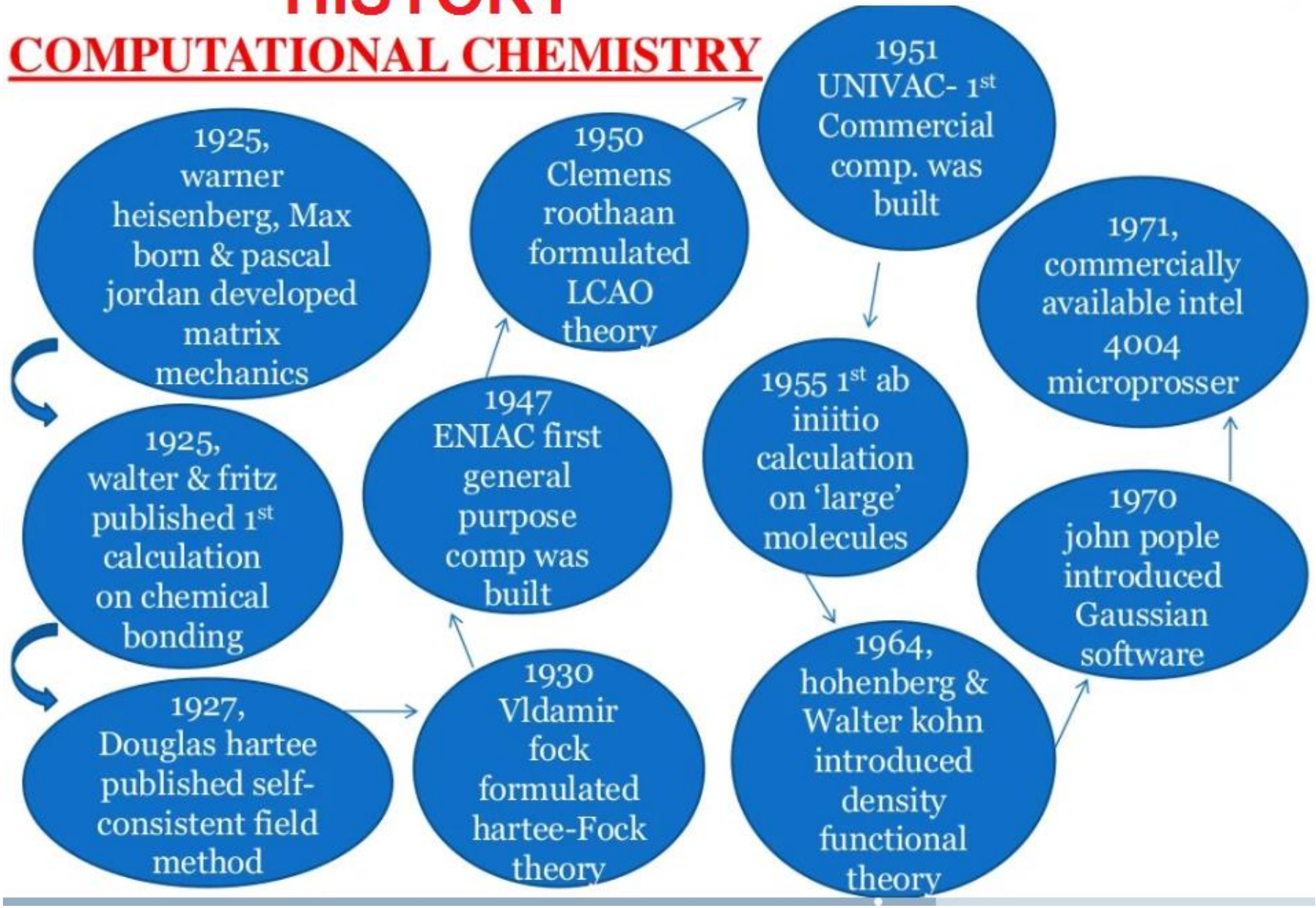
HISTORY OF COMPUTERS IN PHARMACEUTICAL RESEARCH AND DEVELOPMENT

INTRODUCTION

- Today, computers are so ubiquitous in pharmaceutical research and development that it may be hard to imagine a time when there were no computers to assist the medicinal chemist or biologist.
- Computers began to be utilized at pharmaceutical companies as early as the 1940s.
- There were several scientific and engineering advances that made possible a computational approach to design and develop a molecule.

HISTORY

COMPUTATIONAL CHEMISTRY



A Little History of Computer Aided Drug Design

- 1960's - Viz - review the target - drug interaction
- 1980's- Automation - high trhoughput target/drug selection
- 1980's- Databases (information technology) - combinatorial libraries
- 1980's- Fast computers - docking
- 1990's- Fast computers - genome assembly - genomic based target selection
- 2000's- Vast information handling - pharmacogenomics

- One fundamental concept understood by chemists was that chemical structure is related to molecular properties including biological activity.
- Hence if one could predict properties by calculations, one might be able to predict which structures should be investigated in the laboratory.
- Another fundamental, well-established concept was that a drug would exert its biological activity by binding to and/or inhibiting some biomolecule in the body. (This concept stems from Fischer's famous lock-and-key hypothesis)
- Pioneering research in the 1950s attacked the problem of linking electronic structure and biological activity.
- A good part of this work was collected in the 1963 book by Bernard and Alberte Pullman of Paris, France, which fired the imagination of what might be possible with calculations on biomolecules .

- The earliest papers that attempted to mathematically relate chemical structure and biological activity were published in Scotland in the middle of the nineteenth century .
- This work and a couple of other papers were forerunners(pecursor) to modern quantitative structureactivity relationships (QSAR).
- The early computers were designed for military and accounting applications, but gradually it became apparent that computers would have a vast number of uses.

COMPUTATIONAL CHEMISTRY: THE BEGINNINGS AT LILLY

- In the late 1950s or early 1960s, the first computers to have stored programs of scientific interest were acquired.
- One of these was an IBM 650; it had a rotating magnetic drum memory consisting of 2000 accessible registers.
- The programs, the data input, and the output were all in the form of IBM punched cards.
- It was carried out by Lilly's research statistics group under Dr. Edgar King.
- It was not until 1968, when Don Boyd joined the second theoretical chemist in the group, that the computers at Lilly started to reach a level of size, speed, and sophistication to be able to handle some of the computational requirements of various evaluation and design efforts.
- Don brought with him Hoffmann's EHT program from Harvard and Cornell.

Recent Applications of computers in Pharmacy

- Drug information storage and retrieval,
- Pharmacokinetics, Mathematical model in Drug design,
- Electronic Prescribing and discharge systems,
- Barcode medicine identification and automated dispensing of drugs,
- Mobile technology and adherence monitoring
- Diagnostic System, Lab-diagnostic System, Patient Monitoring System,
- Pharma Information System
- Bioinformatics
- Computers as data analysis in Preclinical development
- The design of new drug molecules using molecular modeling software
- Molecular docking
- Computer-aided formulation development Pharmacodynamics
- Computer Simulations in Pharmacokinetics and
- Artificial Intelligence, Robotics and Computational fluid
- Electronic records and digital
- Pharmaceutical Automation, Computerized system validation

Table 1. Marketed Pharmaceuticals who's Discovery were performed by Computers

Generic Name	Brand Name	Discovery Assisted by	Activity	Year of approved in US
Norfloxacin	Noroxin	QSAR	Antibacterial	1983
Losartan	Cozaar	CADD	Anti-hypertensive	1994
Dorzolamide	Trusopt	CADD/SBDD	Antiglaucoma	1995
Ritonavir	Norvir	CADD	Antiviral	1996
Donepezil	Aricept	QSAR	Anti-Alzheimer's	1997
Lopinavir	Aluviran	SBDD	Antiviral	2000
Ximelagatran	Exanta	SBDD	Anticoagulant	2004

IMPORTANCE OF COMPUTERS IN PHARMA INDUSTRY

1-DECREASE MANUAL WORK
2-SMOOTH & EASE OF WORK FLOW

3-HIGH LEVEL OF SECURITY AS COMPARE TO PAPER WORK

4-REDUCE PAPER WORK
5-TIME EFFICIENT

Computers in Medicine

1970

Early ECG & diagnosis

1980

Administrative, imaging (CT)

1990

Clinical systems

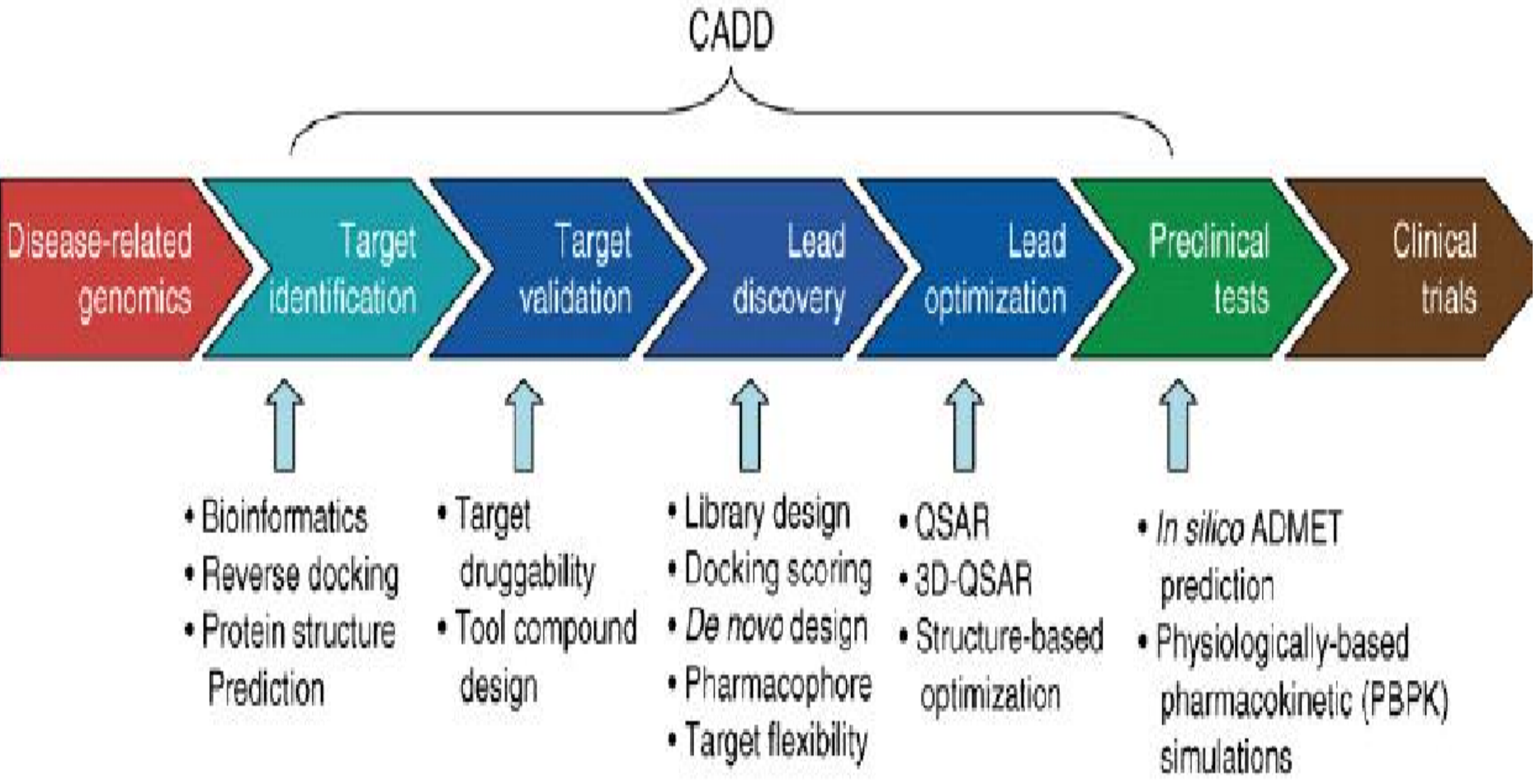
2000

Communication, research

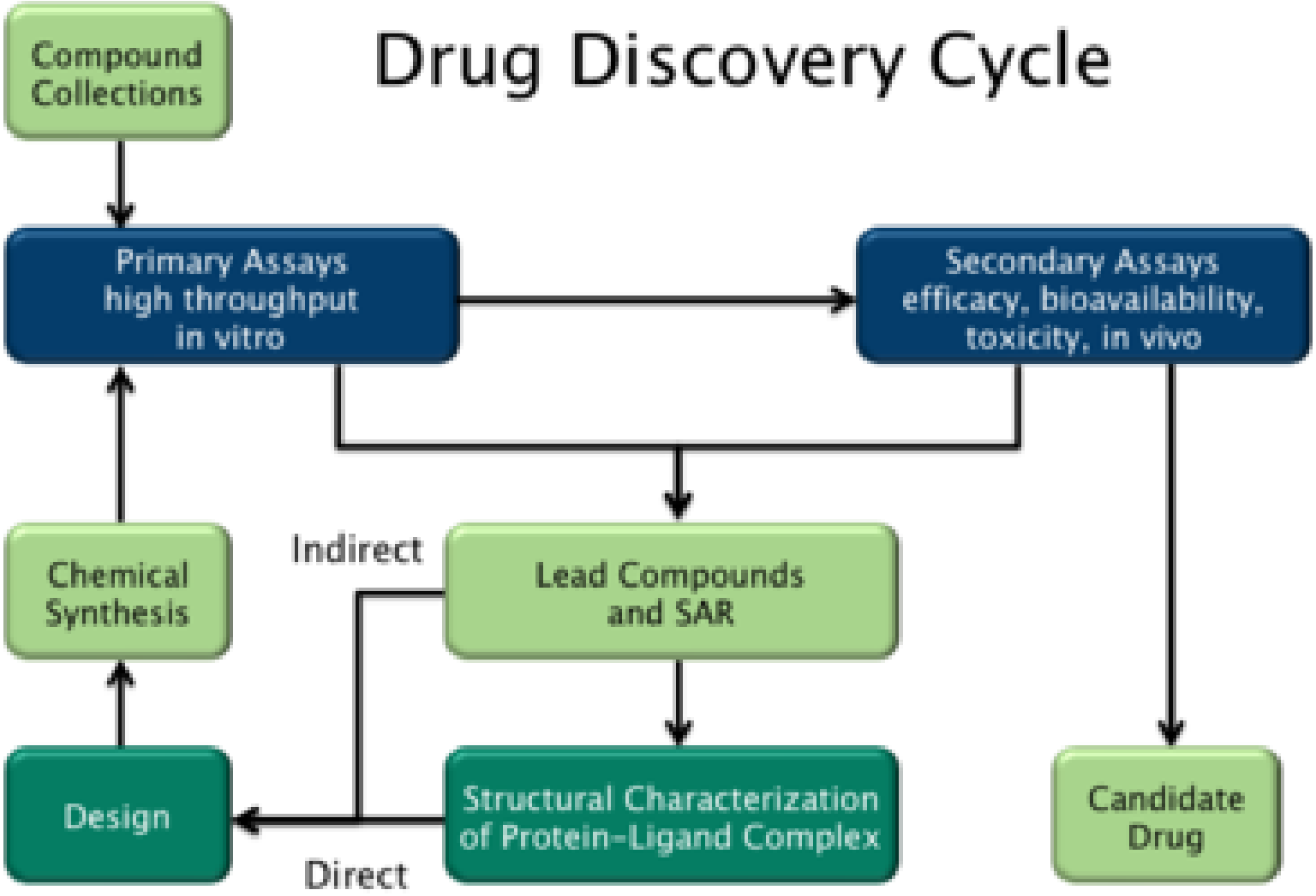
2011

HITECH

COMPUTER-AIDED DRUG DESIGN (CADD):



Drug Discovery Cycle



- **REVIEW ARTICLE**

- History of Computers in Pharmaceutical Research and Development by ClinSkill | Dec 19, 2017 | Pharmaceutical Research

- **BOOK**

- **Computer Applications in Pharmaceutical Research and Development – "S.Ekins (Wiley, 2006) WW".**

- **IMAGES TAKEN FROM GOOGLE & SOURCE OF SLIDE NUMBER 14 IS LINKED WITH HYPERLINK INTO IT.**