Computer-aided Healthcare

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ADVANCED REVIEW

WIREs DATA MINING AND KNOWLEDGE DISCOVERY

WILEY

Computational resources in healthcare

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Abstract

Healthcare is the most important component in the life of all human beings as each individual wish to have happy, healthy, and wealthy life-span. Most of the branches of science are dedicated to improve the healthcare. In the era of knowledge mining, informatics is playing a crucial role in different branches of research. Thus, a wide range of informatics-based fields have emerged in the last three decades that include medical informatics, bioinformatics, cheminformatics, pharmacoinformatics, immunoinformatics, and clinical informatics. In the past, a number of reviews have been focused on the application of an informatics-based field in the healthcare. In this review, an attempt is

HOME | GENOMICS | PROTEOMICS | DRUG INFO | MEDINFO | VACCINFO | RESOURCES (A-Z) | CONTACT US

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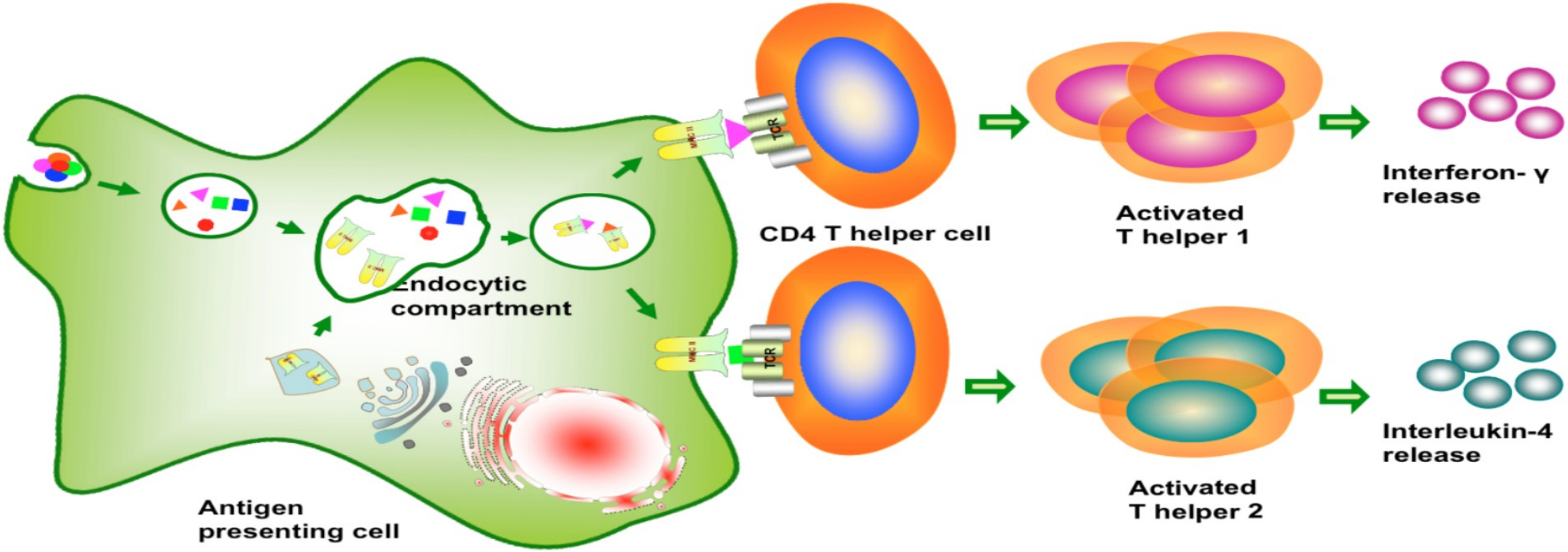

(2021) Computational resources in healthcare. WIREs: Data Mining and Knowledge Discovery, e1437

PHI: PORTAL FOR HEALTH INFORMATICS

Genomics

This section list compuational tools and web server in the field of genomics. This includes genome annotation, genome-based medicine, Cancer genomics and genome based biomarkers.

Annotations

This section host servers that is important for annotating genome (or nucleotide) sequences (directly or indirectly). These tools cover wide range of applications that includes; i) genome wide similarity search, ii) repeats in nucleotide sequence, iii) identification of protein coding regions or genes, iv) classification of RNA families and v) designing siRNA and miRNA.

Cancer Genomics

One of major challenges in handling cancer is to annotate big data in the the field of cancer genomics. Aim of this module is to provide in silico solutions for cancer biologists. This page manitain tools and databases developed in the field of cancer informatics, it includes; i) drug resistance databases, ii) genome based cancer biomarkers (e.g., stage classification), iii) epitope-based vaccines, iv) databases.

Genome Medicine

Personalised medicine is a new concept in the field of drug or vaccine design. In this module our focus is to utilise genomic or genetic information for designing medicine against disease like cancer, tuberculosis. This page maintain wide range of computational resources, like i) prioritization of drugs based on genomic information, ii) personalised vaccine agains cancer, iii) strain-specific vaccines

Genome Biomarkers

One of the major challenges in the field oh health sciences is to design genome based biomarkers, as these biomarkers are more sensitive and accurate than traditional tests. Here, aim is to develop computational tools to predict wide range of biomrakers from genomic information. These resources can be classified in following categories; i) disease identification, ii) disease progression, iii) drug biomarkers.

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Proteomics

This section provides services related to proteomics that includes mainly annotation of proteins and peptides.

Protein Function

How to assign function of a newly sequenced protein is a most important task for bioinformaticians. In this module, we list servers important for assigning function of proteins from its amino acid sequence. Broadly, these servers can be divided in following categories; i) subcellular localisation ii) identification of specific class of proteins, iii) functional annotation.

Structural Proteomics

Broadly structure of protein is responsible for its function, thus structural annotation is one of major challenges in the field of computational biology. This page list of wide range of web server that includes servers for predicting i) tertiary structure, ii) secondary structure, iii) super secondary structure, iii) surface accessibility and iv) residue-residue contact in a protein.

Molecular Interactions

Personalised medicine is a new concept in the field of drug or vaccine design. In this module our focus is to utilise genomic or genetic information for designing medicine against disease like cancer, tuberculosis. This page maintain wide range of computational resources, like i) prioritization of drugs based on genomic information, ii) personalised vaccine agains

Peptide Informatics

In the last few decades, based drug designing ha choice of most of the s world wide because of toxicity and high specifici page resources developed group for predicting f peptide properties; i) delivery, ii) epitope-based iii) antibacterial, iv) toxi stability in body fluids structural features.

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Drug Informatics

Drug informatics cover wide range of tools, we grouped these tools based on their function.

Drug Targets

Identification of drug targets in human (for disorder related disease, like cancer) and targets in pathogen (for pathogen associated disease) is crucial for designing medicine. In past, large number of in silico tools have been developed for identification of drug targets, following are major types; i) prediction of receptors (e.g., GPCR), ii) cytokines, iii) enzymes

Molecular Docking

After identification of drug target, next challenge is to design drug or inhibitor against target. Molecular docking is not only important for designing drug against a target but also required for predicting binding between molecules. This page provides list of computational resources developed for molecular docking particularly for predicting inhibitors against drug targets.

Bio-Therapeutics

In the era of drug-resistance, peptides are alternate to small-molecules based drugs. Peptides have wide-range of properties (like cell-penetration, tumour homing, antihypertensive, antibacterial, anticancer) that is used by researchers for designing peptide-based therapeutics. This page provides web servers developed for designing therapeutics based

Chem/Pharma-Informatics

How to bring down cost of drug discovery is one of the major challenges to develop affordable drugs. Most of exiting drug discovery software are commercial, most of researchers can not afford these software. In order to provide alternate to commercial software, our group have developed number of open source software in the filed of

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Medical Informatics

Personalized Medicine

Every living organism have unique genetic features, thus personalised medicine based on genetic features may be more useful than generalised medicine. Numerous computational resources have been developed in group that can be used for designing person-specific or disease causing pathogen-specific medicines. These resources may facilitate: i)

Disease Biomarkers

It is well known fact that treating a disease is easy if we are able to detect it in early phase. In order to develop sensitive biomarkers, it is important to utilise genetic information. This page contains servers which will be helpful in designing biomarkers for different diseases. These servers can be used to differentiate between cancer and normal patients,

Clinical Informatics

Clinical informatics or health care informatics or health informatics plays an important role in provide all information required for improving quality of life. This page will provide servers and software important for clinicians.

Disease Forecasting

It contains servers which will be able to assist in the forecasting of a particular plant or animal disease based on the properties of the analysis of curated data. These will be useful to prevent and mitigate and control the spread of disease.

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Vaccine Informatics

Epitope (B cell & T-cell)

There is a tremendous change in strategy of designing vaccines, it is moving from minimisation to micro-minimization (whole pathogen to antigen to antigenic peptides). This server list severs developed for predicting compete path of antigen processing (endogenous & exogenous). It include methods for predicting; i) MHC or HLA binders, ii) helper T-cell epitopes, iii) CTL epitopes, iv) TAP binders.

Cytokine-specific Epitopes

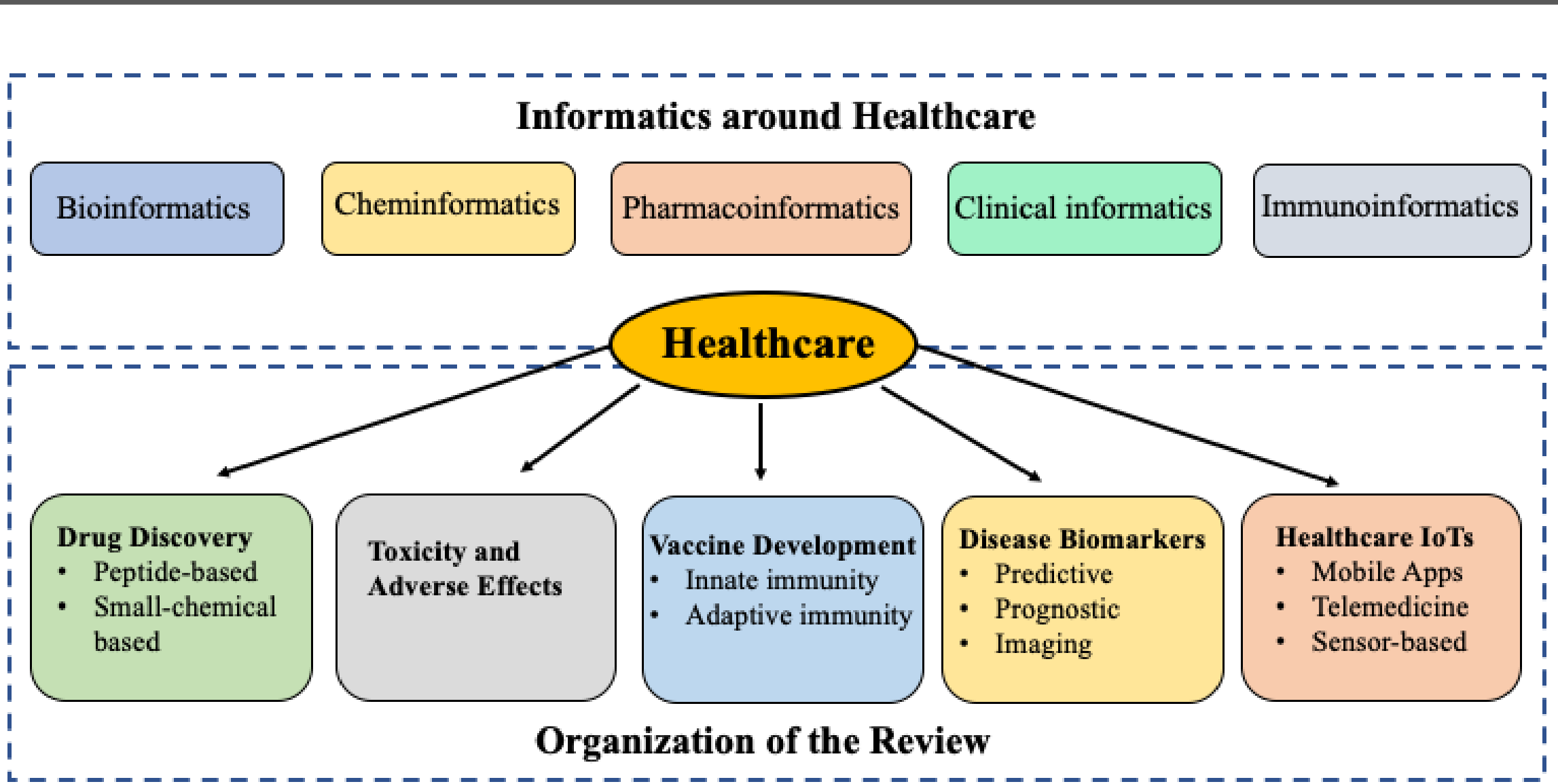
Numerous software have been developed in the filed of immunoinformatics in last two decades. In initial phase,researchers focused on prediction of peptides that can activate B- or T-cells. Recently, researcher are developing methods for predicting peptides that can activate specific class of interleukins or cytokines. This page provides link to these servers, they will be very useful in

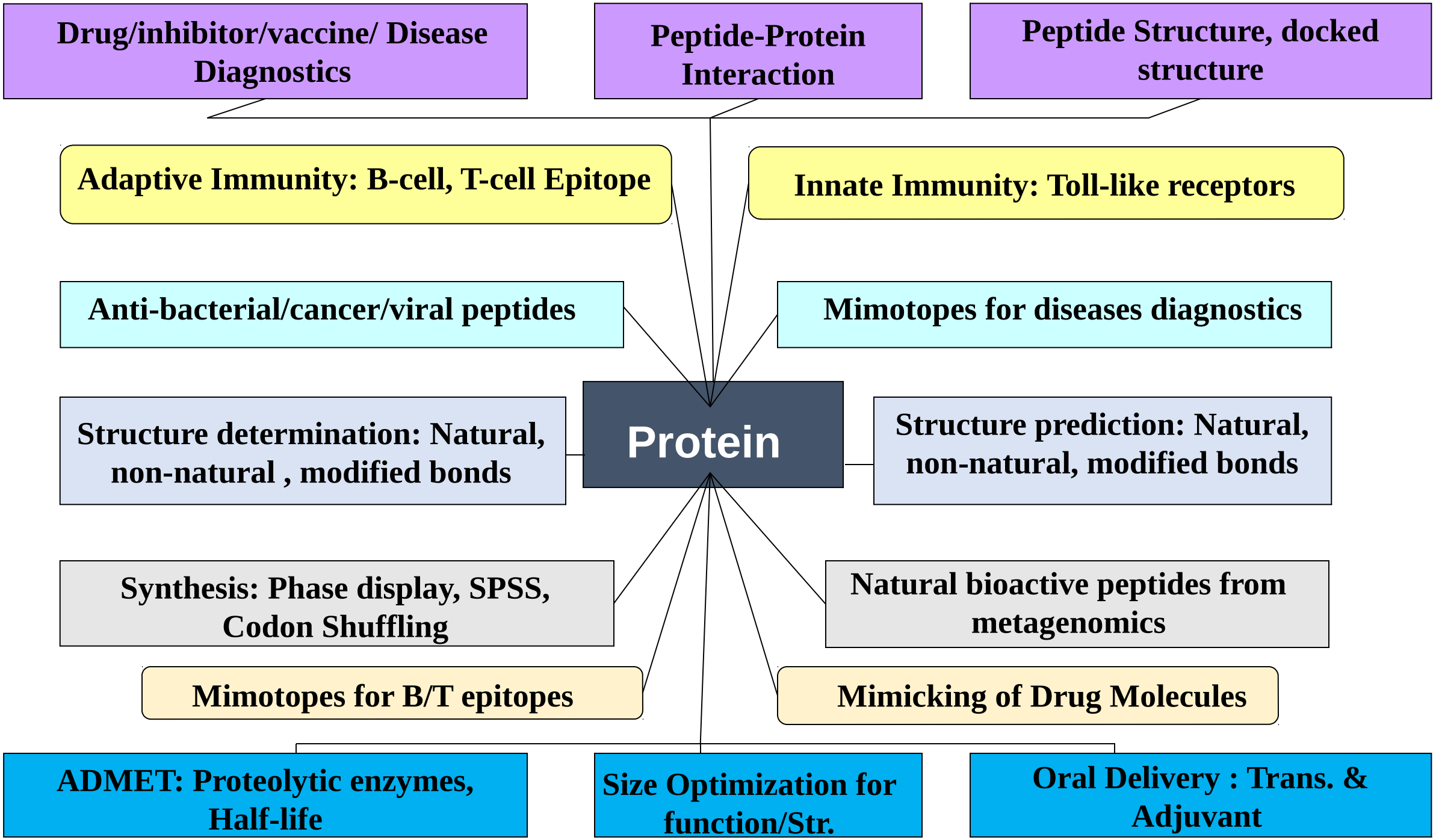
Vaccine Adjuvants

Both arms of immune system (innate and adaptive), plays an important role in protection and elimination of a disease. Most of tools developed in past address problems associated with adaptive immune system. In addition to adaptive immune system our group also developed computational tools to predict biomolecules that can activate innate immunity. These tools can be used to design vaccine

Personalized Vaccine

Despite tremendous advances in science, researches failed to develop vaccine against number of diseases (like cancer, tuberculosis and HIV) as they try to design one vaccine against one disease without considering genomic variation in host/human and in disease-associated pathogens. In order to overcome this problem, our group have developed number of computational resources for designing personalised or strain-


Informatics around Healthcare
Bioinformatics
Cheminformatics
Pharmacoinformatics
Clinical informatics
Immunoinformatics
Healthcare
Drug Discovery
• Peptide-based
• Small-chemical based
Toxicity and Adverse Effects
Vaccine Development
• Innate immunity
• Adaptive immunity
Disease Biomarkers
• Predictive
• Prognostic
• Imaging
Healthcare IoTs
• Mobile Apps
• Telemedicine
• Sensor-based
Organization of the Review


Drug/inhibitor/vaccine/ Disease Diagnostics
Peptide-Protein Interaction
Peptide Structure, docked structure
Adaptive Immunity: B-cell, T-cell Epitope
Innate Immunity: Toll-like receptors
Anti-bacterial/cancer/viral peptides
Mimotopes for diseases diagnostics
Structure determination: Natural, non-natural , modified bonds
Protein
Structure prediction: Natural, non-natural, modified bonds
Synthesis: Phase display, SPSS, Codon Shuffling
Natural bioactive peptides from metagenomics
Mimotopes for B/T epitopes
Mimicking of Drug Molecules
ADMET: Proteolytic enzymes, Half-life
Size Optimization for function/Str.
Oral Delivery : Trans. & Adjuvant

THPdb

A database of FDA approved therapeutic peptides and proteins

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

Welcome to Home Page of THPdb

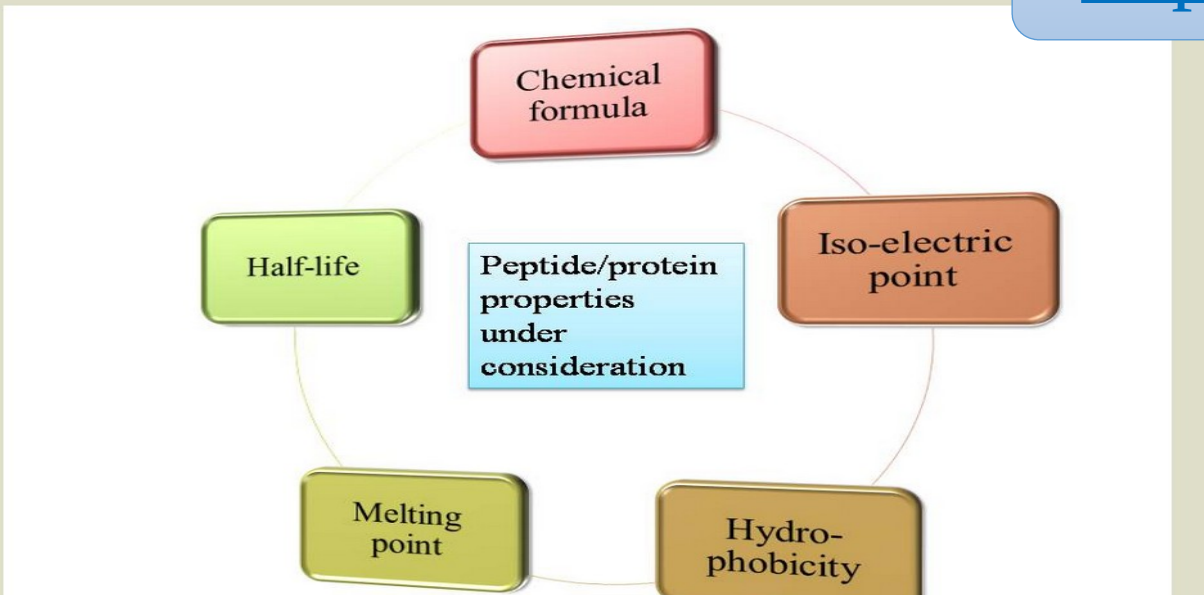
Therapeutic Proteins

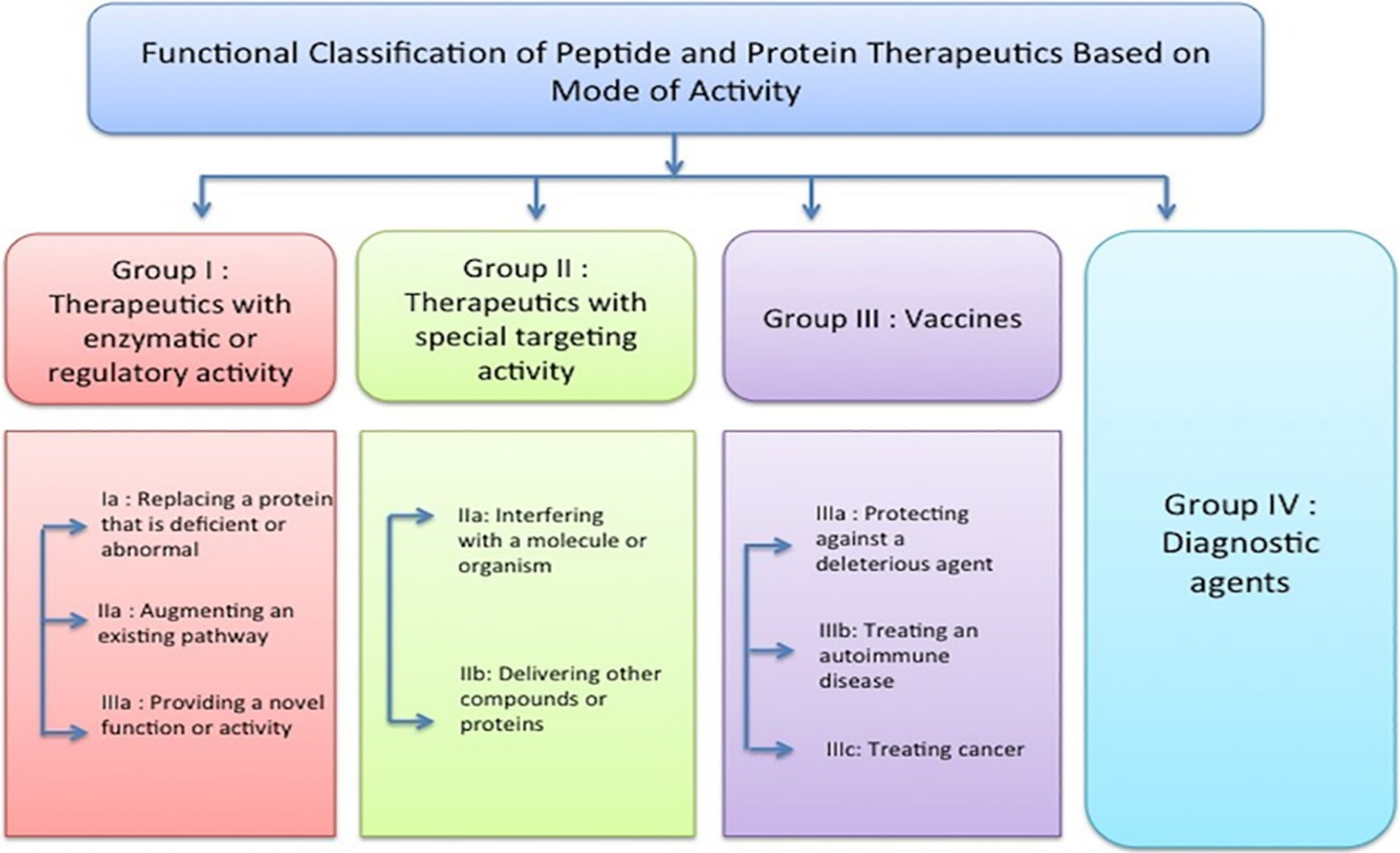
On therapeutic prespective, there is tremendous opportunity in terms of harnessing protein therapeutics to alleviate disease. Once a rarely used subset of medical treatments, protein therapeutics have increased dramatically in number and frequency of use since the introduction of the first recombinant 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/



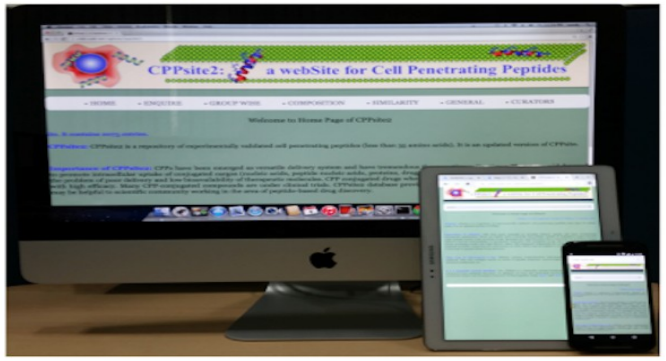

Functional Classification of Peptide and Protein Therapeutics Based on Mode of Activity
Group I : Therapeutics with enzymatic or regulatory activity
Group II : Therapeutics with special targeting activity
Group III : Vaccines
Group IV : Diagnostic agents
Ia : Replacing a protein that is deficient or 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

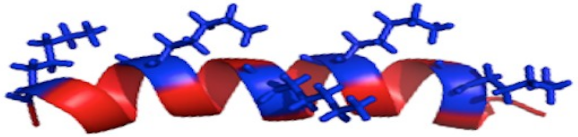
Drug Delivery

Research articles

Patents

Responsive website
(compatible for desktop, smartphone and tablets)





CPPsite 2.0

Entries Peptides
1855 1700

Major Tools

- **Search** — Keyword, Complex, SMILES
- **Browse** — Chirality, Modifications, Nature, Cargo types
- **Analysis** — BAST, Smith-waterman, Structure similarity

Peptide Types

L	D	Mix
1564	63	32

Linear	Cyclic
1753	102

Major Fields

- Chirality
- Localization
- Chem. modification
- Uptake efficiency
- Uptake mechanism
- In vitro/ in vivo
- Cargo types

Structure Annotation

3D-Structures	Number
PDB	58
I-TASSER	89
PEPstrMOD	1415
Total	1562

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

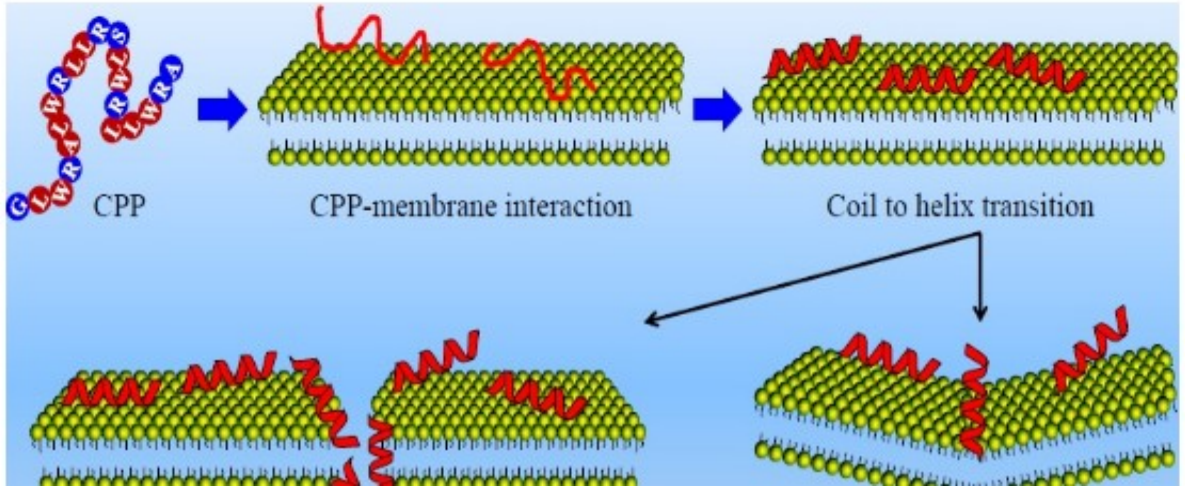
utam *et al.*: *In silico* approaches for designing highly effective cell penetrating peptides. *Journal of Translational Medicine* 3 11:74.Link

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

TopicalPdb

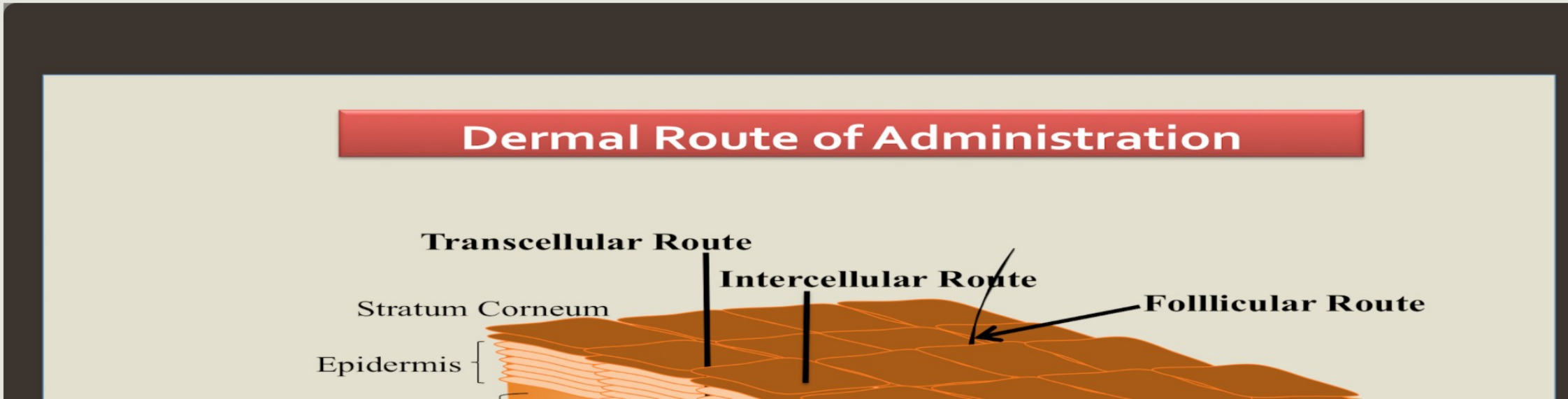
TOPICALLY DELIVERED PEPTIDE DATABASE

HOME | QUERY | EXPLORE | ANALYZE | MISCELLANEOUS | TEAM

Welcome to TopicalPdb

=== Mathur et al., (2018) TopicalPdb: A database of topically delivered peptides. PLoS One. 2018 Feb 12;13(2):e0190134 ===

TopicalPdb: Database of Topically Administered Peptide. It contains 657 peptide entries alongwith their secondary & tertiary structure. This database maintains experimentally validated peptides that are topically and non-invasively administered via transdermal, occular and nasal routes.



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.

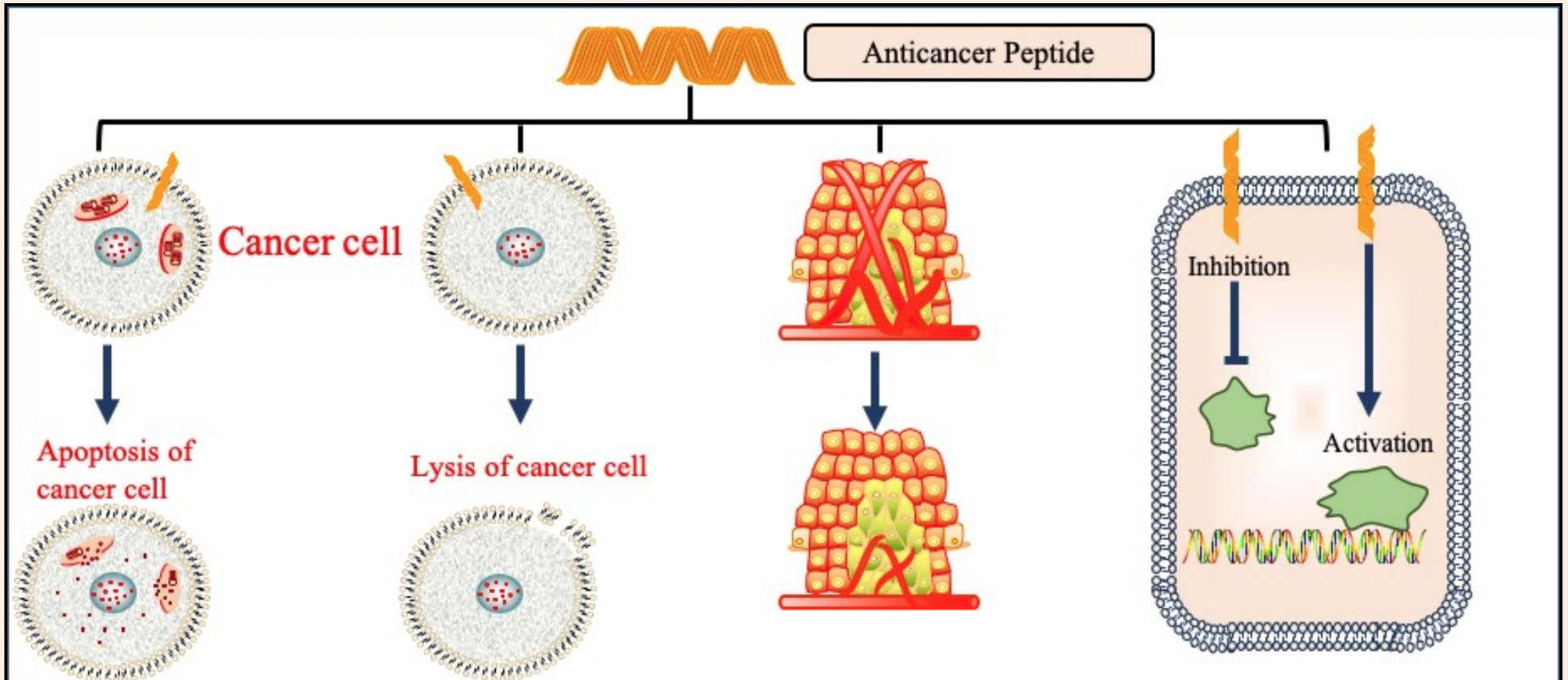
Developed by: Bioinformatics Centre, Institute of Microbial Technology, Sec-39A, Chandigarh,

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

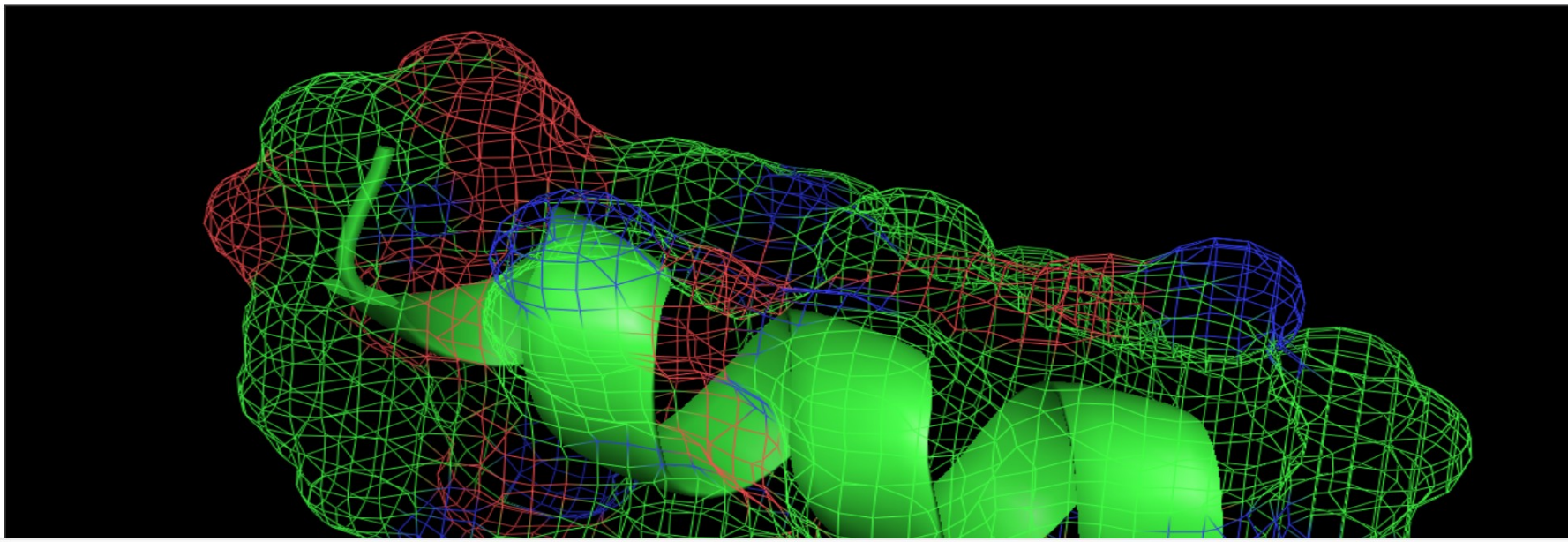
ANTIHYPERTENSIVE PEPTIDE INHIBITORS

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 based Inhibitors

AntiBP2 : Server for antibacterial peptide prediction

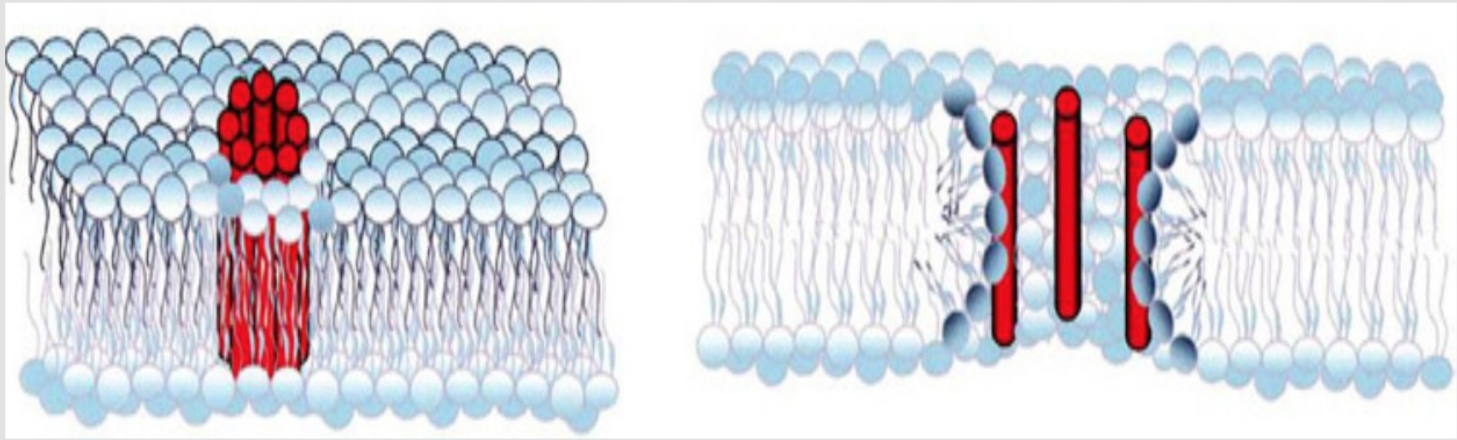
- Home
- Algorithm
- Submission
- Help
- Team
- Contact

Antibp : Our previous version for the prediction of antibacterial peptides for given protein sequence.

Sneh Lata, B K Sharma, GPS Raghava. **Analysis and prediction of antibacterial peptides. *BMC Bioinformatics* 2007,8:263**

About AntiBP2

Antibacterial peptides are important components of innate immune system, used by the host to protect itself from different types of pathogenic bacteria. Antimicrobial peptides have broad spectrum of activity against bacteria, fungai, viruses and even cancer cells.



AntiBP2 server predicts the antibacterial peptides in a protein sequence. Prediction can be done by using Support Vector Machine (SVM) based method using coposition of peptide sequences and overall accuracy of this server is ~92.14%. This server can also predict the source of these antibacterial peptides with ~98.52% accuracy. If the source of these antibacterial peptides are insect, frog or mammal then it gives the information of its family also. This server can help in finding and designing of peptides based antibiotics.

If You are using this server, please site:
Lata, S., Mishra, N.K. and Raghava, G. P. S. (2009) AntiBP2: Improved version of antibacterial peptide prediction. **BMC Bioinformatics 11:S19** .

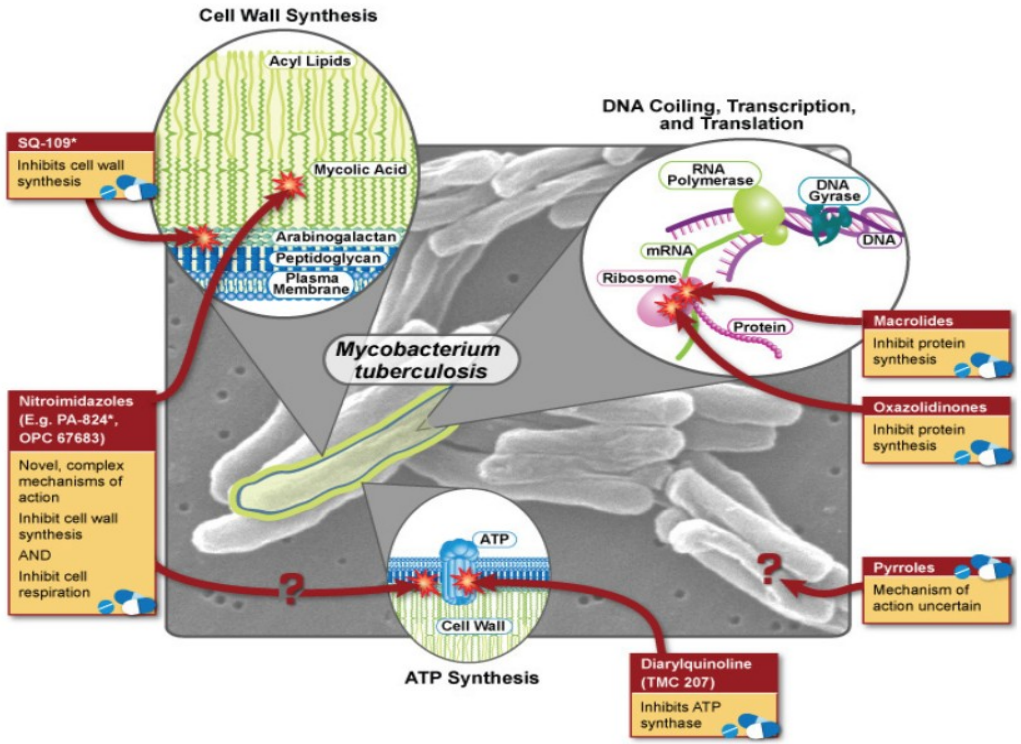
Peptide based Inhibitors

AntiTbPred: Prediction of antitubercular peptides

Home | Predict | Design | Protein Scan | Downloads | Help | Developers | Contact

Welcome to AntiTbPred

eference: Usmani S.S., Bhalla S. and Raghava, G.P.S. (2018) Prediction of Antitubercular Peptides From Sequence Information Using Ensemble Classifier and Hybrid Features Front. F



Source: NIAID

In past number of methods have been developed to predict antimicrobial or antibacterial activity of a peptide. But an common antibectreial peptide will also have bactericidal activity against Mycobacterium, is not so sure. Our analysis reveals amino acid compositional differences as well as prefernce of certain specific residues in anti-tubercular peptides than common antibacterial and non-antibactreial peptides.

This webserver is designed to predict peptides having effective bactreicidal activity against Mycobacteruium species. These peptides are commonly known as antitubercular or antimycobacterial peptides.

Peptide Stability

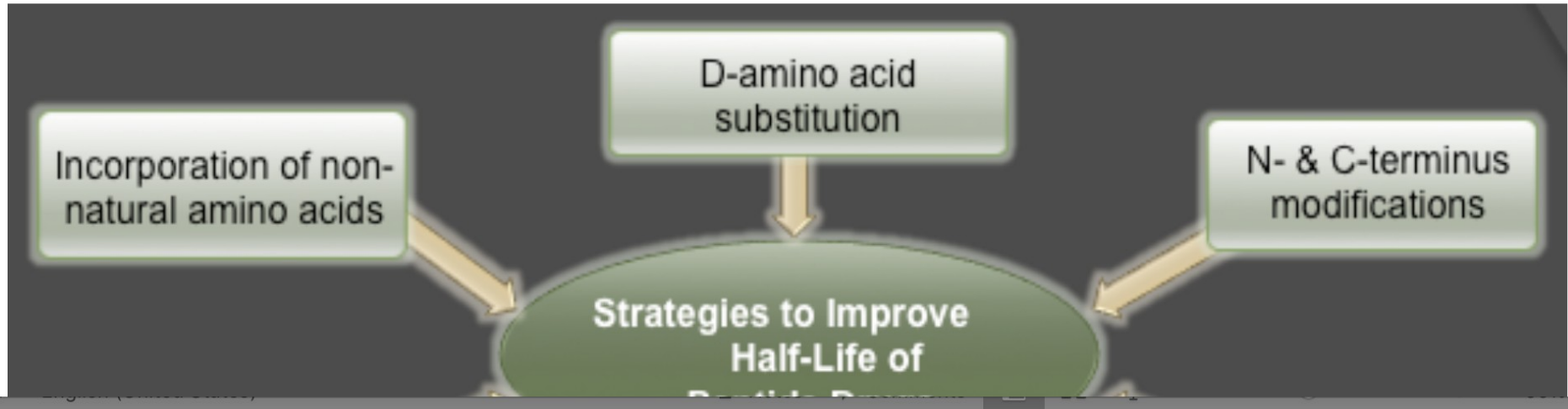
PEPlife

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



CellPPD-MOD Modified Cell Penetrating Peptides Prediction Server

Welcome to CellPPD-Mod

CellPPD-Mod is an in silico method, which is developed to predict efficient modified cell penetrating peptides (CellPPD-Mods). The main dataset used in this method consists of 732 experimentally validated Modified CPPs as well as Non-CPPs.

Major Features include:

(1) Prediction: This module is the main module which allows user to predict whether a given modified peptide is CPP or non-CPP.This module accept the pdb file as input file. User can provide its own structure or we will advice user to predict the structure using PepStrMOD.

(2) Subsidiary Module: We have also provided the provision of predicting CPP or non-CPP using peptide sequence. Link of this page is provided in our main prediction module.

(3) Mutational Series: We have also provided the provision of generating analogs of submitted peptide and its prediction as CPP or non-CPP. Link of this page is provided in our main prediction module.

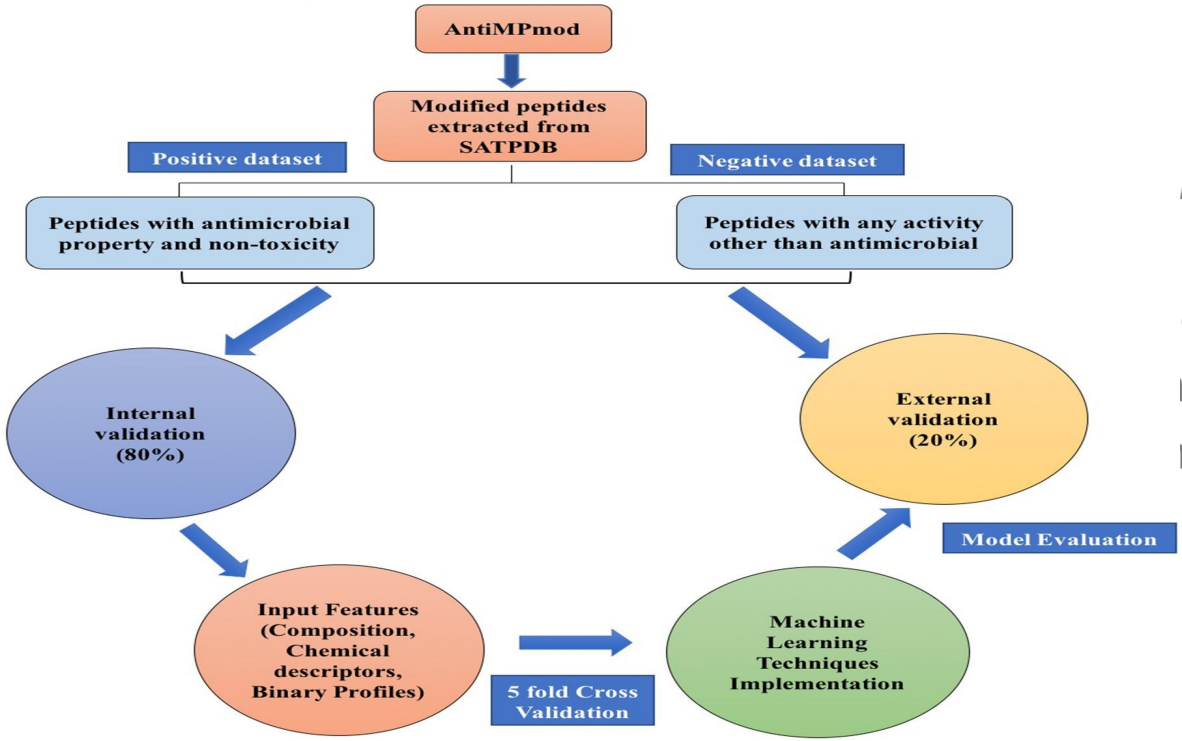
(4) Download: This module of CellPPD-Mod allows user to download the dataset used in this study.

Peptide based Inhibitors

AntiMPmod

Modified Antimicrobial Peptides Prediction Server

Home Prediction Download Help Team Contact



Welcome To AntiMPmod

in silico method, which is developed to predict
antimicrobial peptides (ModAMP). The main dataset
od consists of 948 modified AMPs and 931 non-
taset was divided into two parts (i) Training dataset
dataset.

Structure of Chemically Modified Peptides

- Home PEPstrMOD
- Natural Peptides
- D Amino Acids
- Terminal Modification
- Peptide Cyclization
  - N-C Cyclization
  - Disulfide Bridge (S-S)
  - Structure Modification
- Non-Natural Residue
- PTMs of Residue
- Advance Modification
- Structure Simulations
- Download
- General

Welcome to Peptide Cyclization Module for N-C cyclization

This page is designed to predict the peptide structure with N-to-C terminal cyclization. The peptide is made cyclic by incorporating a bond between Nitrogen atom of N-terminal residue and Carbon atom of C-terminal residue. For more information click help

Peptide Sequence Submission Form

Peptide sequence in plain text format Example Sequence

Email Address:

Advanced Options: CLICK

Reset or clear form Submit sequence for prediction

Review > Adv Protein Chem Struct Biol. 2018;112:221-263. doi: 10.1016/bs.apcsb.2018.01.006.
Epub 2018 Mar 5.

In Silico Tools and Databases for Designing Peptide-Based Vaccine and Drugs

Salman Sadullah Usmani [1], Rajesh Kumar [1], Sherry Bhalla [2], Vinod Kumar [1], Gajendra P S Raghava [3]

Affiliations + expand

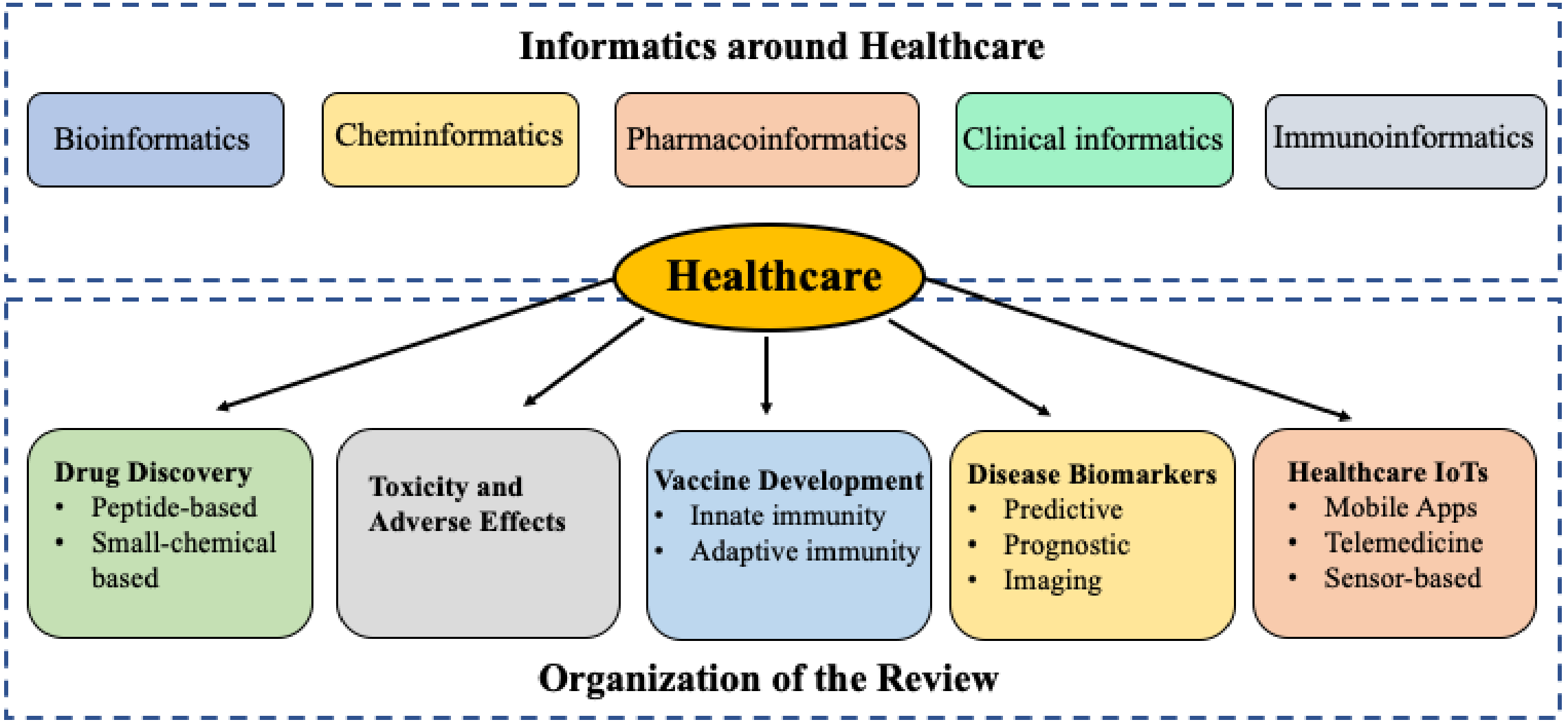
PMID: 29680238 DOI: 10.1016/bs.apcsb.2018.01.006

Abstract

The prolonged conventional approaches of drug screening and vaccine designing prerequisite patience, vigorous effort, outrageous cost as well as additional manpower. Screening and experimentally validating thousands of molecules for a specific therapeutic property never proved to be an easy task. Similarly, traditional way of vaccination includes administration of either whole

Peptide based

Tool	Description (Link)
AniAMPpred	Prediction of antimicrobial peptides in animal kingdom (https://aniamppred.anvil.app/)
B3Pdb	Compilation of Blood Brain Barrier Penetrating Peptides (https://webs.iiitd.edu.in/raghava/b3pdb/)
B3Pred	Blood-Brain Barrier penetrating peptides prediction (https://webs.iiitd.edu.in/raghava/b3pred/)
AlgPred 2.0	Highly accurate method for predicting allergic proteins (https://webs.iiitd.edu.in/raghava/algpred2 /)
AntiCP 2.0	Improved method for identification of anticancer peptides (https://webs.iiitd.edu.in/raghava/anticp2/)
HemoPI-MOD	Hemolytic potency of chemically modified peptides (https://webs.iiitd.edu.in/raghava/hemopimod/)
Antifp	Prediction of antifungal peptides (https://webs.iiitd.edu.in/raghava/antifp/)
AntiMPmod	Antimicrobial potential of chemically modified peptides (https://webs.iiitd.edu.in/raghava/antimpmod/)
AntiTbPred	Prediction of antitubercular peptides (https://webs.iiitd.edu.in/raghava/antitbpred/)
CellPPD-MOD	Computation of chemically modified cell penetrating peptides (https://webs.iiitd.edu.in/raghava/cellppdmod/)
PlifePred	Estimation of half-life of peptides in blood (https://webs.iiitd.edu.in/raghava/plifepred/)
TopicalPdb	Repository of topically delivered peptides (https://webs.iiitd.edu.in/raghava/topicalpdb/)
THPdb	Compilation of peptide/protein based therapeutic molecules (https://webs.iiitd.edu.in/raghava/thpdb/)
CPPSite2	Database of cell-penetrating peptides (https://webs.iiitd.edu.in/raghava/cppsite/)
AHTpin	Designing antihypertensive peptides (https://webs.iiitd.edu.in/raghava/ahtpin/)
AntiAngioPred	Prediction of anti-angiogenic peptides (http://clri.res.in/subramanian/tools/antiangiopred/)
CancerPPD	Database of anticancer peptides and proteins (https://webs.iiitd.edu.in/raghava/cancerppd/)


Informatics around Healthcare
Bioinformatics
Cheminformatics
Pharmacoinformatics
Clinical informatics
Immunoinformatics
Healthcare
Drug Discovery
• Peptide-based
• Small-chemical based
Toxicity and Adverse Effects
Vaccine Development
• Innate immunity
• Adaptive immunity
Disease Biomarkers
• Predictive
• Prognostic
• Imaging
Healthcare IoTs
• Mobile Apps
• Telemedicine
• Sensor-based
Organization of the Review

Drug Discovery and Design

- **Plants or Natural Product**
  - Plant and Natural products were source for medical substance
  - Example: foxglove used to treat congestive heart failure
  - Foxglove contain digitalis and cardiotonic glycoside
  - Identification of active component
- **Accidental Observations**
  - Penicillin is one good example
  - Alexander Fleming observed the effect of mold
  - Mold(Penicillium) produce substance penicillin
  - Discovery of penicillin lead to large scale screening
  - Soil micoorganism were grown and tested
  - Streptomycin, neomycin, gentamicin, tetracyclines etc.

Drug Discovery and Design

- **Chemical Modification of Known Drugs**
  - Drug improvement by chemical modification
  - Pencillin G -> Methicillin; morphine->nalorphine
- **Receptor Based drug design**
  - Receptor is the target (usually a protein)
  - Drug molecule binds to cause biological effects
  - It is also called lock and key system
  - Structure determination of receptor is important
- **Ligand-based drug design**
  - Search a lead ocompound or active ligand
  - Structure of ligand guide the drug design process

Current Topics in Medicinal Chemistry, 2013, *13*, 1172-1191

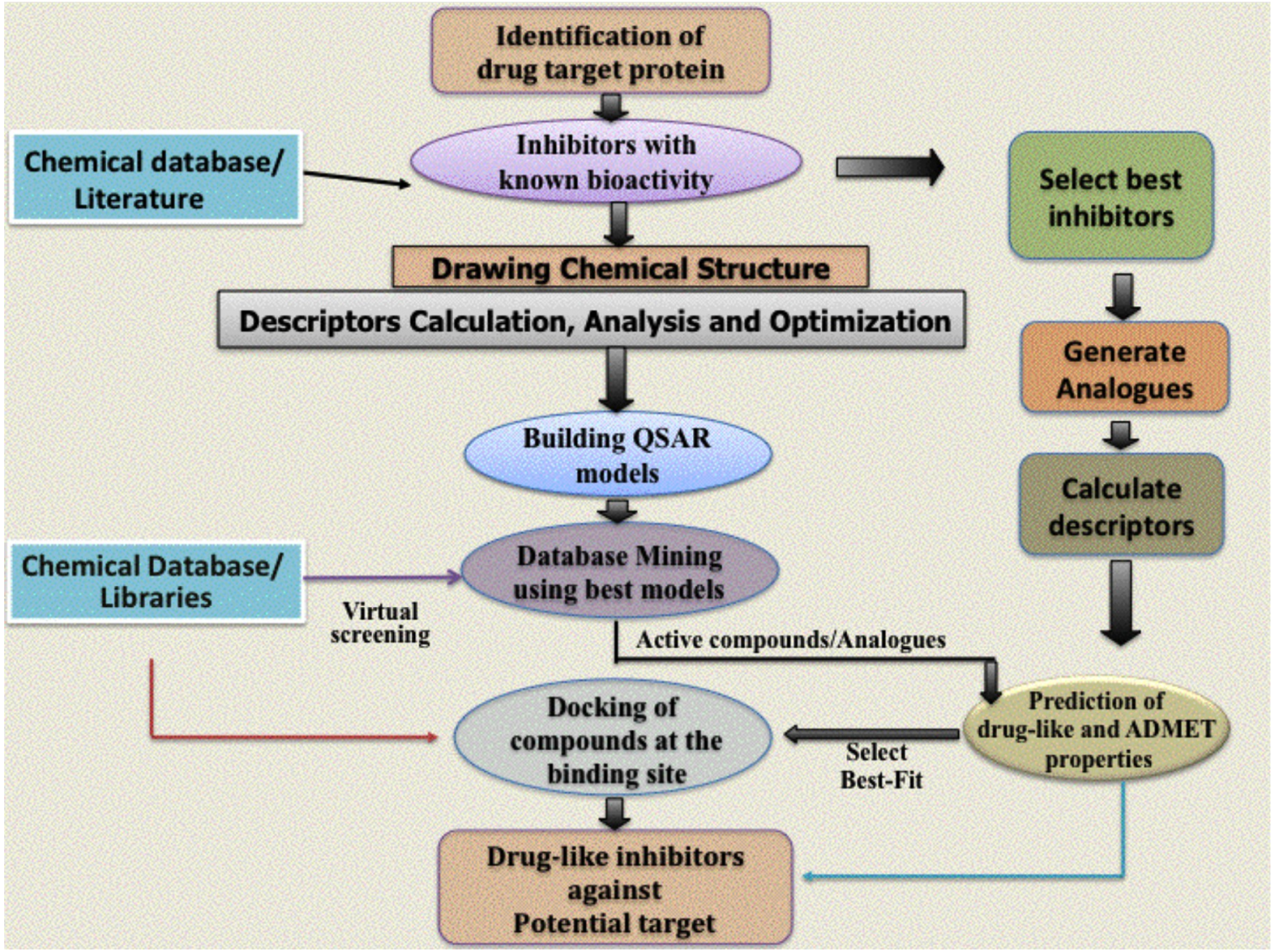
Open Source Software and Web Services for Designing Therapeutic Molecules

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



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/)

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,*]

[1]*Center for Computational Biology, Indraprastha Institute of Information Technology, New Delhi, India;* [2]*CSIR-Institute of Microbial Technology, Chandigarh, India*

ARTICLE HISTORY

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DOI:
10.2174/1568026618666180816155131

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.

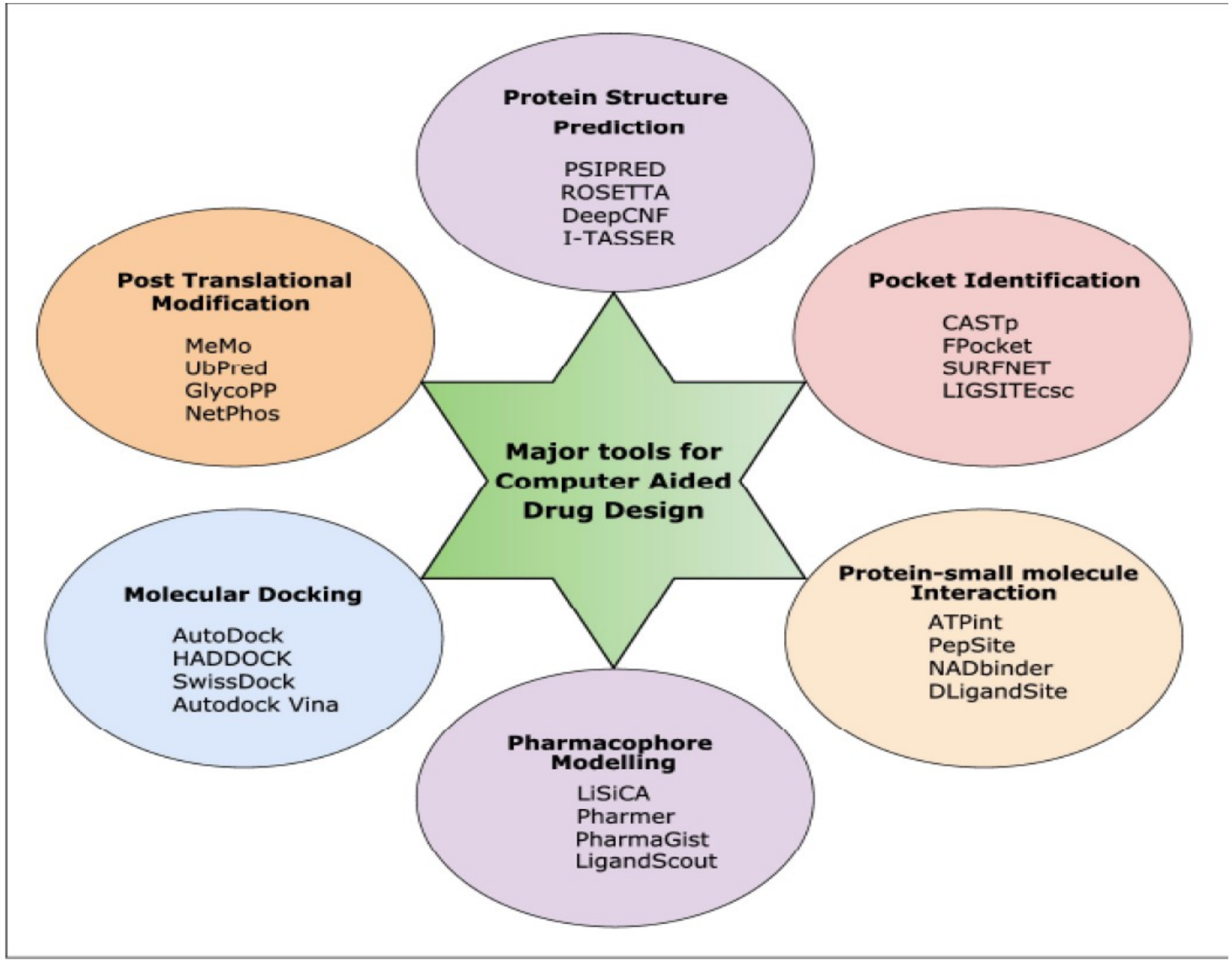


Fig. (1). Shows major categories of freely available computational tools reviewed in this manuscript and popular tools in each category.

Small Chemical-based Drug Discovery

Tool	Description (Link)
PubChem	Database of bioassays, compounds and substances (https://pubchem.ncbi.nlm.nih.gov/)
ChEMBL	Database of drug like molecules (https://www.ebi.ac.uk/chembldb)
Zinc15	Database of commercially-available compounds for virtual screening (http://zinc.docking.org/)
DrugBank	Comprehensive information about drugs (https://go.drugbank.com/)
BindingDB	Binding affinity of PDB ligands (http://www.bindingdb.org/)
SuperDRUG2	Database of approved/marketed drugs (http://cheminfo.charite.de/superdrug2/)
PaDEL	1D, 2D, 3D and fingerprints calculation (http://padel.nus.edu.sg/software/padeldescriptor)
CDK	Chemistry Development Kit (http://cdk.sourceforge.net)
Mordred	Molecular descriptor calculator (https://github.com/mordred-descriptor/mordred)
Dock 6	Standalone software for molecular docking (http://dock.compbio.ucsf.edu/)
AutoDock Vina	Program for molecular docking and virtual screening (http://vina.scripps.edu/)
Autodock	Molecular modelling simulation software (http://autodock.scripps.edu/)
QSAR-Co	Classification-based QSAR model development (https://sites.google.com/view/qsar-co)
DPubChem	Web tool for QSAR modeling and high-throughput virtual screening (https://www.cbrc.kaust.edu.sa/dpubchem/)
Weka	Collection of machine learning algorithm for the development of QSAR based models (https://www.cs.waikato.ac.nz/~ml/weka/)
TINKER	Software tools for molecular design (http://dasher.wustl.edu/tinker/))
Frog	Generation of free online drug conformation (

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

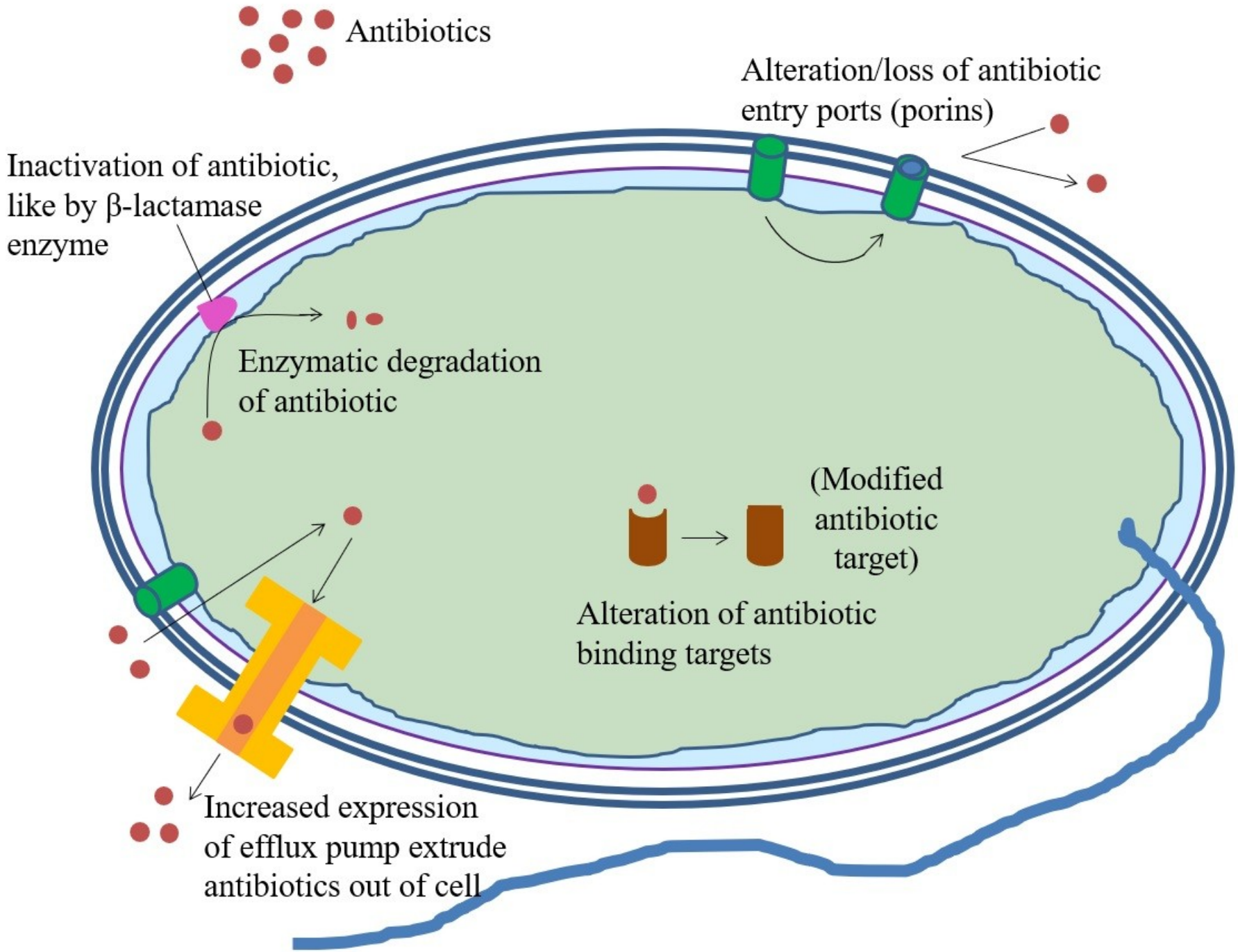
KEYNOTE (GREEN)

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

ChAlPred: A web server for prediction of allergenicity of chemical compounds

Neelam Sharma, Sumeet Patiyal, Anjali Dhall, Naorem Leimarembi Devi, Gajendra P. S. Raghava *

Department of Computational Biology, Indraprastha Institute of Information Technology, Okhla Phase 3, New Delhi, 110020, India

A R T I C L E I N F O

Keywords:
Chemical allergens
Allergy
Machine learning
PaDEL
FDA-approved drugs
DrugBank
IEDB
ChEBI
Chemical descriptors
Fingerprints

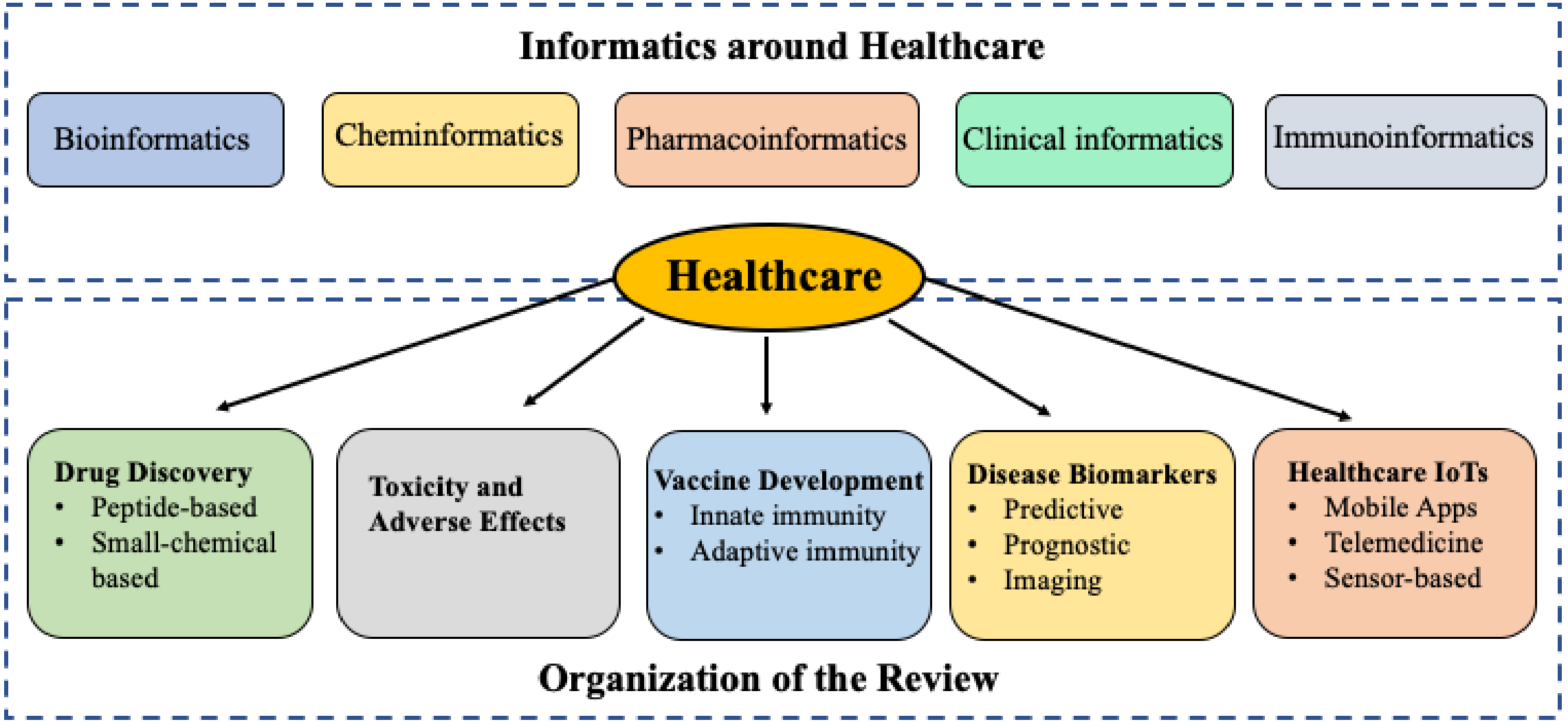
A B S T R A C T

Background: Allergy is the abrupt reaction of the immune system that may occur after the exposure to allergens such as proteins, peptides, or chemicals. In the past, various methods have been generated for predicting allergenicity of proteins and peptides. In contrast, there is no method that can predict allergenic potential of chemicals. In this paper, we described a method ChAlPred developed for predicting chemical allergens as well as for designing chemical analogs with desired allergenicity.

Method: In this study, we have used 403 allergenic and 1074 non-allergenic chemical compounds obtained from IEDB database. The PaDEL software was used to compute the molecular descriptors of the chemical compounds to develop different prediction models. All the models were trained and tested on the 80% training data and evaluated on the 20% validation data using the 2D, 3D and FP descriptors.

Results: In this study, we have developed different prediction models using several machine learning approaches. It was observed that the Random Forest based model developed using hybrid descriptors performed the best, and achieved the maximum accuracy of 83.39% and AUC of 0.93 on validation dataset. The fingerprint analysis of the dataset indicates that certain chemical fingerprints are more abundant in allergens that include PubChemFP129 and GraphFP1014. We have also predicted allergenicity potential of FDA-approved drugs using our best model and identified the drugs causing allergic symptoms (e.g., Cefuroxime, Spironolactone, Tioconazole). Our results agreed with allergenicity of these drugs reported in literature.

Conclusions: To aid the research community, we developed a smart-device compatible web server ChAlPred (https://webs.iiitd.edu.in/raghava/chalpred/) that allows to predict and design the chemicals with allergenic properties.


Informatics around Healthcare
Bioinformatics
Cheminformatics
Pharmacoinformatics
Clinical informatics
Immunoinformatics
Healthcare
Drug Discovery
• Peptide-based
• Small-chemical based
Toxicity and Adverse Effects
Vaccine Development
• Innate immunity
• Adaptive immunity
Disease Biomarkers
• Predictive
• Prognostic
• Imaging
Healthcare IoTs
• Mobile Apps
• Telemedicine
• Sensor-based
Organization of the Review

Toxicity

crdd.osdd.net/raghava/toxinpred/

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

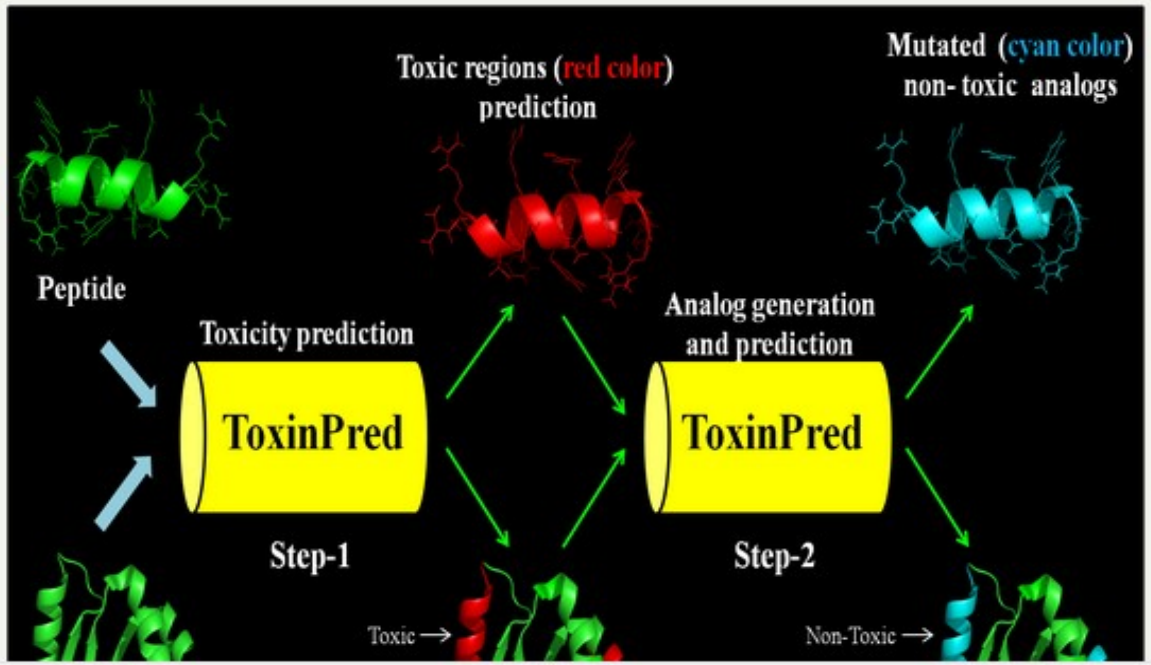
ToxinPred

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.

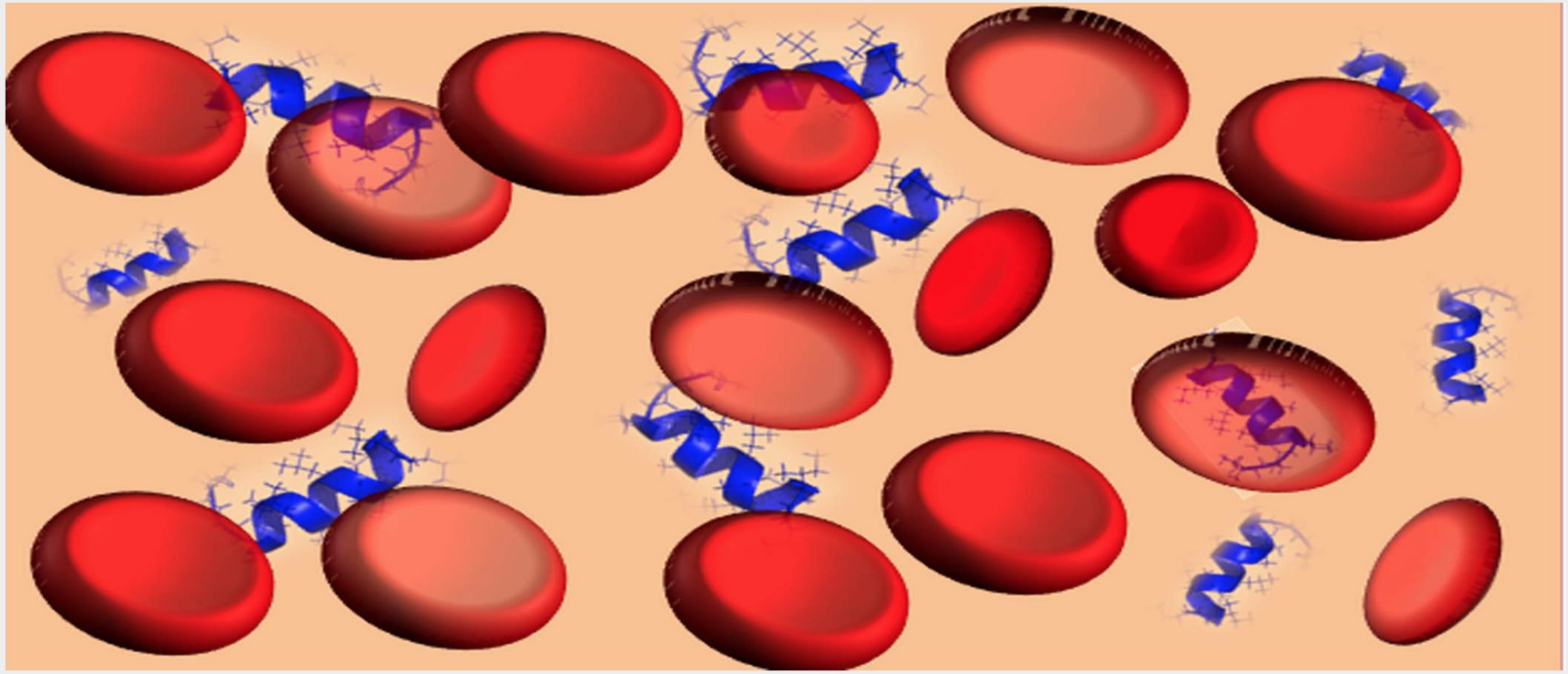
(4) **QMS Calculator:** This tool allows the users to submit query peptide in FASTA format and to optimize the peptide sequence to get maximum/minimum/desired toxicity based upon the Quantitative Matrix based position specific scores. It will help the user to tweak any residue from the predecessor peptide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

Toxicity

HemoPI: Hemolytic Peptide Identification Server

Reference: Chaudhary et., al., (2016) A Web Server and Mobile App for Computing Hemolytic Potency of Peptides. Sci Rep. 2016.

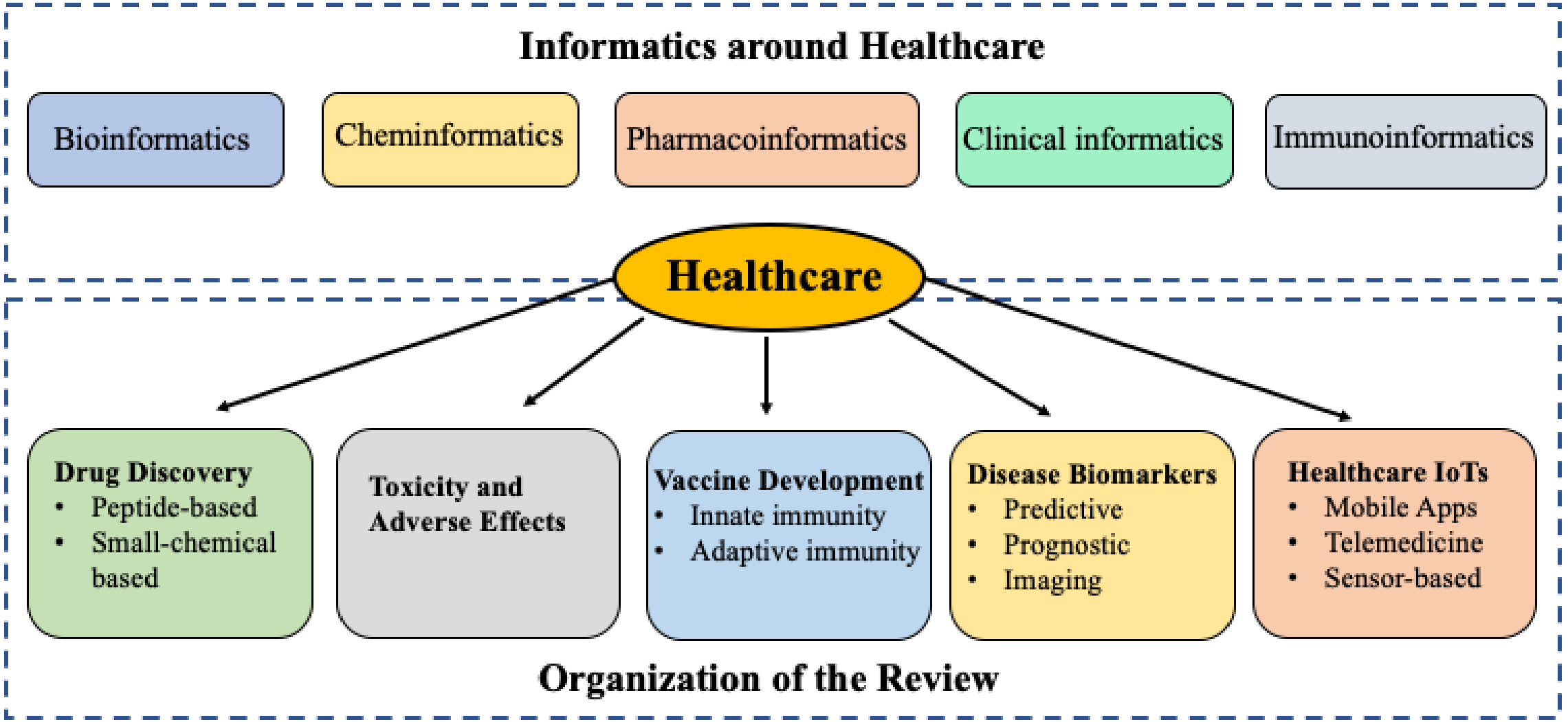
Welcome to HemoPI



Major features of HemoPI

Toxicity of molecules and macromolecules

Tool	Description (Link)
admetSAR 2.0	Tool to predict the chemical ADMET properties (http://lmmd.ecust.edu.cn/admetsar2/)
ADMETopt	Optimization of lead compounds and ADMET screening (http://lmmd.ecust.edu.cn/admetsar2/admetopt/)
ADMETlab	Web-service for systematic ADMET evaluation of chemicals http://admet.scbdd.com/
DrugMint	Computation of drug-like molecules (https://webs.iiitd.edu.in/oscadd/drugmint/)
MetaPred	Prediction of drug metabolizing CYP450 isoforms (https://webs.iiitd.edu.in/raghava/metapred/)
SwissADME	Tool to assess pharmacokinetics, drug-likeness and related parameters of small molecules (http://www.swissadme.ch)
vNN	Webserver for ADMET predictions https://vnnadmet.bhsai.org/
ADVERpred	Web-service for prediction of adverse effects of drugs (http://www.way2drug.com/adverpred/)
BTXpred	Prediction of bacterial toxins (https://webs.iiitd.edu.in/raghava/btxpred/)
ChAlPred	Computation of allergenicity of chemical compounds (https://webs.iiitd.edu.in/raghava/chalpred/)
CTD	The comparative toxicogenomics database (http://ctdbase.org/)
eToxPred	Calculate toxicity and synthetic accessibility of compounds (https://github.com/pulimeng/etoxpred/)
NTXpred	Webserver for predicting neurotoxins (https://webs.iiitd.edu.in/raghava/ntxpred/)
Pred-hERG	Computational tool for predicting cardiac toxicity (http://labmol.farmacia.ufg.br/predherg/)
Pred-Skin	Web portal for accurate prediction of human skin sensitizers (http://labmol.com.br/predskin/)


Informatics around Healthcare
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• Adaptive immunity
Disease Biomarkers
• Predictive
• Prognostic
• Imaging
Healthcare IoTs
• Mobile Apps
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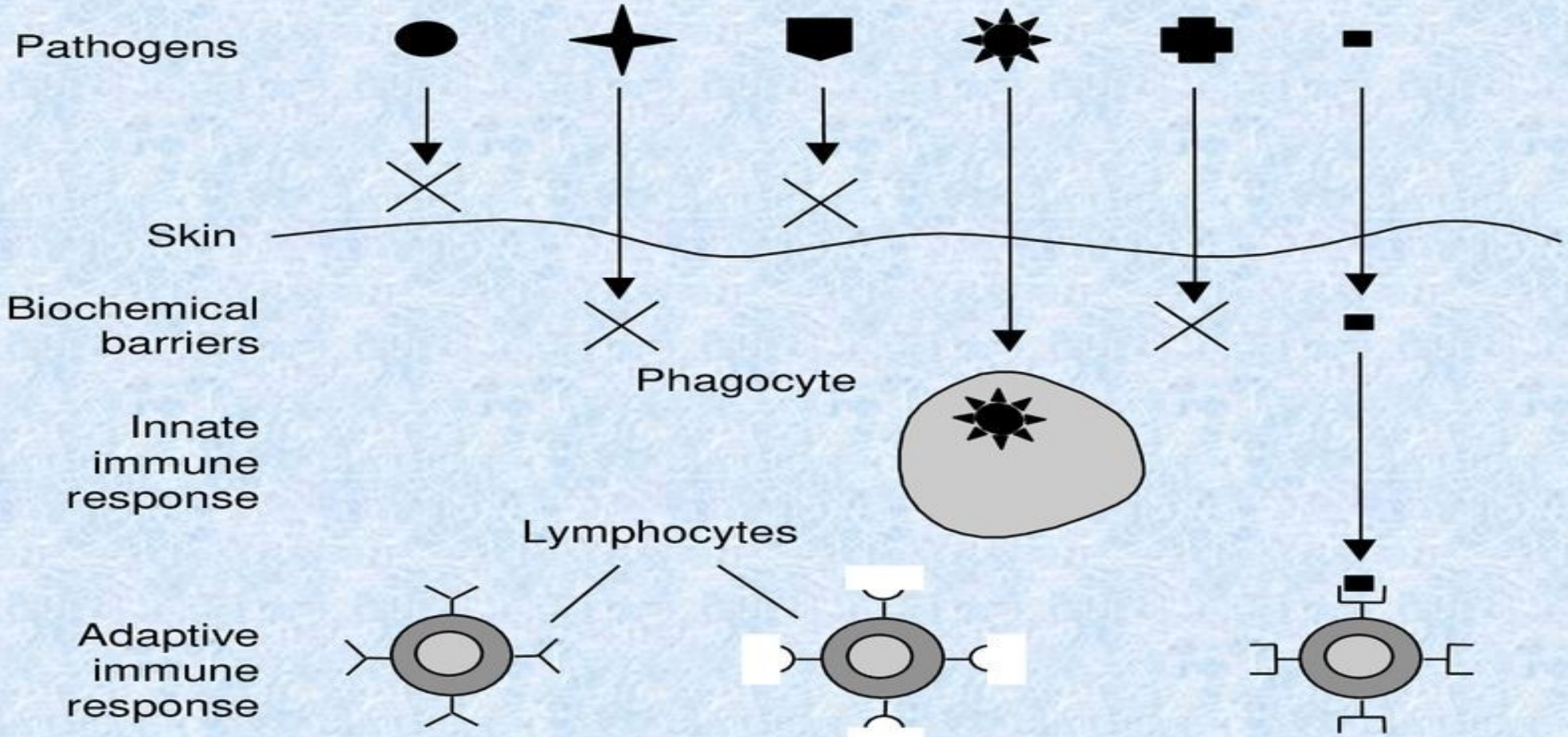
• Sensor-based
Organization of the Review

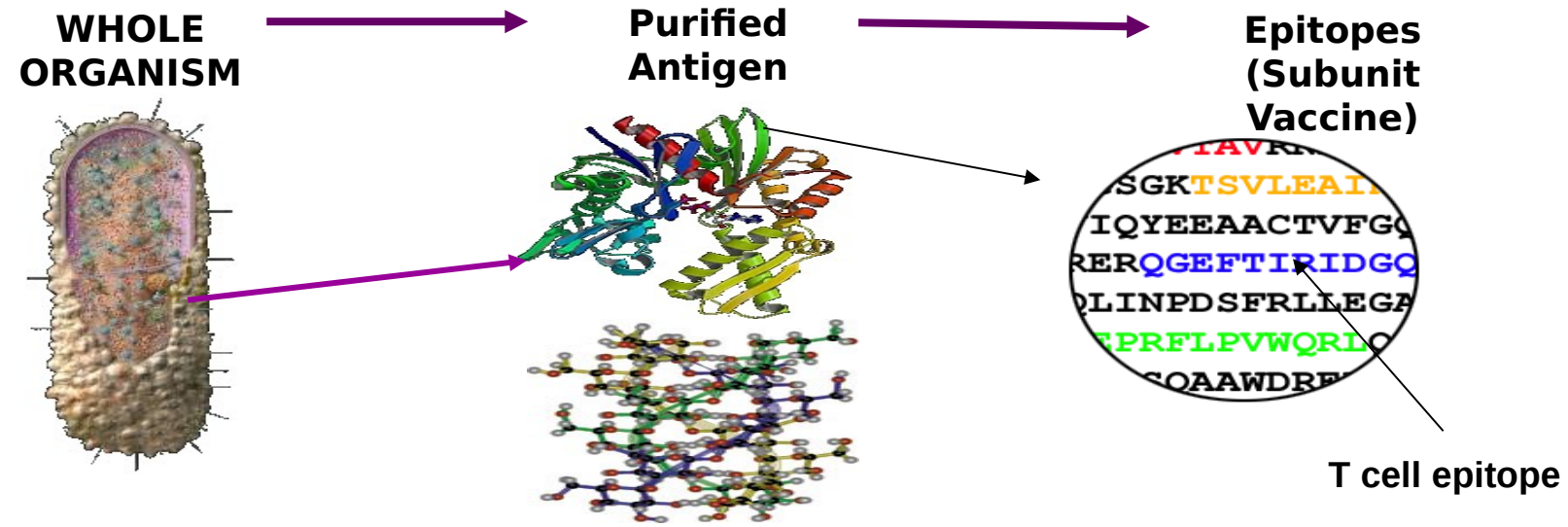
History of Immunization

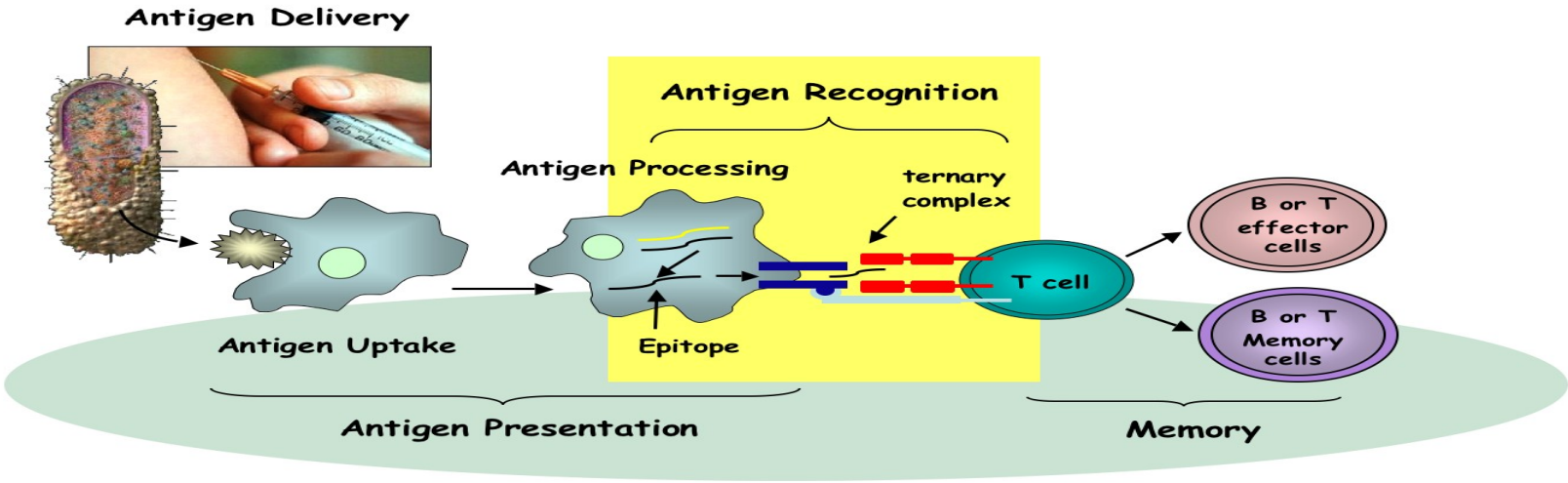
- Children protected who recovered from smallpox
- Immunity induce, a process known as variolation
- Variolation spread to England and America
- Stopped due to the risk of death
- Edward Jenner found that protection against smallpox
- Inoculation with material from an individual infected with cowpox
- This process was called vaccination (cowpox is vaccina)

Multiple layers of the immune system



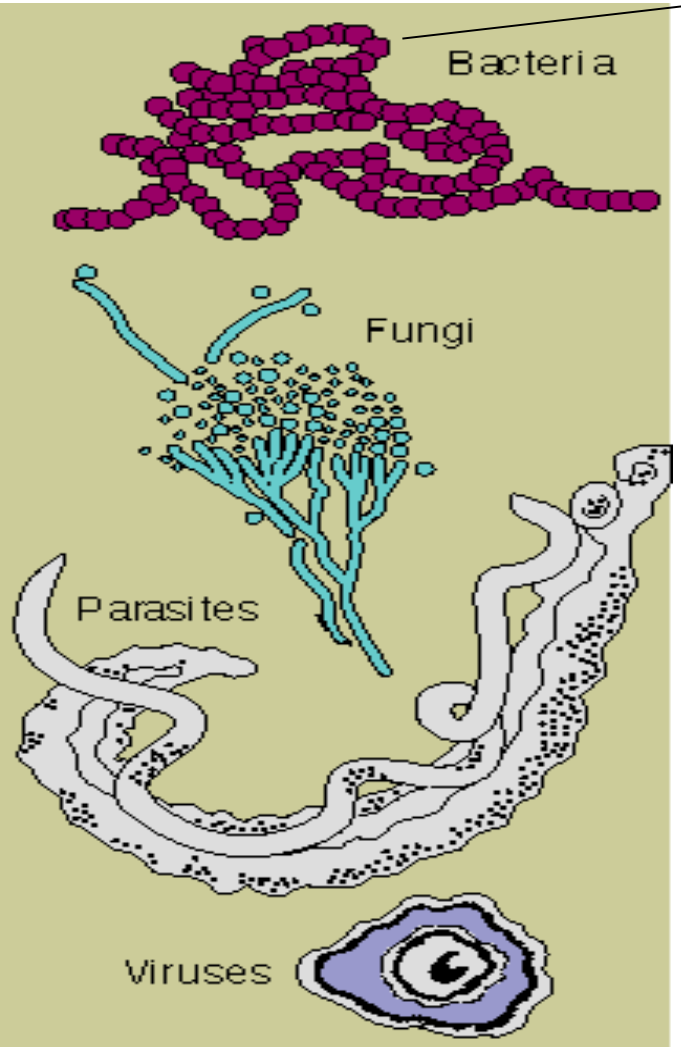
Biomolecules Based Vaccines





Different arms of Immune System

Disease Causing Agents



Pathogens/Invac

Host Immune Defense System
For Microbial (Pathogens) Attack

Non-Specific Defense
(Innate Immunity)

Specific Defense
Adaptive Immunity
Responsible for Generating
Memory B & T Cells

TOLL LIKE RECEPTORS
PATHOGEN ASSOCIATED
MOLECULAR PATTERNS

Humoral Immunity
(B-Lymphocytes)

Cell-Mediated Immunity
(T-Lymphocytes)

B-Cell Epitopes
Antibody Prod.
Neutralization

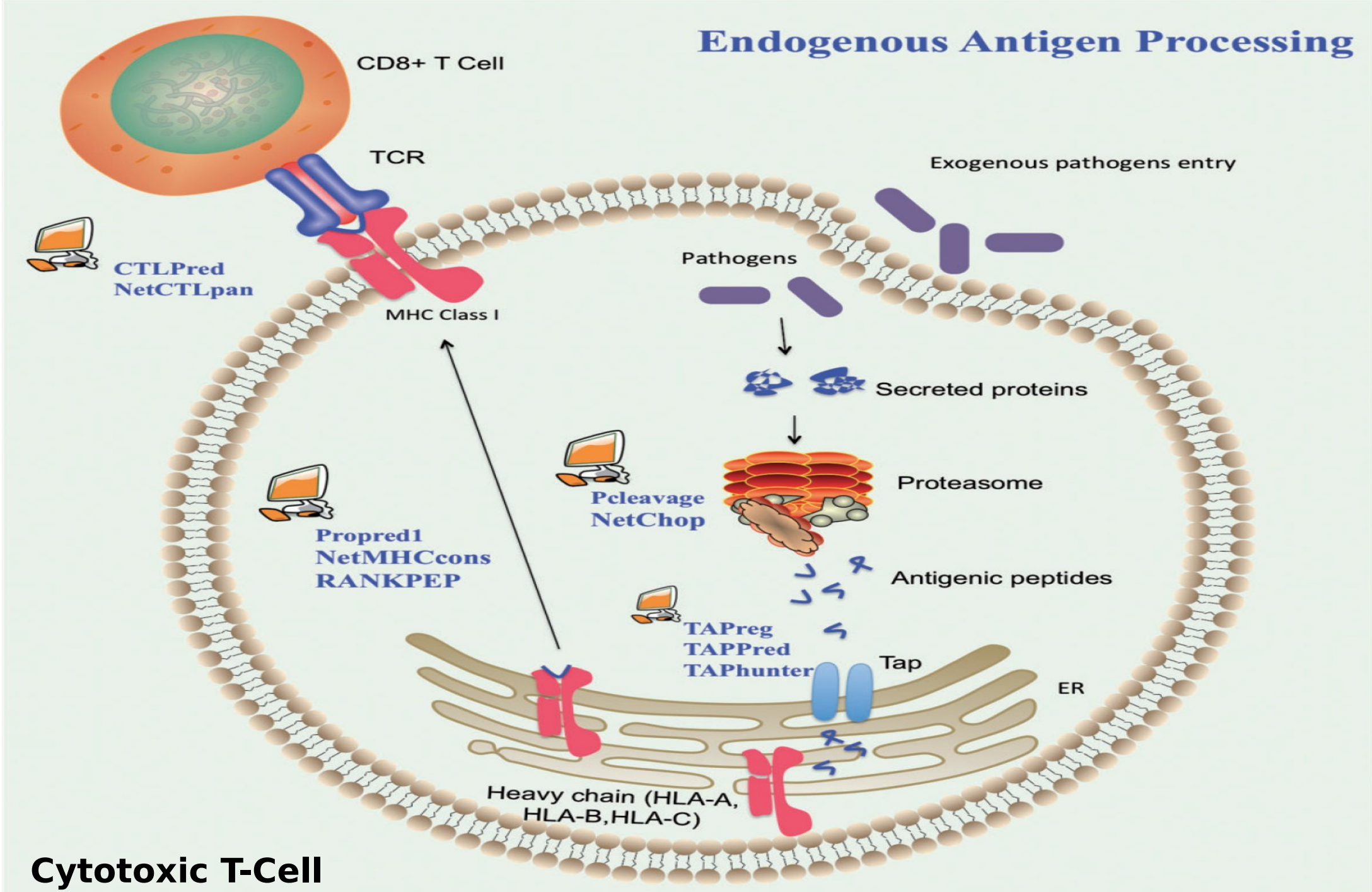
Endogenous Antigen Processing

Exogenous Antigen Processing

CTL Epitopes
MHC I binders
TAP Binders
P. Cleavage Sites

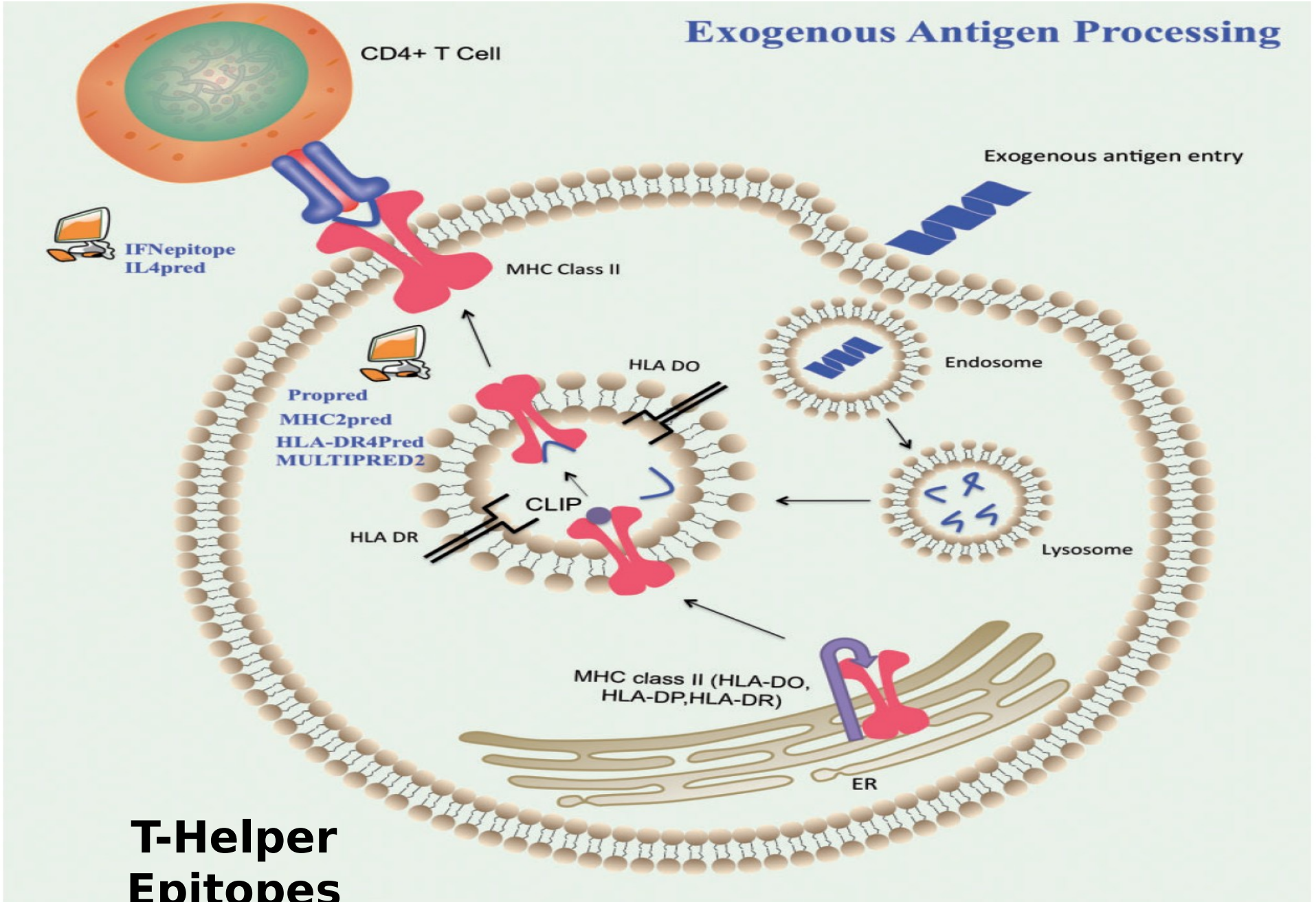
T-Helper Epitopes
MHC II binders

Cell Mediated Immunity (T-cell Epitopes)

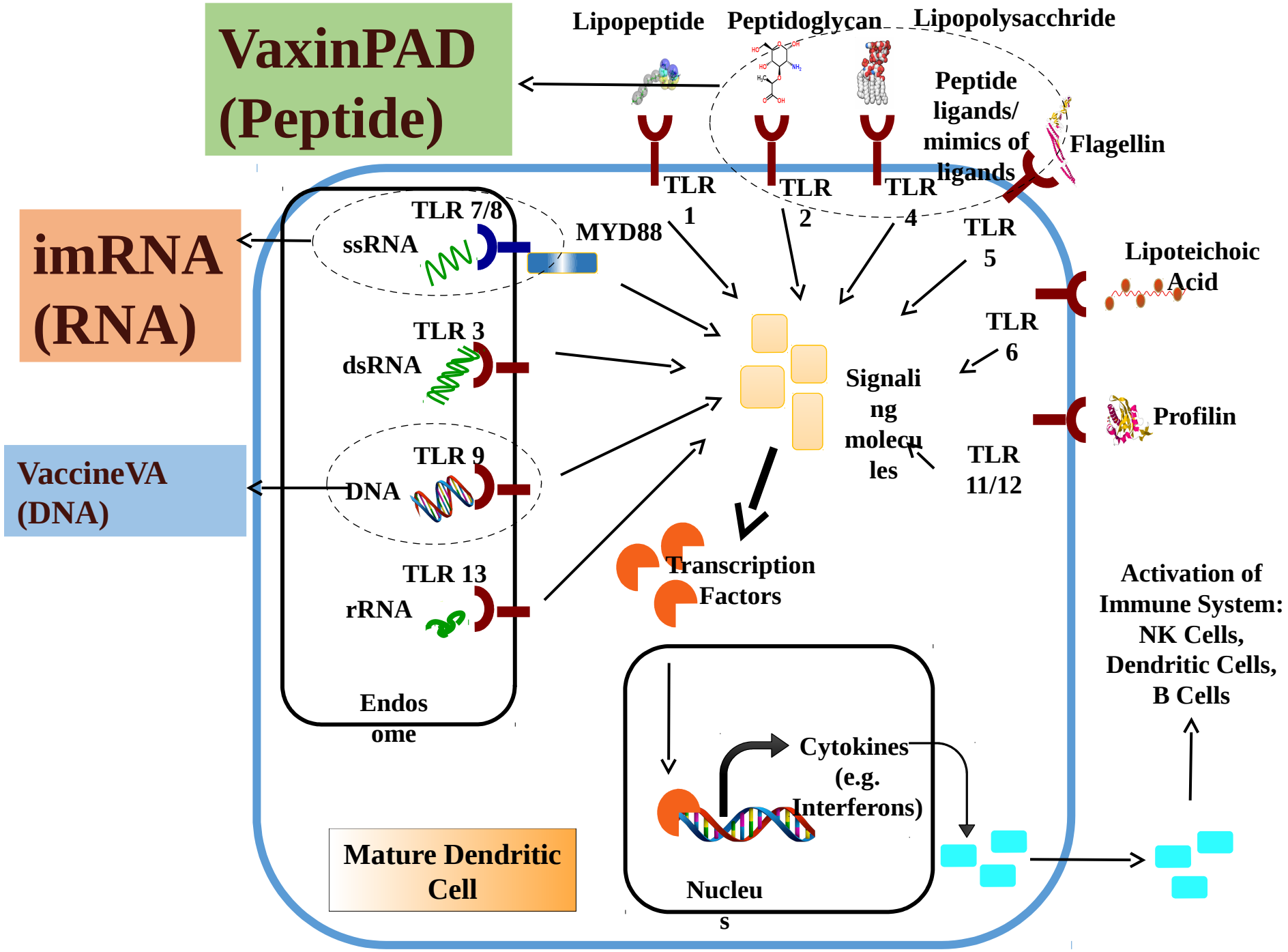


Cytotoxic T-Cell Epitopes

Cell Mediated Immunity (T-cell Epitopes)



T-Helper Epitopes

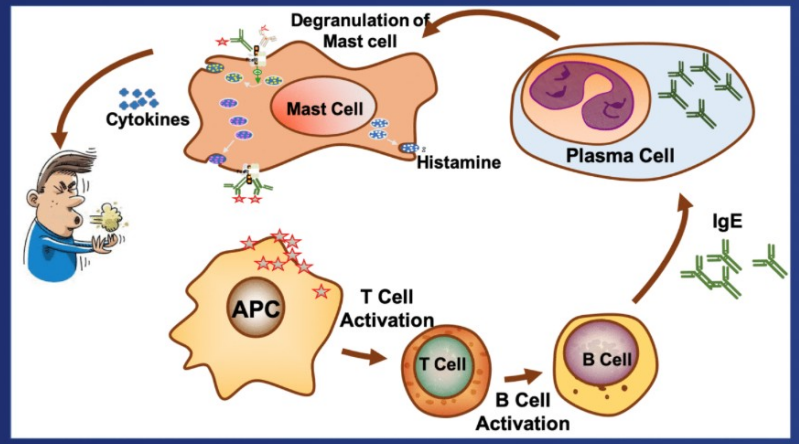

VaxinPAD (Peptide)
imRNA (RNA)
VaccineVA (DNA)
Lipopeptide
Peptidoglycan
Lipopolysacchride
Peptide ligands/ mimics of ligands
Flagellin
TLR 1
TLR 2
TLR 4
TLR 5
TLR 6
TLR 7/8
ssRNA
TLR 3
dsRNA
TLR 9
DNA
TLR 13
rRNA
MYD88
Signaling molecules
Lipoteichoic Acid
Profilin
TLR 11/12
Transcription Factors
Endosome
Cytokines (e.g. Interferons)
Nucleus
Mature Dendritic Cell
Activation of Immune System: NK Cells, Dendritic Cells, B Cells

AlgPred 2.0

Home Prediction IgE epitope Mapping Motif Scan BLAST Search General

Welcome to AlgPred 2.0

A web server for predicting allergens and mapping of IgE epitopes



Cite: Sharma et al. (2020) AlgPred 2.0: an improved method for predicting allergenic proteins and mapping of IgE epitopes, Briefings in Bioinformatics,22(4): bbaa294.

Major Features

AlgPred 2.0 is an updated version of our old server **AlgPred** developed for predicting allergenic proteins (See Nucleic Acids Res. 2006; 34 : W202–W209). It utilize wide range of information and techniques for prediction that includes machine learning techniques, BLAST, MEME/MAST and IgE epitope mapping. Our models have been trained on large dataset that contain 10075 allergens and 10075 non-allergens. This server allow user to map 10451 IgE epitopes as well as blast search against these IgE

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

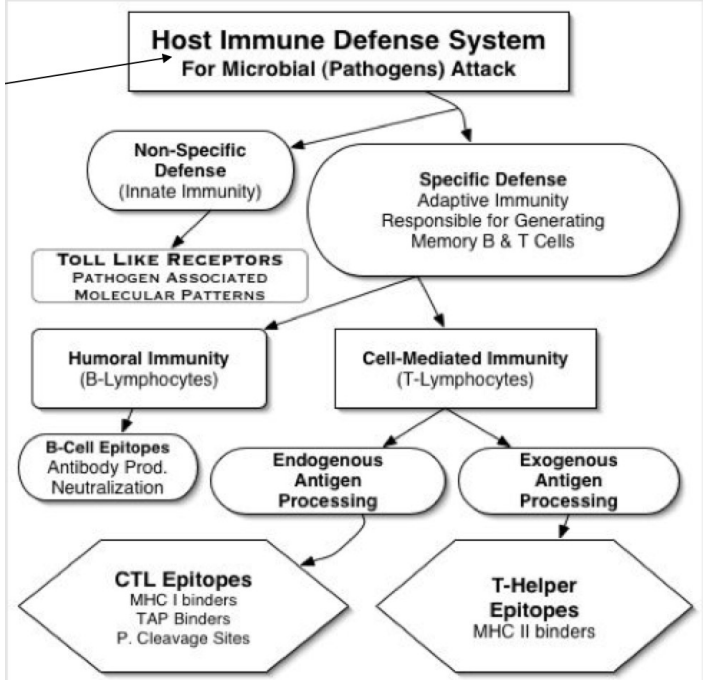
PRRDB: A database of PRRs & ligands

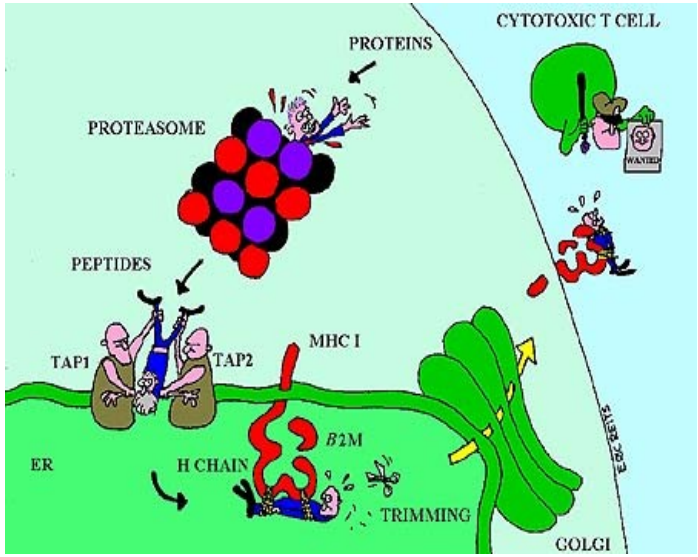
VaccineDA: DNA-based adjuvants

imRNA: Immunomulatory RNAs

VaccinePAD: Peptide-based adjuvants

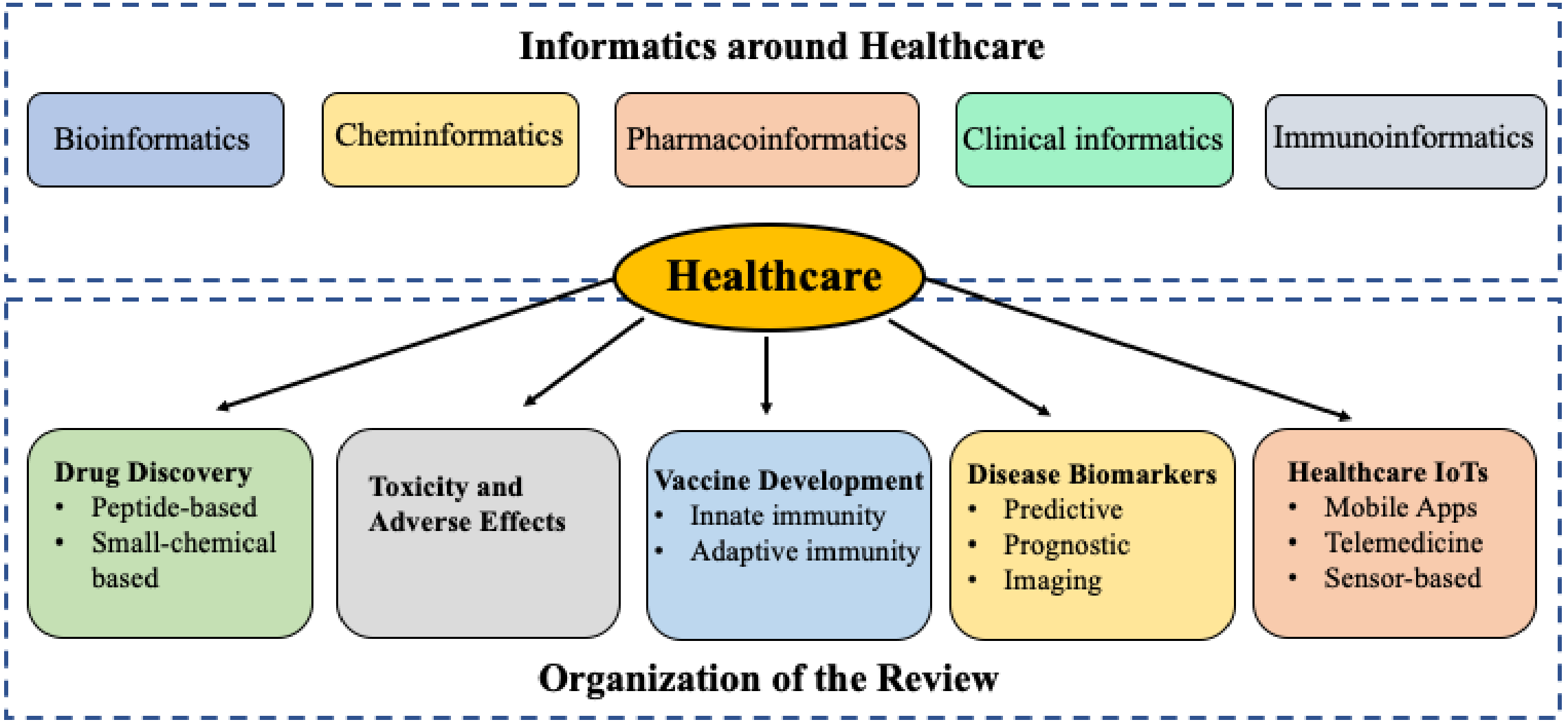
PolysacDB: Polysaccharide antigens



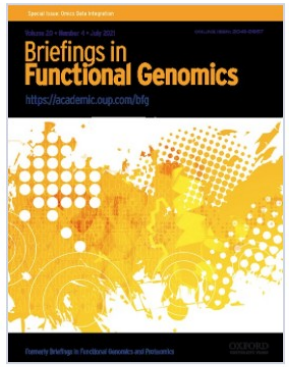


Computer-aided vaccine design

Tool	Description (Link)
pVACtools	Computational toolkit to identify cancer neoantigens (https://pvactools.readthedocs.io/)
IL-6pred	Prediction of interleukin-6 inducing peptides (https://webs.iiitd.edu.in/raghava/il6pred/)
IEDB	Database of immune epitopes and analysis resources (http://www.iedb.org/)
NetMHCIIpan 3.2	Prediction of MHC class II molecules (http://www.cbs.dtu.dk/services/NetMHCIIpan-3.2/)
NetMHCpan 4.0	Prediction MHC class I molecules (http://www.cbs.dtu.dk/services/NetMHCpan-4.0/)
IL-10pred	Identification of interleukin-10 Inducing peptides (https://webs.iiitd.edu.in/raghava/il10pred/)
IL4pred	Prediction of interleukin-4 Inducing peptides (https://webs.iiitd.edu.in/raghava/il4pred/)
IFNepitope	Interferon-gamma inducing epitopes (https://webs.iiitd.edu.in/raghava/ifnepitope/)
LBtope	Predicting linear B-cell epitopes (https://webs.iiitd.edu.in/raghava/lbtope/)
IgPred	B-cell epitopes for different class of antibodies (https://webs.iiitd.edu.in/raghava/igpred/)
DiscoTope 2.0	Discontinuous B cell epitopes (http://www.cbs.dtu.dk/services/DiscoTope/)
Cbtope	Prediction of conformational B-cell epitope (https://webs.iiitd.edu.in/raghava/cbtope/)
ABCpred	ANN based method for predicting B cell epitopes (https://webs.iiitd.edu.in/raghava/abcpred/)
Pcleavage	Proteasomal cleavage sites in a protein (https://webs.iiitd.edu.in/raghava/pcleavage/)
CTLPred	A direct method for prediction of CTL epitopes (https://webs.iiitd.edu.in/raghava/ctlpred/)


Informatics around Healthcare
Bioinformatics
Cheminformatics
Pharmacoinformatics
Clinical informatics
Immunoinformatics
Healthcare
Drug Discovery
• Peptide-based
• Small-chemical based
Toxicity and Adverse Effects
Vaccine Development
• Innate immunity
• Adaptive immunity
Disease Biomarkers
• Predictive
• Prognostic
• Imaging
Healthcare IoTs
• Mobile Apps
• Telemedicine
• Sensor-based
Organization of the Review

Briefings in Functional Genomics



Volume 20, Issue 4
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Article Contents

EDITOR'S CHOICE

Computational resources for identification of cancer biomarkers from omics data FREE

Harpreet Kaur, Rajesh Kumar, Anjali Lathwal, Gajendra P S Raghava ✉ Author Notes

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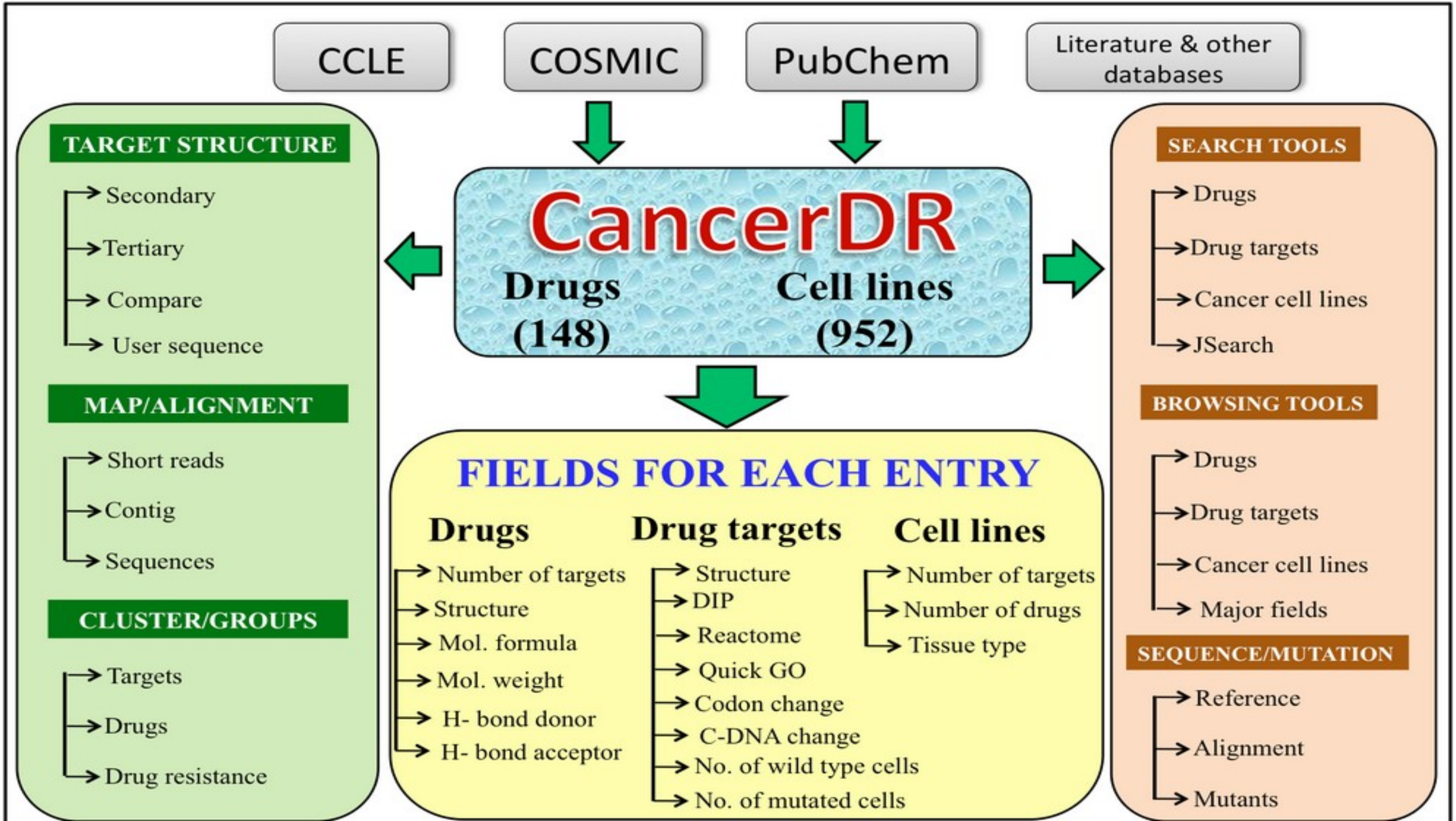
Published: 01 April 2021 **Article history** ▾

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


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

OvirusTdb - A Resource To Explore The Therapeutic Potential Of Oncolytic Viruses

Cancer is the leading cause of death worldwide. According to GLOBOCAN database of world health organization (WHO) report 2018, the glob Scientists and researchers wo Drugs such as paclitaxel, vinc hibitor, mitotic disruptor, HDA(current cancer treatment is th ith several side effects. Cancer as interleukin-2 (IL) based the in tumor cells without affectir **e therapeutic potential of c** and manages information on ses.

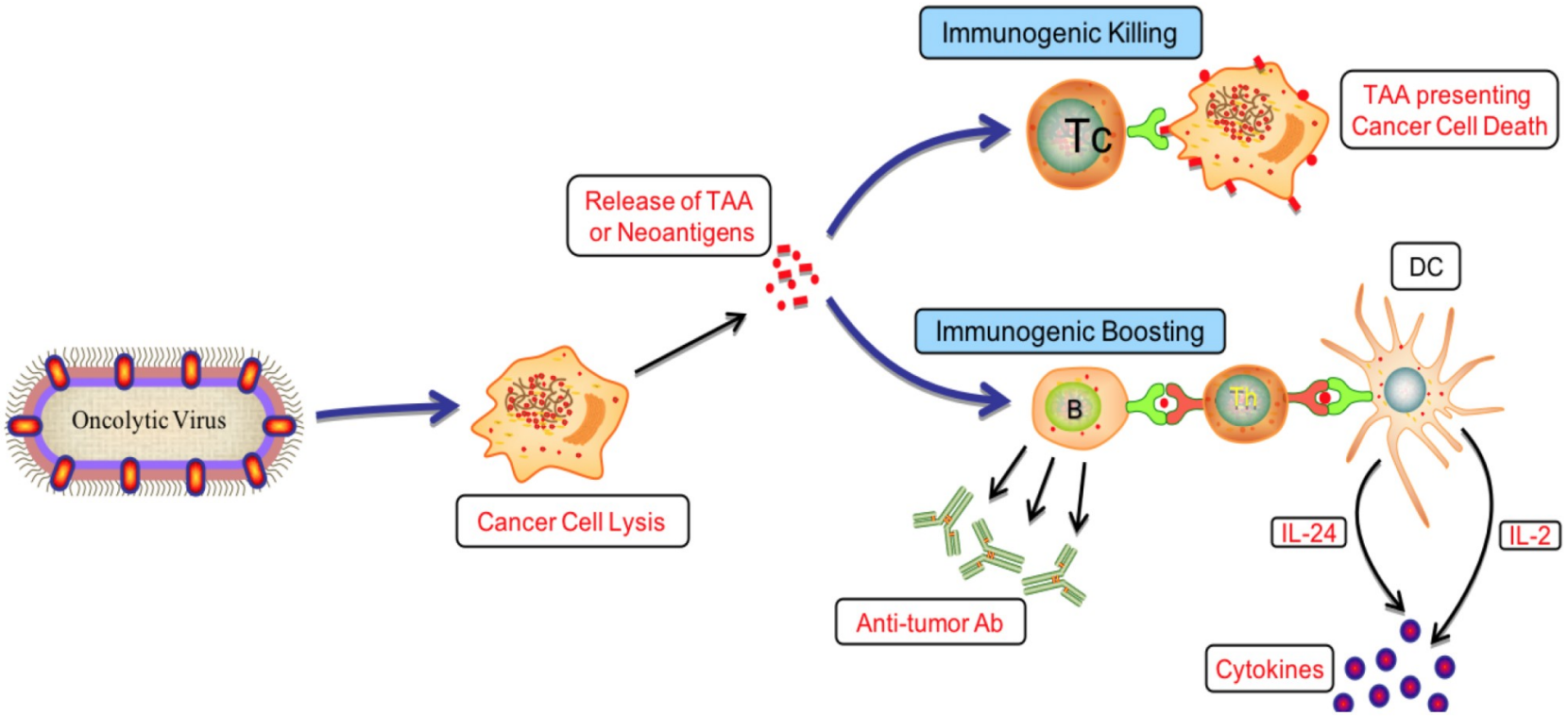
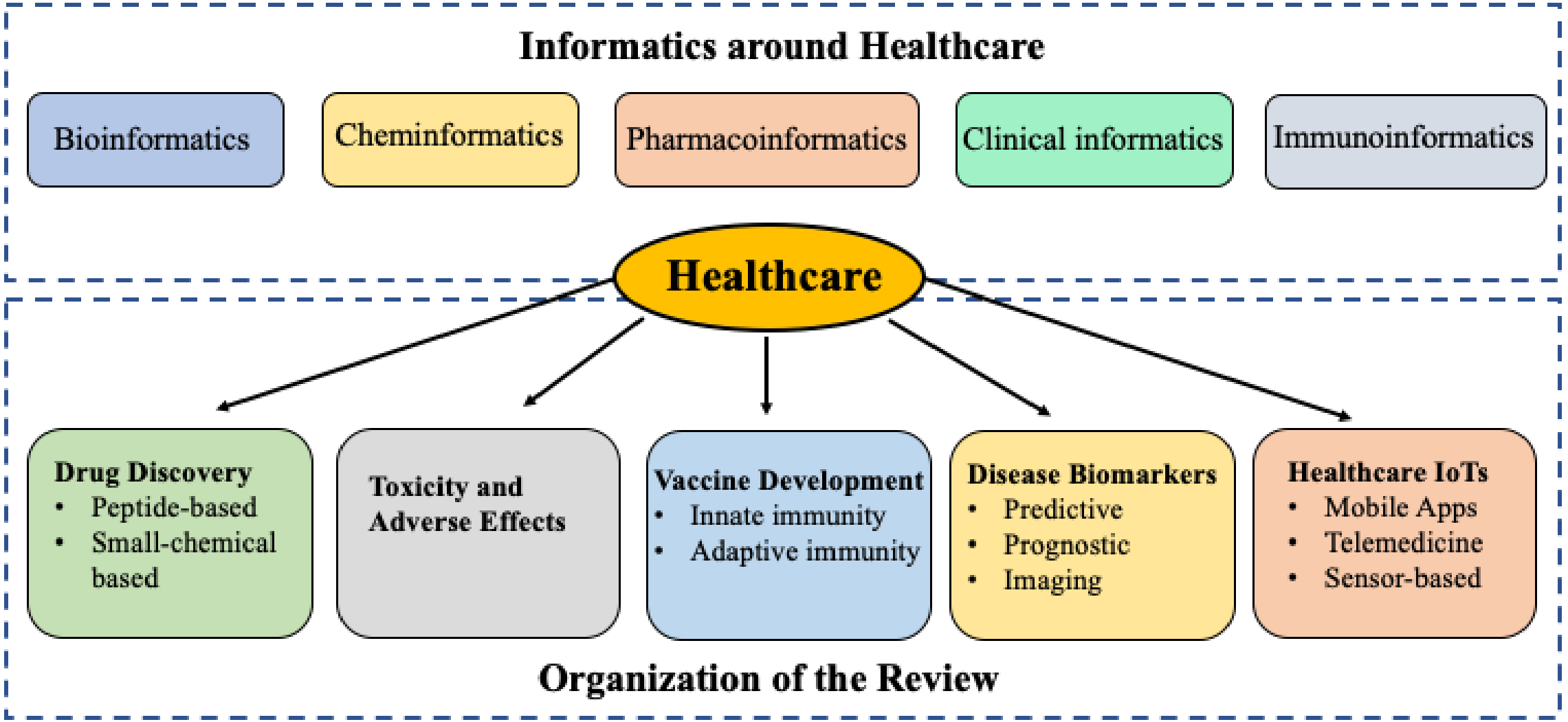


Figure illustrating mechanism of oncolysis and immunogenic effect induced by Oncolytic virus

Disease biomarkers based on genomic profiles

Tool	Description (Link)
CancerCSP	Classification of early and late stages of CCRC (https://webs.iiitd.edu.in/raghava/cancercsp/)
CancerEnD	Database of cancer associated enhancers (https://webs.iiitd.edu.in/raghava/cancerend/)
CancerLivER	Repository of liver cancer-specific biomarkers (https://webs.iiitd.edu.in/raghava/cancerliver/)
CancerLSP	Identification of early-stage liver cancer patients (http://webs.iiitd.edu.in/raghava/cancerlsp/)
CancerTSP	Prediction of early-stage thyroid cancer (http://webs.iiitd.edu.in/raghava/cancertsp/)
CRC-EBD	Database for epigenetic biomarkers on colorectal cancer (http://www.sysbio.org.cn/EBD/)
MarkerDB	Database of molecular biomarkers (https://markerdb.ca/)
PTSDDB	Database for post-traumatic stress disorder biomarkers (https://ptsd.scai.fraunhofer.de/)
CMcrpred	Survival risk in cutaneous melanoma patients (https://webs.iiitd.edu.in/raghava/cmcrpred/)
CRCRpred	Prediction of risk scores of colorectal cancer patients (https://webs.iiitd.edu.in/raghava/crcrpred/)
SKCMhrp	Classification of high-risk cutaneous melanoma patients (https://webs.iiitd.edu.in/raghava/skcmhrp/)
SurvExpres	Survival analysis from expression data (http://bioinformatica.mty.itesm.mx/SurvExpress)
ePAD	Quantitative imaging biomarkers of cancer treatment response (http://epad.stanford.edu/)
LIFEx	Freeware to extract radiomic features (https://www.lifexsoft.org/)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Vaccine Development
• Innate immunity
• Adaptive immunity
Disease Biomarkers
• Predictive
• Prognostic
• Imaging
Healthcare IoTs
• Mobile Apps
• Telemedicine
• Sensor-based
Organization of the Review

Mobile apps for Health & Telemedicine

Tool	Description (Link)
mg	An online pharmacy with a wide range of prescription (https://www.1mg.com/)
arogya Setu	Fight against coronavirus infection in India (https://www.aarogyasetu.gov.in/)
IIMS-WHO CC NBC	App for nursing colleagues and neonatologist across small hospitals (https://play.google.com/store/apps/details?id=drdeorari.aiims.enc)
abylon health	All-in-one healthcare on phone (https://www.babylonhealth.com/)
oDysAn	A telemedicine tool for patients (http://www.codysan.eu/)
omarch ealthcare	A wide range of healthcare solutions (https://www.comarch.com/healthcare/)
SanjeevaniOP	A teleconsultation service ttps://esanjeevaniopd.in/)
ybrate	Consult doctors online (https://www.lybrate.com/)
lanageMyHea h	Comprehensive telemedicine solution (https://www.managemyhealth.co.nz/m/)
ational ealth Portal ndia	A single point access for health information (https://www.india.gov.in)