Computer-aided Peptide Therapeutics

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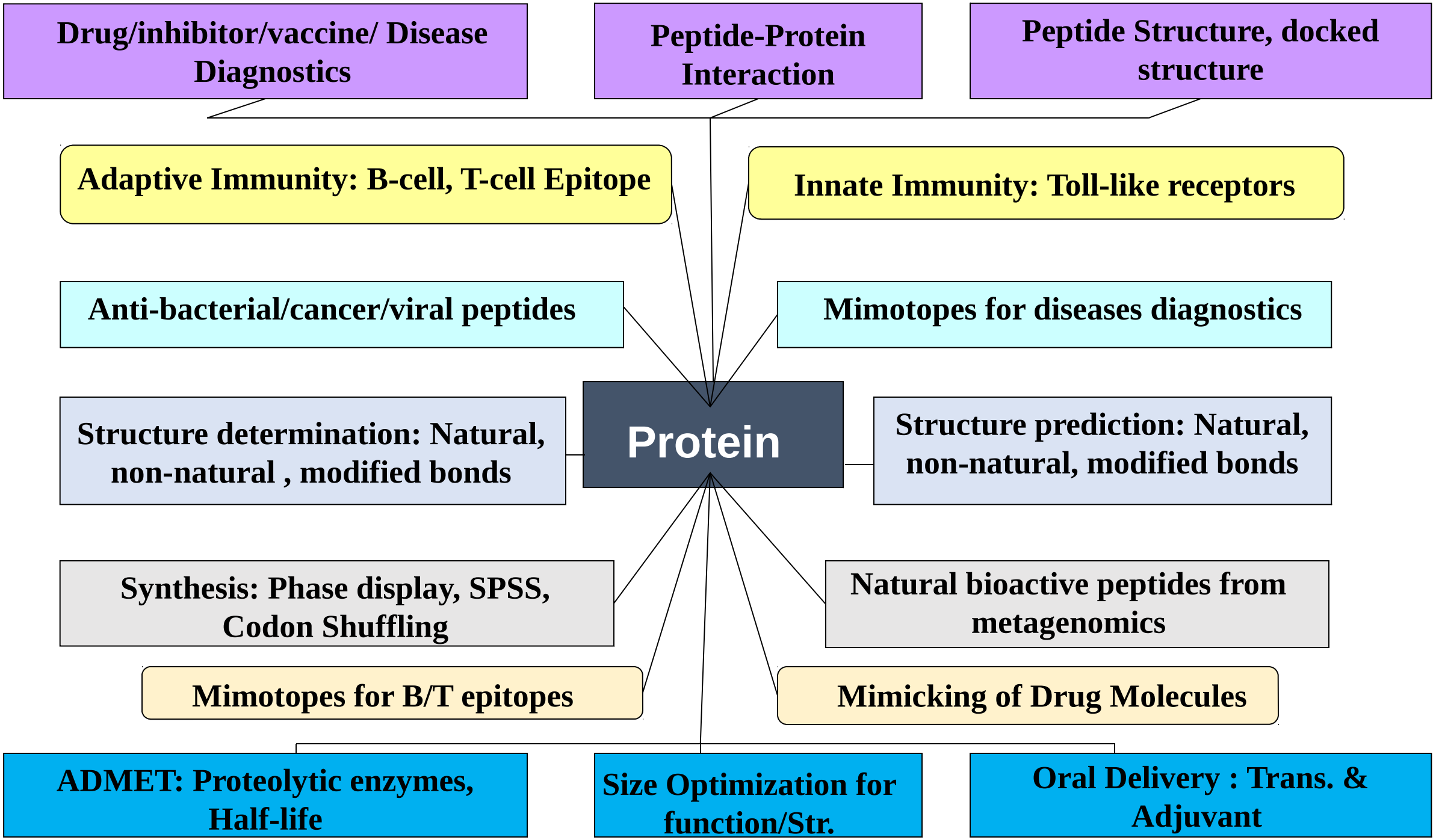
DELHI

Web Site:
http://webs.iiitd.edu.in/raghava/


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

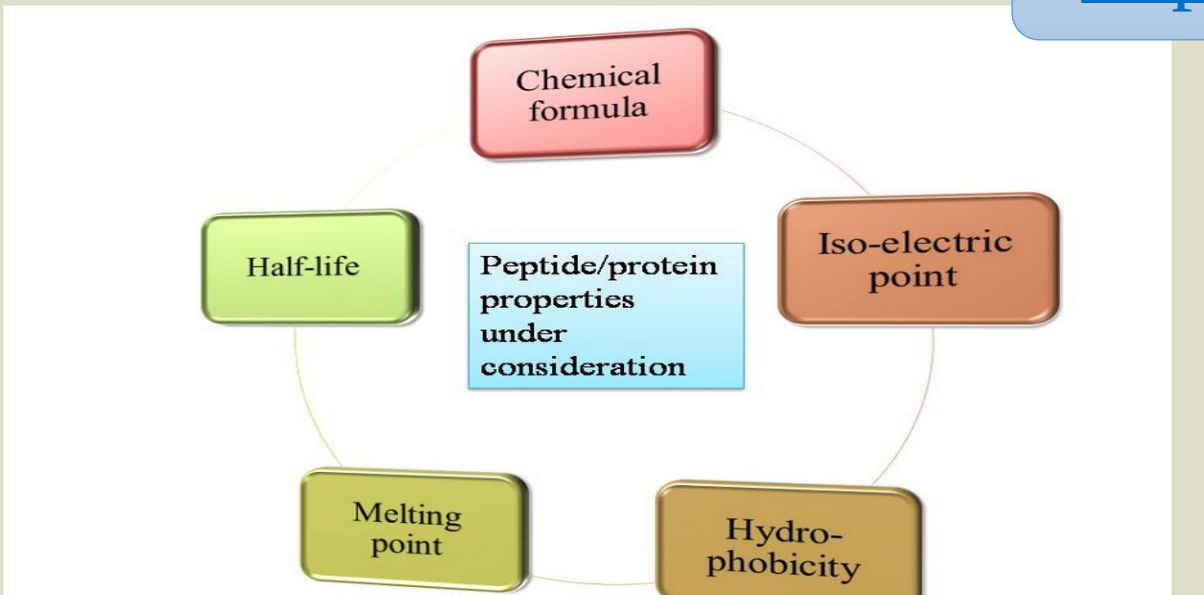
Therapeutic Proteins

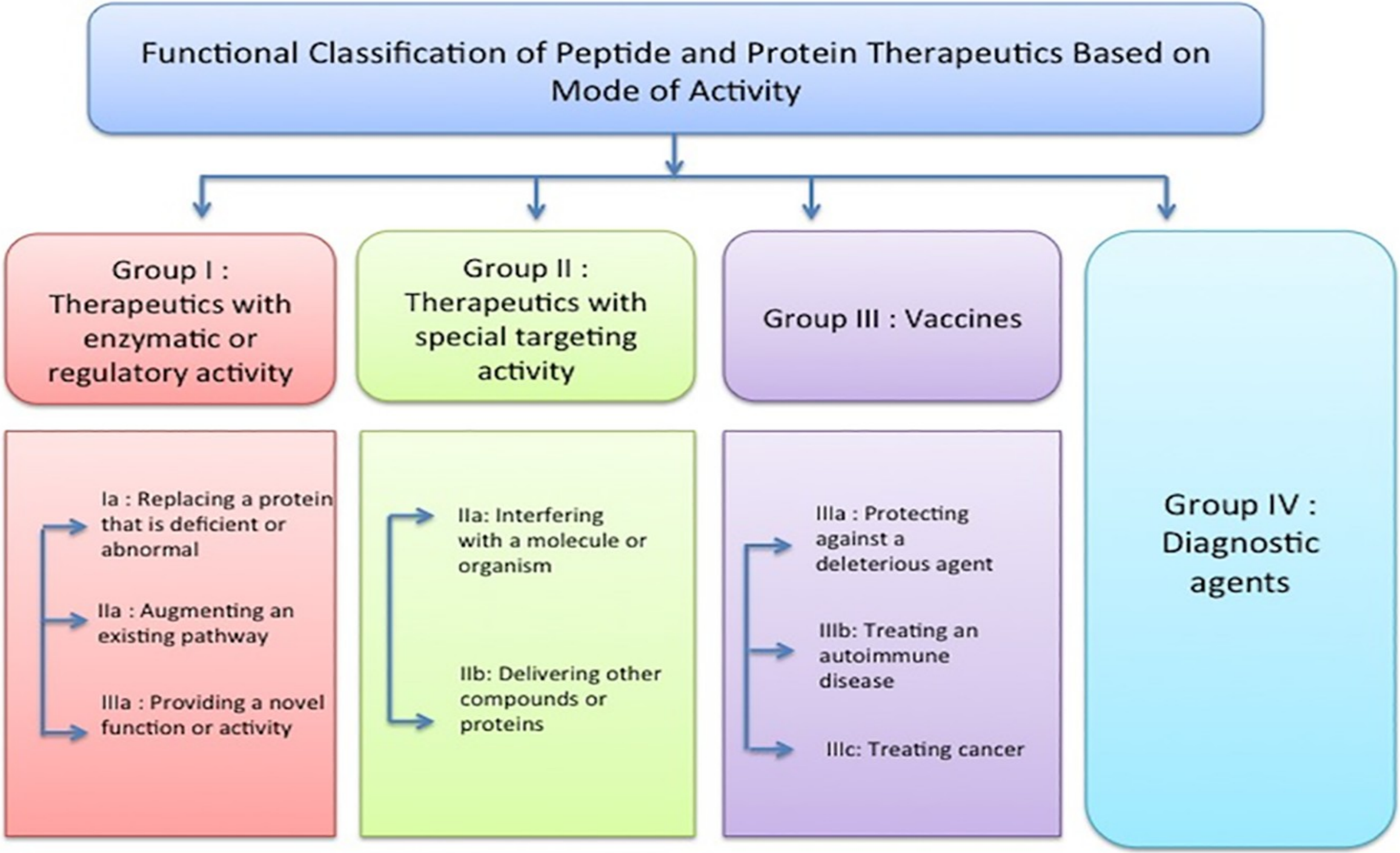
On therapeutic prespective, there is tremendous opportunity in terms of harnessing protein therapeutics to alleviate disease. Once a rarely used subset of medical treatments, protein therapeutics have increased dramatically in number and frequency of use since the introduction of the first recombinant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

Concept of Drug and Vaccine

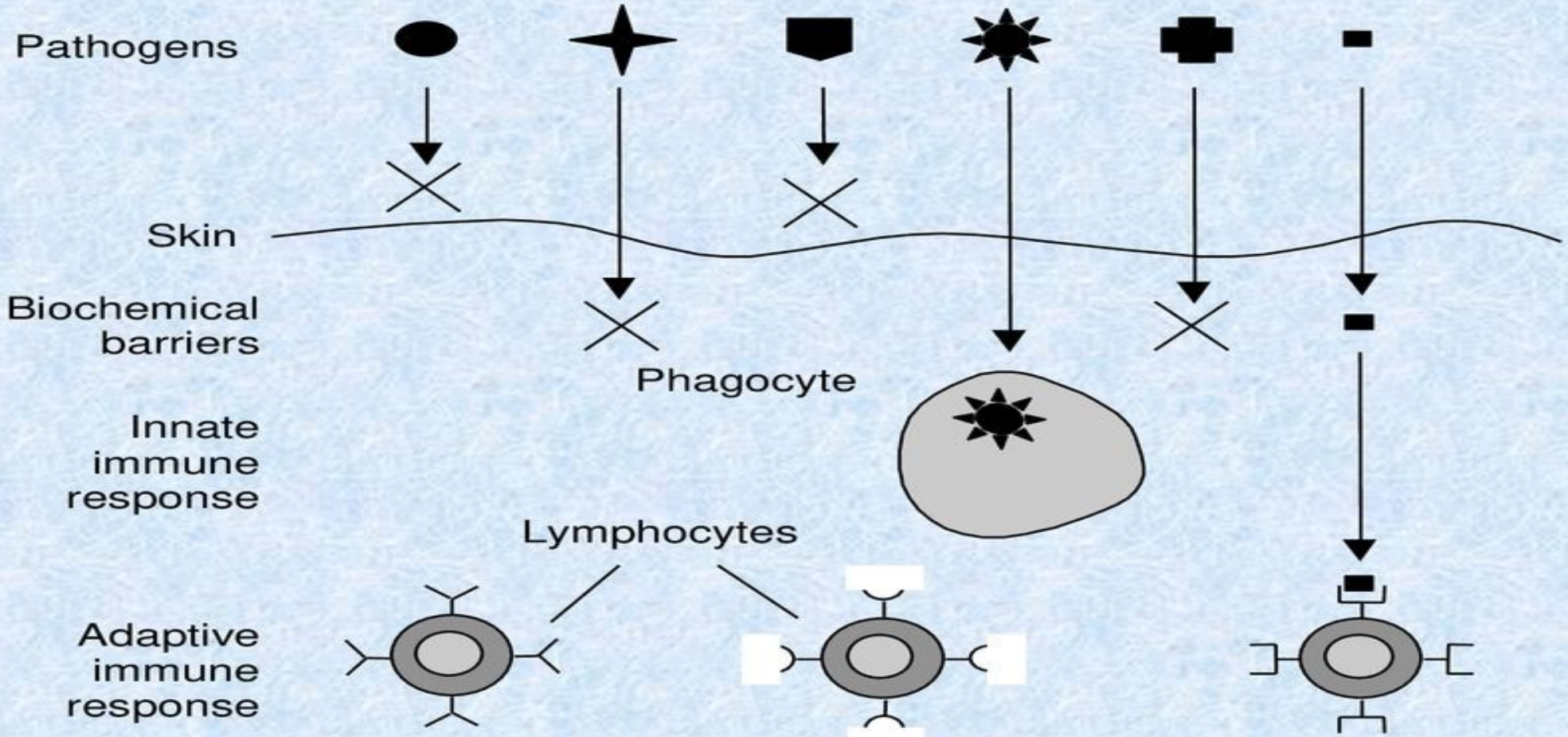
- **Concept of Drug**
  - Kill invaders of foreign pathogens
  - Inhibit the growth of pathogens

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

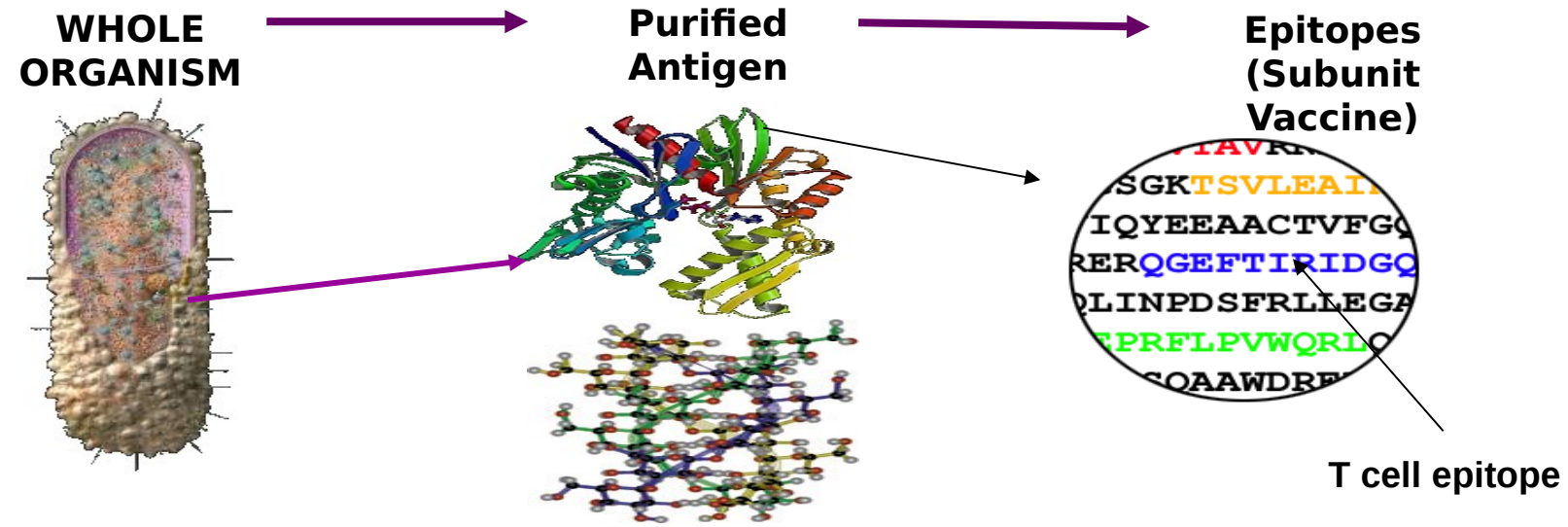
History of Immunization

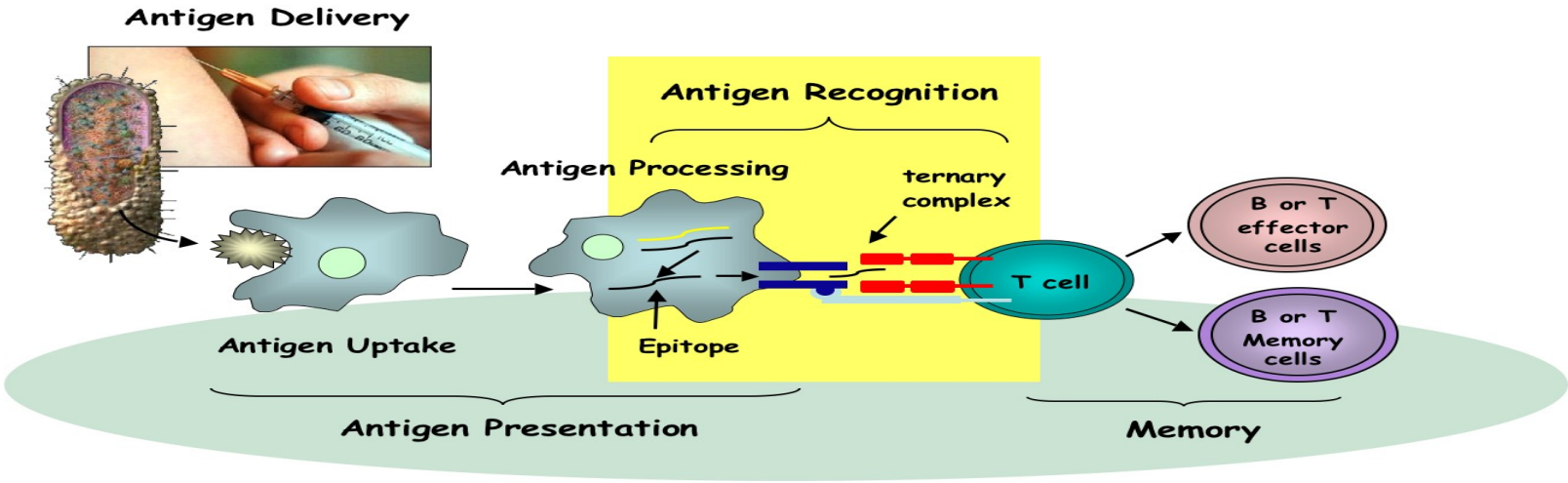
- Children protected who recovered from smallpox
- Immunity induce, a process known as variolation
- Variolation spread to England and America
- Stopped due to the risk of death
- Edward Jenner found that protection against smallpox
- Inoculation with material from an individual infected with cowpox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

Multiple layers of the immune system



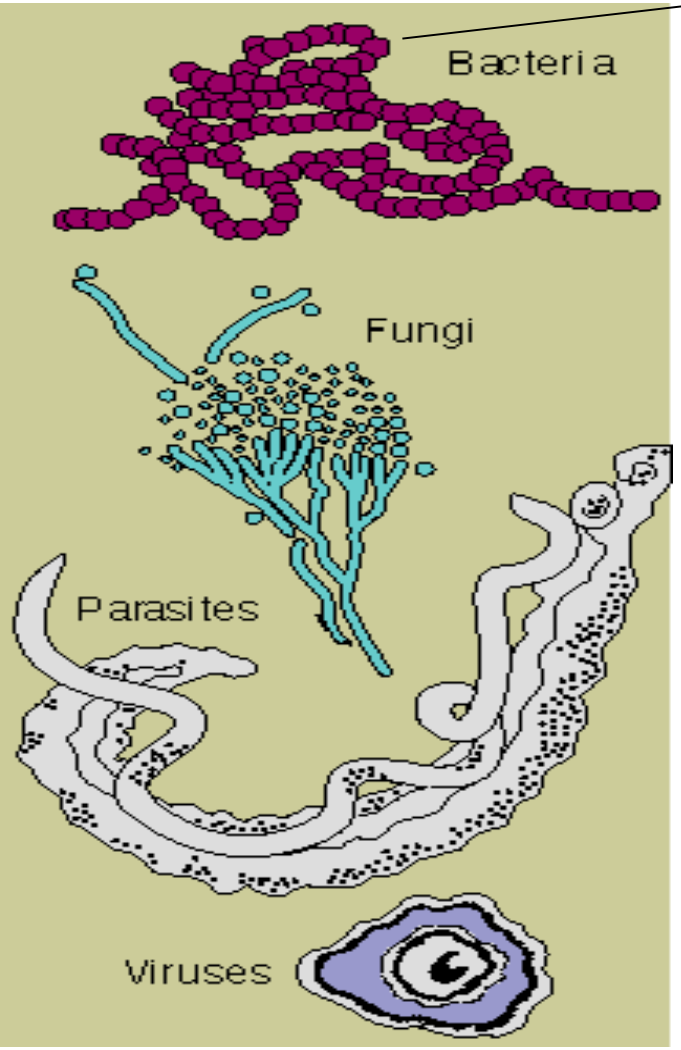
Biomolecules Based Vaccines





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

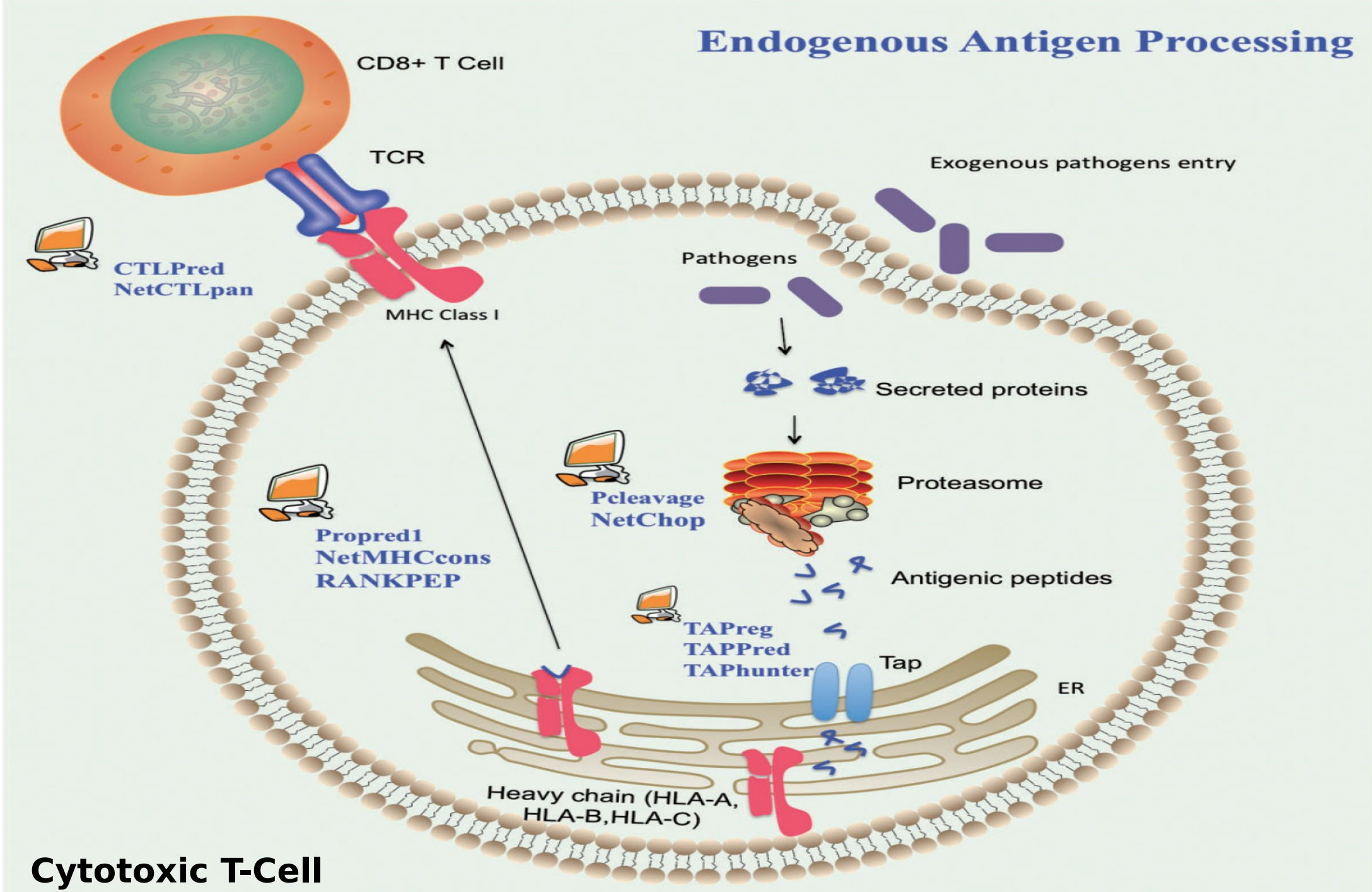
Endogenous Antigen Processing

Exogenous Antigen Processing

CTL Epitopes
MHC I binders
TAP Binders
P. Cleavage Sites

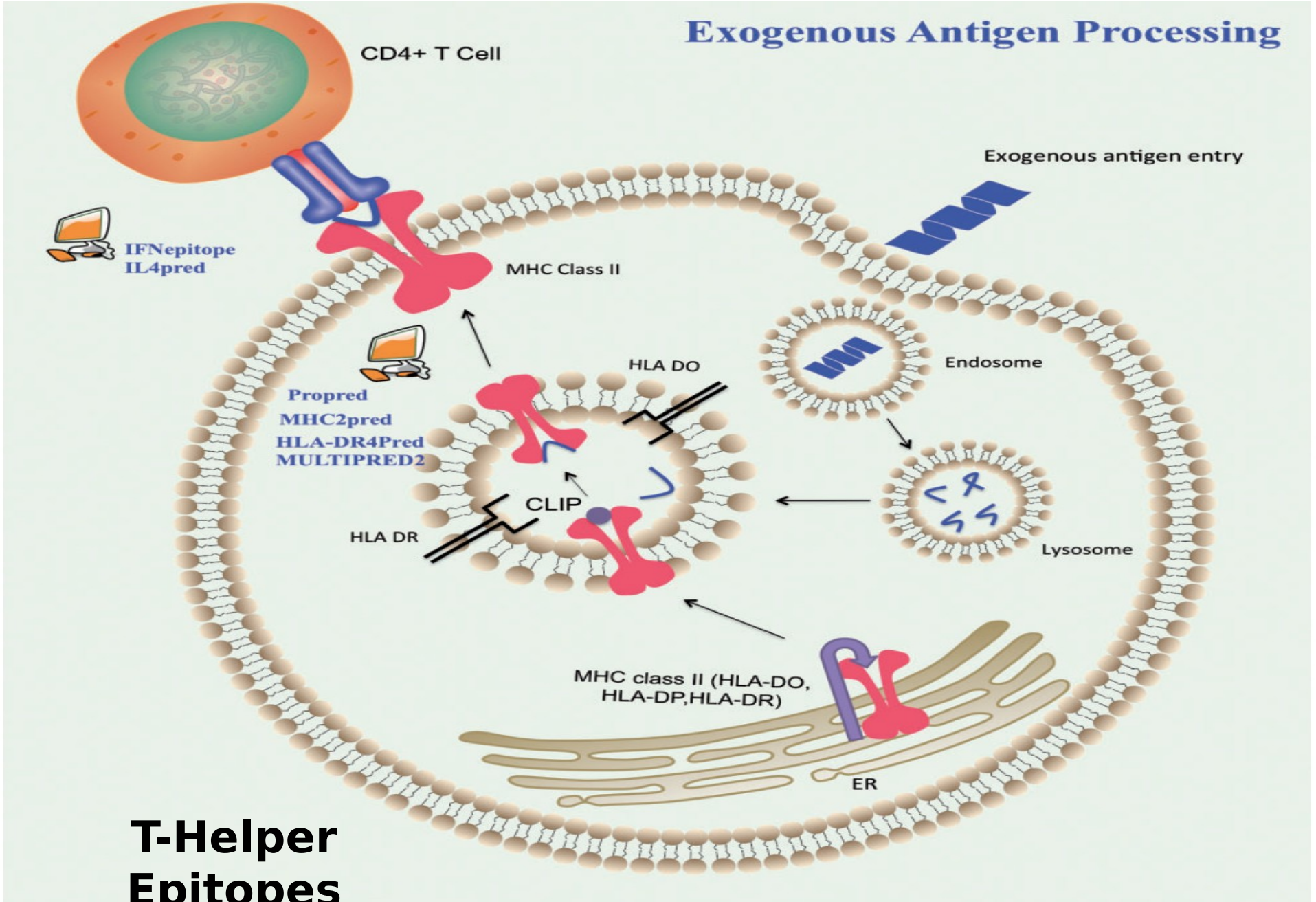
T-Helper Epitopes
MHC II binders

Cell Mediated Immunity (T-cell Epitopes)



Cytotoxic T-Cell Epitopes

Cell Mediated Immunity (T-cell Epitopes)



T-Helper Epitopes

Bioinformatics Center

ProPred.
MHC Class-II Binding Peptide Prediction Server

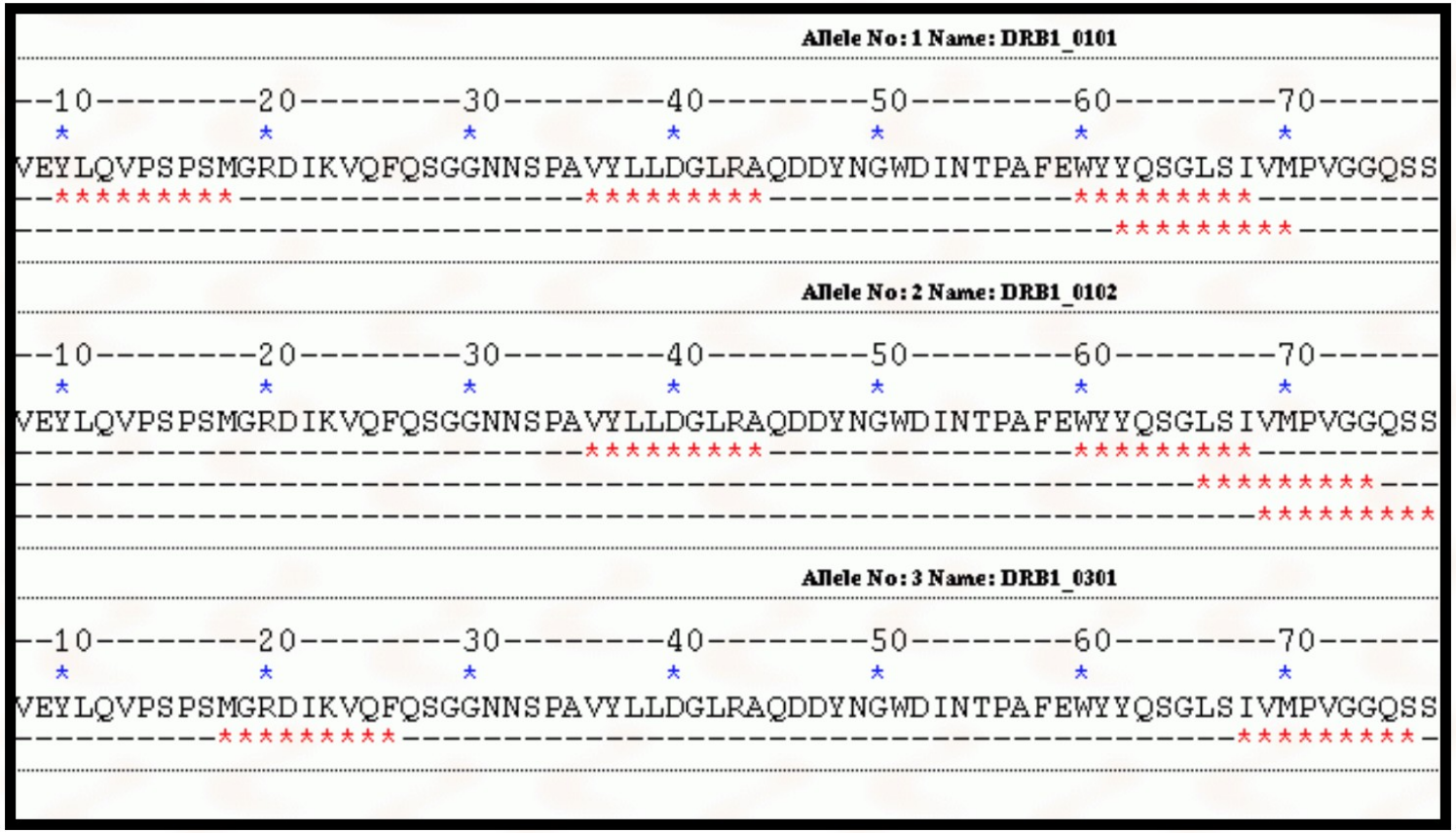
- Prediction Method
- MHC and Prediction Algorithms
- Help
- Virtual matrices
- Related Links
- ProPred Team

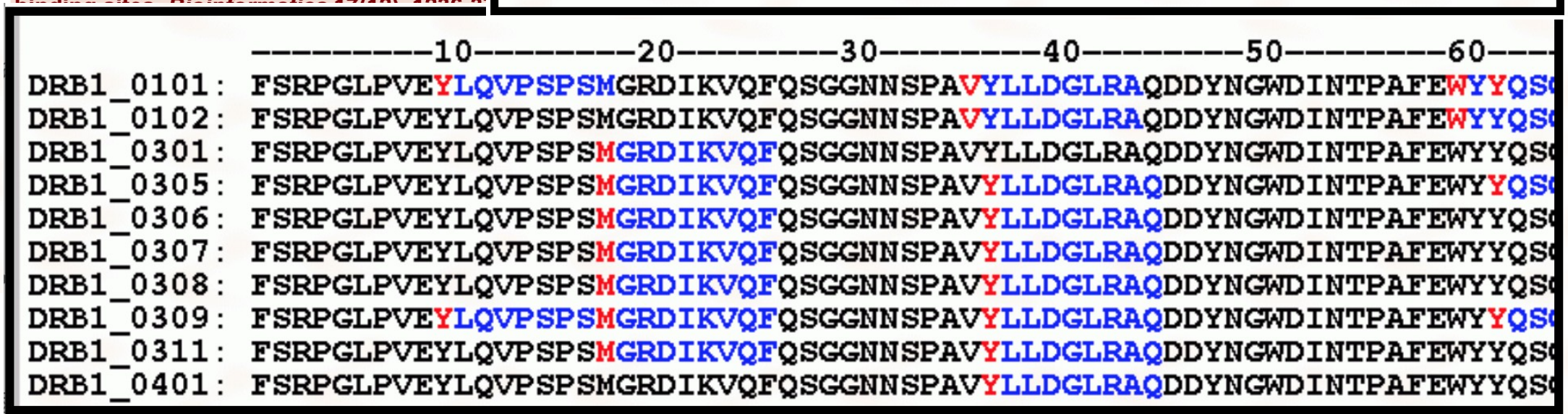
OSDDlinux for Standalone,

Purpose: The aim of this server is to predict M
regions in an antigen sequence, using quantita
from published literature by Sturniolo et. al., 19
in locating promiscuous binding regions that ar
vaccine candidates.

If you are using the results for publication,

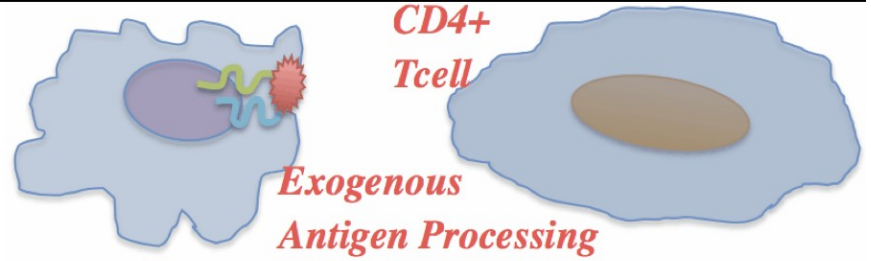
Singh,H. and Raghava,G.P.S.(2001) ProPred





IFNepitope

A server for predicting and designing interferon-gamma inducing epitopes



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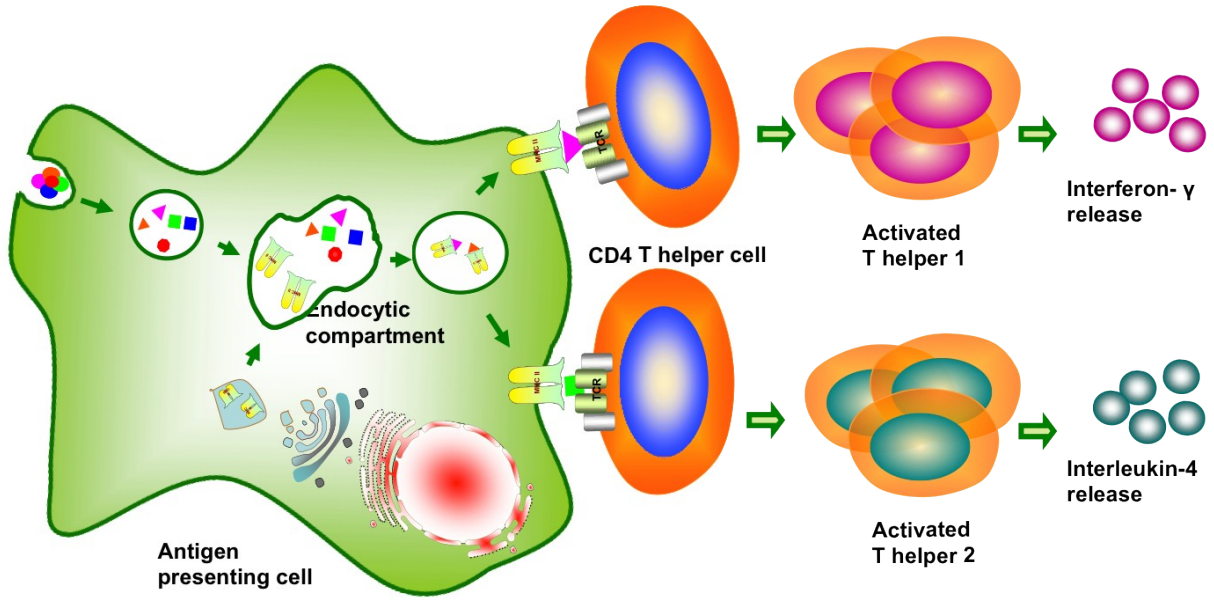
Welcome to IFNepitope Home Page

ında *et. al* 2013: Designing of interferon-gamma inducing MHC class-II binders. Biology Direct 2013



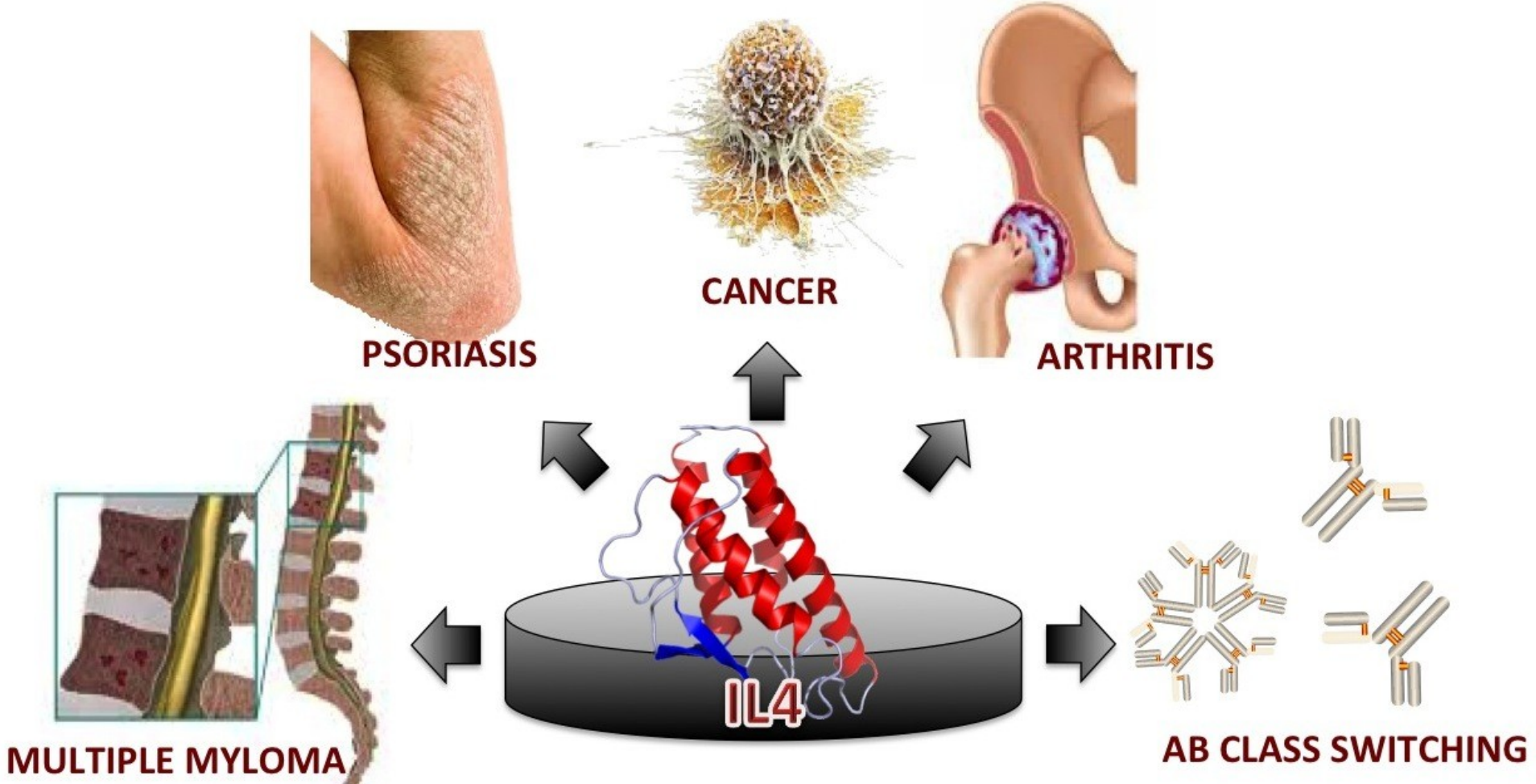
IFN-γ inducing peptides

IFN-γ non-inducing peptides

IL4pred

In Silico Platform for Designing and Disovering of Interleukin-4 inducing peptides

Welcome to Home Page of IL4pred

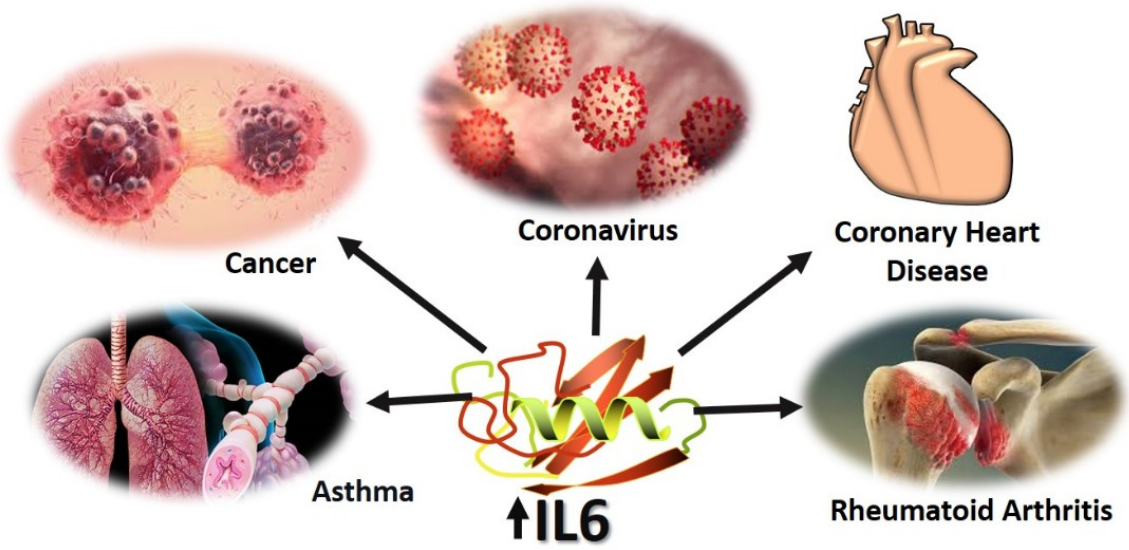


IL-6Pred: Prediction of Interleukin-6 inducing peptides

Home | Predict | Design | Protein Scan | Motif Scan | BLAST Scan | General

Welcome to IL-6Pred

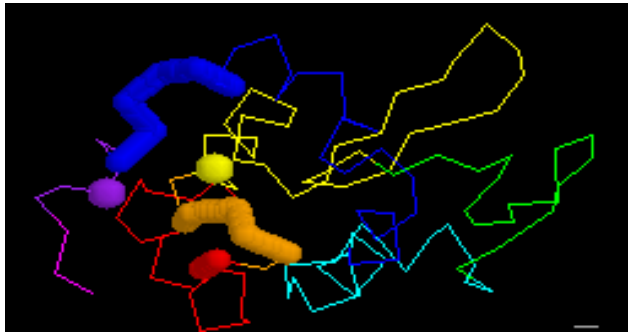
SS, Raghava GPS (2020) Computer-aided prediction and design of IL-6 inducing peptides: IL-6 plays a crucial role in COVID-19 Briefings in Bioinformatics, dx.doi.org/10.1093/bib/bbaa2



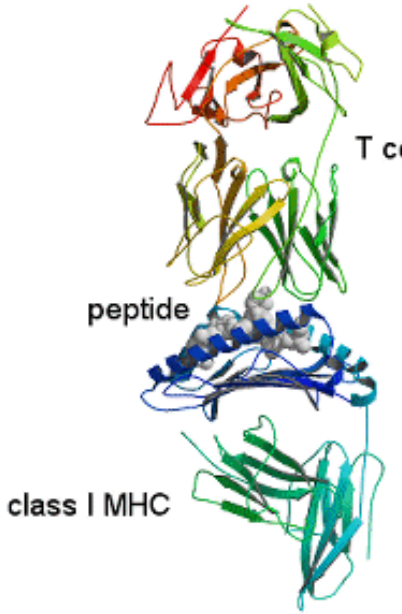
Several methods have been developed for the prediction of the antigenic regions for subunit vaccines designing. Interleukin-6 (IL-6) is a rapidly produced proinflammatory cytokine generated as an immune response in various infections and tissue injuries. Many studies show that high levels of IL-6 are related to a high risk of cancer and other disease conditions such as insulin resistance, asthma, coronary heart disease, advanced-stage cancer. The elevated level of IL-6 causes cytokine release syndrome(CRS) in severe COVID-19 patients. Thus, it is essential to check the subunit vaccine candidate provided to a COVID-19 patient must not be IL-6 inducing peptide. Based on our knowledge, we develop an in silico tool that allows the user to predict, scan, and map the IL-6 inducing/non-inducing peptides.

Types of epitopes

B cell Epitope



- Conformational
- Non-Conformational
  - Linear B cell Epitope
  - T cell Epitope



CTL epitope

Class I MHCs

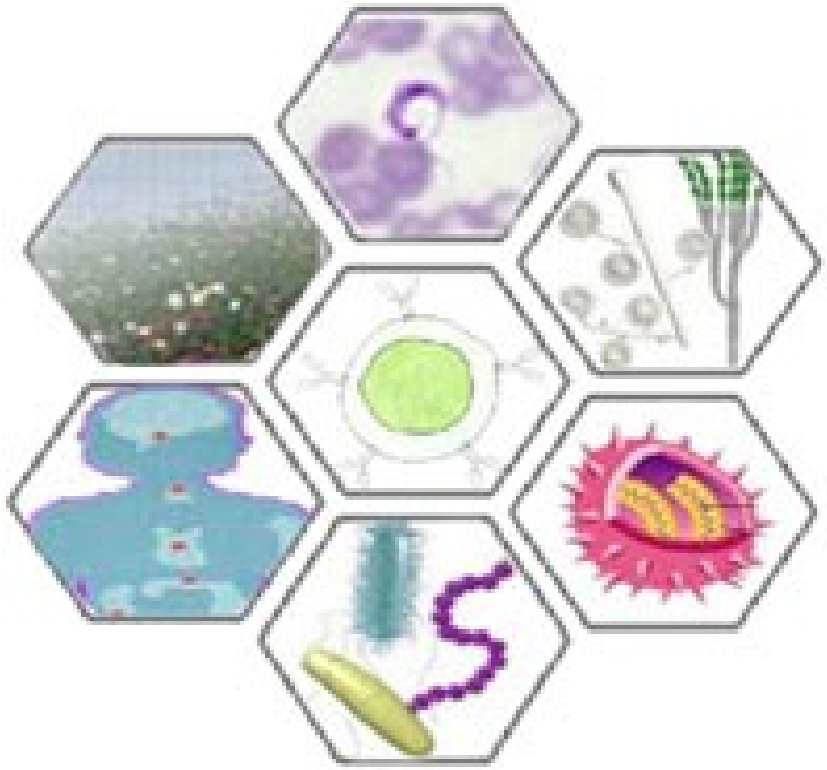
Endogenous Antigen Processing

Helper T cell epitope

Class II MHCs

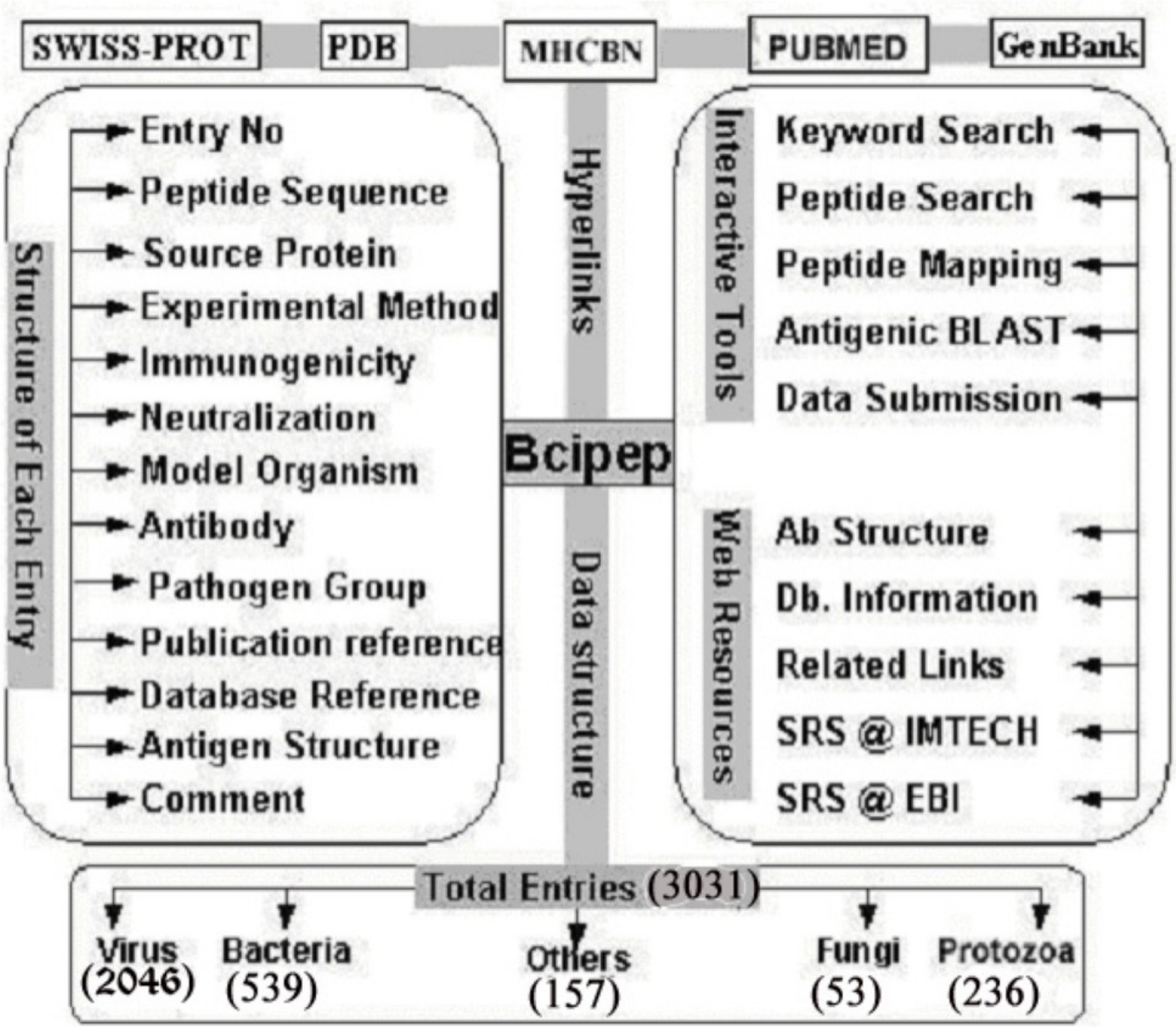
Exogenous Antigen Processing

BCIPEP: A database of B-cell epitopes.



Saha et al.(2005) BMC Genomics 6:79.

Saha et al. (2006) NAR (Online)

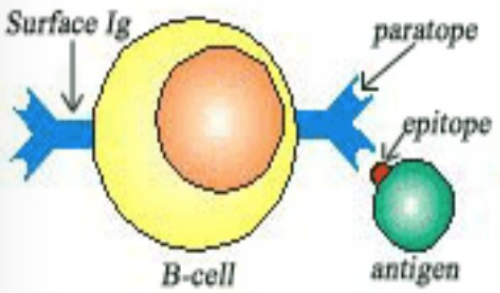


BCEpred: Benchmarking of physicocemical properties used in existing B-cell epitope prediction methods

In 2003, we evaluate parmeters on 1029 non-redudant B-cell epitopes obtained from BCIpep and 1029 random peptide. Saha and Raghava (2004) ICARIS 197-204

Physico-chemical Properties	Threshold	Sensitivity	Specificity	Accuracy% (Max)
Hydrophilicity [1]## (Parker et al., 1986)**	2.00	33	76	54.47
Accessibility[2](Emini et al., 1985)	2.00	65	46	55.49
Flexibility [3] (Karplus and Schulz, 1985)	**1.90**	**47**	**68**	**57.53**
Surface [4] (Janin and Wodak, 1978)	2.40	37	74	55.73
Polarity [5](Ponnuswamy et al., 1980)	2.30	2.8	81	54.08
Turns [6] (Pellequer et al., 199)	1.90	17	89	52.92
Antigenic Scale [7] (Kolaskar and Tongaonkar, 1990)	1.80	59	52	55.59
[3]+[1]+[5]+[4]	**2.38**	**56**	**61**	**58.70**

Residue property number, for each property a number is assigned. [3]+[1] means combination of Flexibility and Hydrophilicity



OSDDlinux for Standalone, Galaxy & Local version

Bcepred: Prediction of linear B-cell epitopes, using physico-chemical properties

We evaluated the performance of existing linear B-cell epitope prediction methods based on physico-chemical properties on a non-redundant dataset. The dataset consists of 1029 B-cell epitopes obtained from Bcipep database and equally number of non-epitopes obtained randomly from Swiss-Prot database. The prediction accuracy for models based of various properties varies from 52.92% and 57.53%. We achived highest accuracy of 58.70% at threshold 2.38, when we combined four amino acid properties(hydrophilicity, flexibility, polarity and exposed surface).

Based on our evaluation and analysis we have developed a web server Bcepred for predicting linear B-cell epitopes in a protein sequence. This server allows users to predict B-cell epitopes using any of the physico-chemical properties (**hydrophilicity, flexibility/mobility, accessibility, polarity, exposed surface** and **turns**) or combination of properties.

It presents the results in graphical and tabular frame. In case of graphical frame, this server plot the residue properties along protein backbone, which assist the users in rapid visulaziation of B-cell epitope on protein. The peak of the amino acid residue segment above the threshold value (default is 2.38) is considered as predicted B-cell epitope. The tabular output is in the form of a table, which will give the normalized score of the selected properties with the corresponding amino acid residue of a protein along with the maximum, minimum and averages values of the combined methods, selected.

ABCpred

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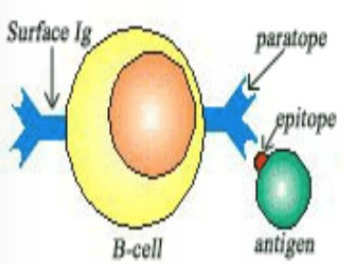
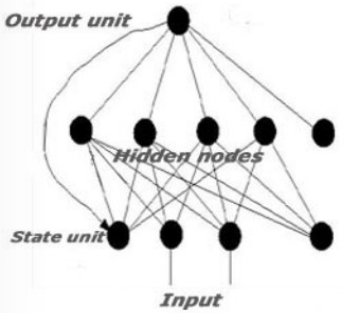
Artificial neural network based B-cell epitope prediction server

Home | Submission | Help | Method | Team

Datasets



B-cell and epitope of antigen



Recurrent neural network

The aim of ABCpred server is to predict *B cell epitope(s)* in an antigen sequence, using artificial neural network. This is the first server developed based on recurrent neural network (machine based technique) using fixed length patterns.

Algorithm: The machine-learning technique need fixed length patterns for training or testing whereas B-cell epitopes vary 5 to 30 residues as reported in literature(Bcipep database **Bcipep**). In order to overcome this problem we made an attempt to create datasets of fixed length patterns from B-cell epitopes by eliminating or adding residues at terminals. The dataset used for training and testing consists of 700 B-cell epitopes and 700 non B-cell epitopes (random peptides) of maximum length of 20 residues. We tried different neural networks and achived an accuracy of 65.93% using recurrent neural network.

Users can select window length of 10, 12, 14, 16 and 20 as predicted epitope length. It presents the results in graphical and tabular frame. In case of graphical frame, this server plot the epitopes in blue color along protein backbone (black color), which assist the users in rapid visulaziation of B-cell epitope on protein. The tabular output is in the form of a table, which will provide the aminoacids length from N-terminal to C-terminal in a protein predicted by the server.

The server is able to predict epitopes with **65.93% accuracy** using recurrent neural network.

Please cite following paper if you are using ABCpred server

Saha, S and Raghava G.P.S. (2006) Prediction of Continuous B-cell Epitopes in an Antigen Using Recurrent Neural Network. Proteins,**65(1)**,40-48 PMID: 16894596

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CBTOPE- Conformational B-cell Epitope Prediction

CBTOPE-Menu

- Home
- Submit Sequence
- Algorithm
- Developers
- Help
- Supplementary Data
- Contact Us
- Standalone CBTOPE 

About CBTOPE

It has been observed that conformational B cell epitopes (~90% of all B cell epitopes) are more complex and hard to define than sequential epitopes. Several methods do exist for the prediction of conformational B cell epitope but they require antigen 3D structure or homology based model of the amino acid sequence. So far no method is available which can predict conformational B cell epitope using antigen primary sequence in the absence of any homology with the known structures. In the present study using amino acid composition as an input feature for Support vector machine (SVM) we developed a model with prediction accuracy of more than 85% and Area under curve (AUC) 0.9.

If you are using this webserver, please cite:

Hifzur Rahman Ansari and Gajendra PS Raghava. **Identification of conformational B-cell Epitopes in an antigen from its primary sequence.**
Immunome Research 2010, 6:6.

LBtope: Linear B-cell Epitope Prediction Server

Prediction of Epitopes

Antigen sequence

Multiple peptides

Peptide mutatants

Important B-cell epitope server

Abcpred

Bcepred

BCPREDS

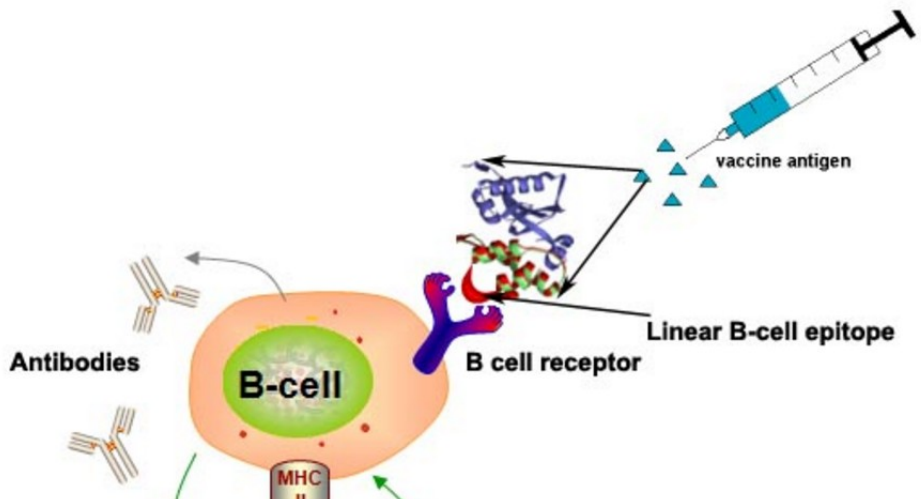
COBEpro

BepiPred

OSDDlinux for Standalone, Galaxy & Local version

LBtope : Prediction of Linear B-cell Epitopes

Predict of B-cell epitopes (antigenic region) with high accuracy is one of the major challenges in designing subunit/peptide vaccine or immunotherapy. In past number of methods have been developed for predicting linear or continious B-cell epitopes like ABCpred. These existing methods have two major limitations, first they developed on small dataset, second random peptides were used as non B-cell epitopes in these methods.



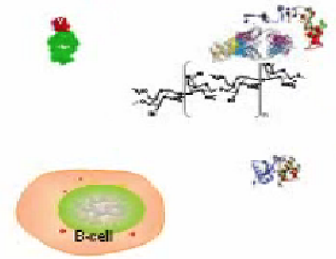
IgPred

Prediction of Antibody-specific B-cell epitopes

**** If you are using this server please cite Gupta et al. (2013) Identification of B-cell epitopes in an antigen for inducing specific class of antibodies. **Biology Direct 8:27** ***** || ***** OSDDlinux for Standalone & Local version ******

********Click here to download Debian file for OSDDlinux-standalone of IgPred********

IgPred is a web server developed for predicting different types of B-cell epitopes that can induce different class of Antibodies like IgG, IgE and IgA. In past large number of methods have been developed for predicting B-cell epitopes but no method have been developed for predicting antibody-specific epitopes. One of the major features of this server is that it assist users in designing B-cell epitopes using rational technique of mutation.



All models implemented in IgPred, were developed on experimentally validated non-redundant dataset and evaluated using five-fold cross validation technique. In addition, performance of these models were also evaluated on an indepenandent dataset. The performance of these models in term of accuracy is around 80% .

This is a user-friendly web server developed for researchers working in the field vaccinology or immunology. In order to provide efficient service to community we classify serivices in following five modules.

- **Epitopes Prediction:** This module allows users to predict whether a peptide is B-cell epitope or not. If a peptide is a B-cell epitope then what class of antibody it will induce. This module has options for predicting antibody-class specific B-cell epitopes for **variable length** and for **fixed length** peptides. This module is designed for virtual scanning, selecting desired B-cell epitopes in a set of peptides.

- **Protein Scan:** This module assists users to identify antigenic regions in a protein or antigen sequences. It has two options for model selection namely **Variable length**: for user defined window length and **Fixed length**: for fixed length window This module simply scan a protein to identify IgG-, IgA- or IgE-specific B-cell eptopes.

- **Epitope Mapping:** The module is designed for **mapping experimentally validated B-cell** epitopes in an antigen or protein sequence. This module identify antibody-specific B-cell epitopes availble in IEDB in users query sequence.

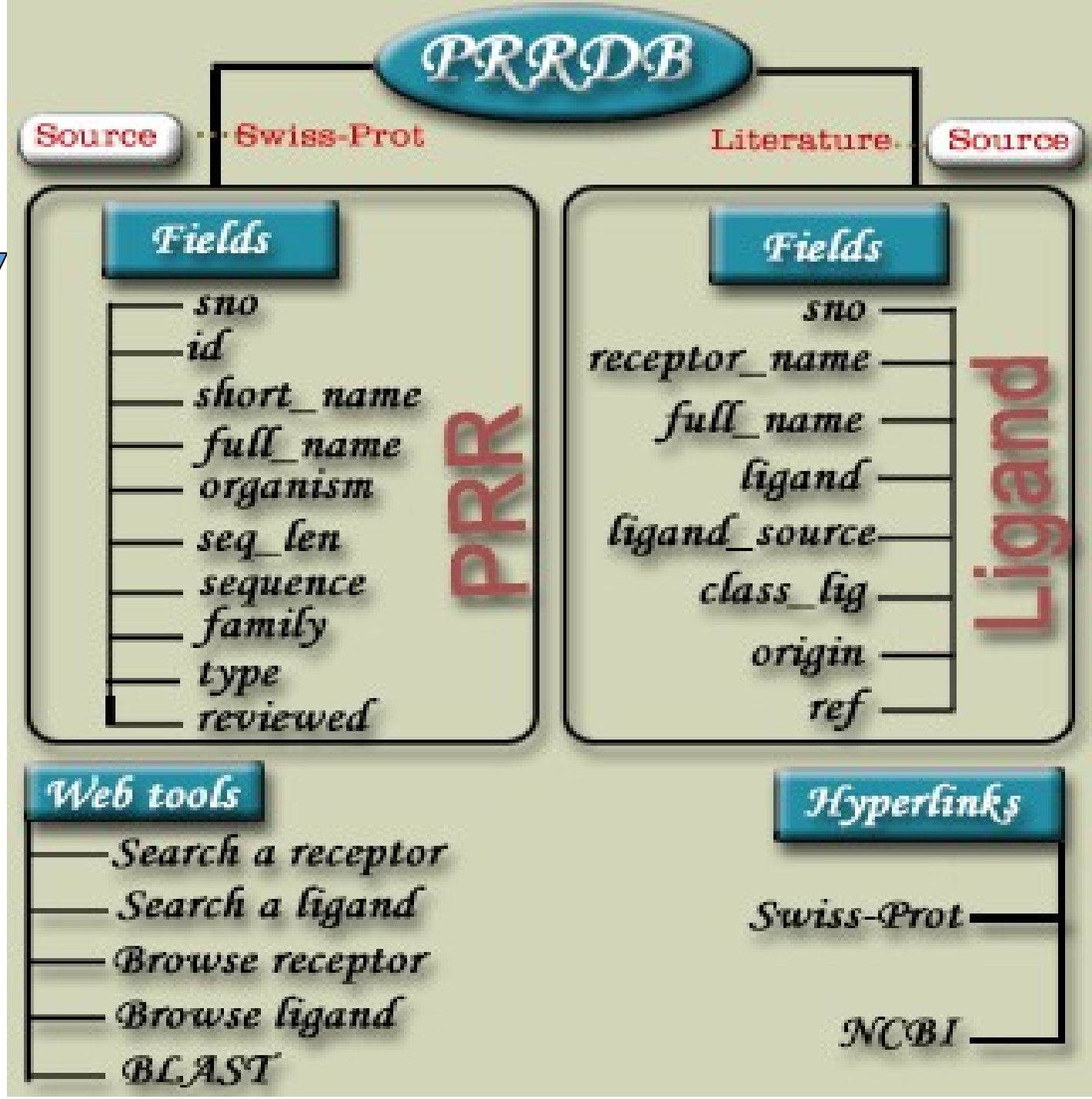
PRRDB is a database of pattern recognition receptors and their ligands

~500 Pattern-recognition Receptors

228 ligands (PAMPs)

77 distinct organisms

720 entries

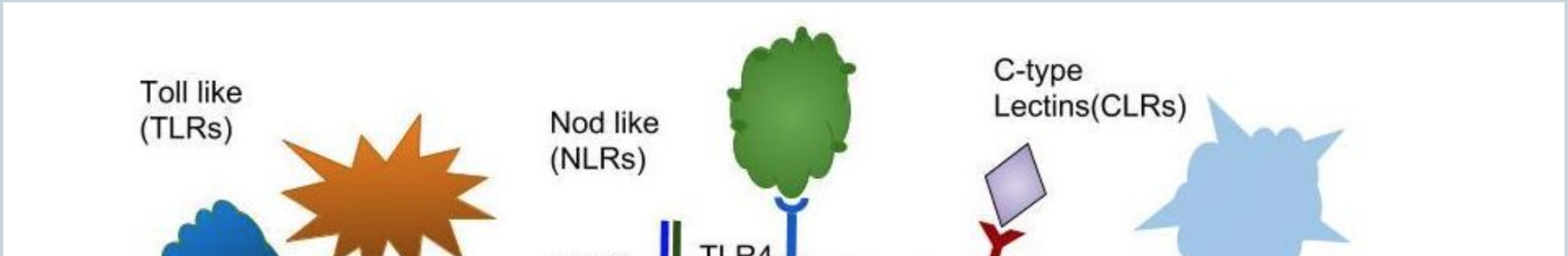


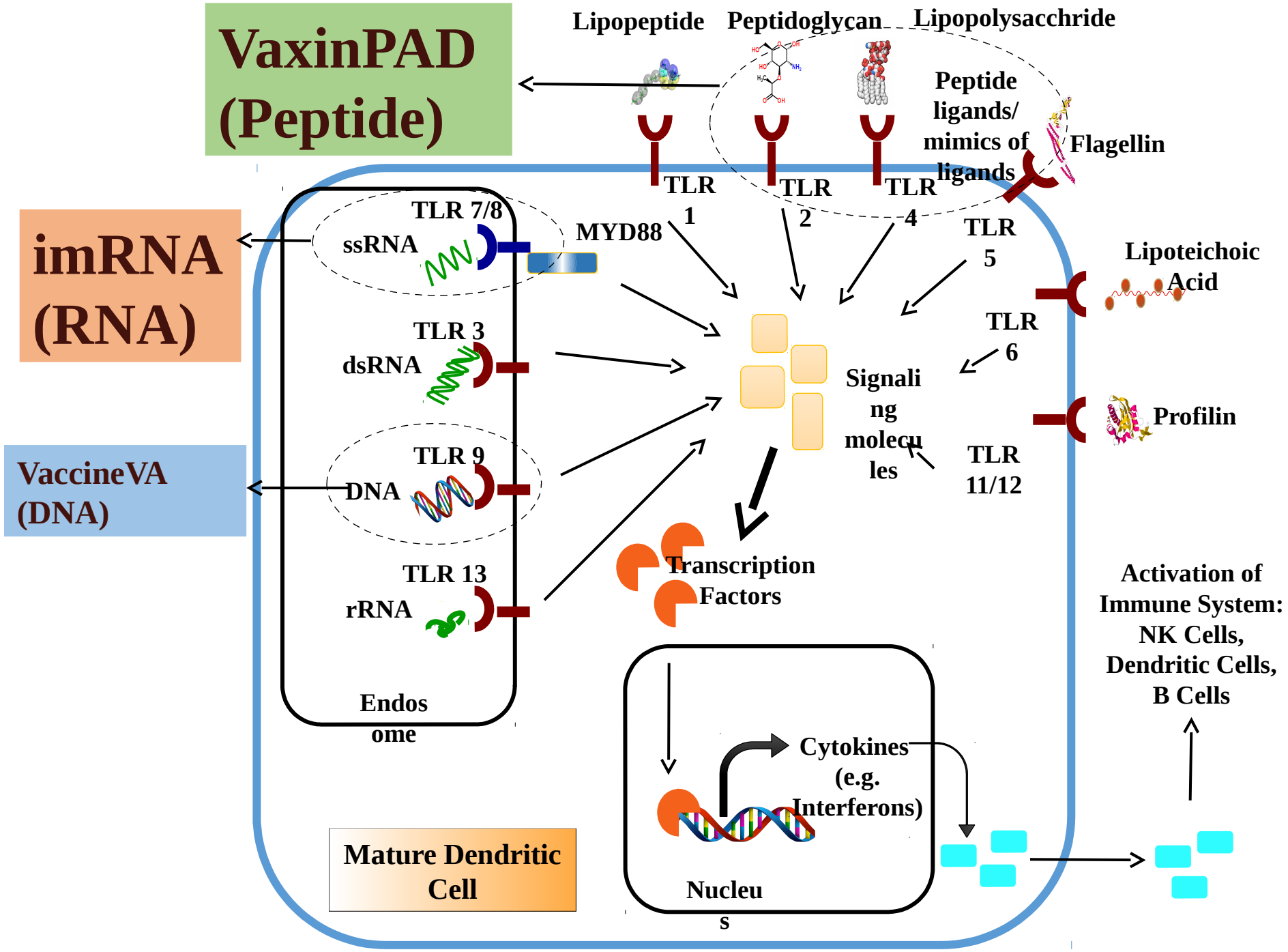
PRRDB 2.0 : Pattern Recognition Receptor Database

Welcome to PRRDB 2.0

ference: Kaur et al., (2019) PRRDB 2.0: a comprehensive database of pattern-recognition receptors and their ligands. Database, Volume 2(

PRRDB2.0 is a comprehensive database of pattern recognition receptors and their ligands. This is an updated version of the database PRRDB. It contains extensive information about 467 unique pattern-recognition receptors and 827 ligands manually extracted from ~600 research articles. This is a manually curated database where information about PRRs and their ligands is extracted manually from research articles and public databases.




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

Menu
Home
Submission
Help
Algorithm
Supplementary
Related Links
Acknowledgements

AlgPred: Prediction of Allergenic Proteins and Mapping of IgE Epitopes

Introduction

Mirror site at UAMS

The prediction of allergenic proteins is becoming very important in present time due to use of modified proteins in foods (genetically modified foods), therapeutics, bio-pharmaceuticals etc. World Health Organization (WHO) and Food and Agriculture Organization (FAO) realize the importance of prediction and proposed guidelines to assess the potential allergenicity of proteins. In past, number of approaches and methods has been developed to predict allergens; each has their own merits and demerits. In AlgPred a systematic attempt has been made to integrate various approaches in order to predict allergenic proteins with high accuracy.

The salient features of AlgPred server are,

- **Algpred allows prediction of allergens based on similarity of known epitope with any region of protein.**
- **The mapping of IgE epitope(s) feature of server allows user to locate the position of epitope in their protein.**
- **Server search MEME/MAST allergen motifs using MAST and assign a protein allergen if it have any motif.**
- **Allows to predict allergens based on SVM modules using amino acid or dipeptide composition.**
- **It facilitates BLAST search against 2890 allergen-representative peptides (ARPs) obtained from Bjorklund et al 2005 and assign a protein allergen if it have a BLAST hit..**
- **Hybrid option of server allows to predict allergen using combined approach (SVMc + IgE epitope + ARPs BLAST + MAST).**

World Health Organization (WHO) and Food and Agriculture Organization (FAO) proposed guidelines to assess the potential allergenicity of protein are available from http://www.fao.org/es/ESN/food/pdf/allergygm.pdf.

Please cite following paper if you are using Algpred:

Saha, S. and Raghava, G.P.S. (2006) AlgPred: prediction of allergenic proteins and mapping of IgE epitopes. Nucleic Acids Research, Volume 34, W202-W209.

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

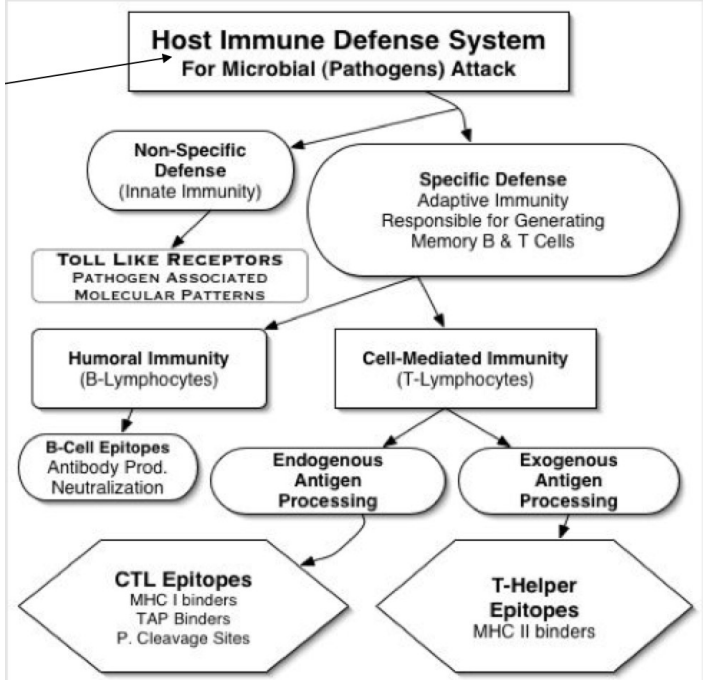
PRRDB: A database of PRRs & ligands

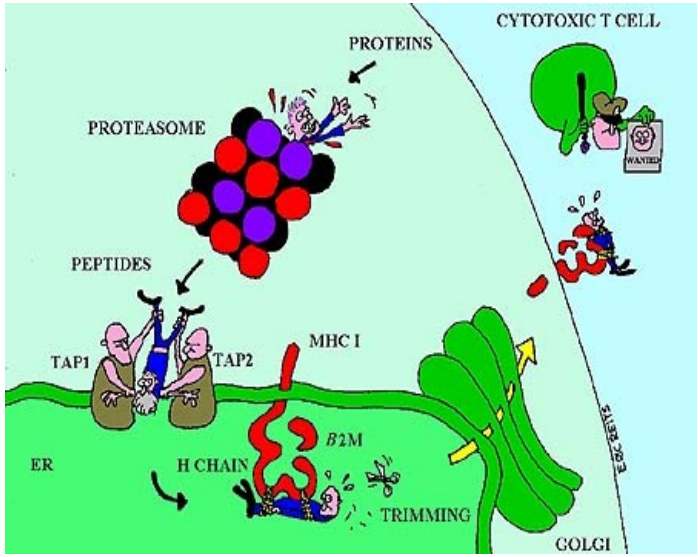
VaccineDA: DNA-based adjuvants

imRNA: Immunomulatory RNAs

VaccinePAD: Peptide-based adjuvants

PolysacDB: Polysaccharide antigens



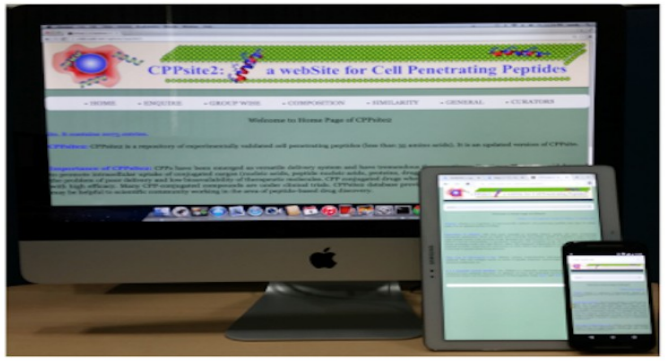


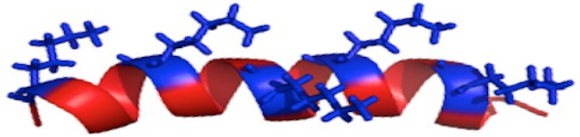
Drug Delivery

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

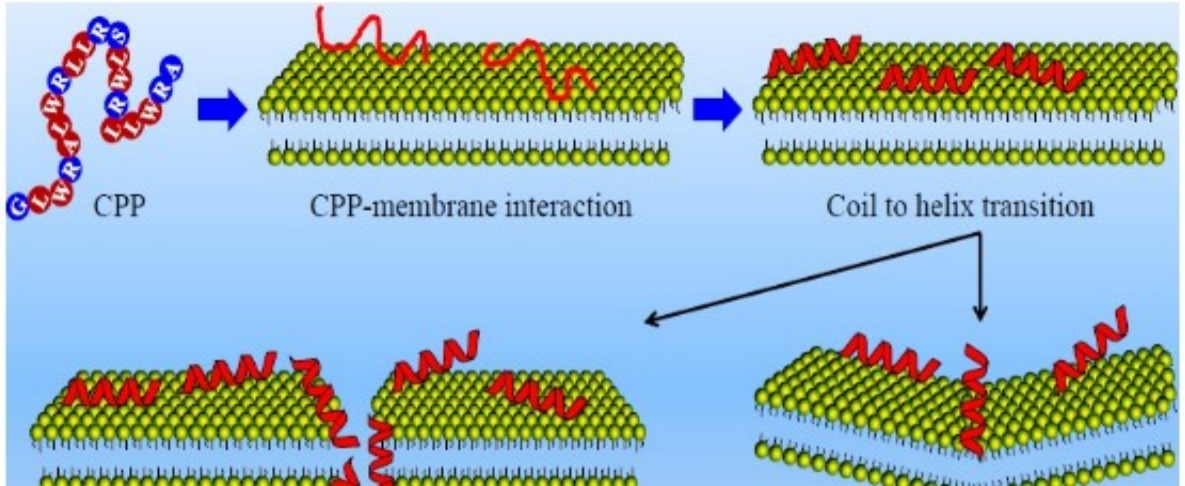
utam *et al.*: *In silico* approaches for designing highly effective cell penetrating peptides. *Journal of Translational Medicine* 3 11:74.Link

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

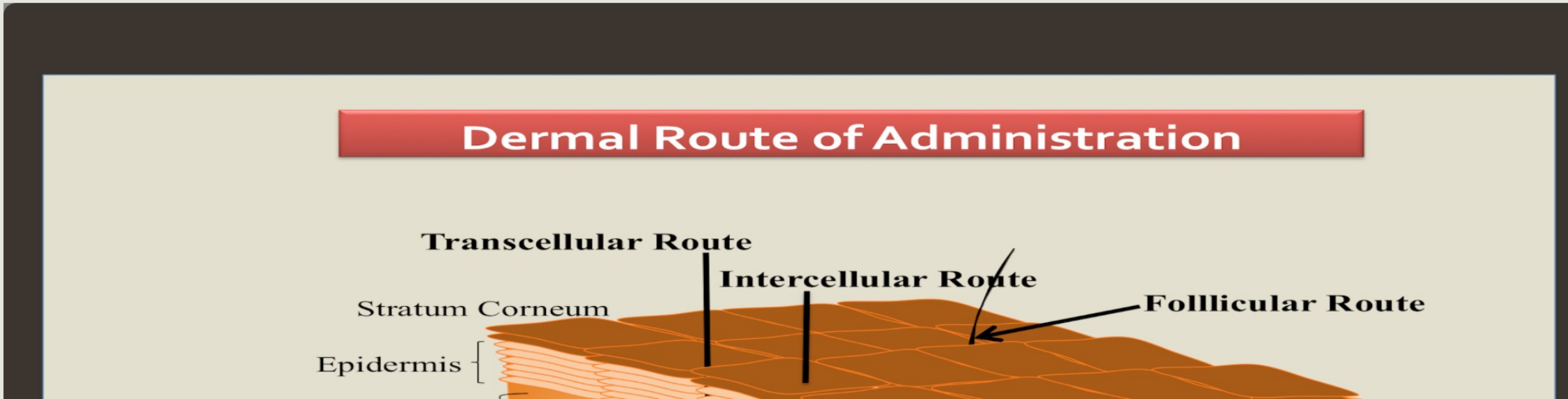
TOPICALLY DELIVERED PEPTIDE DATABASE

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.

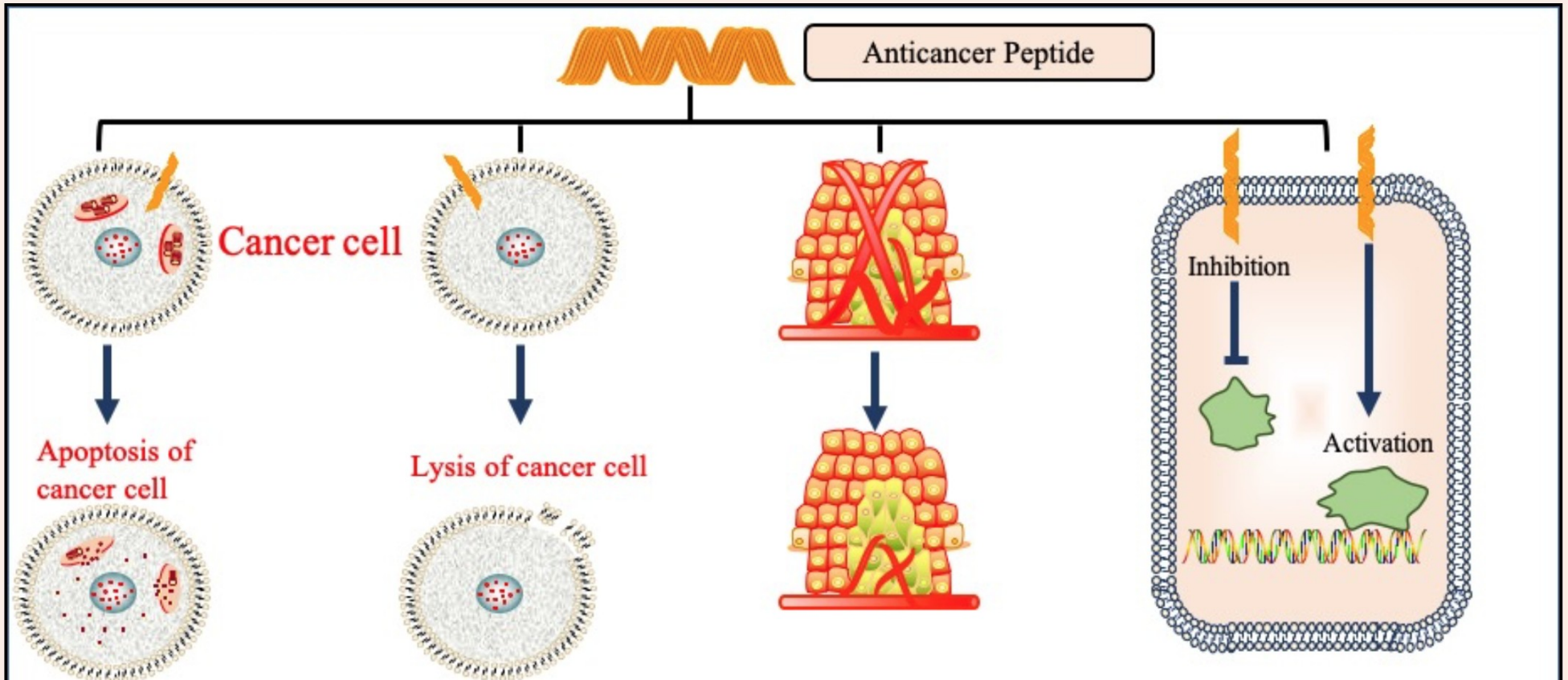
Developed by: Bioinformatics Centre, Institute of Microbial Technology, Sec-39A, Chandigarh,

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

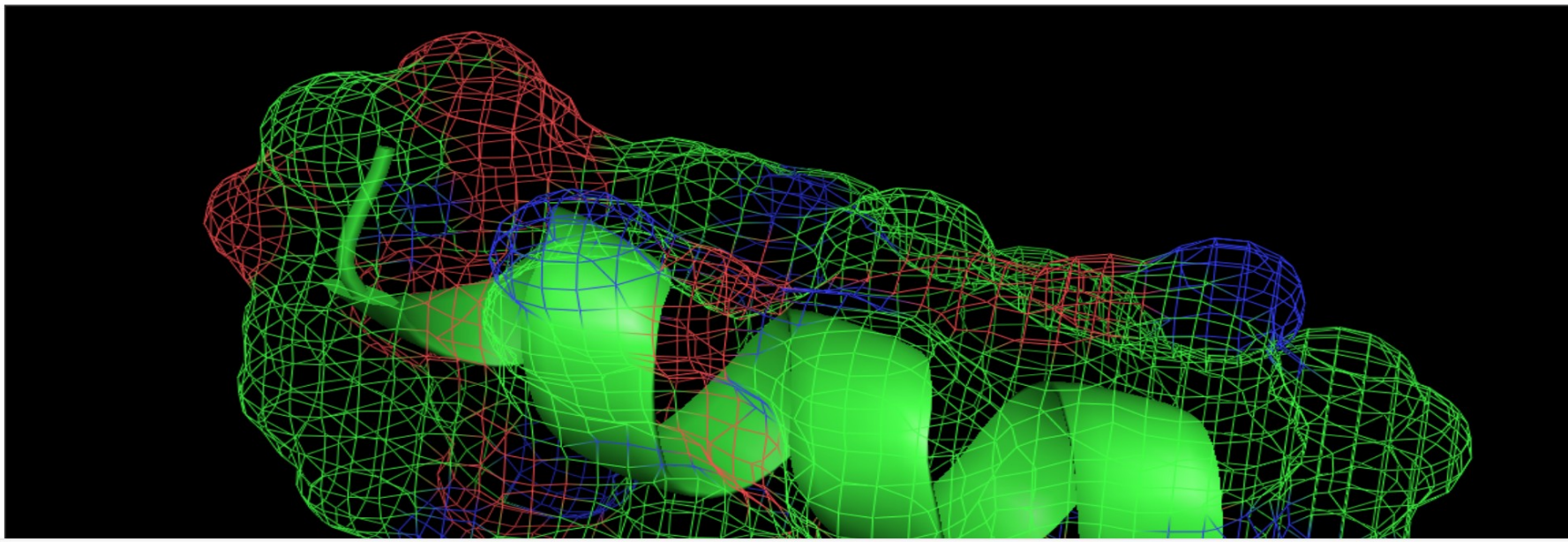
ANTIHYPERTENSIVE PEPTIDE INHIBITORS

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

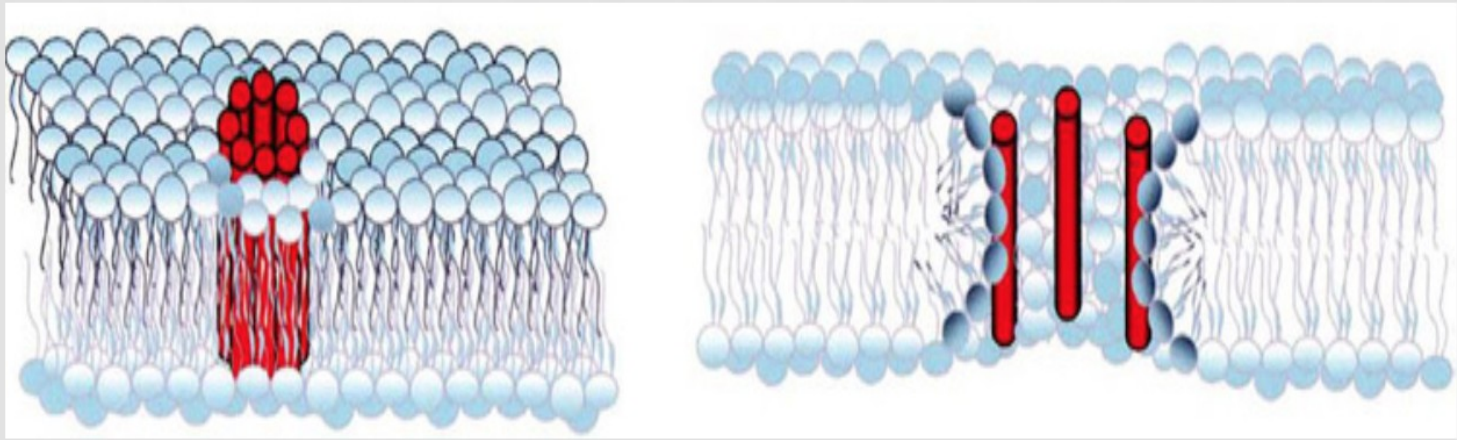
- Home
- Algorithm
- Submission
- Help
- Team
- Contact

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** .

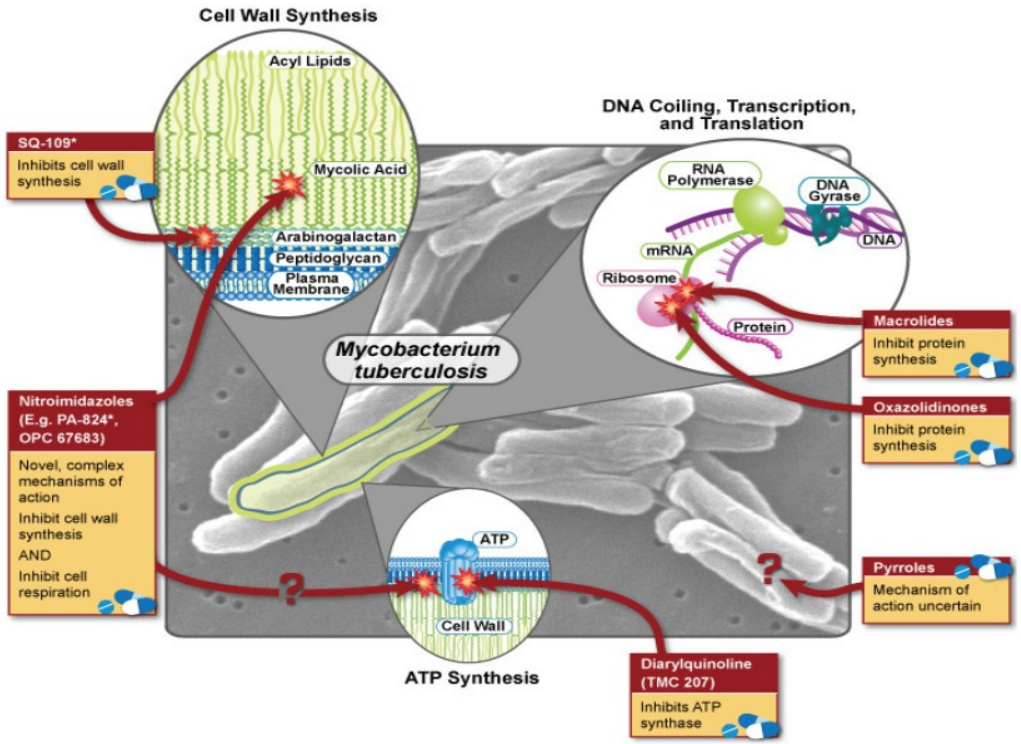
Peptide based Inhibitors

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

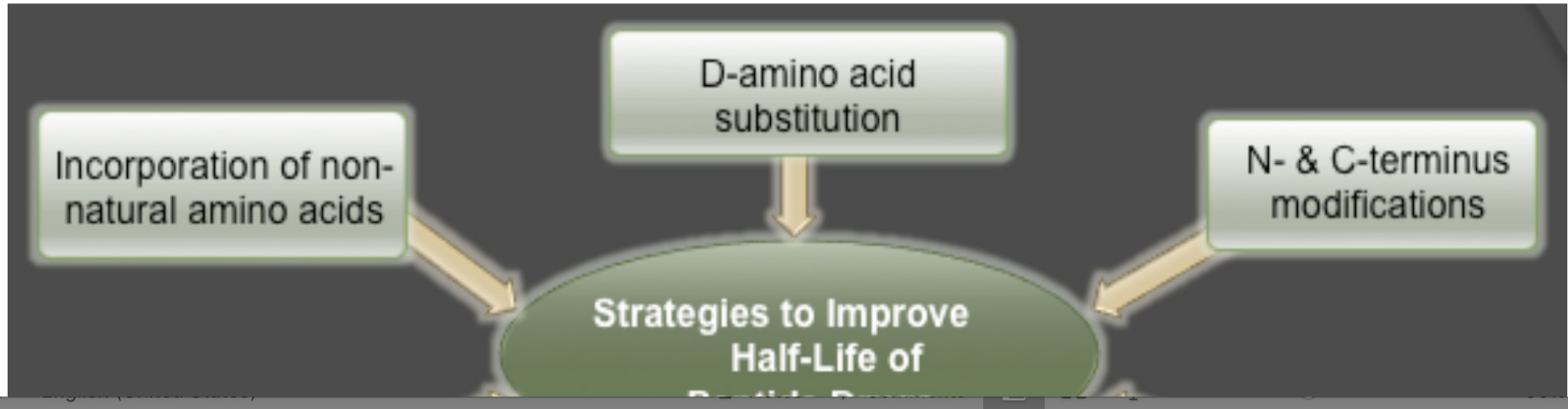
PEPlife

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



Toxicity

crdd.osdd.net/raghava/toxinpred/

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

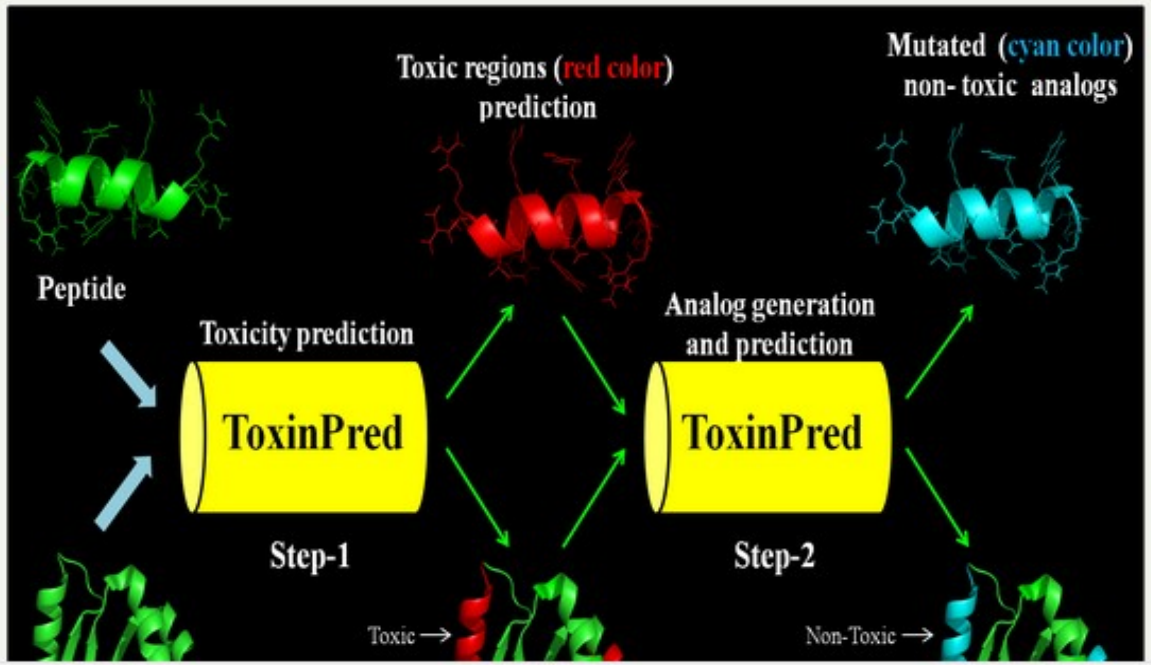
ToxinPred

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.

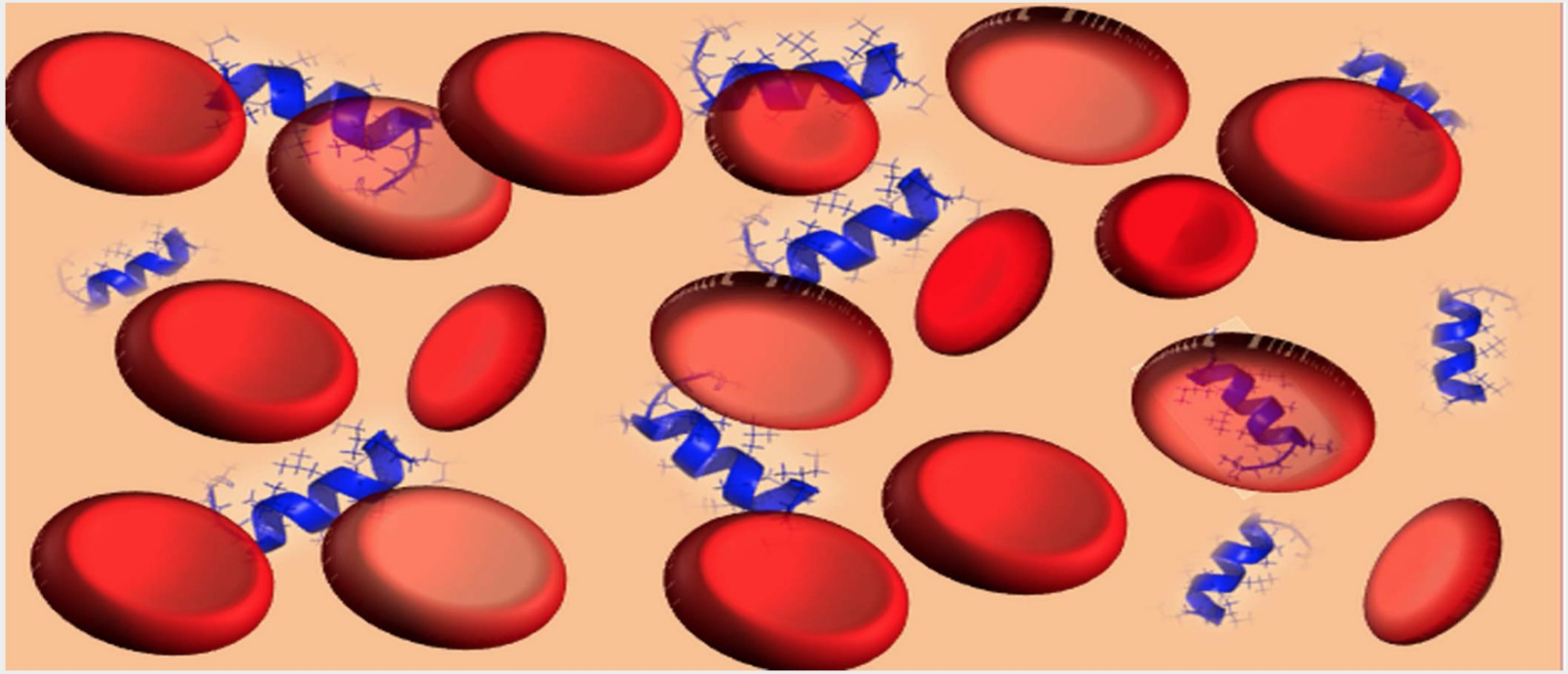
(4) **QMS Calculator:** This tool allows the users to submit query peptide in FASTA format and to optimize the peptide sequence to get maximum/minimum/desired toxicity based upon the Quantitative Matrix based position specific scores. It will help the user to tweak any residue from the predecessor peptide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

Peptide Structure

PEPstr: PEPTIDE TERTIARY STRUCTURE PREDICTION SERVER

Bioinformatics Centre, Institute of Microbial Technology, Chandigarh

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[HOME] [PREDICTION METHOD] [PERFORMANCE] [HELP] [REFERENCES] [TEAM]

The Pepstr server predicts the tertiary structure of small peptides with sequence length varying between 7 to 25 residues. The prediction strategy is based on the realization that β-turn is an important and consistent feature of small peptides in addition to regular structures. Thus, the methods uses both the regular secondary structure information predicted from PSIPRED and β-turns information predicted from BetaTurns. The side-chain abgles are placed using standard backbone-dependent rotamer library. The structure is further refined with energy minimization and molecular dynamic simulations using Amber *version6*.

Usage: Paste your one-letter amino acid sequence in the textarea provided below..

Sequence name :

Choose the peptide environment: Vacuum

Paste the peptide sequence below : Help

Enter your e-mail address:

SUBMIT CLEAR

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.

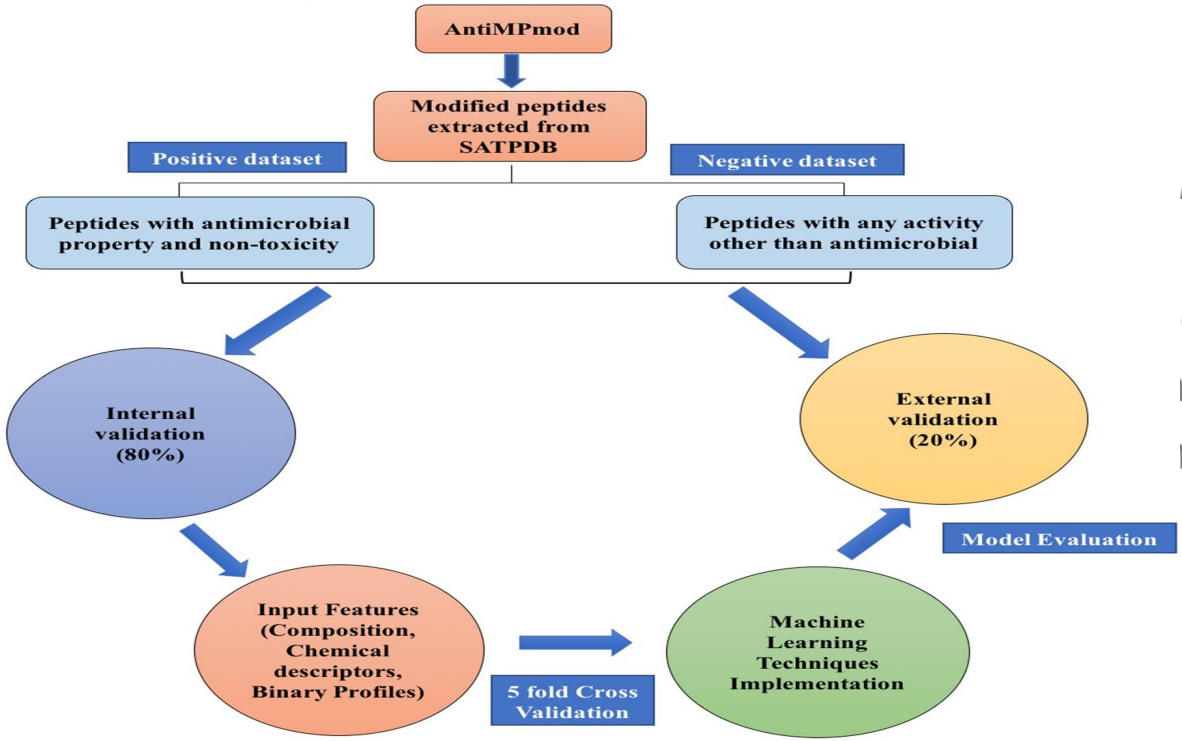
(4) Download: This module of CellPPD-Mod allows user to download the dataset used in this study.

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:

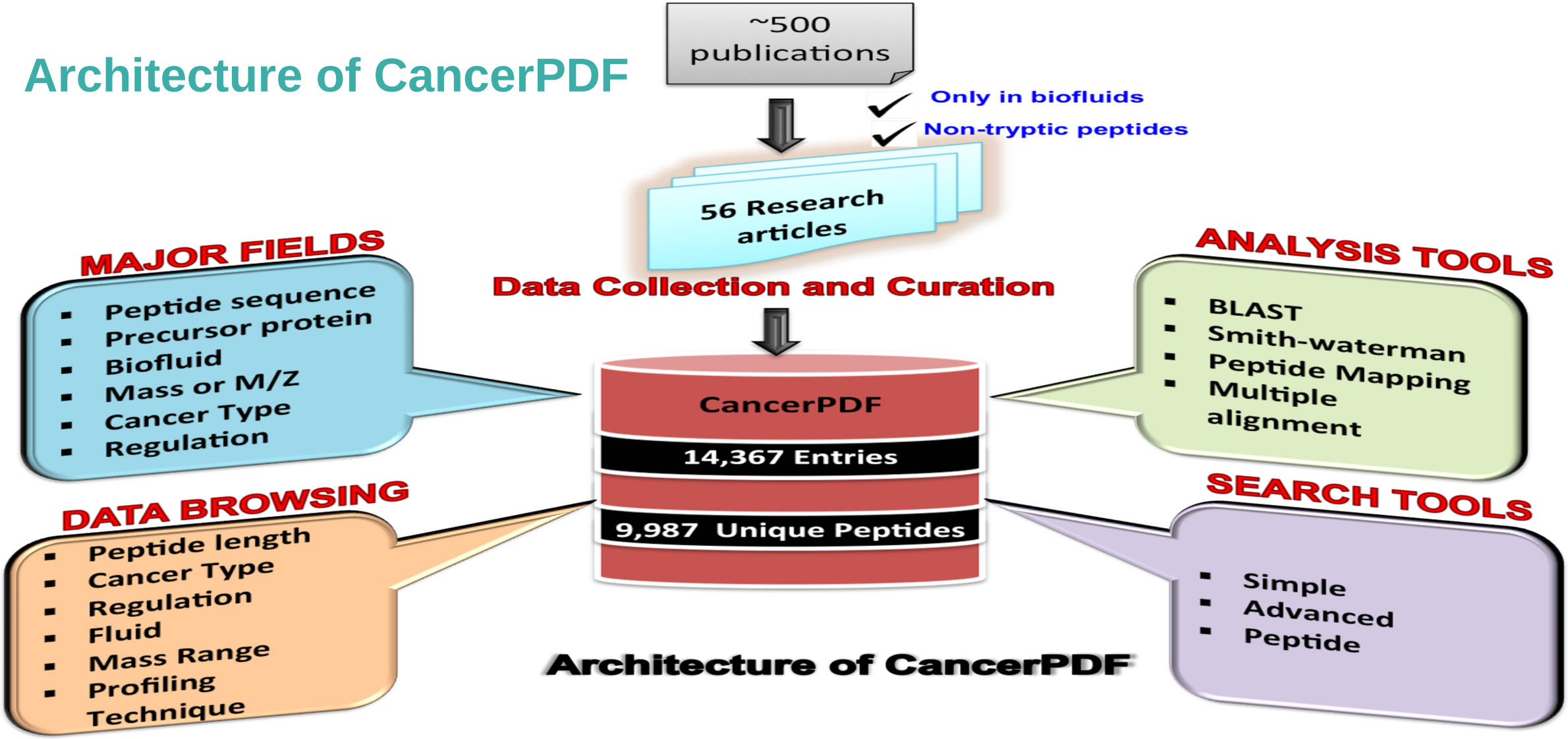
Advanced Options: CLICK

Reset or clear form Submit sequence for prediction

Peptide as Diagnostics

CancerPDF: A repository of cancer-associated peptidome found in human biofluids

Architecture of CancerPDF



Cancertope

In silico Platform for designing genome-based Personalized immunotherapy or Vaccine against Cancer

- Home Page
- **Cancer-specific?**
  - Epitope Search
  - Data Retrieval
  - Browse Gene
  - Browse Tissue
  - Sequence Similarity
- **Partially Personalized?**
  - Submit a Protein
  - Vaccine Target
  - Proteome Data
  - NGS data
  - BLAST & Predict
- **Fully Personalized?**
  - Proteins Pair
  - Proteome Pair
- **Advanced Tools**
  - Epitope Mapping
  - Cross Reactivity
- **Important Information**
  - Acknowledgement
  - Algorithm
  - Help

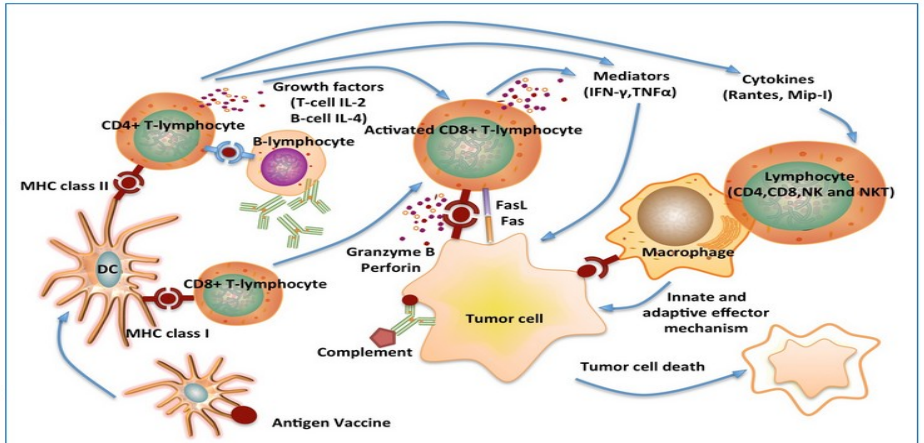
Welcome to Cancertope

Challenges in Development of Cancer Vaccines: It is one of the most difficult jobs to generate immunity or design vaccine against cancer in comparison to pathogens, since cancer cells are part of our body. Due to cross reactivity, it is difficult to design vaccine against cancer. In addition, the studies show a wide variation in genetic profile of cancer patients, which further complicate the situation.

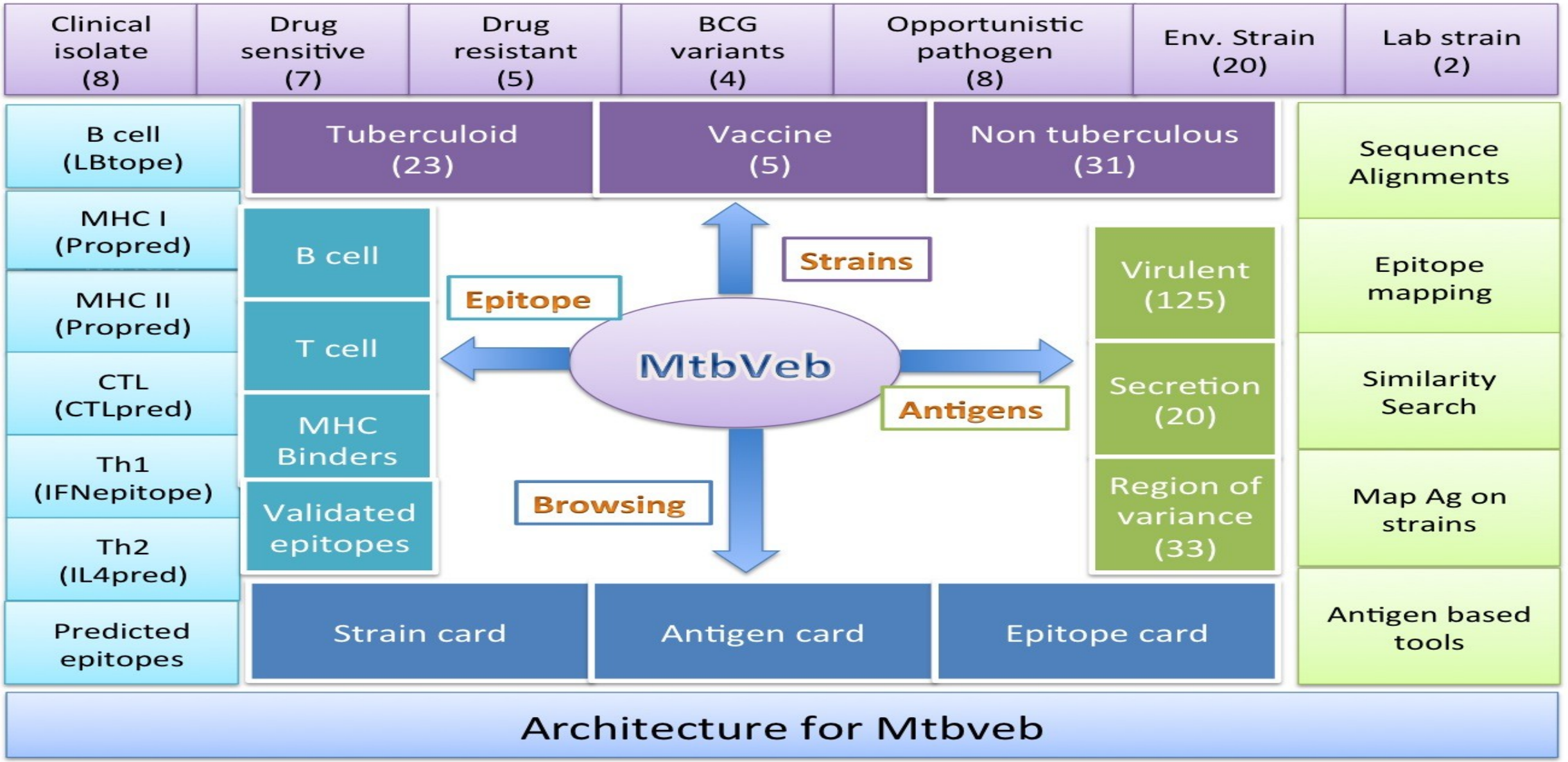
Advancement in Technology: In last two decades, there is a tremendous advancement in the field of genome sequencing, immunology and in immuno-informatics. Due to advancement in the field of genome sequencing, important genes of more than thousands of cancer cell-lines have been sequenced. Generation of immunotherapy against any antigen is routine due to advancement in immunology. Similarly, a large number of web-based servers have been developed in the field of immuno-informatics to predict antigenic or immunogenic regions for activating all arms of adaptive immunity.

***In Silico* Platform or Workbench**: Aim of this platform is to assist researchers in designing and discovering suitable epitopes/antigens for cancer vaccine/immunotherapy. This workbench takes full advantage of genomic data generated from cancer cell lines over the years. Following are three major modules of this workbench:

- **Cancer-Specific Epitopes:** This module is designed to identify "antigenic/epitopic" regions suitable to design vaccine against a specific type of cancer or cell line. Basically, it is a database of epitopes (B-cell, T-helper and CD8+) generated from around 60 cancer vaccine targets belonging to 905 cancer cell lines. A large number of web-based tools has been integrated to retrieve desired epitopic regions.
- **Partially Personalized Immunotherapy:** This module is designed to identify best vaccine antigen or epitope for a patient based on genome profile of its cancerous cells. In this module, server compares cancer genome of a patient with reference human genome and identifies



MtbVeb – A web portal for M. tuberculosis Vaccine



Architecture for Mtbveb

CoronaVIR: Computational Resources on Novel Coronavirus (SARS-CoV-2 or COVID-19)

Home Page CoronaVIR

Aim of this web site is to facilitate the scientific community to fight against severe pandemic disease COVID-19 caused by SARS-CoV-2. Here, We have collected and organized information related to novel strain of coronavirus, i.e. SARS-CoV-2.and its resulting disease COVID-19 from the literature and other resources from the Internet. We are providing links to appropriate literature. Moreover, we are Bioinformatics Group, based on our knowledge and expertise, we are also proposing potential diagnostics primers, peptide and RNA based vaccine candidates and potential drug molecules. These are predicted candidates, need to be validated by experimental Researchers, who have appropriate infrastructure. It is an integrated multi-omics repository dedicated to current genomic, proteomic, diagnostic and therapeutic knowledge about coronaviruses particularly the recent strain, i.e. SARS-CoV-2 or 2019-nCoV. This web resource will be helpful for the researchers engaged in the development of therapies and drugs for the COVID-19. The information is collected from various available resources.

Cite: Patiyal, Sumeet, et al. "A Web-based Platform on COVID-19 to Maintain Predicted Diagnostic, Drug and Vaccine Candidates." OSF Preprints, 6 Apr. 2020. Doi:10.31219/osf.io/xegzu

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

Web Sites for India

- Ministry of Health
- **Drug: Hydroxy-Chloroquine**
- **Test Labs**
- **Private Labs**
- ICMR Update

Status of COVID-19

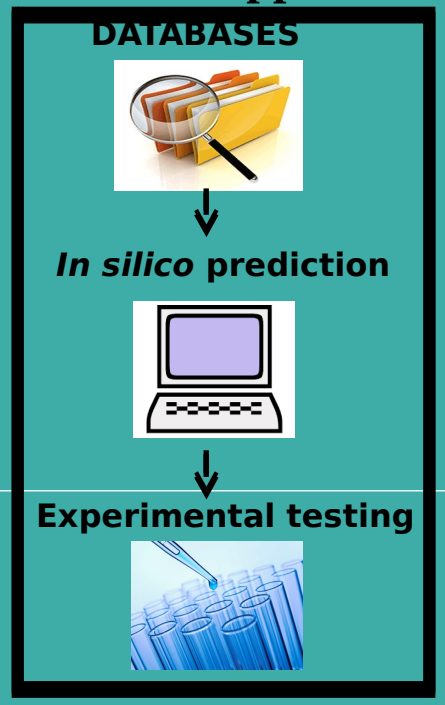
State-wise in India

Status in World

- WHO Update
- Coronavirus Update
- Global Prevention
- Six Steps
- 10 things to mange

Cell-Penetrating Peptide for Drug Delivery

Overall Approach



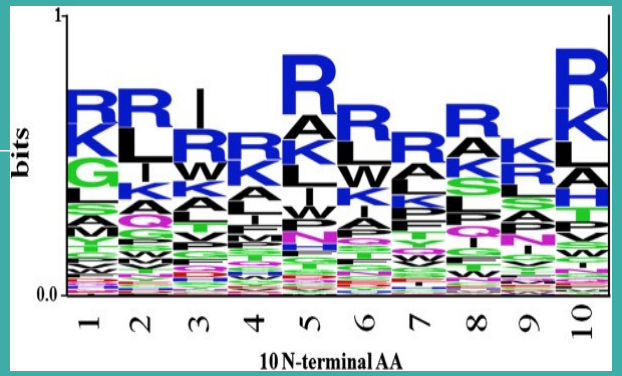
CPPs Collection and Compilation

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)

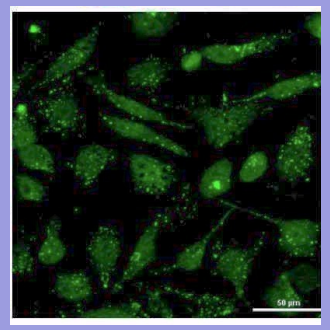


Virtual Screening

IMT-P8 (Patented*)

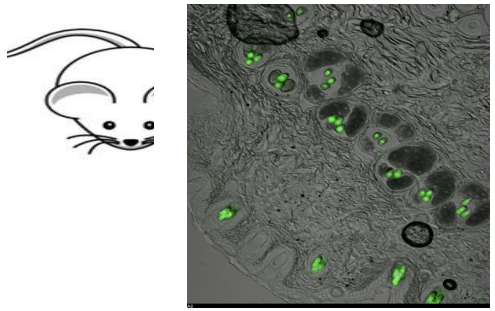
Experimental Validation

Delivery in Cancer Cells



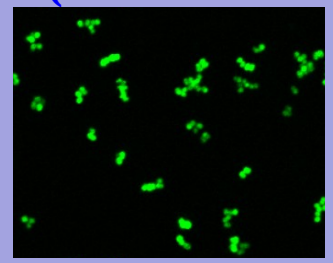
Eur J Pharm Biopharm. 2015;89:93-106

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)

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,*]

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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.

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

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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

Table 2 List of In Silico Tools for Predicting Epitopes Involved Humoral-Mediated Immunity

alt-text: Table 2

Name	Description	Method	Year
Sequence-based B-cell prediction			
ABCPred (Saha & Raghava, 2006)	http://www.imtech.res.in/raghava/abcpred/ Predict B-cell epitope in an antigen sequence	Artificial neural network	2006
BepiPred (Larsen, Lund, & Nielsen, 2006)	http://www.cbs.dtu.dk/services/BepiPred/ Predict the location of linear B-cell epitopes using a combination	Hidden Markov model (HMM) and a propensity scale method	2006
Bcepred (Saha & Raghava, 2007)	http://webs.iiitd.edu.in/raghava/bcepred/ Prediction of B-cell epitopes	Physicochemical properties matrices	2007
BCPREDS (EL-Manzalawy, Dobbs, & Honavar, 2008)	http://ailab.ist.psu.edu/bcpred/ Predict flexible length B-cell epitopes	Support vector machine and string kernels	2008
COBEPro (Sweredoski & Baldi, 2009)	http://scratch.proteomics.ics.uci.edu Predict B-cell epitopes	Support vector machine	2009
SVMTriP (Yao, Zhang, Liang, & Zhang, 2012)	http://sysbio.unl.edu/SVMTriP/ Predict antigenic epitopes 2012	Support vector machine and tri-peptide similarity propensity score	2012
Lbtope (Singh, Ansari, & Raghava, 2013)	http://webs.iiitd.edu.in/raghava/lbtope/ Predict B-cell epitope of fixed and variable length using datasets from IEDB	Support vector machine and K-nearest neighbor algorithm	2013
APCPred (Shen et al., 2015)	http://ccb.bmi.ac.cn/APCpred/ Predict B-cell epitope in an antigen sequence 2015	Support vector machine	2015
BepiPred 2.0 (Jespersen, Peters, Nielsen, & Marcatili, 2017)	http://www.cbs.dtu.dk/services/BepiPred/ Predict B-cell epitope from antigen sequences	Random forest	2017
Structure-based B-cell epitope prediction			
CEP (Kulkarni-Kale, Bhosle, & Kolaskar, 2005)	http://196.1.114.49/cgi-bin/cep.pl Conformational B-cell epitope prediction	CEP algorithm	2005
BEpro (Sweredoski & Baldi, 2008)	http://pepito.proteomics.ics.uci.edu/ Discontinuous B-cell epitope prediction	Based on multiple distance threshold and half-sphere exposure method	2008
ElliPro (Ponomarenko et al., 2008)	http://tools.immuneepitope.org/ellipro/ Identifying discontinuous antibody epitopes in the protein regions of the antigen	Thornton's method residue clustering algorithm	2008

Table 3 List of Significant Computational Methods Available for Predicting MHC Binders and Cell-Mediated Immunity

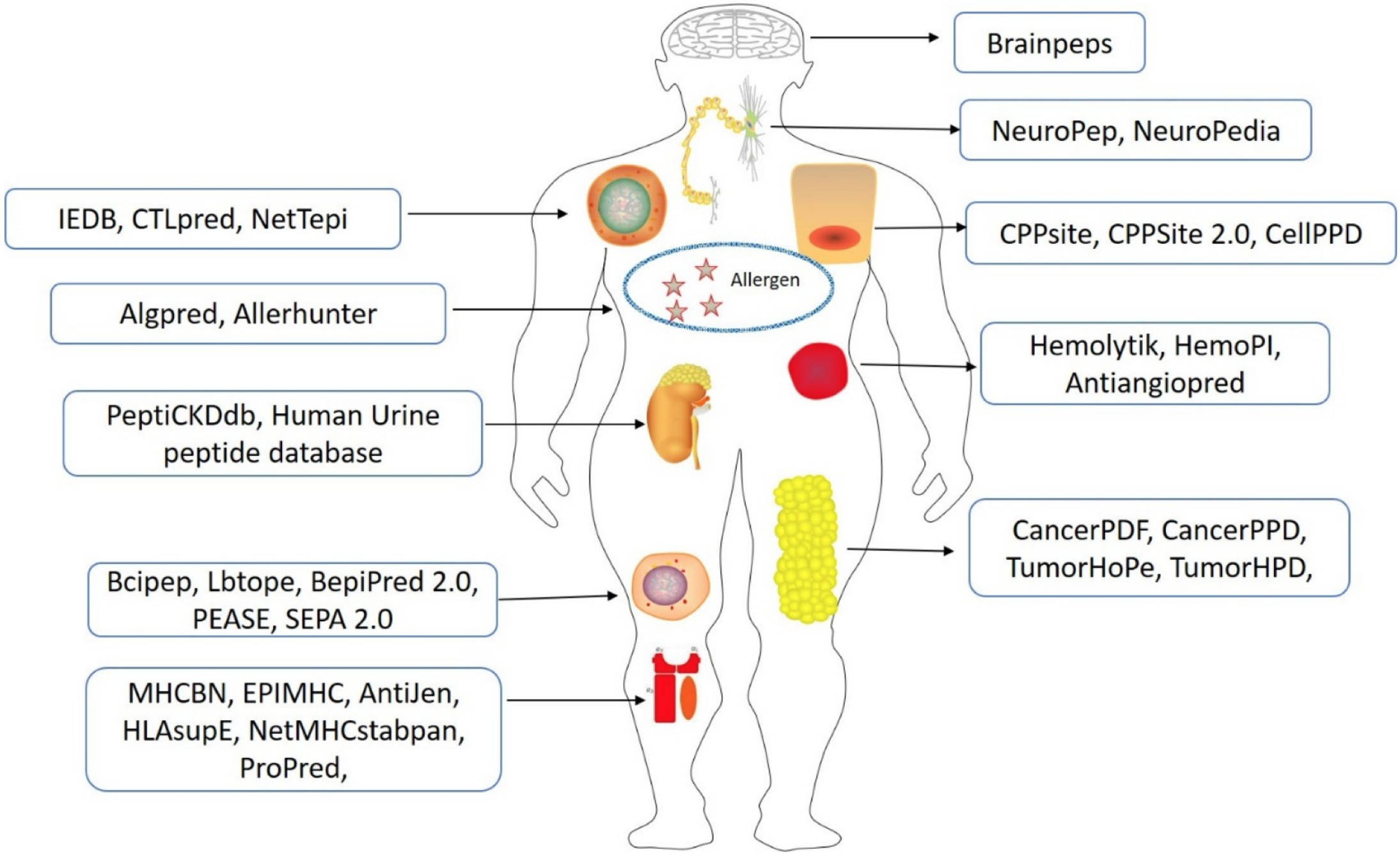
alt-text: Table 3

Name	Description	Method	Year
Tools to predict MHC-I binders			
ProPred 1 (Mustafa & Shaban, 2006)	http://webs.iiitd.edu.in/raghava/propred1/ Promiscuous MHC-I binding prediction server	Matrix based	2003
MmbPred (Bhasin & Raghava, 2003)	http://webs.iiitd.edu.in/raghava/mmbpred/ Mutated MHC binders prediction server	Quantitative matrix based	2003
nHLAPred (Bhasin & Raghava, 2007)	http://webs.iiitd.edu.in/raghava/nhlapred/ MHC-I binding prediction server	Artificial neural network	2006
RANKPEP (Reche, Glutting, Zhang, & Reinherz, 2004)	http://imed.med.ucm.es/Tools/rankpep.html Predict peptide binders to MHC-I and MHC-II molecules from protein sequence/s	Position-specific scoring matrices (PSSMs)	2007
POPI (Tung & Ho, 2007)	http://iclab.life.nctu.edu.tw/POPI/ Server for predicting immunogenicity of MHC class I and II binding peptides	Support vector machine	2007
NetCTLpan (Stranzl et al., 2010)	http://www.cbs.dtu.dk/services/NetCTLpan/ Pan-specific MHC class I pathway epitope prediction	Artificial neural network	2010
NetMHCcons (Karosiene, Lundegaard, Lund, & Nielsen, 2012)	http://www.cbs.dtu.dk/services/NetMHCcons/ Consensus method for MHC-I binding prediction	Combination of ANN-based NetMHC, NetMHCpan, and matrix-based PickPocket	2012
NetMHCstab (Jørgensen, Rasmussen, Buus, & Nielsen, 2014)	http://www.cbs.dtu.dk/services/NetMHCstab/ Predict stability of peptide–MHC-I complexes	Artificial neural network	2014
NetMHCstabpan (Rasmussen et al., 2016)	http://www.cbs.dtu.dk/services/NetMHCstabpan/ Predicts binding stability of peptides to any known MHC molecule	Artificial neural network	2016
Tools to predict MHC-II binders			
Propred (Singh & Raghava, 2001)	http://webs.iiitd.edu.in/raghava/propred/ Predict MHC class II binding regions in an antigen sequence	Quantitative matrices based	2001
HLA-DR4Pred (Bhasin and Raghava, 2004a)	http://webs.iiitd.edu.in/raghava/hladr4pred/ Prediction of HLA-DRB1*0401 binding peptides in an antigen sequence	Support vector machine and artificial neural network	2004

Table 4 List of Computational Methods Available to Assist in Peptide-Based Drug Development

alt-text: Table 4

Name	Description	Method	Year
Based on protein–peptide interaction			
PeptideMine (Shameer, Madan, Veeranna, Gopal, & Sowdhamini, 2010)	http://caps.ncbs.res.in/peptidemine/ A webserver for the design of peptides for protein–peptide binding studies derived from protein–protein interactomes	Inteacting sequence space and bioinformatics mashup approach	2010
PepSite (Trabuco, Lise, Petsalaki, & Russell, 2012)	http://pepsite2.russelllab.org/ Prediction of peptide-binding site on protein surface	Protein–peptide interaction based on 3D structure	2012
DockoMatic 2.0 (Bullock et al., 2013)	Standalone	Homology modeling	2013
EPI-Peptide (Viart et al., 2016)	http://www.biocomp.icb.ufmg.br/biocomp/ Tool for designing peptide ligand libraries based on epitope–paratope interactions	I2R interaction	2016
SPRINT (Taherzadeh, Yang, Zhang, Liew, & Zhou, 2016)	http://sparks-lab.org/ Sequence-based prediction of protein–peptide binding sites	Support vector machine	2016
Sequence and structure-based method			
AVPpred (Thakur, Qureshi, & Kumar, 2012)	http://crdd.osdd.net/servers/avppred/ Prediction and designing of antiviral peptides	Support vector machine	2012
CellPPD (Gautam et al., 2013)	http://webs.iiitd.edu.in/raghava/cellppd/ Prediction and designing of highly cell-penetrating peptide	Support vector machine	2013
Peptimap (Lavi et al., 2013)	Standalone Detection of peptide-binding sites on protein surfaces	Ab-initio and FTMap approach	2013
QSPpred (Rajput, Gupta, & Kumar, 2015)	http://crdd.osdd.net/servers/qsppred/ Predicting and designing quorum sensing peptide	Support vector machine	2015
PEPstrMOD (Singh et al., 2015)	http://webs.iiitd.edu.in/raghava/pepstrmod/ Predicts the tertiary structure of small peptides with sequence length varying between 7 and 25 residues	Support vector machine	2015
iACP (Chen, Ding, Feng, Lin, & Chou, 2016)	lin.uestc.edu.cn/server/iACP/ Sequence-based anticancer peptide prediction	Support vector machine	2016
In silico approaches for antimicrobial peptide prediction			
AntiBP2 (Lata, Mishra, & Raghava, 2010)	http://crdd.osdd.net/raghava/antibp2/index.html Antibacterial peptide prediction	Support vector machine	2010


Brainpeps
NeuroPep, NeuroPedia
IEDB, CTLpred, NetTepi
CPPsite, CPPSite 2.0, CellPPD
Allergen
Algpred, Allerhunter
Hemolytik, HemoPI, Antiangiopred
PeptiCKDdb, Human Urine peptide database
CancerPDF, CancerPPD, TumorHoPe, TumorHPD,
Bcipep, Lbtope, BepiPred 2.0, PEASE, SEPA 2.0
MHCBN, EPIMHC, AntiJen, HLAsupE, NetMHCstabpan, ProPred,

Thank You