Computational Resources for Computer-Aided Drug Discovery

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Brief History of Group

1986: Simple computer services

- Joined as computer scientist (1986)
- Developed databases (COBOL, Dbase)
- DIC/BIC under BTISNET of DBT (1987)
- Setup communication via NICNET
- EMAIL facility via ERNET

1992: Initiating research activities

- First paper on customize curve fitting
- General software for biological methods
- Ph.D. (1996) Protein structure prediction

1996: International presence

- 1996-8: PDF at Oxford University, UK
- Sequence/Structure alignment algorithm
- Successfully compete in CASP
- Web-based service & mirror sites

2000: Target prediction for Drug/vaccine

- Research group started (Ph.D. students)
- 2002-7: CSIR-Mega project (45 core)
- Identification of drug & vaccine targets
- Setup BIC at UAMS, Little Rock, USA
- Visiting prof. at POSTECH, South Korea

2008: Open source drug discovery

- CRDD: Comp. resources for drug discovery
- Freeware in Chemo/pharma informatics
- Assembling & annotation of NGS data

2012-: In silico models for healthcare

- 2012: GENESIS project (50 crore)
- Exp. validation of therapeutic peptides
- Customize OS for drug discovery
- Genome-based personalize medicine

Concept of Drug and Vaccine

- **Concept of Drug**
  - Kill invaders of foreign pathogens
  - Inhibit the growth of pathogens

- Concept of Vaccine
  - Generate memory cells
  - Trained immune system to face various existing disease agents

Web servers for designing epitope-based vaccine

T-Cell Epitopes

Propred: Promiscuous MHC-II binders

MHCBN: Database of MHC

IL4Pred: Prediction of interleukin-4

Propred1: for promiscuous MHC I binders

Pcleavage: Proteome cleavage sites

TAPpred: for predicting TAP binders

CTLpred: Prediction of CTL epitopes

B-Cell Epitopes

BCIpep: Database of B-cell eptioes;

Lbtope: Prediction of B-cell epitopes

ALGpred: Allergens and IgE eptopes

IgPred: Antibody-specific epitopes

Vaccine Adjuvants

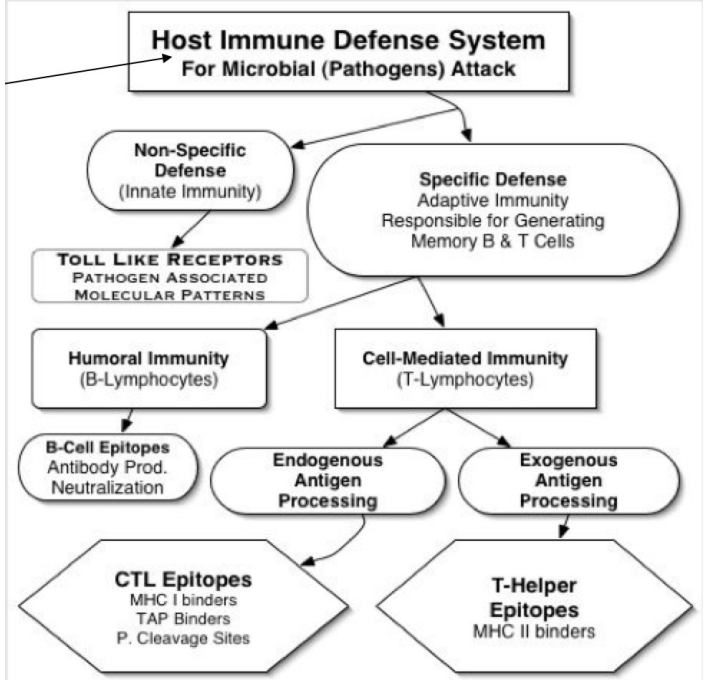
PRRDB: A database of PRRs & ligands

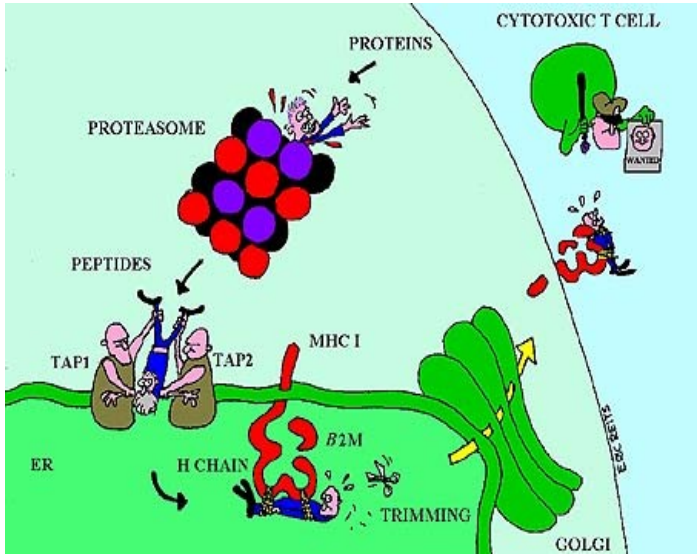
VaccineDA: DNA-based adjuvants

imRNA: Immunomulatory RNAs

VaccinePAD: Peptide-based adjuvants

PolysacDB: Polysaccharide antigens





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Software Review

Novel *in silico* tools for designing peptide-based subunit vaccines and immunotherapeutics

Sandeep Kumar Dhanda, Salman Sadullah Usmani, Piyush Agrawal, Gandharva Nagpal, Ankur Gautam and Gajendra P.S. Raghava

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Web servers for drug targets

Genome Annotation

FTGpred: Prediction of Prokaryotic genes
EGpred: Prediction of eukaryotic genes
GeneBench: Benchmarking of gene finders
SRF: Spectral Repeat finder

Comparative genomics

GWFASTA: Genome-Wide FASTA Search
GWBLAST: Genome wide BLAST search
COPID: Composition based similarity search
LGEpred: Gene from protein sequence

Subcellular Localization Methods

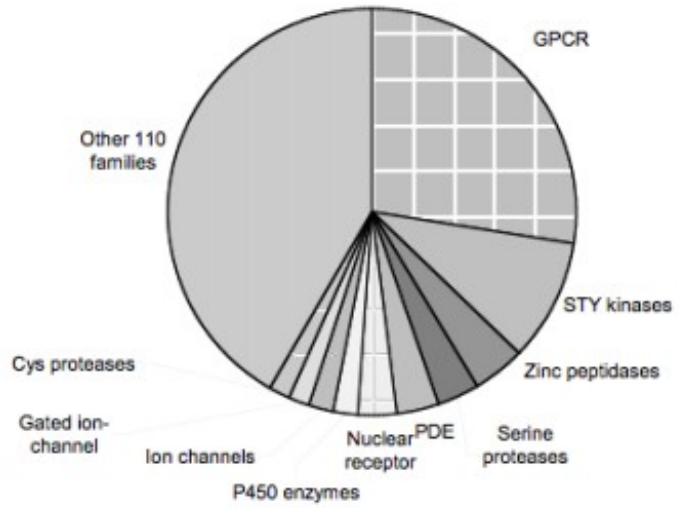
PSLpred: localization of prokaryotic proteins
ESLpred: localization of Eukaryotic proteins
HSLpred: localization of Human proteins
MITpred: Prediction of Mitochndrial proteins
TBpred: Localization of mycobacterial

Prediction of drugable proteins

NRpred: Classification of nuclear receptors
GPCRpred: Prediction of G-protein-coupled receptors
GPCRsclass: Amine type of GPCR
VGIchan: Voltage gated ion channel
Pprint: RNA interacting residues in proteins

Protein Structure Prediction

APSSP2: protein secondary structure prediction
Betatpred: Consensus method for β-turns prediction
BetaTurns: Prediction of β-turn types in proteins
Turn Predictions: Prediction of α/ β/γ -turns in proteins
BhairPred: Prediction of Beta Hairpins
TBBpred: Prediction of trans membrane beta barrel proteins
SARpred: Prediction of surface accessibility (real accessibility)
PepStr: Prediction of tertiary structure of Bioactive peptides



Computational Resources for Drug Discovery

CSIR

Target Identification

Genome Annotation
Proteome Annotation
Potential Targets
Protein Structure

Virtual Screening

QSAR Techniques
Docking & QSAR
Chemoinformatics
siRNA/miRNA

Drug Design

Lead Optimization
Pharmainformatics
ADMET
Clinical Informatics

How to Contribute?

Expermentalists
Virtual Trainees/Jobs
Software Developers

Computational Resources

Library Interfaces
Meta Servers
Publishing Document
Data on *M.tb.*

**** Prediction of cytochrome P450 isoform responsible for metabolizing a drug molecule ****

Computational Resources for Drug Discovery

OSDD Forum is an initiative with a vision to provide affordable healthcare to the developing world. The OSDD concept aims to synergize the power of genomics, computational technologies and facilitate the participation of young and brilliant talent from Universities and industry. It seeks to provide a global platform where the best brains can collaborate and collectively endeavor to solve the complex problems associated with discovering novel therapies for neglected diseases like Tuberculosis.

CRDD (Computational Resources for Drug Discovery) is an important module of the *in silico* module of OSDD. The CRDD web portal provides computer resources related to drug discovery on a single platform. Following are major features of CRDD:

- **CRDD provides computational resources for researchers in the field of computer-aided drug design.**
- **CRDD allows users to discuss their problem with other members.**
- **CRDD gives equal opportunity to those willing to solve these problems.**
- **CRDD Wiki maintain wikipedia related to drug discovery.**
- **Contributors may host their database or web server on CRDD portal.**

Thus, CRDD provides a platform for researchers having limited resources.

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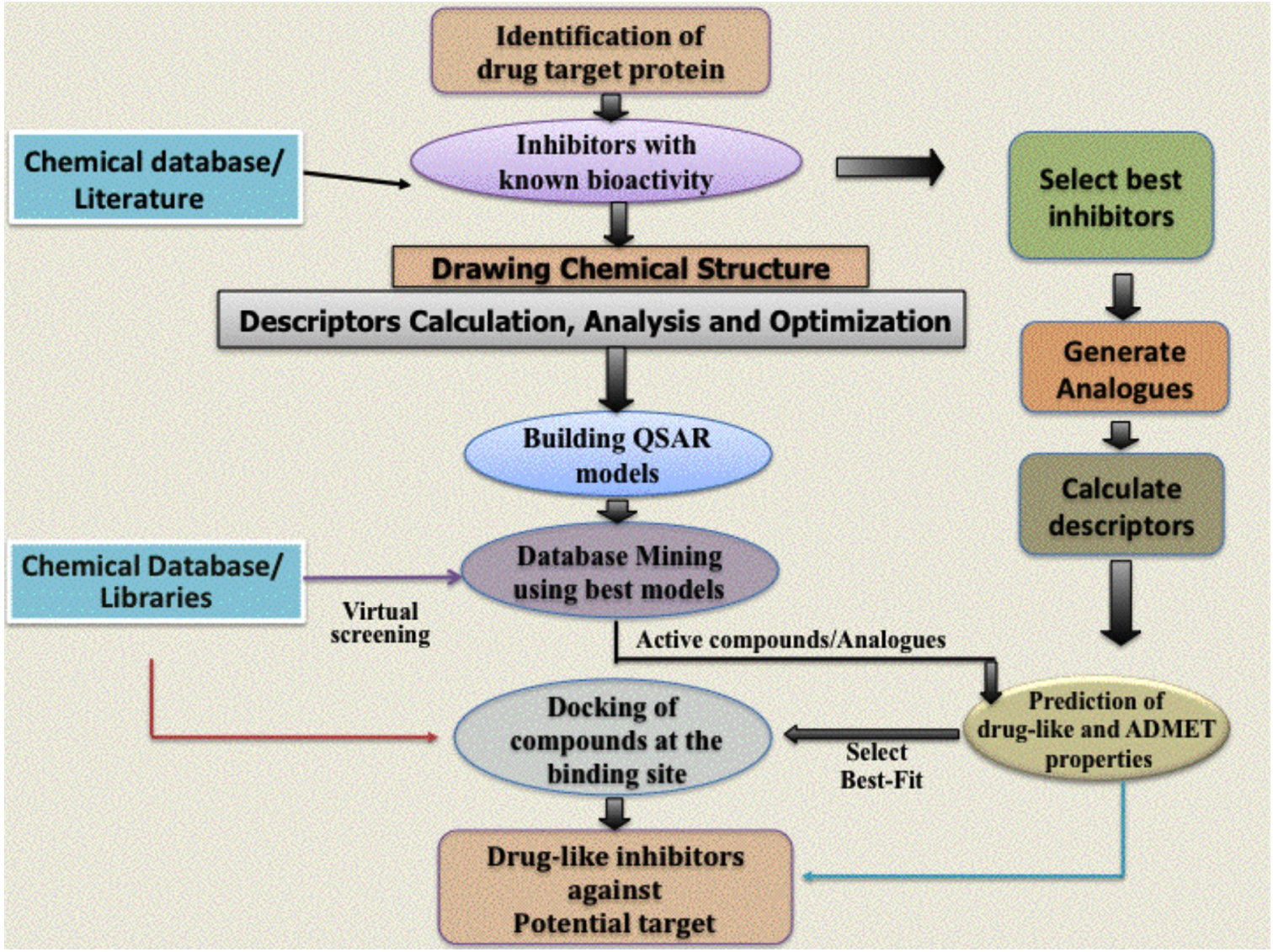
Open Source Software and Web Services for Designing Therapeutic Molecules

Deepak Singla[1,2], Sandeep Kumar Dhanda[1], Jagat Singh Chauhan[1], Anshu Bhardwaj[3], Samir K. Brahmachari[3,4], Open Source Drug Discovery Consortium[3] and Gajendra P.S. Raghava[1,*]

[1]*Bioinformatics Centre, CSIR-Institute of Microbial Technology, Chandigarh, India;* [2]*Centre for Microbial Biotechnology, Panjab University, Chandigarh, India;* [3]*CSIR-Open Source Drug Discovery Unit, New Delhi, India;* [4]*CSIR-Institute of Genomics and Integrative Biology, New Delhi, India*

Abstract: Despite the tremendous progress in the field of drug designing, discovering a new drug molecule is still a challenging task. Drug discovery and development is a costly, time consuming and complex process that requires millions of dollar and 10-15 years to bring new drug molecules in the market. This huge investment and long-term process are attributed to high failure rate, complexity of the problem and strict regulatory rules, in addition to other factors. Given the availability of 'big' data with ever improving computing power, it is now possible to model systems which is expected to provide time and cost effectiveness to drug discovery process. Computer Aided Drug Designing (CADD) has emerged as a fast alternative method to bring down the cost involved in discovering a new drug. In past, numerous computer programs have been developed across the globe to assist the researchers working in the field of drug discovery. Broadly, these programs can be classified in three categories, freeware, shareware and commercial software. In this review, we have described freeware or open-source software that are commonly used for designing therapeutic molecules. Major emphasis will be on software and web services in the field of chemo- or pharmaco-informatics that includes *in silico* tools used for computing molecular descriptors, inhibitors designing against drug targets, building QSAR models, and ADMET properties.

An overview of the workflow of *in silico* drug designing process



Important Points

1. Source of Molecules (databases or repositories)
2. Molecular Editors (editing & viewing existing molecules)
3. Analog Generators (software used to generate analogs)
4. Structure Optimization (Energy/geometry of molecules)
5. Calculation of Molecular Descriptors
6. Chemical Similarity Search
7. Development of QSAR/QSPR Models
8. Classification and Clustering of Small Molecules
9. Docking Small Molecules in Macromolecules
10. Pharmacophore Tools/Search
11. Software for ADMET Techniques
12. Designing of Inhibitors
13. Major Initiatives towards affordable drugs

Databases and resources managing and hosting chemical compounds

Database	Brief Description with URL
PubChem	A comprehensive database of bioassays, compounds and substances (http://pubchem.ncbi.nlm.nih.gov/)
ChEMBL	Database of drug like molecules (https://www.ebi.ac.uk/chembldb)
Zinc	Maintain commercially-available compounds for virtual screening (http://zinc.docking.org/)
ChemDB	Collection of small-molecules (http://cdb.ics.uci.edu/)
ChemSpider	A chemical database (http://www.chemspider.com/)
MMsINC	Commercial compounds (http://mms.dsfarm.unipd.it/MMsINC/)
KEGG	Maintain comprehensive information (http://www.genome.jp/kegg/)
SMPDB	Small molecule Pathway database (http://www.smpdb.ca)
HMDB	Human Metabolites (http://www.hmdb.ca/)
PDBeChem	Dictionary of chemical components refered in PDB entries (http://www.ebi.ac.uk/pdbe-srv/pdbechem/)
PDB-Bind	Binding affinity information for PDB Ligands (http://sw16.im.med.umich.edu/databases/pdbbind/index.jsp)
BindingDB	Binding affinity of PDB Ligands (http://www.bindingdb.org/)
NCI	Small molecules related to cancer (http://cactus.nci.nih.gov/ncidb2.1/)

List of major molecular editors, frequently used for drawing and editing molecules

Editors	Brief description
BKchem	**Python based free 2D molecule editor (http://bkchem.zirael.org/)**
PubChem Sketcher [*117*]	**A web-based tool for sketching, integrated in PubChem (http://pubchem.ncbi.nlm.nih.gov/edit2/index.html)**
ChemSketch	**ACD/ChemSketch Freeware is a free software for drawing chemicals** (http://www.acdlabs.com/resources/freeware/chemsketch/)
JChemPaint	**Editor for 2D chemical structures (http://jchempaint.github.com/)**
Accelrys Draw	**Draw and edit complex molecules, no fee for academic community (http://accelrys.com/products/informatics/cheminformatics/draw/index.html)**
XDrawChem	**Molecule drawing program (http://xdrawchem.sourceforge.net/)**
MedChem Designer	**Drawing molecules and integration with ADMET property. (http://simplus-downloads.com/)**
JME	**JME Molecular Editor** (http://www.molinspiration.com/jme/)

Analogs generation softwares

Software	Brief description
SmiLib [*118*]	**Enumerates combinatorial libraries with very high rate (http://gecco.org.chemie.uni-frankfurt.de/smilib/)**
GLARE [*119*]	**Generate combinatorial library (http://glare.sourceforge.net/)**
Library synthesizer	**Virtual chemical enumeration (http://tripod.nih.gov/?p=370)**
CLEVER [*120*]	**Chemical Library Editing, Visualization and Enumerating Resource (http://datam.i2r.a-star.edu.sg/clever/)**
Newlead [*121*]	**Generate of combinatorial library from bioactive conformations (http://www.ccl.net/cca/software/MAC/index.shtml)**

REVIEW ARTICLE

Overview of Free Software Developed for Designing Drugs Based on Protein-Small Molecules Interaction

Piyush Agrawal[1,2], Pawan Kumar Raghav[1], Sherry Bhalla[1], Neelam Sharma[1], and Gajendra P.S. Raghava[1,2,*]

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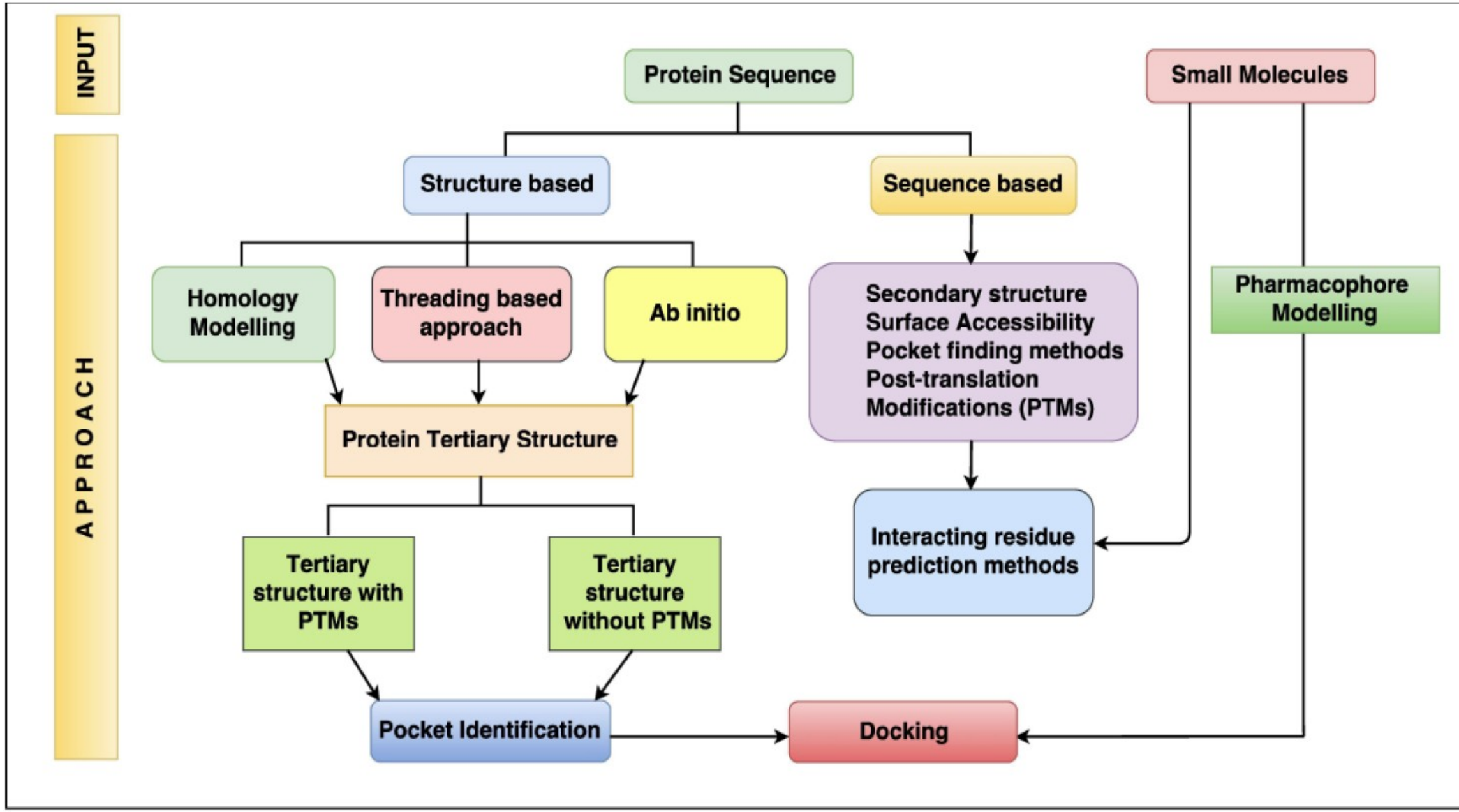
Abstract: One of the fundamental challenges in designing drug molecule against a disease target or protein is to predict binding affinity between target and drug or small molecule. In this review, our focus will be on advancement in the field of protein-small molecule interaction. This review has been divided into four major sections. In the first section, we will cover software developed for protein structure prediction. This will include prediction of binding pockets and post-translation modifications in proteins. In the second section, we will discuss software packages developed for predicting small-molecule interacting residues in a protein. Advances in the field of docking particularly advancement in the knowledge-based force fields will be discussed in the third part of the review. This section will also cover the method developed for predicting affinity between protein and drug molecules. The fourth section of the review will describe miscellaneous techniques used for designing drug molecules, like pharmacophore modelling. Our major emphasis in this review will be on computational tools that are available free for academic use

Keywords: Protein-small molecule interaction, Structure Prediction, Docking, Pharmacophore, Molecular Dynamics, Post Translational Modifications.



(3). Schematic representation of CADD.

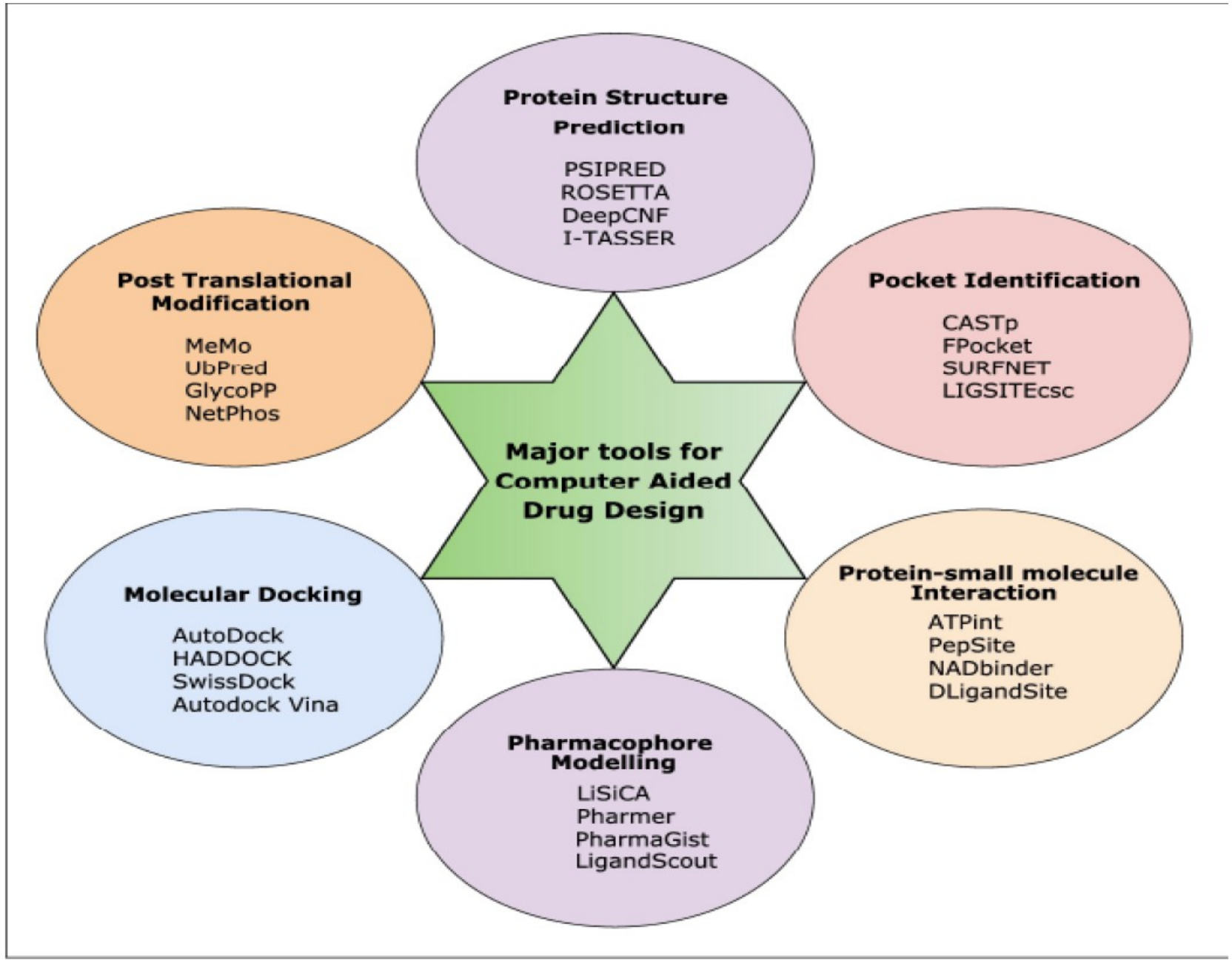


Fig. (1). Shows major categories of freely available computational tools reviewed in this manuscript and popular tools in each category.

Table 1. List of web servers and standalone software for predicting tertiary structure of proteins and are freely available for public use.

Name of Tool [Reference]	Description of Tool [Web Link]
PHYRE2[#] [30]	It uses HMM technique for tertiary structure prediction. [http://www.sbg.bio.ic.ac.uk/phyre2/]
CPHModels[#] [31]	It is based on secondary structure-guided profile alignment and exposure prediction. [http://www.cbs.dtu.dk/services/CPHmodels/]
SWISS MODEL[#] [32]	A fully automated protein structure homology-modelling server. [https://swissmodel.expasy.org/]
I-TASSER[###] [33]	Prediction of protein tertiary structure using threading approach. [http://zhanglab.ccmb.med.umich.edu/I-TASSER/]
EsyPred3D[#] [34]	It obtains the alignment using neural network technique and final model is built using MODELLER. [http://www.unamur.be/sciences/biologie/urbm/bioinfo/esypred/]
(PS)2[#] [35]	Protein tertiary structure prediction using comparative modelling. [http://ps2v3.life.nctu.edu.tw/]
AS2TS[#] [36]	Homology-based approach for predicting protein structure directly based on amino acid sequence. [http://proteinmodel.org/AS2TS/AS2TS/as2ts.html]
RaptorX[#] [37]	Nonlinear scoring function for predicting the structure of non-homologous proteins. [http://raptorx.uchicago.edu/StructurePrediction/predict/]
IntFOLD-TS[#] [38]	It uses single-template local consensus fold recognition approach for tertiary structure prediction. [http://www.reading.ac.uk/bioinf/IntFOLD/IntFOLD3_form.html]
Robetta[#] [39]	Comparative and de novo methods are used for prediction. [http://robetta.bakerlab.org/]

Table 2. Standalone software and web servers developed for predicting important component of protein structure like secondary structure, surface accessibility.

Name of Tool [Reference]	Description of Tool [Web Link]
APPSP2[###] [55]	A combination of nearest neighbour and neural network for secondary structure prediction. [http://webs.iiitd.edu.in/raghava/apssp2/]
YASPIN[#] [56]	Hidden Neural Network based approach for prediction. [http://www.ibi.vu.nl/programs/yaspinwww/]
CFSSP[#] [57]	Predict secondary structure using Chou Fasman Algorithm. [http://www.biogem.org/tool/chou-fasman/]
PSIPRED[###] [58]	Utilize the evolutionary information in the form of alignment profile for prediction. [http://bioinf.cs.ucl.ac.uk/psipred/]
Jpred4[#] [59]	It predicts secondary structure using Jnet algorithm. [http://www.compbio.dundee.ac.uk/jpred/]
DSC[#] [60]	It uses simple and linear statistical method for prediction. [https://npsa-prabi.ibcp.fr/cgi-bin/npsa_automat.pl?page=/NPSA/npsa_dsc.html]
PREDATOR[#] [61]	This method is based on recognition of potentially hydrogen-bonded residues in a single amino acid sequence. [https://npsa-prabi.ibcp.fr/cgi-bin/npsa_automat.pl?page=/NPSA/npsa_predator.html]
GOR V[#] [62]	A statistical method that utilizes evolutionary information. [http://gor.bb.iastate.edu/]
NetSurfP[###] [63]	Predicts secondary structure as well as surface accessibility. [http://www.cbs.dtu.dk/services/NetSurfP/]

Table 3. List of software and web servers developed for predicting binding pockets on the surface of a protein.

Name of Tool [Reference]	Description of Tool [Web Link]
PockDrug[#] [82]	It uses physio-chemical and geometry based descriptors to find the pocket. [http://pockdrug.rpbs.univ-paris-diderot.fr/]
SURFNET[##] [83]	It uses PDB 3D coordinates to generate molecular surfaces and gaps. [http://www.ebi.ac.uk/thornton-srv/software/SURFNET/]
Q-siteFinder[#] [84]	Locate energetically favourable binding sites in a protein. [http://www.bioinformatics.leeds.ac.uk/qsitefinder]
CASTp[#] [85]	Identification of surface accessible pockets and interior inaccessible cavities in a protein. [http://sts.bioe.uic.edu/castp/]
PASS[##] [86]	It utilizes geometry to characterize regions of buried volume in proteins. [http://www.ccl.net/cca/software/UNIX/pass/overview.html]
LIGSITEcsc[###] [87]	LIGSITEcsc is based on the notion of surface-solvent-surface events and the degree of conservation of the involved surface residues. [http://projects.biotec.tu-dresden.de/pocket/]
bSiteFinder[#] [88]	Predicts binding sites on a protein using multiple techniques. [http://binfo.shmtu.edu.cn/bsitefinder/]
AutoSite[###] [89]	It identifies binding pockets using energetic aspects. [http://adfr.scripps.edu/AutoDockFR/autosite.html]

Table 5. List of computational methods developed for predicting ligand interacting residues in a protein.

Name of Tool [Reference]	Description of Tool [Web Link]
ATPint[###] [169]	Prediction of ATP interacting residues in a protein. [http://webs.iiitd.edu.in/raghava/atpint/]
TargetATPsite[##] [170]	A template-free method for predicting residues in ATP binding sites. [http://www.csbio.sjtu.edu.cn:8080/TargetATPsite/]
ATPsite[#] [171]	Sequence-based method for predicting ATP-binding residues. [http://biomine.ece.ualberta.ca/ATPsite/]
GTPbinder[###] [172]	Prediction of GTP binding residue in a protein sequence. [http://webs.iiitd.edu.in/raghava/gtpbinder/]
NADbinder[###] [173]	Prediction of NAD interacting residues in a protein. [http://webs.iiitd.edu.in/raghava/nadbinder/]
FADPred[###] [174]	A method for predicting FAD interacting residues in a protein. [http://webs.iiitd.edu.in/raghava/fadpred/]
ProtChemSI[###] [175]	A database of protein-chemical structural interaction derived from PDB. [http://pcidb.russelllab.org/]
STITCH[##] [176]	A database containing information of known and predicted interactions between proteins and chemicals. [http://stitch.embl.de/]
3did[###] [177]	A database of 3-D structural templates for domain-domain and domain-peptide interaction. [http://3did.irbbarcelona.org/]

Table 6. Docking tools categorized based on features, algorithms, scoring functions, availability with URLs.

Name of Tool [Reference]	Description of Tool [Web Link]
Autodock Vina[##] [205]	It is a Monte Carlo based docking software. [http://vina.scripps.edu]
Autodock[###] [206]	Genetic Algorithm based docking software for docking small molecules. [http://autodock.scripps.edu]
BSP-SLIM[#] [207]	Blind low-resolution ligand-protein docking approach. [https://zhanglab.ccmb.med.umich.edu/BSP-SLIM/]
COPICAT[#] [208]	SVM based method for predicting interactions between proteins & ligands. [http://copicat.dna.bio.keio.ac.jp]
DAIM[##] [209]	Fragment-based docking suite. [http://www.biochem-caflisch.uzh.ch/download/]
DARWIN[###] [210]	Prediction of the interaction between a protein and ligand. [http://darwin.cirad.fr/product.php]
Dock Blaster[#] [211]	A web server for virtual screening using structure-based ligand discovery. [http://blaster.docking.org/]
DockingServer[#] [212]	Integrates a number of computational chemistry software for docking. [https://www.dockingserver.com/]
DockoMatic[##] [213]	Automate the creation and management of AutoDock screening jobs. [https://sourceforge.net/projects/dockomatic/]
DockVision[###] [214]	Docking package including algorithms like Monte Carlo, Genetic algorithm, and database screening docking algorithms. [http://dockvision.sness.net/overview/overview.html]

Table 7. List of pharmacophore-based tools.

Name of Tool [Reference]	Description of Tool [Web Link]
Pharmer## [256]	A new computational approach to search the pharmacophore. [http://smoothdock.ccbb.pitt.edu/pharmer/]
PharmaGist# [257]	Freely available web server for pharmacophore detection. [http://bioinfo3d.cs.tau.ac.il/PharmaGist/]
LigandScout## [258]	Tool that derives 3D pharmacophores from structural data of macromolecule/ligand complexes. [http://en.bio-soft.net/3d/LigandScout.html]
CoLibri## [259]	Compound collections used as virtual screening library. [https://www.biosolveit.de/CoLibri/]
DecoyFinder## [260]	A graphical tool which helps in finding sets of decoy molecules for a given group of active ligands. [http://urvnutrigenomica-ctns.github.io/DecoyFinder/]
MOLA## [261]	Free software for virtual screening using AutoDock4/Vina in a computer cluster using non-dedicated multi-platform computers. [http://esa.ipb.pt/biochemcore/index.php/ds/m]
NNScore## [262]	Neural network-based scoring function for the characterization of protein-ligand complexes. [http://rocce-vm0.ucsd.edu/data/sw/hosted/nnscore/]

(Table 7) contd….

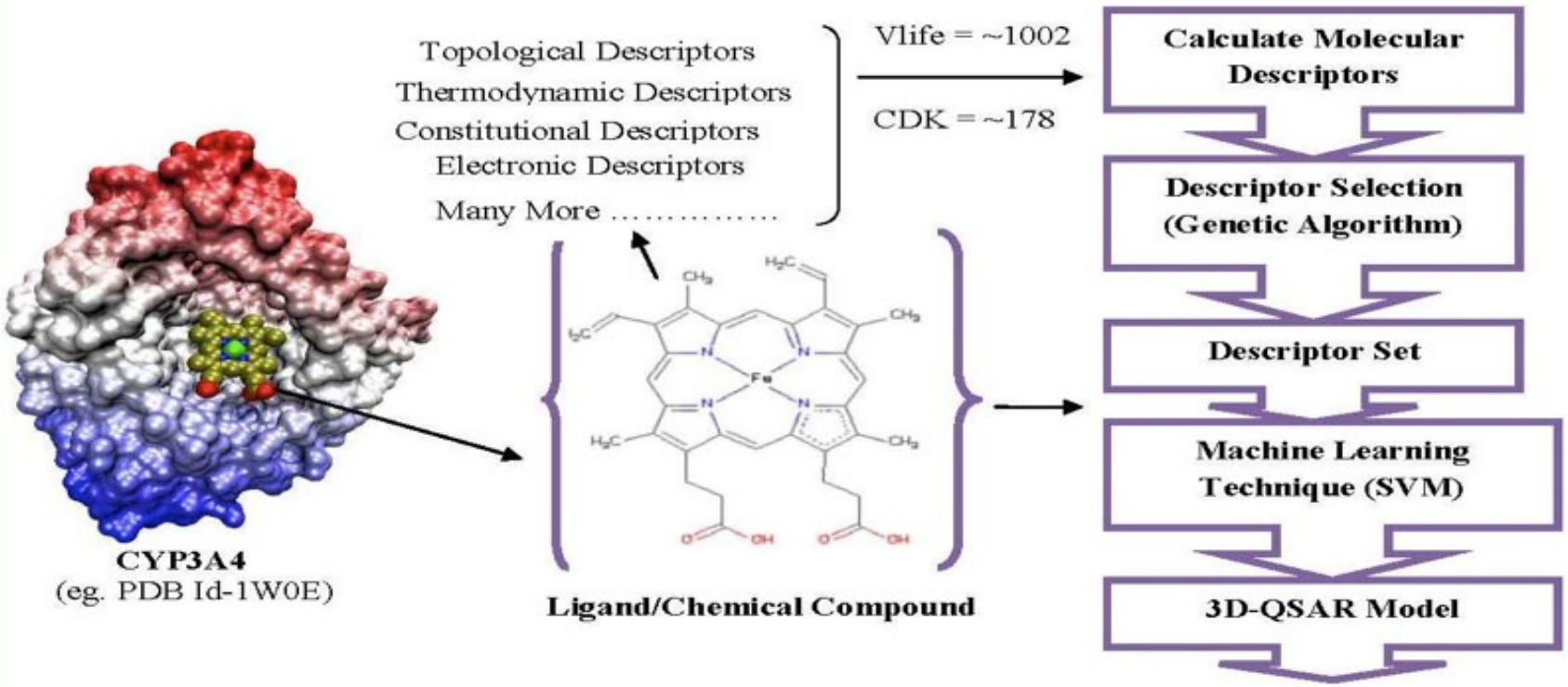
MetaPred:A webserver for the Prediction of Cytochrome P450 Isoform responsible for Metabolizing a Drug Molecule

ver, please cite:: **Prediction of cytochrome P450 isoform responsible for metabolizing a drug molecule** BMC Pharmacolo

» Home
» Submit
» Algorithm
» Developers
» Contact Us
» Help
» Dataset

Cytochrome P450 enzymes (CYPs) are a multi gene family of heme-containing isoenzymes that are involved in oxidative metabolism of drug, steroids and carcinogens. About sixty CYPs are reported in human genome, but more than 90% of all therapeutic drugs are metabolized by five isoforms i.e. CYP1A2, CYP2C9, CYP2C19, CYP2D6 and CYP3A4.

MetaPred Server predict metabolizing CYP isoform of a drug molecule/substrate, based on SVM models developed using CDK descriptors.This server will be helpful for researcher working in the field of drug discovery.This study demonstrates that it is possible to develop free web servers in the field of chemoinformatics. This will encourage other researchers to develop web server for public use, which may lead to decrease the cost of discovering new drug molecules. In the following flow digaram we have given the example of CYP3A4, how this study will be helpful in drug design.



MDRIpred: A webserver for predicting inhibitor against drug tolrent *M.Tuberculosis*

Home OSCADD

Inhibitor Prediction

KiDoQ (Mtb target)

GDoQ (Mtb target)

ABMpred (Mtb target)

eBooster (Mtb target)

MDRIpred (Mtb cell)

CancerIN (Cancer)

ntEGFR (Cancer EGFR)

EGFRpred (Cancer EGFR)

DiPCell (Pancreatic Cancer)

Submission Form

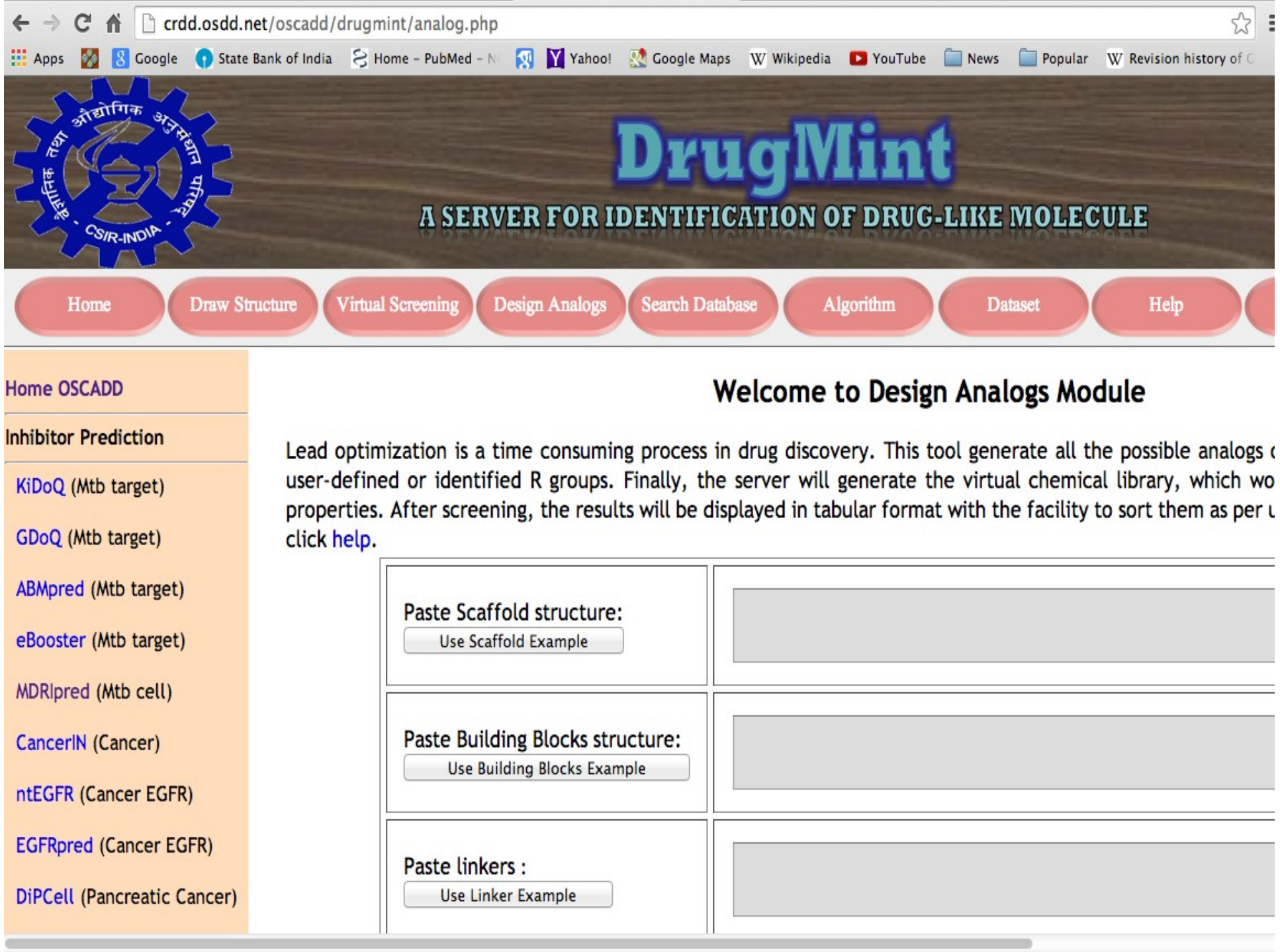
This server allows users to predict inhibitor against different phase of drug tolerant *M.tuberculosi*
methods.
1. Sketch using JME editor.
2. Paste molecules in the box.
3. Upload file containing moleclues in standard format.
Option 2 and 3 allow users to submit more than one molecule (upto 10).

Job Name (Optional)

Email Address (
(Please enter you
via email)

Method 1. **Sketch Structure using JME editor**

Method 2. **Past**
use an example
(Example Test.s


crdd.osdd.net/oscadd/drugmint/analog.php
Apps
Google
State Bank of India
Home - PubMed -
Yahoo!
Google Maps
Wikipedia
YouTube
News
Popular
Revision history of
DrugMint
A SERVER FOR IDENTIFICATION OF DRUG-LIKE MOLECULE
Home
Draw Structure
Virtual Screening
Design Analogs
Search Database
Algorithm
Dataset
Help
Home OSCADD
Inhibitor Prediction
KiDoQ (Mtb target)
GDoQ (Mtb target)
ABMpred (Mtb target)
eBooster (Mtb target)
MDRIpred (Mtb cell)
CancerIN (Cancer)
ntEGFR (Cancer EGFR)
EGFRpred (Cancer EGFR)
DiPCell (Pancreatic Cancer)
Welcome to Design Analogs Module
Lead optimization is a time consuming process in drug discovery. This tool generate all the possible analogs
user-defined or identified R groups. Finally, the server will generate the virtual chemical library, which wo
properties. After screening, the results will be displayed in tabular format with the facility to sort them as per
click help.
Paste Scaffold structure:
Use Scaffold Example
Paste Building Blocks structure:
Use Building Blocks Example
Paste linkers :
Use Linker Example

MetaPred:A webserver for the Prediction of Cytochrome P450 Isoform responsible for Metabolizing a Drug Molecule

Toxipred |KIDoQ | GDoQ | NPTOPE |KetoDrug |CRDD |OSDD |IMTECH | Raghava

ver, please cite:: **Prediction of cytochrome P450 isoform responsible for metabolizing a drug molecule** BMC Pharmacolo

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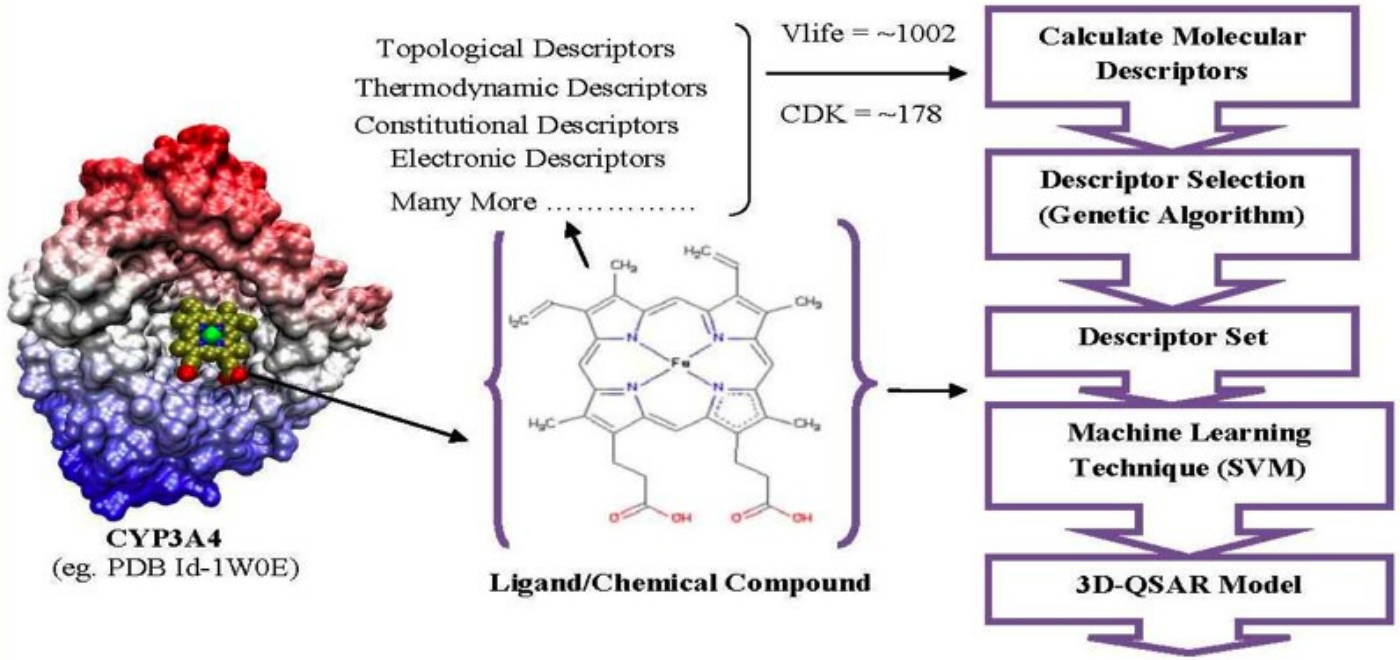
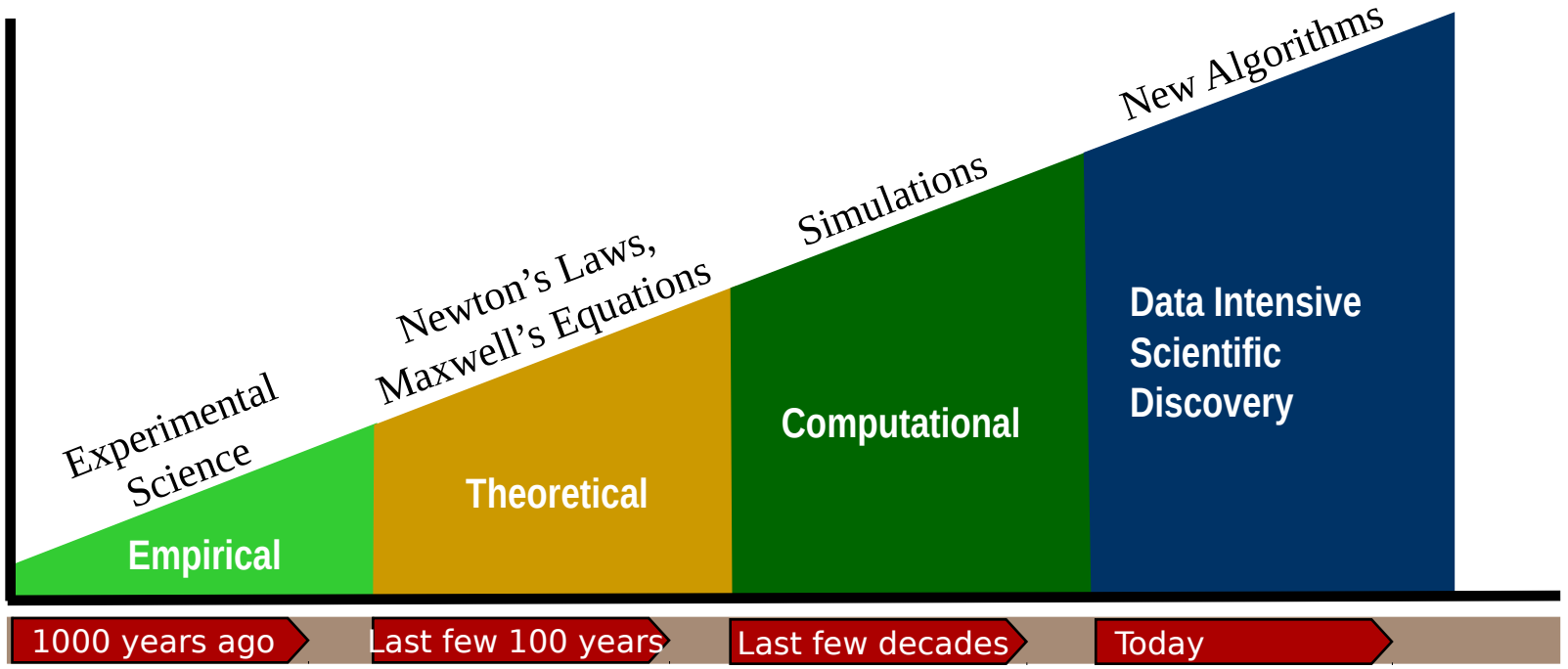
Cytochrome P450 enzymes (CYPs) are a multi gene family of heme-containing isoenzymes that are involved in oxidative metabolism of drug, steroids and carcinogens. About sixty CYPs are reported in human genome, but more than 90% of all therapeutic drugs are metabolized by five isoforms i.e. CYP1A2, CYP2C9, CYP2C19, CYP2D6 and CYP3A4.

MetaPred Server predict metabolizing CYP isoform of a drug molecule/substrate, based on SVM models developed using CDK descriptors.This server will be helpful for researcher working in the field of drug discovery.This study demonstrates that it is possible to develop free web servers in the field of chemoinformatics. This will encourage other researchers to develop web server for public use, which may lead to decrease the cost of discovering new drug molecules. In the following flow digaram we have given the example of CYP3A4, how this study will be helpful in drug design.



INDRA
INFOR
DELHI

What is the Fourth Paradigm of Science



FIRST

- Discovery through Observation of Nature

SECOND

- Development of generalized principles and formulation of Models

THIRD

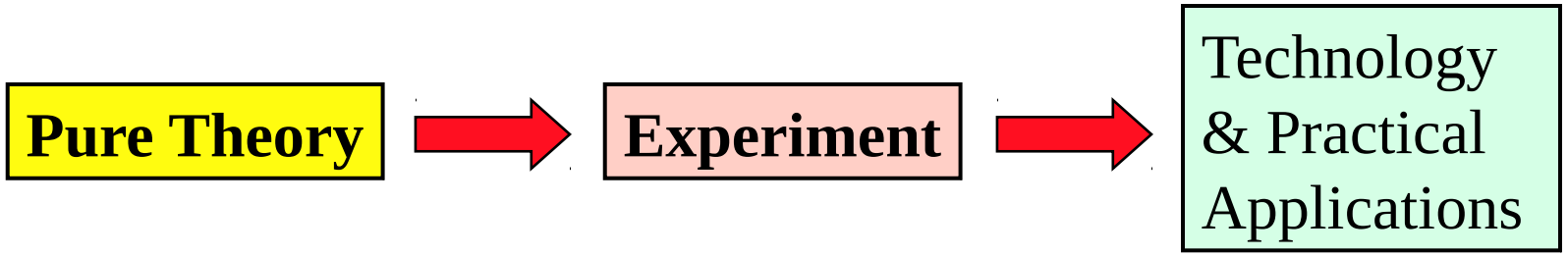
- Modelling and Simulation of complex natural and engineering processes

FOURTH

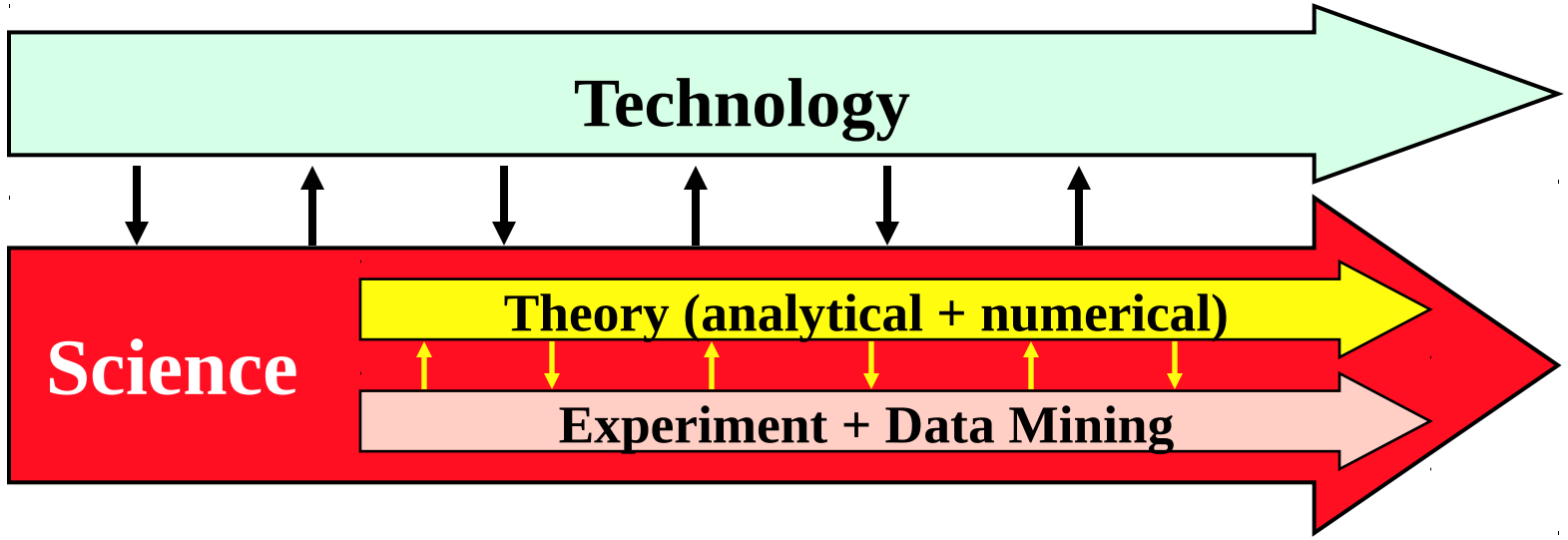
- Unifies theory, experiment and simulation
- Data from observations and/or high fidelity simulations
- Analysis of database using data management and statistics

Scientific and Technological Progress

A traditional, “Platonistic” view:



A more modern and realistic view:

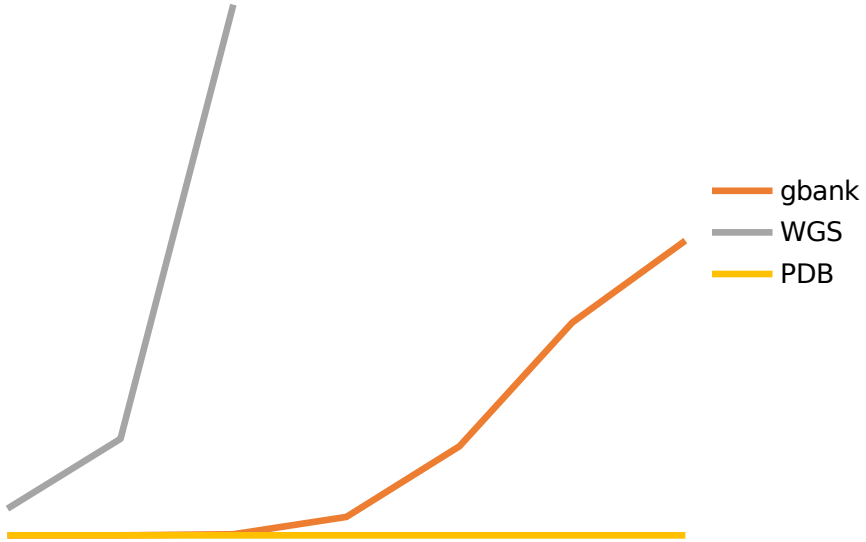


This synergy is stronger than ever and growing;
it is greatly enhanced by the IT/computation

Biological Data is Growing with Exponential Rate (Mining this data is a challenge)

Limitations of traditional tools

- Trained on small & obsolete data
- Unable to utilize modern datamining techniques
- Not suitable for scaling/parallelization
- Lack of precision & speed



Volume
Gene databases are growing with exponential rates

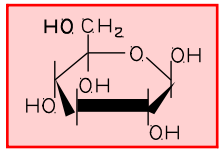
Velocity
Automatic NGS machines are producing data at high rate

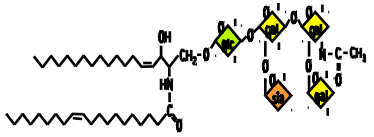
BIG DATA Of Genes

Variety
Type of data from sequence to expression to CNV to SNP etc.

What is Challenge?
Algorithms for dynamic mining for handling data in real life

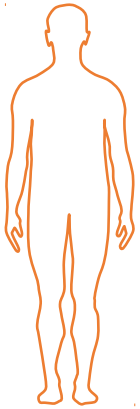
Glycomics (Sugars)

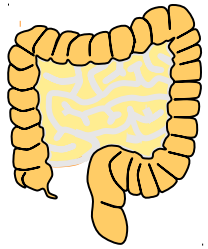




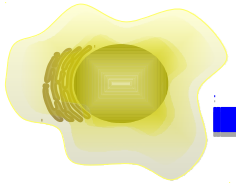
Lipidomics (Lipids)

Metabolomics

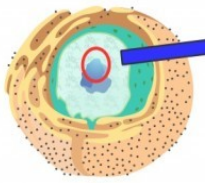




Organ, Tissue

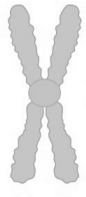


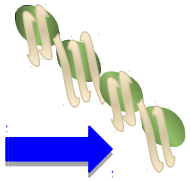
Cell



Nucleus

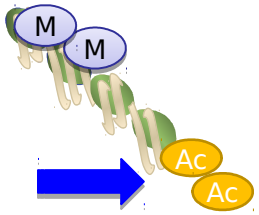
Chromosome (23 pair)

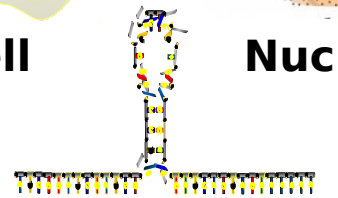




Chromatin

Epigenomics

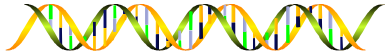




miRNA

Non-coding RNA

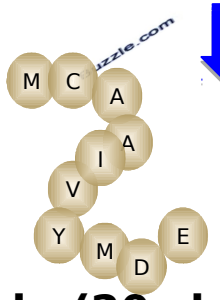
Genomics (3×10⁹)



DNA (4 chemicals: A, T, G, C)

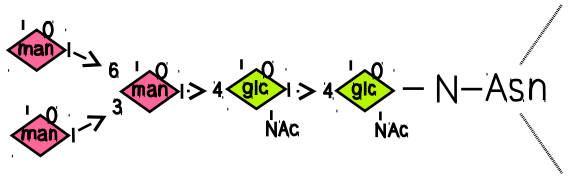
mRNA

Transcriptomics (copies)



Proteomics

Protein (20 chemicals:



Glycomics (Sugars

World of OMICs

Table 1. Different types of omics techniques used in quantifying the genomic architecture of the human genome and their functionalities

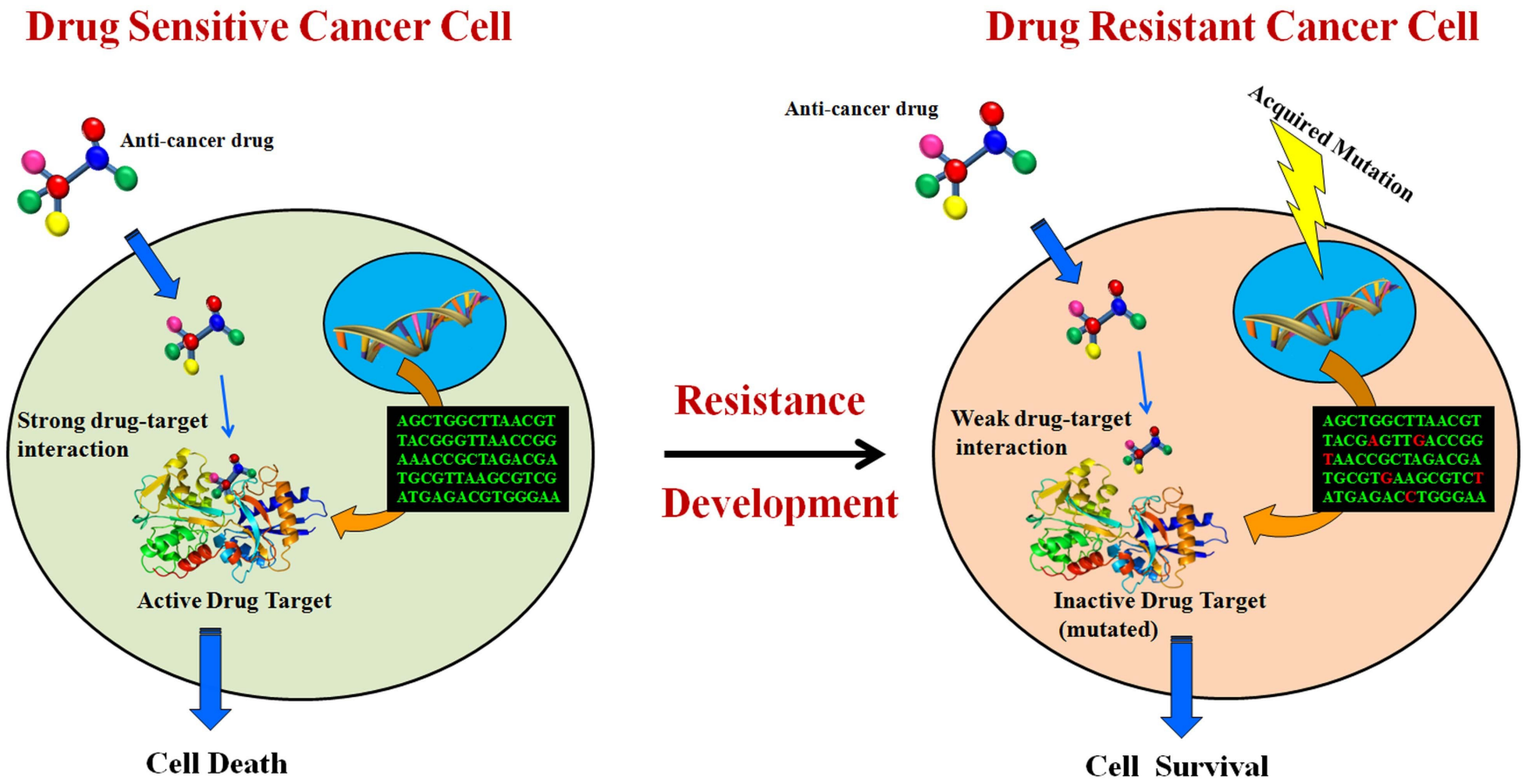
Type of omics	Technique	Description
Genomics	WGS, WES	Used for variant identification at genome or exome level
Epigenomics	ChiP-Seq	Identification for DNA binding site, transcription factor
	DNase-Seq	Identification of regulatory elements
	ChiRP-Seq	Identification of ncRNA, lncRNA and their associated proteins
	WG-bisulphite	Identification of methylation sites in human genome
Transcriptomics	RNA-Seq	Identification of transcripts such as mRNA, miRNA
Proteomics	LC–MS/MS based	Quantify protein abundance within biological condition
	RRPA/SILAC based	Quantify protein abundance within biological condition
Metabolomics	LC–MS based	Identify and quantify metabolites involves in specific pathways

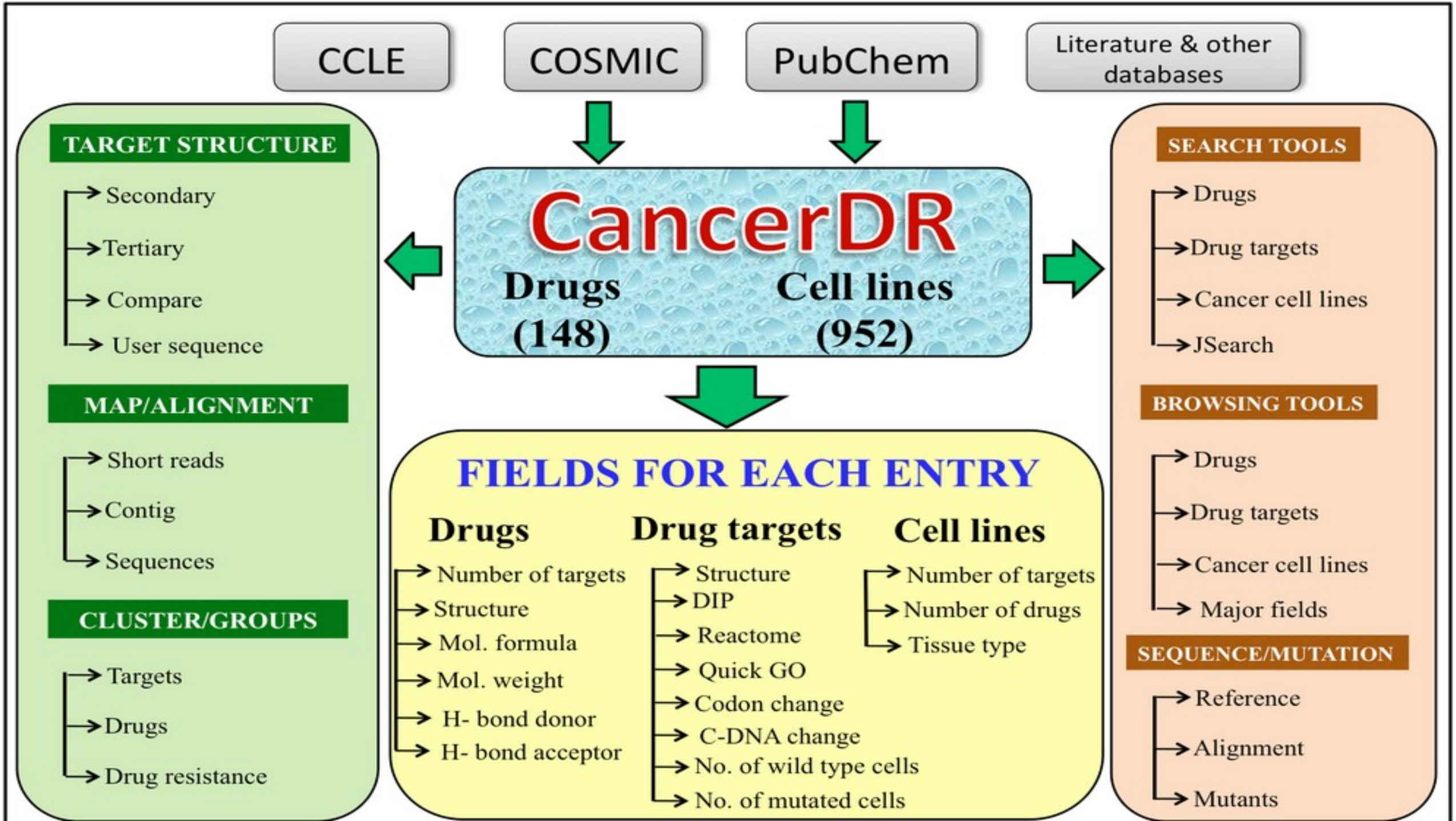
CancerDR: Cancer Drug Resistance Database

CSIR - Institute of Microbial Technology, India

Http://webs.iiitd.edu.in/raghava/cancerdr/

Search
Browse
Alignment/Mutation
Target Structure
Map/Alignment
Clusters/Groups
Downloads




CCLE
COSMIC
PubChem
Literature & other databases
CancerDR
Drugs (148)
Cell lines (952)
TARGET STRUCTURE
Secondary
Tertiary
Compare
User sequence
MAP/ALIGNMENT
Short reads
Contig
Sequences
CLUSTER/GROUPS
Targets
Drugs
Drug resistance
FIELDS FOR EACH ENTRY
Drugs
Number of targets
Structure
Mol. formula
Mol. weight
H- bond donor
H- bond acceptor
Drug targets
Structure
DIP
Reactome
Quick GO
Codon change
C-DNA change
No. of wild type cells
No. of mutated cells
Cell lines
Number of targets
Number of drugs
Tissue type
SEARCH TOOLS
Drugs
Drug targets
Cancer cell lines
JSearch
BROWSING TOOLS
Drugs
Drug targets
Cancer cell lines
Major fields
SEQUENCE/MUTATION
Reference
Alignment
Mutants

Scientific Reports
Sci Rep. 6: 23857

Prioritization of anticancer drugs against a cancer using genomic features of cancer cells: A step towards personalized medicine

Sudheer Gupta[1], Kumardeep Chaudhary[1], Rahul Kumar[1], Ankur Gautam[1], Jagpreet Singh Nanda[1], Sandeep Kumar Dhanda[1], Samir Kumar Brahmachari[2], Gajendra P. S. Raghava[a1]

1. Bioinformatics Centre, CSIR-Institute of Microbial Technology, Sector 39A, Chandigarh, India

2. CSIR-Institute of Genomics and Integrative Biology, Mathura Road, New Delhi-110007, India.

a. raghava@imtech.res.in

DOI: 10.1038/srep23857
Published online: 31 March 2016

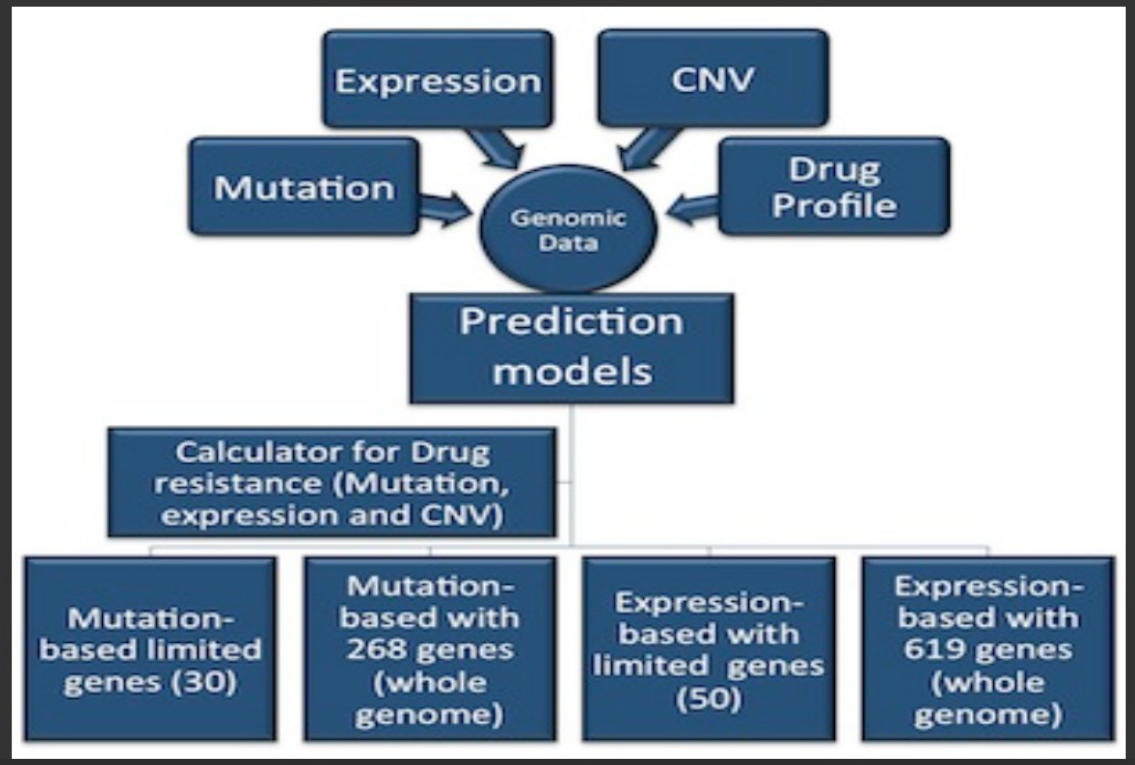
Abstract

In this study, we investigated drug profile of 24 anticancer drugs tested against a large number of cell lines in order to understand the relation between drug resistance and altered genomic features of a cancer cell line. We detected frequent mutations, high expression and high copy number variations of certain genes in both drug resistant cell lines and sensitive cell lines. It was observed that a few drugs, like Panobinostat, are effective against almost all types of cell lines, whereas certain drugs are effective against only a limited type of cell lines. Tissue-specific preference of drugs was also seen where a drug is more effective against cell lines belonging to a specific tissue.

CancerDP

Prioritization Of Anticancer Drugs

CancerDP | Priortization | Drug Calculator | Signatures | Source | Help | Te



Drug Prioritization Prediction

Prioritization: Prediction of drug prioritization based or
mutation/expression/CNV of given genes.

Drug Calculator: Interactive calculation of drug resistar
probability.

Genome Submit: Prediction of anticancer drug based

Signatures: Browsing significant and correlated genes.

rence: Gupta et al. (2016) Prioritization of anticancer drugs against a cancer using genomic features of cancer cells:
rds personalized medicine. Scientific Reports 6, 23857. #####

Figure 1: Illustration of tissue-specific response of 24 anticancer drugs, where right column contains names of drugs and bottom row has names of tissues.

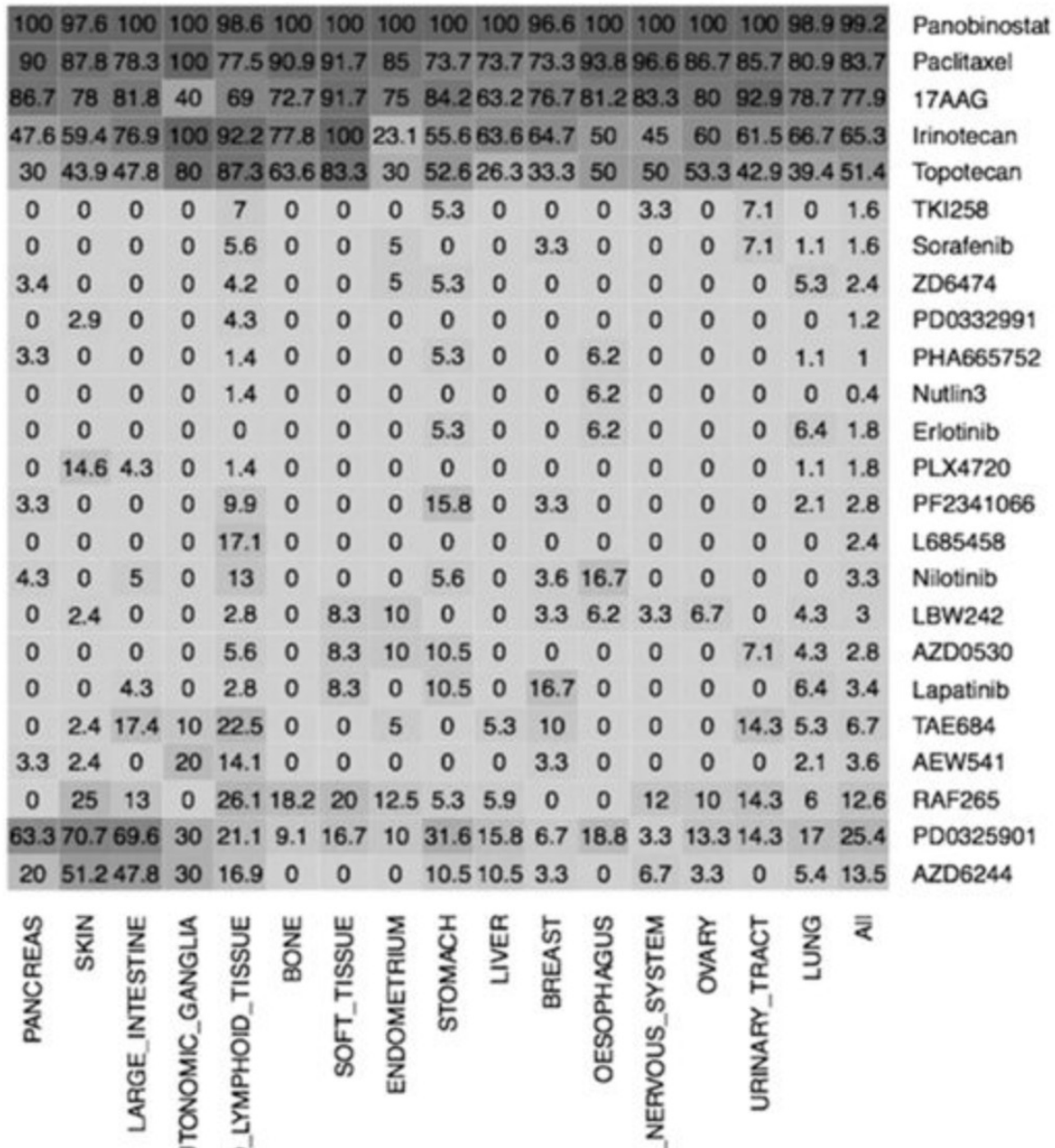


Table 3: The performance of SVM models developed using various genomic features that include mutant genes, variant genes, CNV, expression, hybrid.

From: Prioritization of anticancer drugs against a cancer using genomic features of cancer cells: A step towards personalized medicine

Drug	Mutation	Variation	Expression	CNV	Hybrid	CCLE*
17AAG	0.42	0.55	0.67	0.54	0.76	0.43
AEW541	0.25	0.54	0.69	0.54	0.75	0.33
AZD0530	0.41	0.45	0.65	0.56	0.71	0.19
AZD6244	0.52	0.51	0.81	0.56	0.82	0.59
Erlotinib	0.48	0.56	0.79	0.62	0.82	0.3
Irinotecan	0.58	0.65	0.84	0.56	0.87	0.68
L685458	0.44	0.63	0.82	0.59	0.89	0.48
LBW242	0.44	0.52	0.72	0.52	0.90	0.46
Lapatinib	0.43	0.57	0.75	0.64	0.79	0.09
Nilotinib	0.58	0.53	0.84	0.71	0.77	0.76
Nutlin3	0.24	0.26	0.52	0.33	0.62	0.1
PD0325901	0.54	0.50	0.82	0.55	0.83	0.6
PD0332991	0.42	0.61	0.84	0.51	0.87	0.62
PF2341066	0.38	0.56	0.75	0.61	0.74	0.62
PHA665752	0.37	0.49	0.60	0.49	0.70	0.49
PLX4720	0.68	0.56	0.79	0.68	0.90	0.38
Paclitaxel	0.34	0.51	0.58	0.48	0.73	0.29
Panobinostat	0.46	0.50	0.78	0.58	0.82	0.58
RAF265	0.48	0.49	0.73	0.53	0.78	0.35
Sorafenib	0.37	0.58	0.78	0.44	0.76	0.28
TAE684	0.38	0.42	0.68	0.52	0.74	0.38
TKI258	0.36	0.43	0.72	0.53	0.76	0.3
Topotecan	0.44	0.55	0.75	0.54	0.80	0.58
ZD6474	0.36	0.48	0.71	0.53	0.74	0.22
Average	**0.43**	**0.52**	**0.73**	**0.55**	**0.78**	**0.42**

Briefings in Functional Genomics, 20(4), 2021, 213–222

https://doi.org/10.1093/bfgp/elab021
Advance Access Publication Date: 1 April 2021
Review Paper

Computational resources for identification of cancer biomarkers from omics data

Harpreet Kaur†, Rajesh Kumar†, Anjali Lathwal† and Gajendra P.S. Raghava

Corresponding author: Gajendra P.S. Raghava, Department of Computational Biology, Indraprastha Institute of Information Technology, Okhla Industrial Estate, Phase III, New Delhi 110020, India. Tel.: +91 011 26907444; E-mail address: raghava@iiitd.ac.in
†These authors have contributed equally.

Abstract

Cancer is one of the most prevailing, deadly and challenging diseases worldwide. The advancement in technology led to the generation of different types of omics data at each genome level that may potentially improve the current status of cancer patients. These data have tremendous applications in managing cancer effectively with improved outcome in patients. This review summarizes the various computational resources and tools housing several types of omics data related to cancer. Major categorization of resources includes—cancer-associated multiomics data repositories, visualization/analysis tools for omics data, machine learning-based diagnostic, prognostic, and predictive biomarker tools, and data analysis algorithms employing the multiomics data. The review primarily focuses on providing comprehensive information on the open-source multiomics tools and data repositories, owing to their broader applicability, economic-benefit and usability. Sections including the comparative analysis, tools applicability and possible future directions have also been discussed in detail. We hope that this information will significantly benefit the researchers and clinicians, especially those with no sound background in bioinformatics and who lack sufficient data analysis skills to interpret something from the plethora of cancer-specific data generated nowadays.

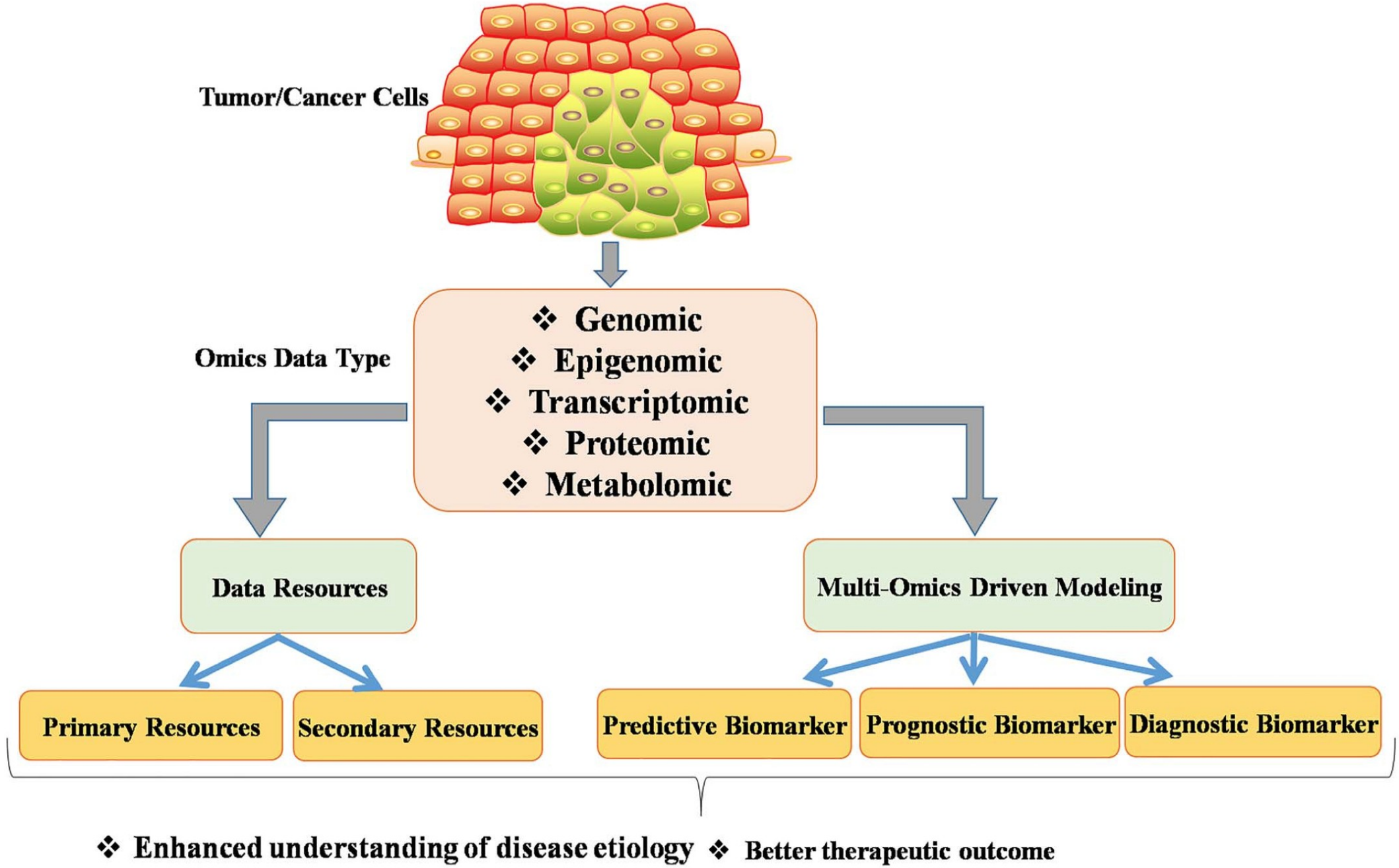


Figure 1. Schematic description of the overall methodology and workflow of the review article.

Drug Discovery Today • Volume xxx, Number xx • xxxx 2021 REVIEWS

KEYNOTE (GREEN)

Computational resources in the management of antibiotic resistance: Speeding up drug discovery

Lubna Maryam [1], **Salman Sadullah Usmani** [1], **Gajendra P.S. Raghava** *

Department of Computational Biology, Indraprastha Institute of Information Technology, New Delhi 110020, India

This article reviews more than 50 computational resources developed in past two decades for forecasting of antibiotic resistance (AR)-associated mutations, genes and genomes. More than 30 databases have been developed for AR-associated information, but only a fraction of them are updated regularly. A large number of methods have been developed to find AR genes, mutations and genomes, with most of them based on similarity-search tools such as BLAST and HMMER. In addition, methods have been developed to predict the inhibition potential of antibiotics against a bacterial strain from the whole-genome data of bacteria. This review also discuss computational resources that can be used to manage the treatment of AR-associated diseases.

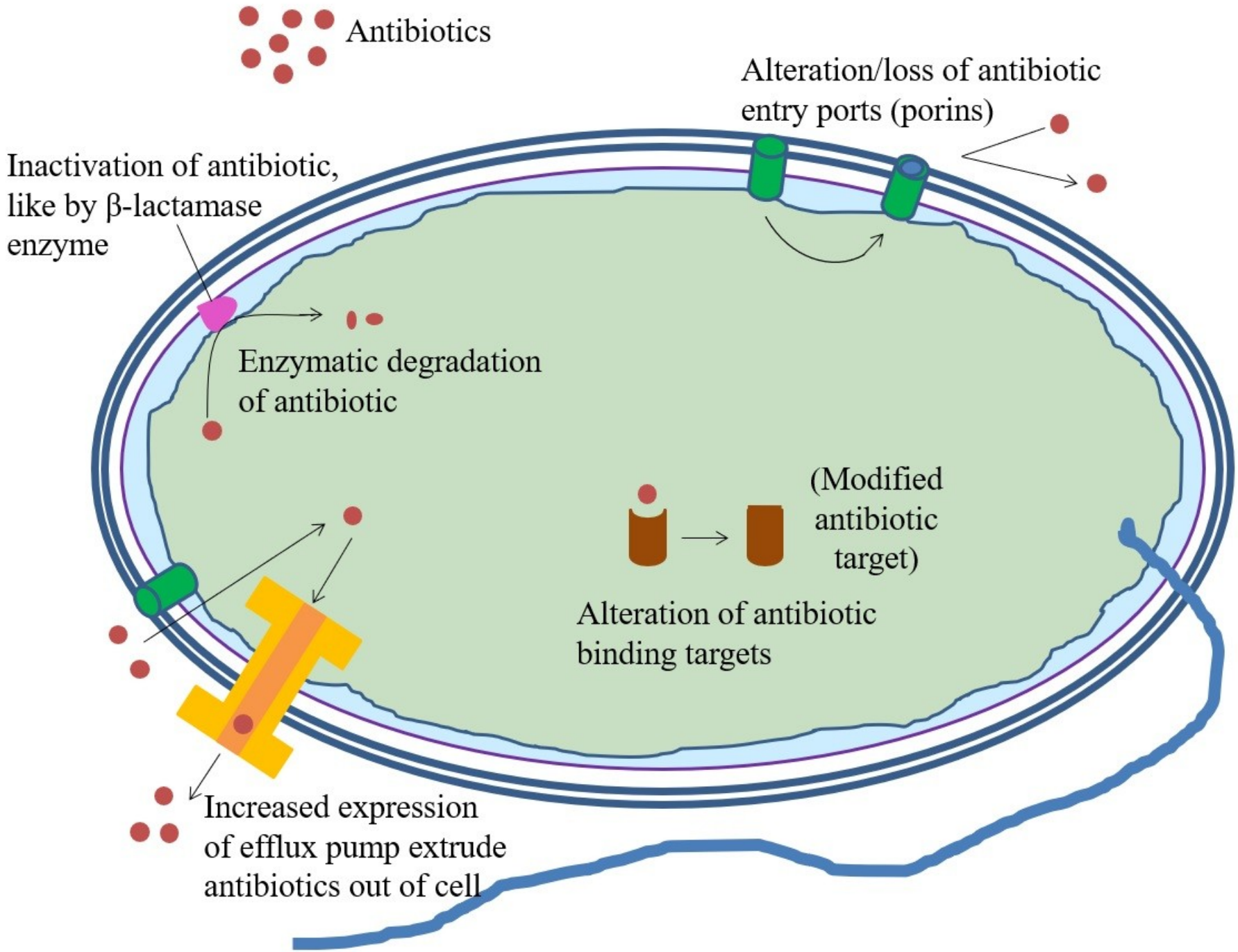

Antibiotics
Alteration/loss of antibiotic entry ports (porins)
Inactivation of antibiotic, like by β-lactamase enzyme
Enzymatic degradation of antibiotic
(Modified antibiotic target)
Alteration of antibiotic binding targets
Increased expression of efflux pump extrude antibiotics out of cell

TABLE 1

List of databases concerned with antibiotic-resistance (AR) genes.

Name and link	Description	Status	Update	Reference
ARGO http://bioinformatics.org/argo/beta/index.php	First database of AR genes	N	N/A	[10]
ARDB http://ardb.cbcb.umd.edu/	Information about AR genes	N	2009	[11]
CARD https://card.mcmaster.ca/	Comprehensive information on AR genes	A	2020	[12]
CARD 2017 https://card.mcmaster.ca/	Comprehensive information on AR genes	A	2020	
CARD 2020 https://card.mcmaster.ca/	Comprehensive information on AR genes	A	2020	[13]
BARRGD https://www.ncbi.nlm.nih.gov/bioproject/313047	Bacterial antibiotic resistance reference gene database.	A	Frequently updated	[15]
NDARO https://www.ncbi.nlm.nih.gov/pathogens/antimicrobial-resistance/	Antimicrobial resistance genes	A	2020	
LacED http://www.laced.uni-stuttgart.de/	Database of TEM-β-lactamases	A	2017	[16]
MBLED http://www.mbled.uni-stuttgart.de/	Contains class B β-lactamases	A	2012	[17]
BLAD	Widely circulated β-lactamases database	A	N/A	[18]
CBMAR http://proteininformatics.org/mkumar/lactamasedb/	Facilitates molecular annotation of β-lactamases	A	2014	[19]
BLDB http://bldb.eu/	Structural and functional information about β-lactamases	A	2020	[20]
β-lactamase database http://ifr48.timone.univ-mrs.fr/beta-lactamase/public/	Sequence, structure, function and phylogenetic tree of β-lactamases	A	N/A	
TBDReaMDB	Tuberculosis drug resistance associated	N	N/A	[21]

THPdb

A database of FDA approved therapeutic peptides and proteins

HOME | SEARCH | BROWSE | TOOLS | INFORMATION | DOWNLOADS | DEVELOPERS | HELP

Welcome to Home Page of THPdb

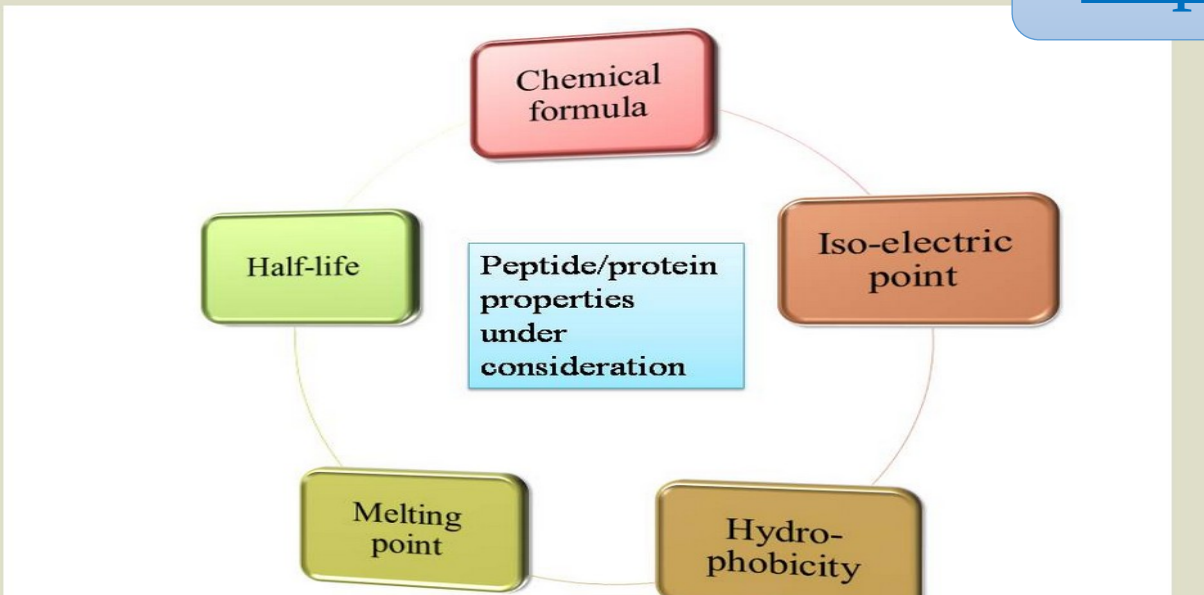
Therapeutic Proteins

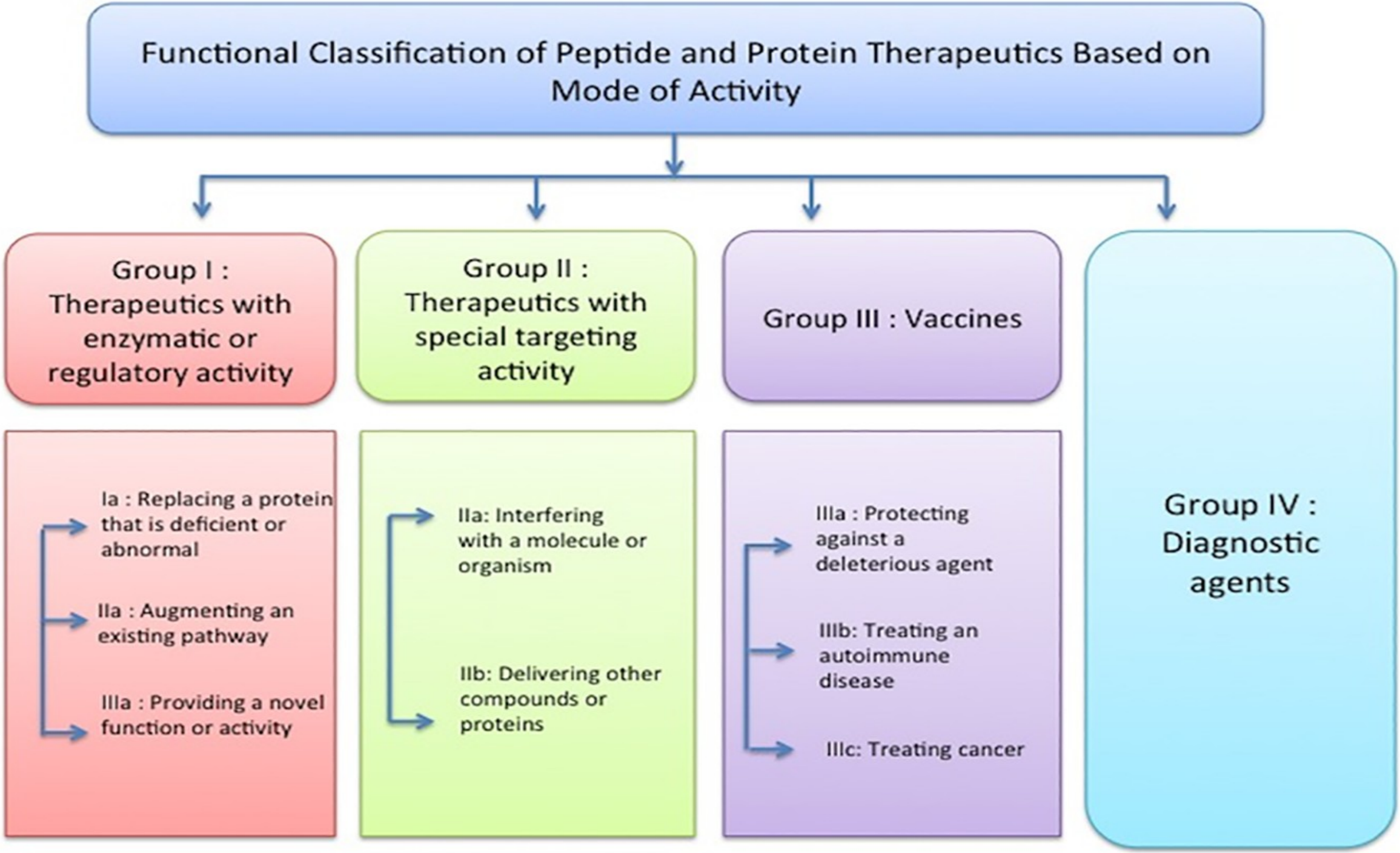
On therapeutic prespective, there is tremendous opportunity in terms of harnessing protein therapeutics to alleviate disease. Once a rarely used subset of medical treatments, protein therapeutics have increased dramatically in number and frequency of use since the introduction of the first recombinant protein therapeutic — human insulin — about 30 years ago. The pharmaceutical industry is viewing therapeutic proteins with a renewed interest. On going research is investigating a myriad of therapeutic peptides to study and improve their availability and efficacy.

What is THPdb?

THPdb is a comprehensive database based on approved and approved/investigational therapeutic peptides compiling important information about these peptides, like their description, sequence, indication, mechanism of action, pharmacodynamics, toxicity, metabolism, absorption, half life, volume of distribution, clearance rate, patent information, interaction with other drugs, targets, physicochemical properties, etc. These peptides have been classified into four categories according to their application, making it easy for the user to access them. Therapeutic peptides are modified in different ways so as to alter their properties and then sold under different brand names by various companies. THPdb provides detailed description of such brands in a user-friendly way to enable quick access of relevant information on the peptides. All information compiled in this database has been extracted from research papers, patents, pharmaceutical company websites catering to product details, drugba

https://webs.iiitd.edu.in/raghava/thpdb/




Functional Classification of Peptide and Protein Therapeutics Based on Mode of Activity
Group I : Therapeutics with enzymatic or regulatory activity
Group II : Therapeutics with special targeting activity
Group III : Vaccines
Group IV : Diagnostic agents
Ia : Replacing a protein that is deficient or abnormal
IIa : Augmenting an existing pathway
IIIa : Providing a novel function or activity
IIa: Interfering with a molecule or organism
IIb: Delivering other compounds or proteins
IIIa : Protecting against a deleterious agent
IIIb: Treating an autoimmune disease
IIIc: Treating cancer

Drug Delivery

crdd.osdd.net/raghava/cellppd/

Google State Bank of India Home - PubMed -

CellPPD: Designing of Cell Penetrating Peptides

Home | Design Peptide | Multiple Peptides | Protein Scaning | Motif Scaning | Motif List | Major Features | Algorithm | Help | Datasets

Welcome to CellPPD

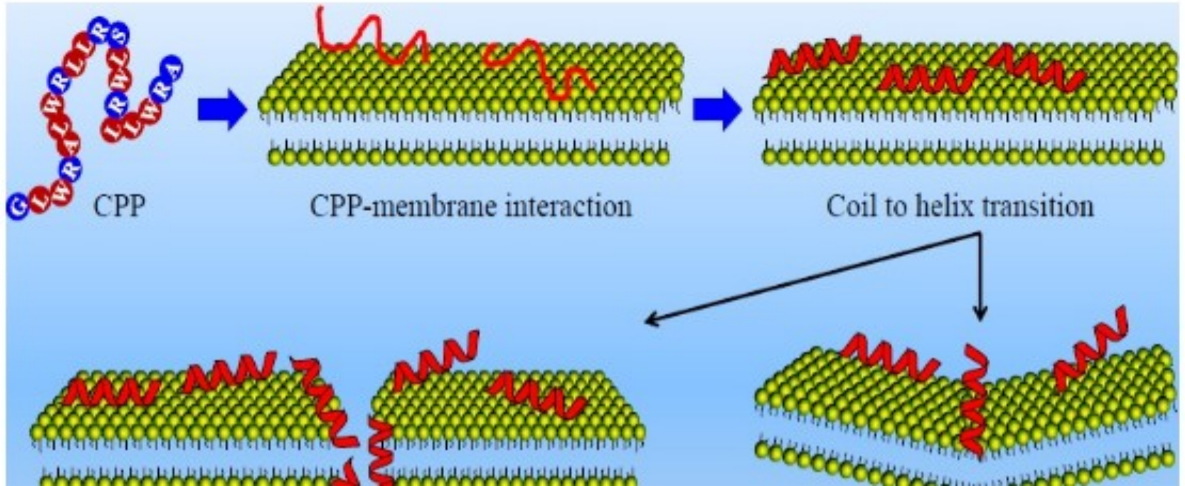
utam *et al.*: *In silico* approaches for designing highly effective cell penetrating peptides. *Journal of Translational Medicine* 3 11:74.Link

CellPPD is an *in silico* method, which is developed to predict and design efficient cell penetrating peptides (CPPs). The main dataset used in this method consists of 708 experimentally validated CPPs.

Major Features include:

(1) **Desing Peptide:** This module allows user to generate all possible single mutant analogues of their peptides and predict whether the analogue is cell penetrating or not.

(2) **Multiple Peptides:** This module of CellPPD allows user to predict number of CPPs in peptides submitted by the user



Drug Delivery

crdd.osdd.net/raghava/tumorhpd/

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TumorHPD: Designing of Tumor Homing Peptides

(Institute of Microbial Technology, Chandigarh, India)

| Home | Peptide | Protein | Batch | Download | Algorithm | Features | Help |

Welcome to TumorHPD

Tumor homing peptides are the short peptides having average length between 7 to 12 residues. These peptides h
bind to tumor cells or tissues. These peptides can be used to deliver target specific drugs and as imaging agents for t
Thus prediction of tumor homing peptide is important for managing cancer treatment effectively.

TumorHPD is a web server for predicting and designing tumor homing peptides. This server is extremely useful fo
the field of therapeutic peptides. This server allows the users to design tumor homing peptides and their mutants
and physicochemical properties.

ference: Sharma, A. et al. Computational approach for designing tumor homing peptides. Sci. Rep. 3, 1607; DOI:10.

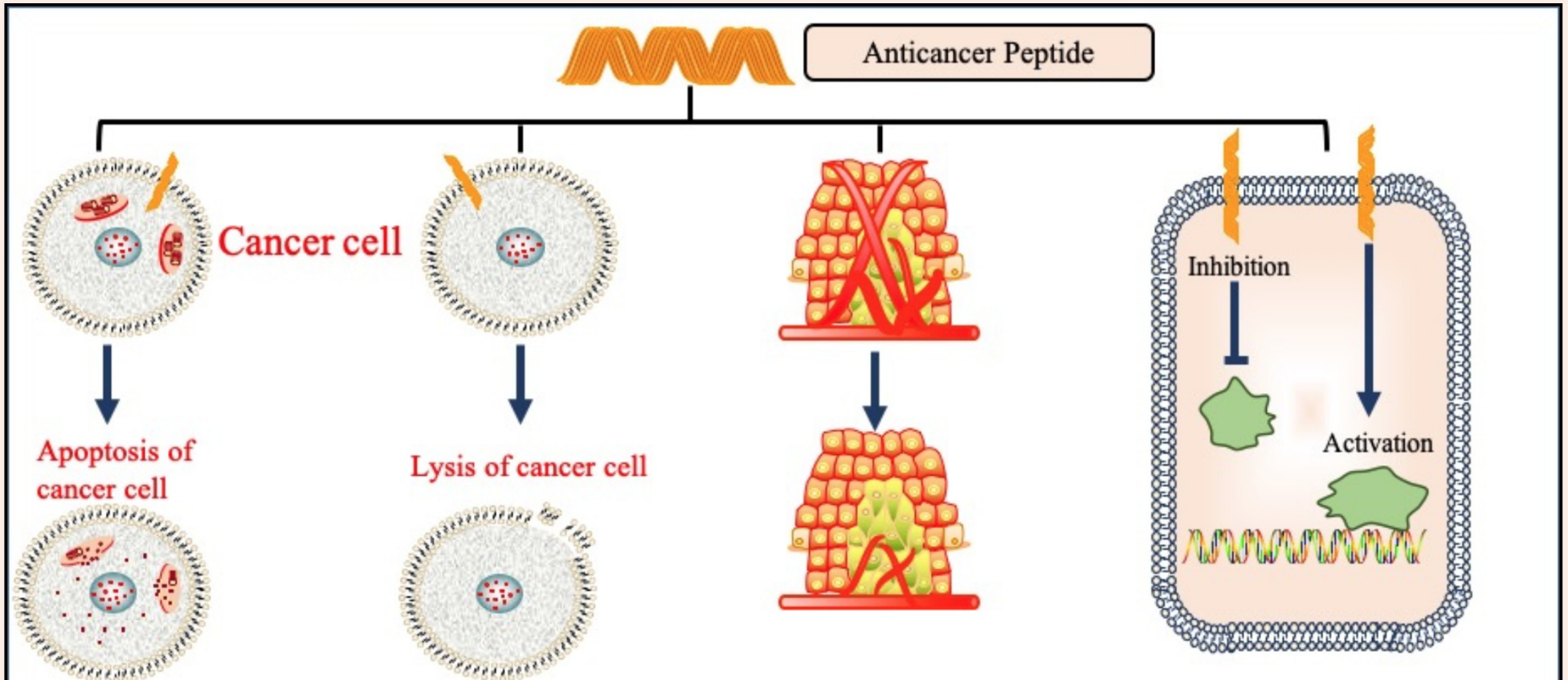
Developed by: Bioinformatics Centre, Institute of Microbial Technology, Sec-39A, Chandigarh,

Peptide based Inhibitors

AntiCP 2.0

Welcome To AntiCP 2.0

AntiCP 2.0 is an updated version of AntiCP, developed to predict and design anticancer peptides with high accuracy. This study utilize largest possible dataset of anticancer and non-anticancer peptides. Main dataset consists of experimentally validated 861 anticancer peptides and 861 non-anticancer or validated antimicrobial peptides. Alternate dataset comprises of 970 anti-cancer peptides and 970 non-anticancer peptides (randomly pickup from Swiss-Prot).



Peptide based Inhibitors

AHTpin

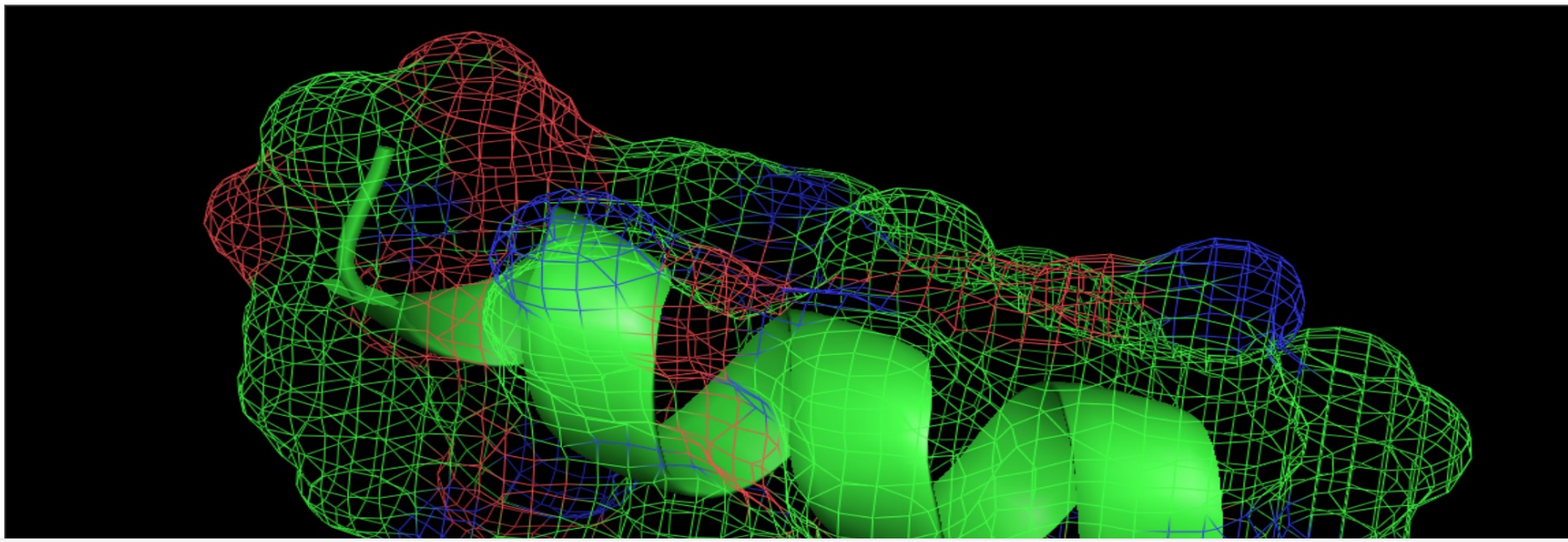
ANTIHYPERTENSIVE PEPTIDE INHIBITORS

HOME ALGORITHM DATASETS HELP TEAM CONTACT

designing of antihypertensive peptides. Sci. Rep. 5, 12512.

- Dipeptide
- Tripeptide
- Tetrapeptide
- Pentapeptide
- Hexapeptide
- 7-12 residues

Welcome to Home Page of AHTpin



Peptide based Inhibitors

Antifp: A Prediction server for Antifungal Peptide

Home | Predict | Mutational Series | sliding Window Prediction | Download | Help | Developers | Contact

Welcome to Antifp

=== If you are using this webserver, please cite, Agrawal et al. (2018) In silico approach for prediction of antifungal peptides. Front. Microbiol., 9:23. ===

Antifp is an in silico method, which is developed to predict and design antifungal peptides. The main dataset used in this method consists of 1459 antifungal peptides.

Major features includes:

1. **Predict :** This module allows user to predict whether the given sequence or number of sequences is antifungal or not.

Peptide Stability

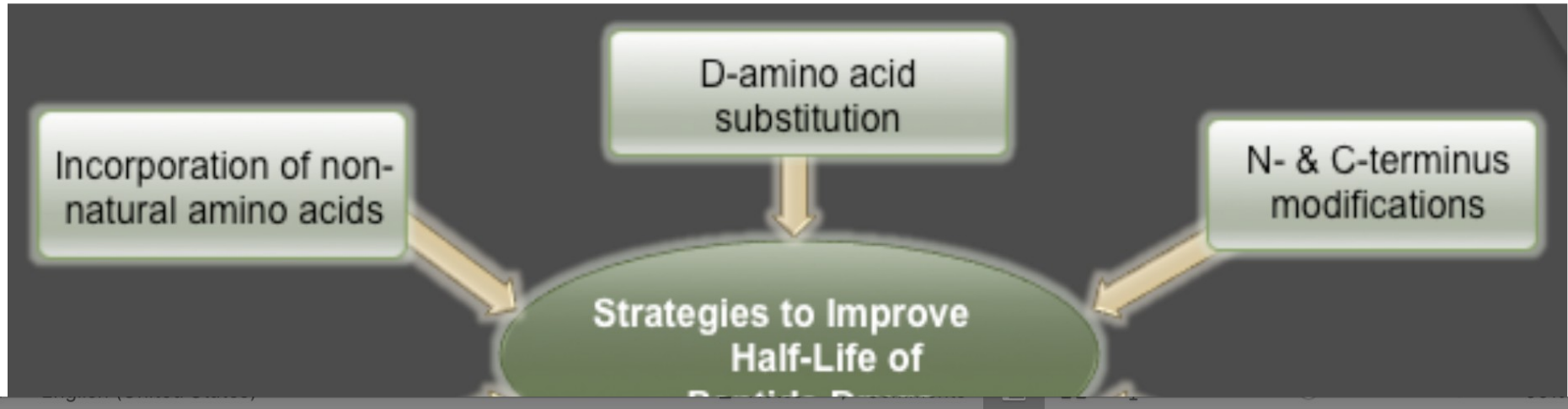
PEPlife

A Database of Half-life of Peptides

Home | Search | Browse | Tools | Download | Important | Team | Contact Us

Welcome to the Home Page of PEPlife

==== If you are using this database, please cite: Mathur, D. et al. PEPlife: A Repository of the Half-life of Peptides. Sci. Rep. 6, 36617; doi: 10.1038/srep36



Toxicity

crdd.osdd.net/raghava/toxinpred/

Google | State Bank of India | Home - PubMed - N

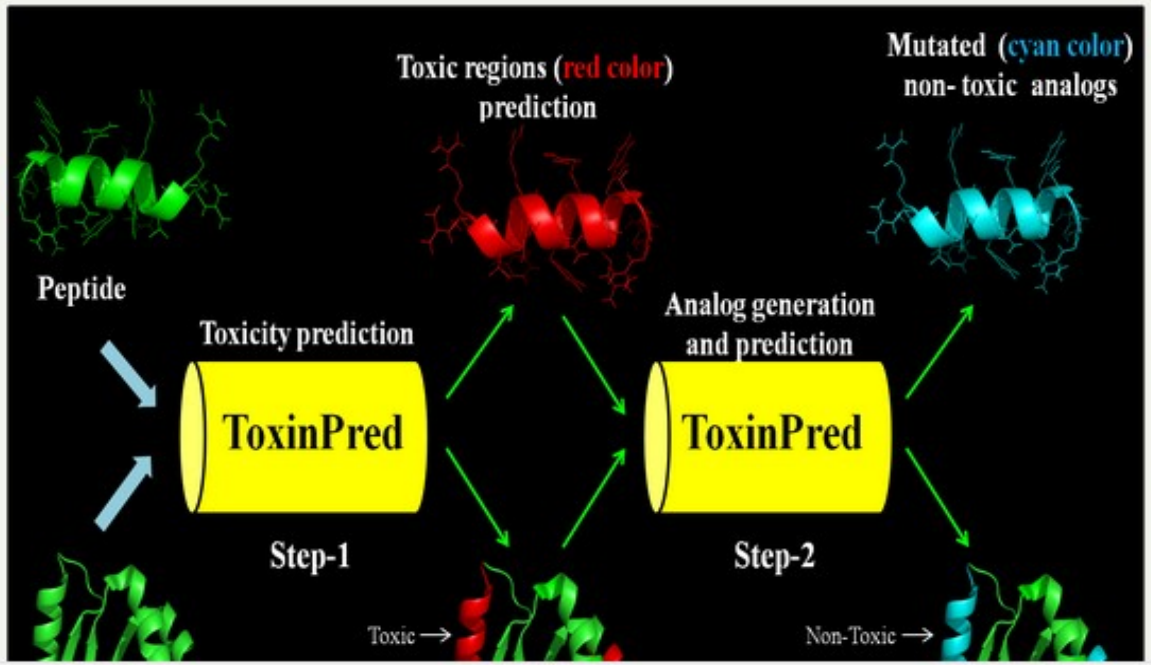
ToxinPred

Designing and prediction of toxic peptides

Home | Design Peptide | Batch Submission | Protein Scanning | Motif Scan | Motif List | QMSCal | Matrices | Algorithm | Help

Welcome to ToxinPred

ToxinPred is an *in silico* method, which is developed to predict and design toxic/non-toxic peptides. The main dataset used in this method consists of 1805 toxic peptides (<=35 residues).



Major Features include:

(1) **Desing Peptide:** This module allows user to generate all possible single mutant analogs of their peptides and predict whether the analog is toxic or not.

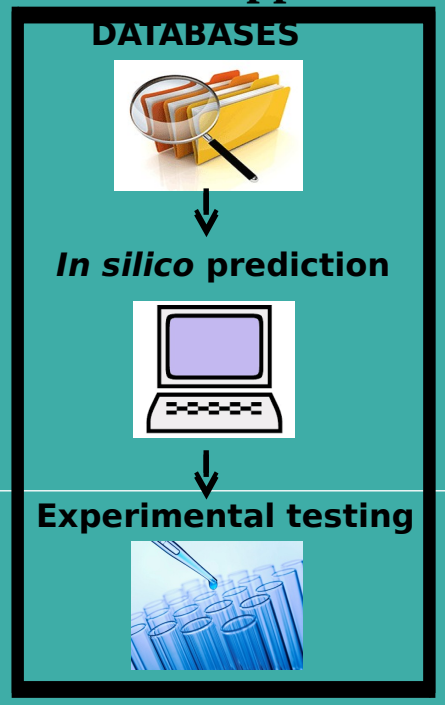
(2) **Batch Submission:** This module of ToxinPred allows user to predict number of toxic peptides submitted by the user.

(3) **Protein Scanning:** This module generates all possible overlapping peptides and their single mutant analogs of protein submitted by the user. It also predicts whether overlapping peptide/analog is toxic or not.

(4) **QMS Calculator:** This tool allows the users to submit query peptide in FASTA format and to optimize the peptide sequence to get maximum/minimum/desired toxicity based upon the Quantitative Matrix based position specific scores. It will help the user to tweak any residue from the predecessor peptide to attain the analog with desired property (highest/lowest toxicity).

Cell-Penetrating Peptide for Drug Delivery

Overall Approach



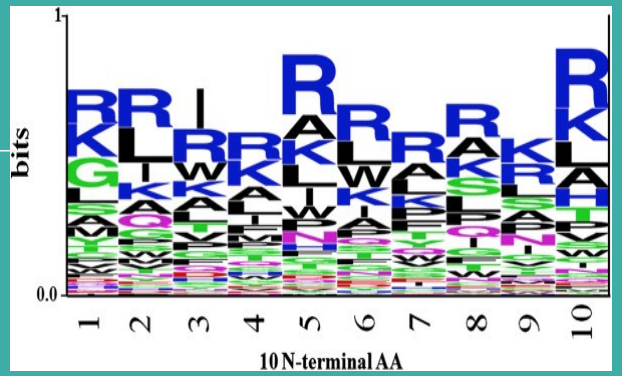
CPPs Collection and Compilation

CPPsite1 (Database (Oxford). 2012; 2012:bas015)

CPPsite2 (Nucleic Acids Res. 2016; 44(D1):D1098-103)

CPP Prediction tool: CellPPD

(J Transl Med. 2013 Mar 22;11:74)

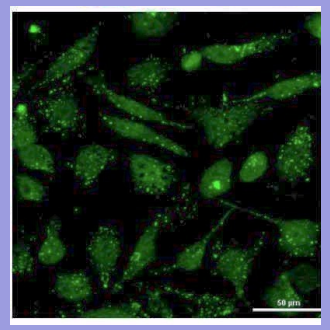


Virtual Screening

IMT-P8 (Patented*)

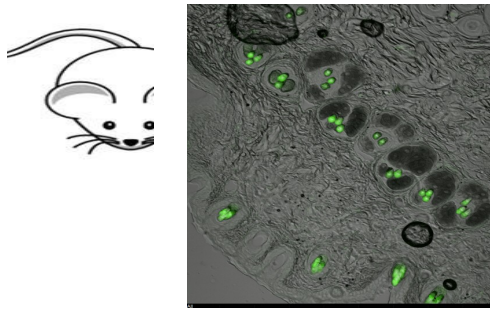
Experimental Validation

Delivery in Cancer Cells



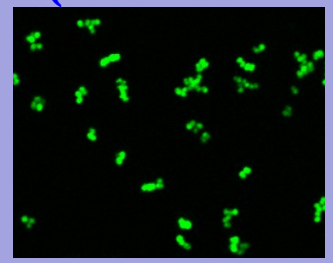
Eur J Pharm Biopharm. 2015;89:93-106

Topical Delivery in Mouse Skin



Scientific Reports 2016

Overcome drug resistance in MRSA (combination therapy)



Appl Microbiol Biotechnol. 2016;(9):4073-83

*Cell Penetrating Peptide for Biomolecule Delivery. (APPL NO. 3380DEL2013)

GPSR

A resource for genomics, proteomics and systems biology

Integration of Computer Programs Developed at

GPS Raghava's Group

Bioinformatics Centre,
Institute of Microbial Technology, Chandigarh

OSDDLinux : A Platform for Open Source Drug Discovery

Introduction

OSDD-Linux integrates open source softwares, libraries , workflows and webservices for creating environment for drug discovery. First attempt made to customize linux to provide services to community of drug discovery. OSDD-Linux may bring down cost as well as increase speed of drug discovery.

Features

- A single platform for bioinformatics and cheminformatics.

- Tools available in three formats e.g. webservers, standalone and galaxy.

Webserver

A separate apache runs all web-servers as local host in the OSDD-Linux CD.

Standalone

Command line tools have been integrated for analysing large scale data.

Softwares

GPSR packages , webservers, standalone, galaxy versions of tools developed in Dr.Rahghava's lab along with third party softwares like rasmol, pymol are integrated

Features

- User can **customize** according to need.
- Easy to install and free of cost.
- It can be launched using LiveCD, Liive server, USB and virttualldesk top like virtualbox.
- Provides source codes for various tools.

third party softwares

Open source softwares used in bioinformatics and cheminformatics have been integrated.

Galaxy

All softwares are integrated in galaxy servers for making the workflows.

System Requirements

The user may use OSDDLinux from portable devices like CD/DVD, USB drive etc or install on local machine or virtual machine depending upon requirement.

Future directions

More webservices, modules, debian packages will be updated on regular basis.

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OSDD LINUX

A Custo
fo

http://osddlinux.osdd.net/

- General Inoformation
- Software Packages
- Install/Download
- Service to Community
- OSDDlinux Online
- Important Resources

Install/Download

- Live DVD/USB
- Full Installation
- Virtual Box
- On existing machine
- Package Repository
- Upgrade/New Packages

General Inoformation

- Major Features
- Installation Guide
- Users Guide
- Drug Discovery manual
- GPSR manual
- Required Package
- List of Packages

Service to Community

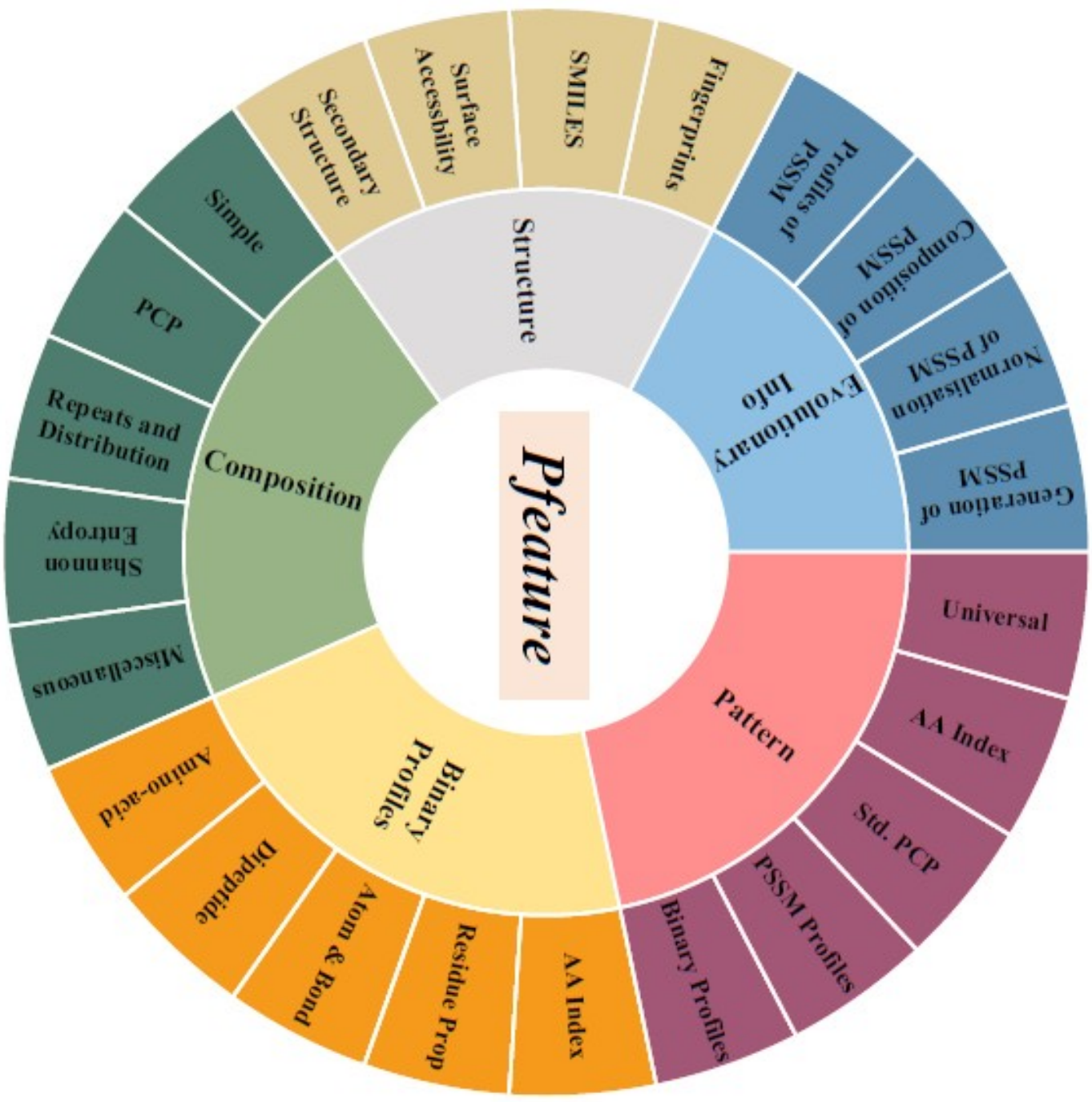
- Command Mode
- Web Services
- Galaxy Portal
- GUI-based Software

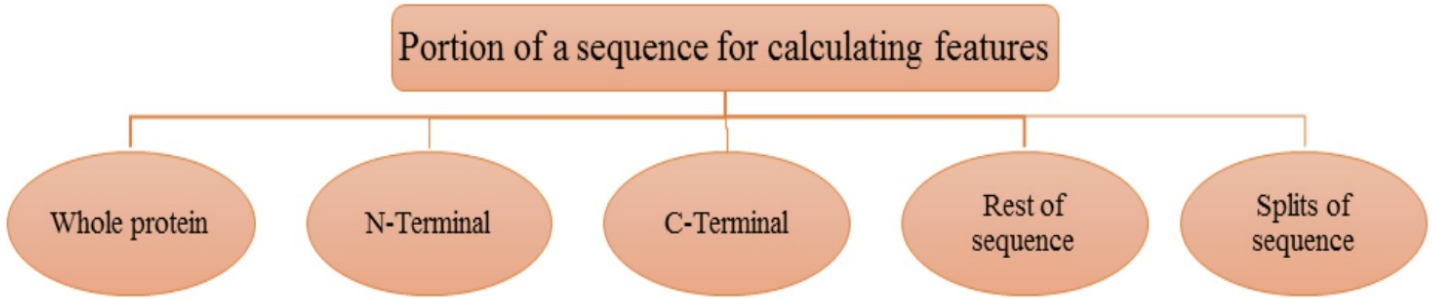
Software Packages

- Bioinformatics
- Vaccine Informatics
- Drug Informatics
- Biotherapeutics
- Analysis of NGS data
- Education & Research
- Basic Scripts

Pfeature: A web server for computing features of proteins and peptides

http://webs.iiitd.edu.in/raghava/pfeature/





Types of Protein/ Peptide Feature Generation

Composition

Simple
Physico-Chemical Prop.
Repeats & Distribution
Shannon Entropy
Miscellaneous

Binary Profiles

Amino Acids
Dipeptides
Atom & Bond
Residue Properties
AA Index

Evolutionary Information

Generation of PSSM
Normalization of PSSM
Composition of PSSM
Profile of PSSM

Structure

Fingerprints
SMILES
Surface Accessibility
Secondary Structure

Pattern

Binary Profiles
PSSM Profile
Standard Physico-Chemical Properties
AA Index
Universal

Simple
Amino acid
Dipeptide
Tripeptide
Atom & Bond

Physico-chemical prop.
Standard
AA Index
Advanced
Structural

Repeats & Distribution
Residue Repeats
Property Repeats
Distance distribution of Residues

Shannon entropy
Protein level
Residue level
Properties

Miscellaneous
Autocorrelation
Conjoint Triad Descriptors (CTD)
Composition enhanced Transition and Distribution (CeTD)
Pseudo Amino Acid Composition (PseAAC)
Amphiphilic Pseudo Amino Acid Composition (A PseAAC)
Quasi-Sequence Order (QSO)
Sequence Order Coupling Number (SOCN)

https://webs.iiitd.edu.in/gpsrdocker/

GPSRdocker

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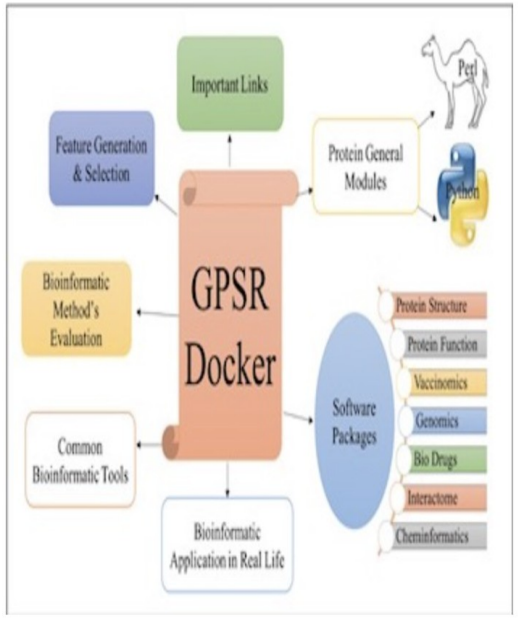
RAGHAVA GROUP

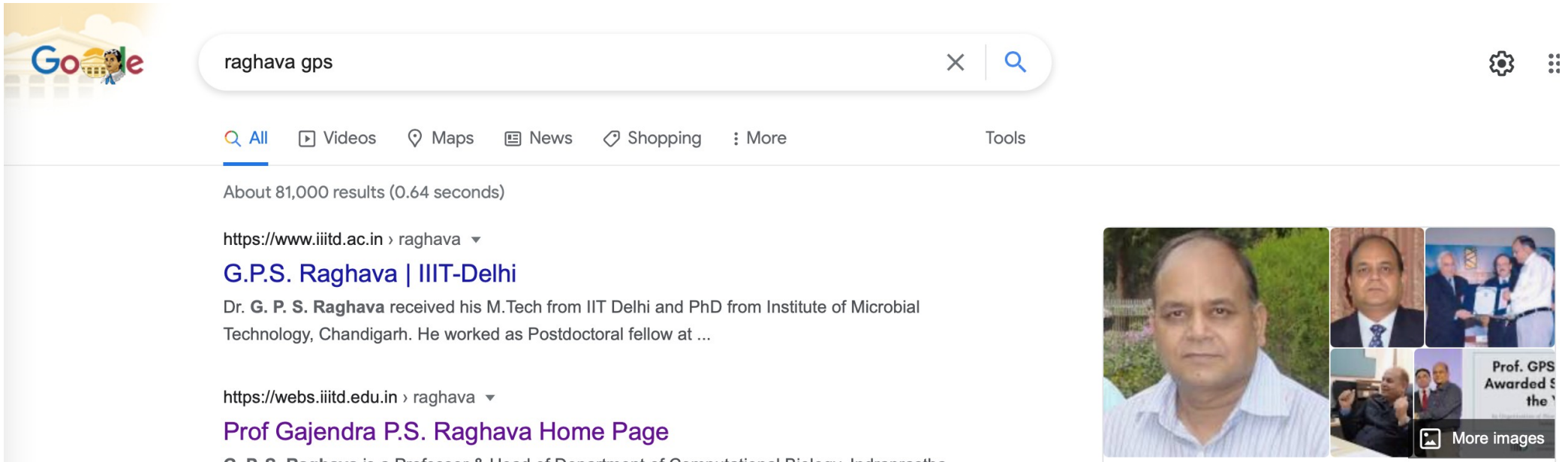


DOWNLOAD GPSRDOCKER MANUAL

Welcome to GPSRdocker *A resource for Genomics, Proteomics and Systems biology*

GPSRdocker is a docker-based container that provides a resources on Genomics, Proteomics and System Biology. In last two decades Prof G. P. S. Raghava group developed more than 200 web-based services, which are heavily used by scientific community. There are number of challenges in utilizing full potential of these services that includes; i) Internet speed, ii) limits on computing power, and iii) security of data. Thus, user needs standlone version of these web-based services, so they can run these services on their local machines. In past group has made attempt to fullfill requirement of users by providing perl script of routine program (GPSR) and customize or virtualize operating system (OSDDlinux). GPSRdocker is another attempt to provide standalone version corresponding to web services at our group. GPSRdocker, is based on docker suite where customized container of all our webservers are available.

Thank You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Maps
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More
Tools
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Dr. G. P. S. Raghava received his M.Tech from IIT Delhi and PhD from Institute of Microbial Technology, Chandigarh. He worked as Postdoctoral fellow at ...
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Prof Gajendra P.S. Raghava Home Page
G. P. S. Raghava is a Professor & Head of Department of Computational Biology, Indraprastha Institute of Information Technology (IIIT-Delhi)
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S Gupta, P Kapoor, K Chaudhary, A Gautam, R Kumar, GPS Raghava, ... PloS one 8 (9), e73957, 2013. 446, 2013. ProPred1: prediction of promiscuous MHC Class-I ...
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G P S Raghava receiving National Bioscience Award from Science and ...
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Gajendra Pal Singh Raghava
Gajendra Pal Singh Raghava is an Indian bio-informatician and head of computational biology at the Indraprastha Institute of Information Technology. Wikipedia
Born: 25 May 1963 (age 58 years), Bulandshahr
Institutions: Indraprastha Institute of Information Technology
Awards: Shanti Swarup Bhatnagar Prize for Science and Technology (2008), MORE