wledge based Drug Design & Open source Web Serv

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Bioinformatics Drug Informatics Vaccine Informatics
Chemoinformatics

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http://crdd.osdd.net/

Exponential Growth of Data: Source of Knowledge

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/)

Example of Open Source Resources

- Operating Systems
  - Linux
  - FreeBSD, OpenBSD, and NetBSD
- Internet
  - Apache (> 50% of the world's web servers)
  - BIND: DNS for the entire Internet.
  - Sendmail (Most email servers)
  - OpenSSL (standard for secure communication)
- Programming Tools
  - Languages (Perl, Python, PHP)
  - GNU compilers and tools (GCC, Make)

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

Open Source Software and Web Services for Designing Therapeutic Molecules

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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.

Software name	Description
AntiCP	Prediction and design of anticancer peptides.
Toxinpred	Prediction and designing of toxic/non-toxic peptides.
AntiBP	Mapping of antibacterial peptides in a protein sequence.
AntiBP2	Advanced server for predicting antibacterial peptides with high precision.
CPPsite	CPPsite is a database of experimentally validated cell penetrating Peptides
CellPPD	Computer-aided Designing of efficient cell penetrating peptides.
TumorHoPe	A comprehensive database experimentally characterized tumor homing peptides.
TumorHPD	Server dedicated for designing tumor homing peptides.
Destamp	Designing of stable antibacterial peptides
HEMOLYTIK	A repository of experimentally validated hemolytic and non-hemolytic peptides.
ParaPep	Compilation of experimentally validated anti-parasitic peptides and their structure

al Conference on Open Source for Computer Aided Drug Discovery (March 22-26, 2009

Computational Resources for Drug Discovery

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

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

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

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

India specific Genomes Sequenced, Assembled and Annotated

Genomes sequence/assemble/annotate at CSIR Institutes

Organism	Discription	Institute	Publication
Acinetobacter baumannii MSP4-16	Isolated from mangrove soil sample from Parangipettai (11°30 N,79° 47'E), Tamil Nadu, India.	CSIR-IMTECH	23558533
Streptomyces gancidicusÂ Strain BKS 13-15	Isolated from mangrove sediment samples collected from the Bhitar Kanika Mangrove Reserve Forest, Odissha, India.	CSIR-IMTECH	23599292
Serratia fonticolaÂ Strain AU-AP2C	Isolated from the Pea Rhizosphere	CSIR-IMTECH	24309742
PantoeaÂ sp. Strain AS-PWVM4	Isolated from the rhizosphere ofÂ Punica granatum, exhibits phosphate solubilization	CSIR-IMTECH	24309733

OSDDLINUX

Customized operating environment for drug discovery pipeline

BIOINFORMATICS

VACCINE INFORMATICS

CHEMINFORMATICS

Live Server

Live CD

Pkg Repository

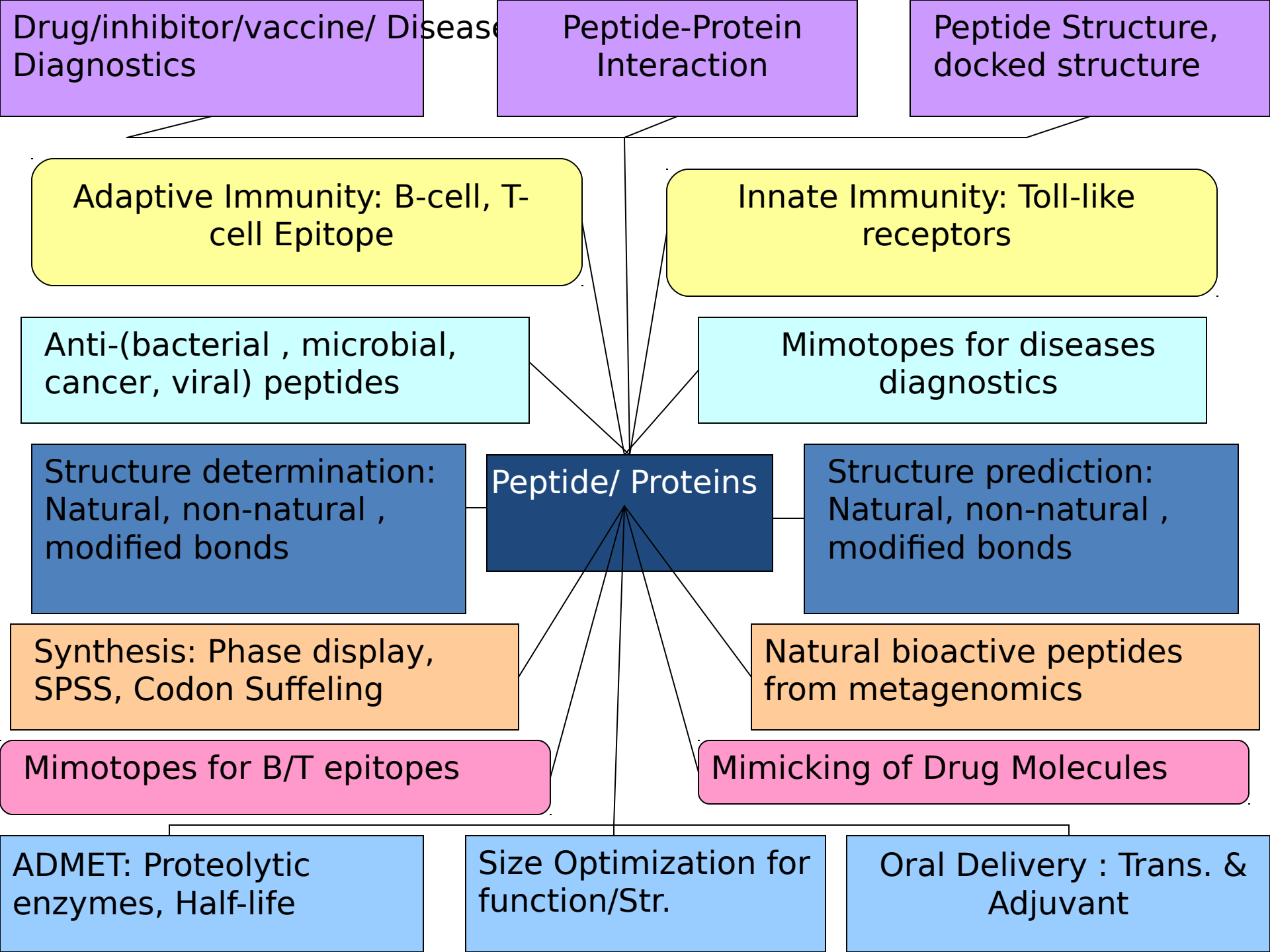
Installation

Webserver

Standalone

Galaxy platform

All in ONE


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 , microbial, cancer, viral) peptides
Mimotopes for diseases diagnostics
Structure determination: Natural, non-natural , modified bonds
Peptide/ Proteins
Structure prediction: Natural, non-natural , modified bonds
Synthesis: Phase display, SPSS, Codon Suffeling
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

Adaptive Immunity

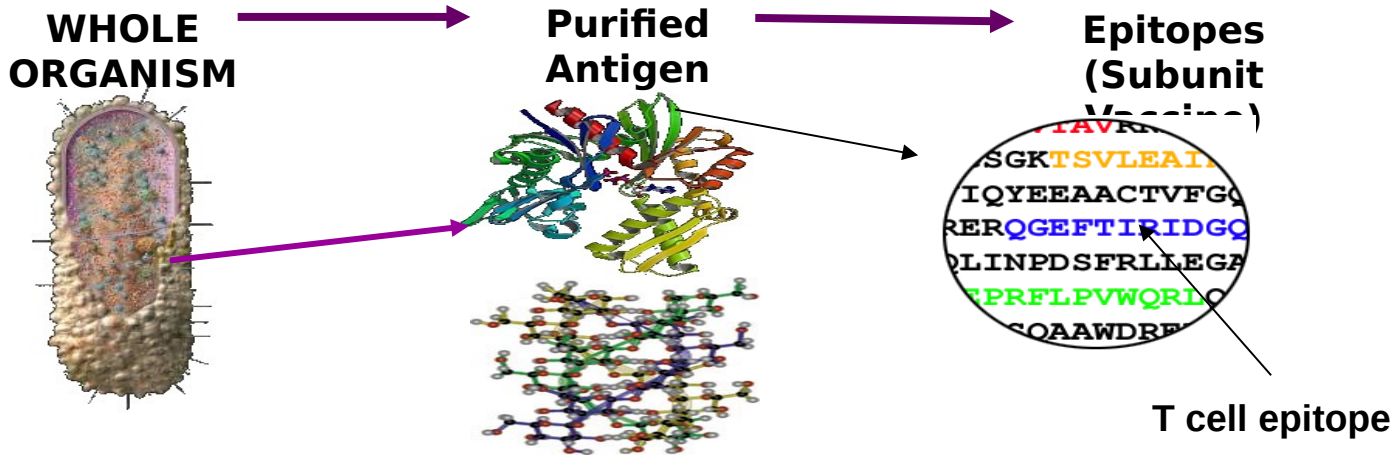
Innate Immunity

Vaccine Informatics

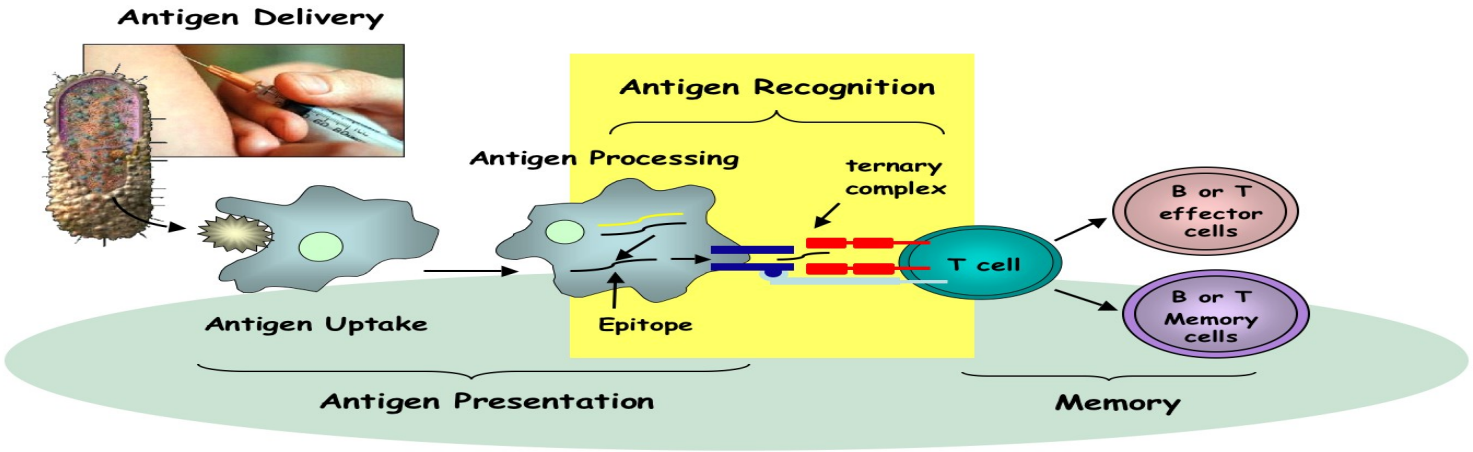
Bioinformatics Centre
IMTECH, Chandigarh

Protective Antigens

Vaccine Delivery



Attenuated



Adaptive Immunity

Innate Immunity

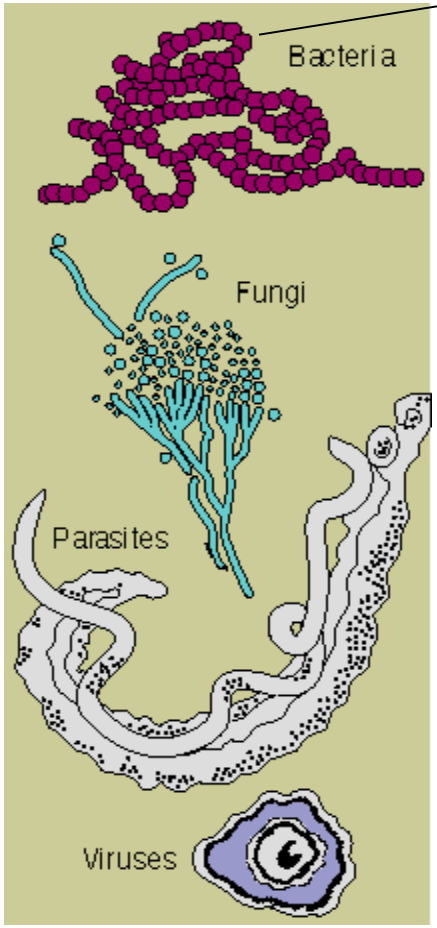
Vaccine Informatics

Bioinformatics Centre
IMTECH, Chandigarh

Protective Antigens

Vaccine Delivery

Disease Causing Agents



Pathogens/Invaders

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

Modelling of Immune System for Designing Epitope-based Vaccines

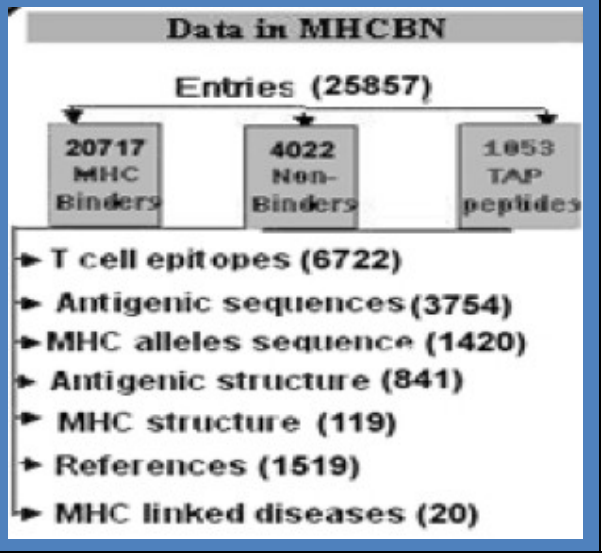
Adaptive Immunity (Cellular Response) : T_{helper} Epitopes

Propred: for promiscuous MHC II binders

MMBpred:for high affinity mutated binders

MHC2pred: SVM based method

MHCBN: A database of MHC/TAP binders and non-binders



Adaptive Immunity (Cellular Response) : CTL Epitopes

Pcleavage: for proteome cleavage sites

TAPpred: for predicting TAP binders

Propred1: for promiscuous MHC I binders

CTLpred: Prediction of CTL epitopes

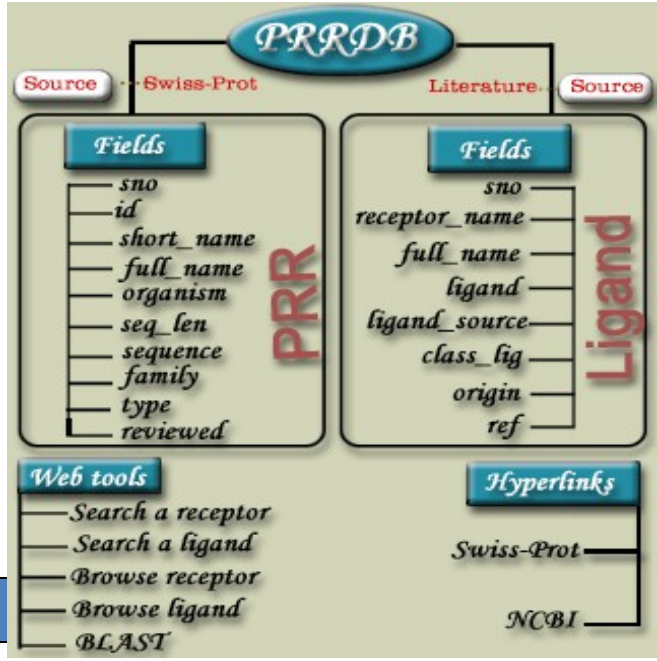
Adaptive Immunity (Humoral Response) :B-cell Epitopes

BCIpep: A database of B-cell eptioes;

ABCpred: for predicting B-cell epitopes

ALGpred: for allergens and IgE eptopes

HaptenDB: A datbase of haptens



Innate Immunity : Pathogen Recognizing Receptors and ligands

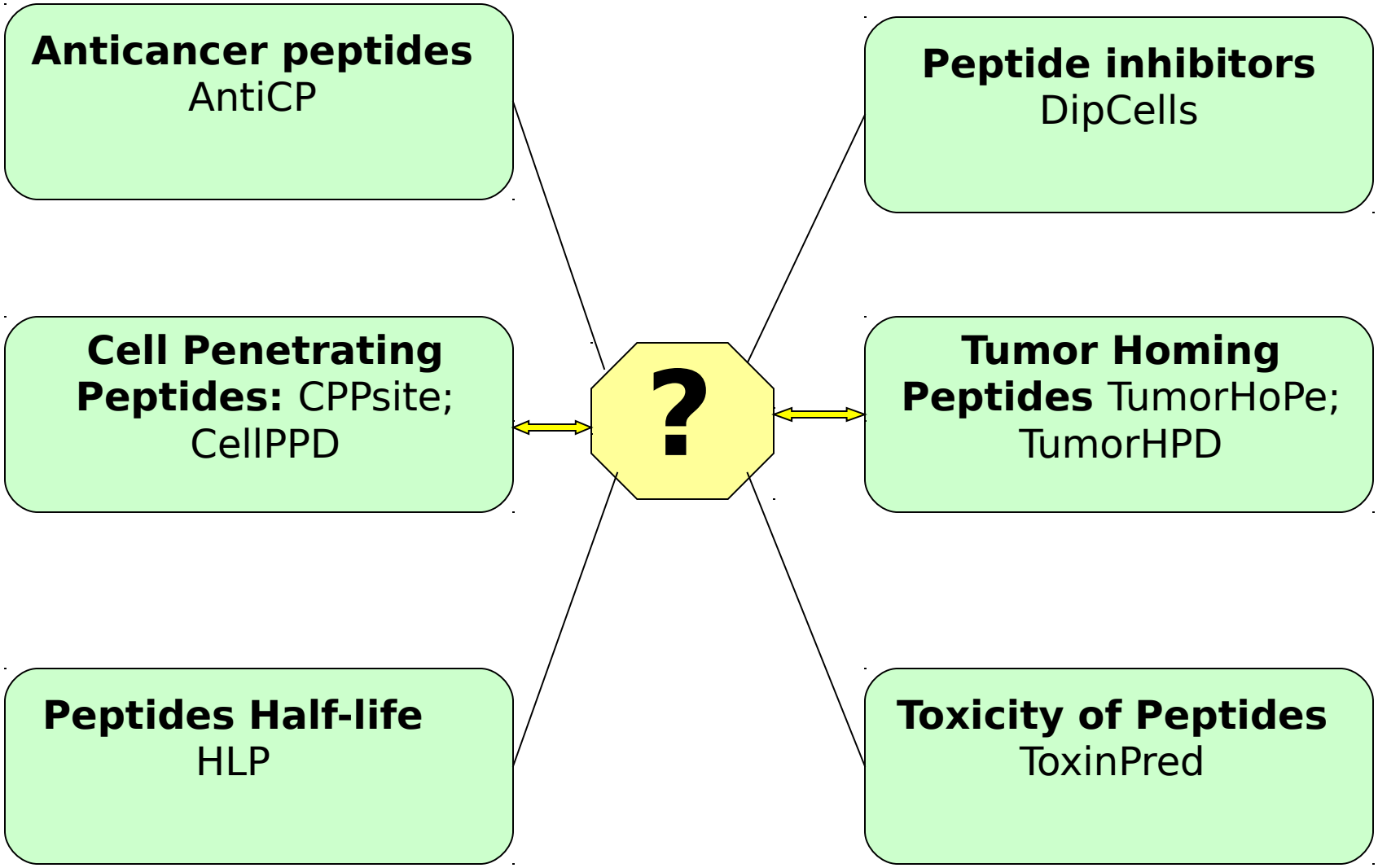
PRRDB: A database of PRRs & ligands

Antibp: for anti-bacterial peptides

Signal transduction in Immune System

Cytopred: for classification of Cytokines

Designing of therapeutic peptides against cancer



TumorHope - Tumor Homing Peptide Database

Home | Search | Browse | Structure | Tools | Important | Help | About Us | Contact Us

Welcome to TumorHope - A comprehensive database of Tumor Homing Peptides

TumorHope is a manually curated comprehensive database of experimentally characterized tumor homing peptides. These peptides recogninze tumor tissues and tumor associated micro environment, including tumor metastasis. Thus, they can be used to deliver drugs selectively in tumors.

Importance of Peptides: Poor selectivity of chemotherapeutic drugs for cancer is a major challenge for successful clinical outcome. Conjugation of drug with homing peptide may enhance the selectivity and efficacy of the therapy. Current efforts are being focused on tumor homing peptides that may target tumor tissues.

Information about Peptides: Tumor Homing Peptide Database has been developed using extensive literature search. It contains detailed information about the tumor targeting/homing peptides. Each entry contains following type of information about a peptide; its sequence, source, target tumor, target cell, biomarker, applications and clones. Experimental details like phage display libraries used, cell lines, *in*

Work in Progress

1. Prediction of CPP 2. Designing CPP 3. Scanning in proteins

TumorHPD: Designing of Tumor Homing Peptides

(Institute of Microbial Technology, Chandigarh, India)

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.

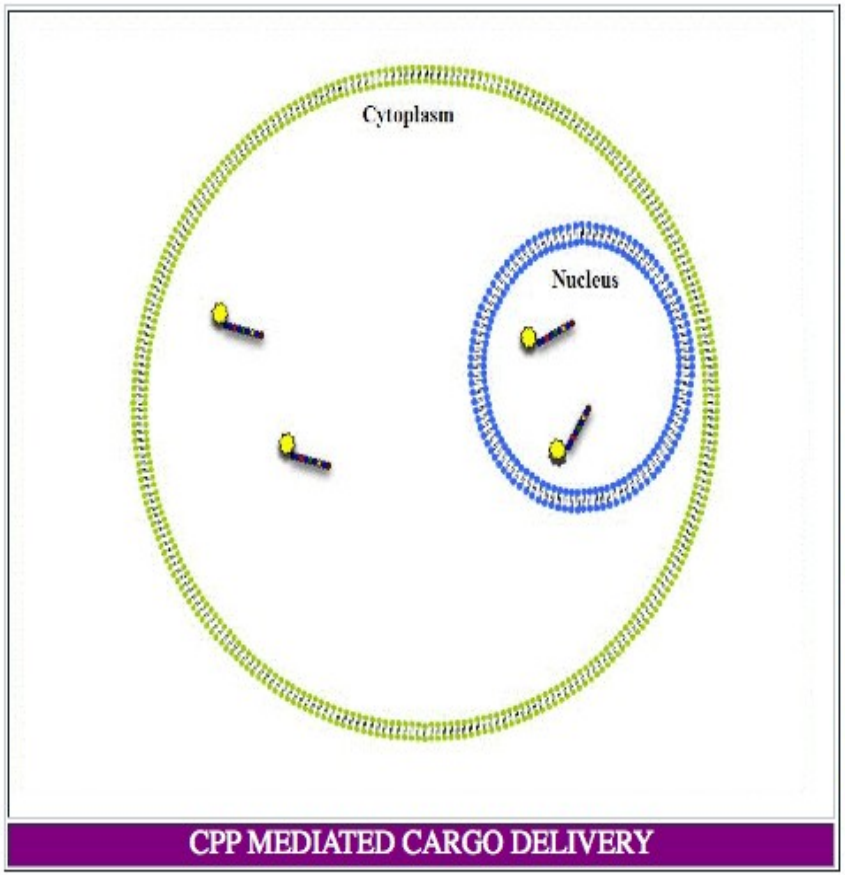
TumorHPD is a web server for predicting and designing tumor homing peptides. This server is extremely useful fo
the field of therapeutic peptides. This server allows the users to design tumor homing peptides and their mutants
and physicochemical properties.

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

CPPsite: a webSite for Cell Penetrating Peptides

Navigation

- Home
- Search
- Browse
- Structure
- Tools
- Important
- Help
- About us
- Contact us



CPP MEDIATED CARGO DELIVERY

CPPsite: CPPsite is a database of experimentally validated Cell Penetrating Peptides (10-30 amino acids).

Importance of CPPsite: CPPs have tremendous therapeutic applications. These are widely used to promote intracellular uptake of conjugated cargos (nucleic acids, peptide nucleic acids, proteins, drugs, liposomes etc.) and thus play role to overcome the problem of poor delivery and low bioavailability of therapeutic molecules. CPP conjugated drugs when delivered *in vivo* have s hown promising results with high efficacy. Many CPP-conjugated compounds are under clinical trials. CPPsite database provides comprehensive information on CPPs, which may be helpful to scientific community working in the area of peptide based drug discovery.

What type of information it has: CPPsite database's current version contains comprehensive information of 843 CPPs with multiple entries in terms of peptide sequence, source/origin, localization, uptake efficiency, uptake mechanism, hydrophobicity, charge etc.

Is it a manually curated database: Yes, we have collected and compiled all the information from published literature. In addition, we have also generated structural information of CPPs. We predicted tertiary and secondary structure of these peptides using PepStr and DSSP.

Work in Progress

1. Prediction of CPP 2. Designing CPP 3. Scanning in proteins

CellPPD: Designing of Cell Penetrating Peptides

Welcome to CellPPD

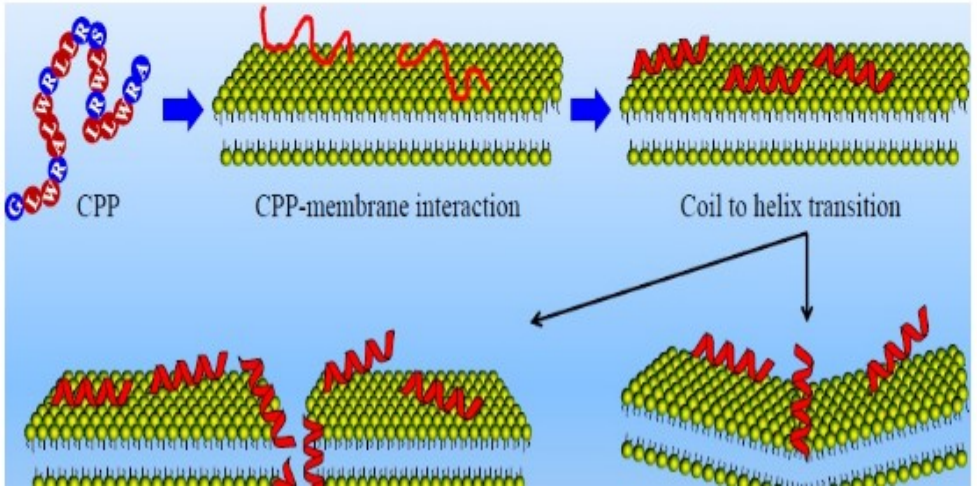
utam *et al.*: *In silico* approaches for designing highly effective cell penetrating peptides. *Journal of Translational Medicine* 13 11:74.Link

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



Peptide Resources/Databases

HMR Base

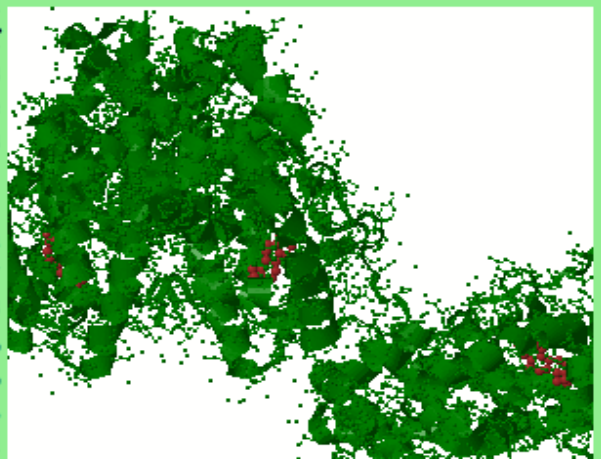
A database of hormones and their receptors

Home	Hormone	Receptor	Tools	Miscellaneous	Contact

Home

Last 90 days Re

Hormones are the chemical messengers of the body which convey the message from one part to another. They are secreted from a particular cell/tissue and act on some distantly located cell/tissue. On the basis of chemical composition, there are two types of hormones: (a) Peptides (b) Non-peptides. The action of both types of hormone is mediated through Receptors which receive the signal and relay it to the destination. Receptors of polypeptide/protein hormones are located in the plasma membrane and regulate various intracellular functions by changing the activity of a particular enzyme. Most of the non-peptide hormones interact with intracellular receptors located in cytoplasm or nucleus and this complex provides the signal.



HMRbase is a manually curated database of Hormones and their Receptors. It is a compilation of sequence data after extensive manual literature search and from publicly available databases. HMRbase can be searched on the basis of a variety of data types such as hormone and receptor description and their names, molecular weight, molecular formula, IUPAC name, smiles, physiochemical properties, post-translational modification, developmental stage, subcellular location, length of the protein sequence, organism name etc. This database has been developed by Dr. GPS Raghava's group at Institute of Microbial

CancerPPD

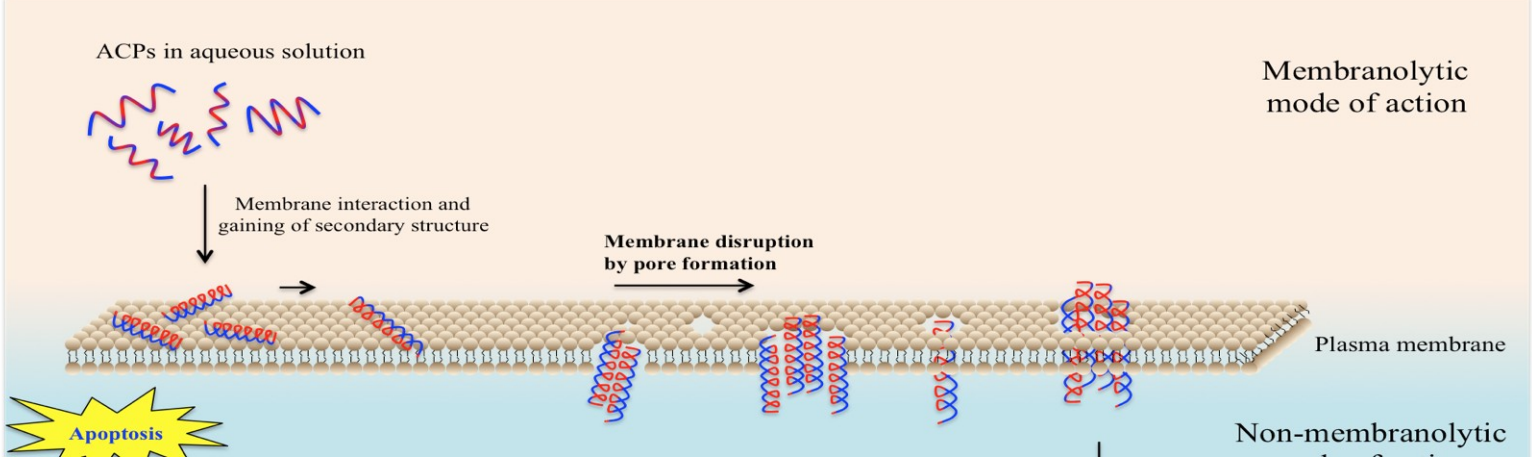
Database of Anticancer Peptides & Proteins

===== Reference: Tyagi et al., (2014) CancerPPD: a database of anticance

CancerPPD is a unique resource of its kind, which provides detailed information related to experimentally verified anticancer peptides (ACPs) and proteins. Data was curated manually from both published articles, patents as well as from other repositories. Since structures play important roles in the anticancer activity, we have predicted tertiary structures of anticancer peptides using state-of-art method PEPstr and secondary structure states are assigned using DSSP. The important feature of cancerPPD is that it also provides information related to various chemical modifications like non-natural, D-amino acids, modified-amino acid like ornithine. The database is cross-linked with various other related resources in order to provide comprehensive information related to ACPs.

Total Peptide Entries : 3491 **Total Cell Lines : 249** **Total Tissue Types : 21**

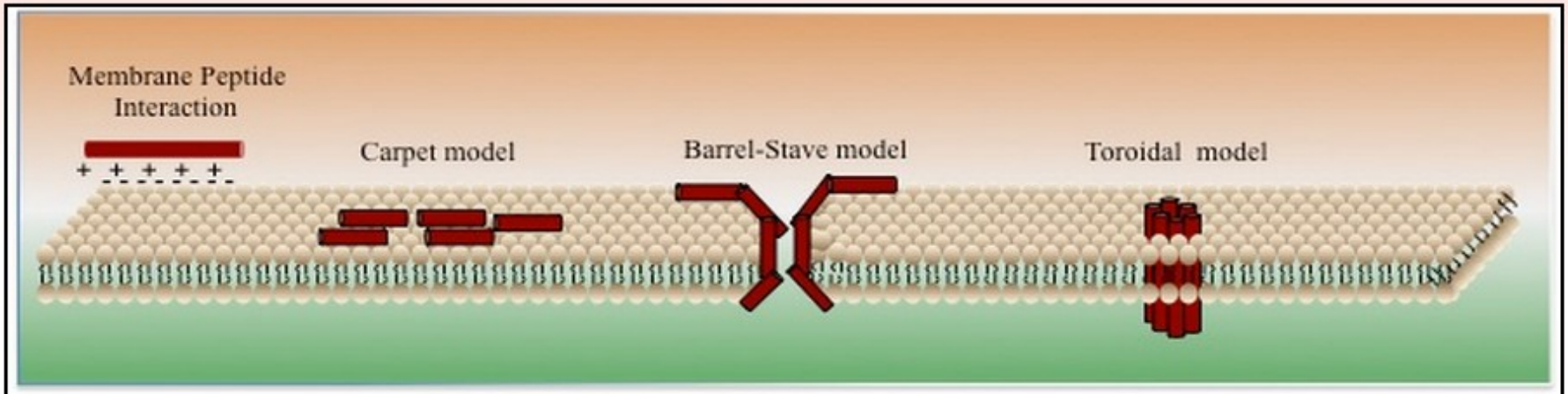
Mechanisms of ACP's action



AntiCP:- Designing of Anticancer Peptides

Institute of Microbial Technology, Chandigarh India

Welcome to AntiCP



Various models of membrane permeation by anti-cancer peptides

AntiCP is web based prediction server for Anticancer peptides. SVM models developed are based on amino acid composition and binary profile features. Positive dataset consists of 225 antimicrobial peptides with anticancer properties. This server is extremely useful for the researchers working in the field of Anticancer peptides. This server allows the users to design ACPs and their mutants with

AHTPDB: Database of Antihypertensive Peptides

CSIR – Institute of Microbial Technology, India

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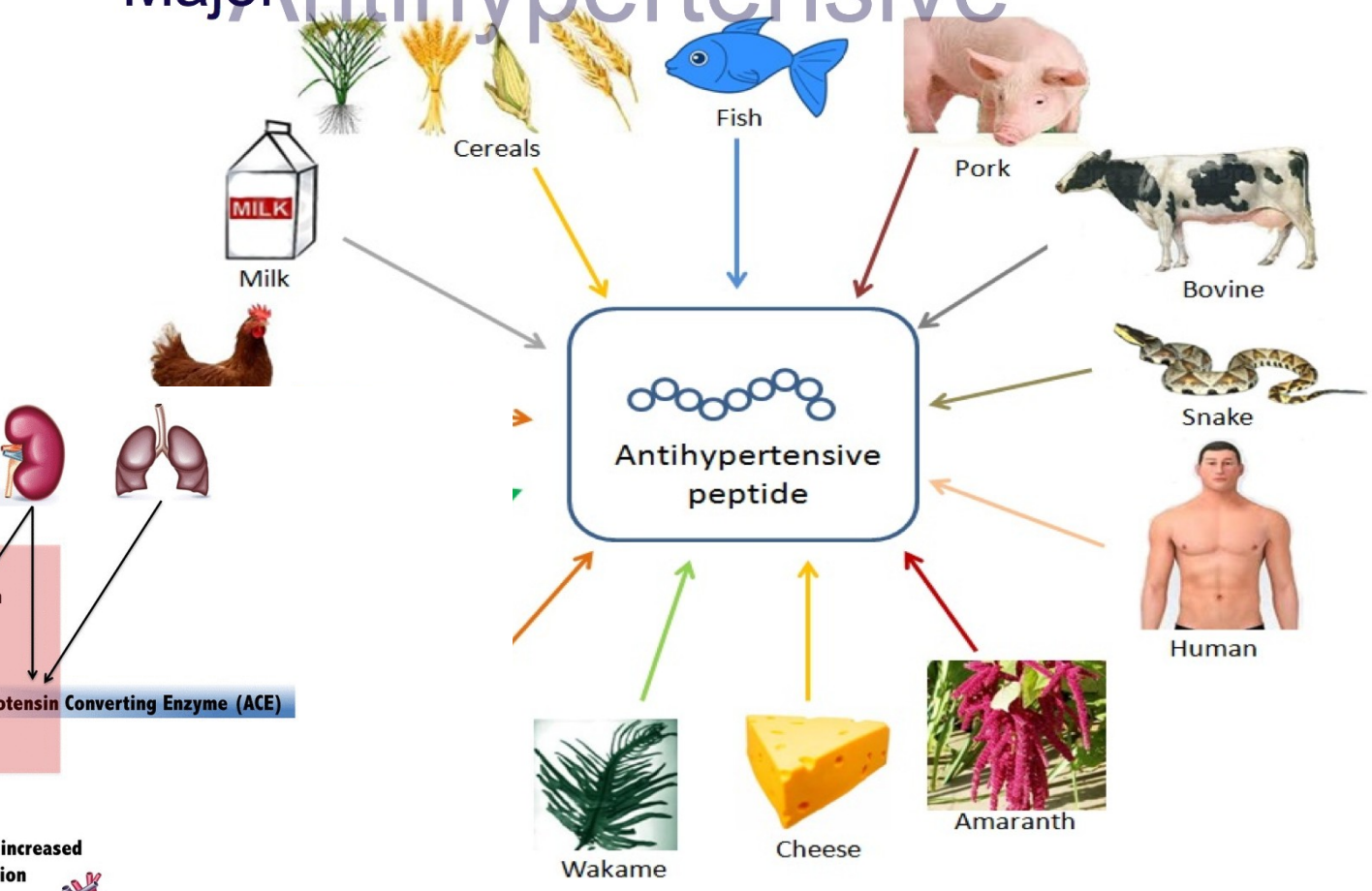
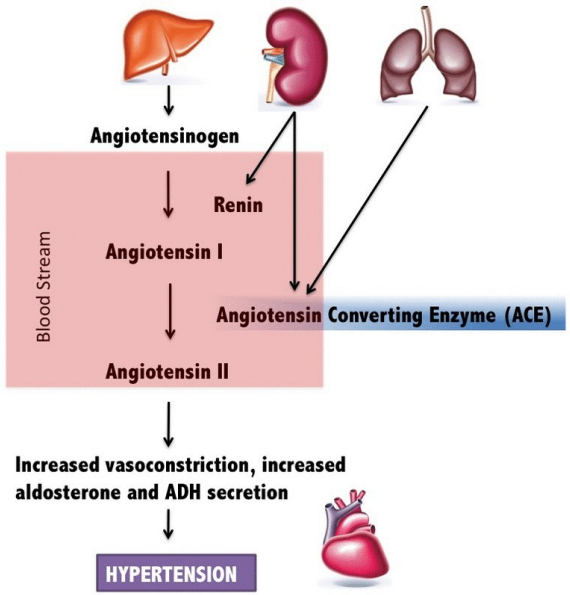
- QUERY
- EXPLORE
- FACILITY
- PROPERTY
- STRUCTURE
- IMPORTANT

Major Antihypertensive





ParaPep -A Database of Anti-parasitic peptides

Home Page of ParaPep

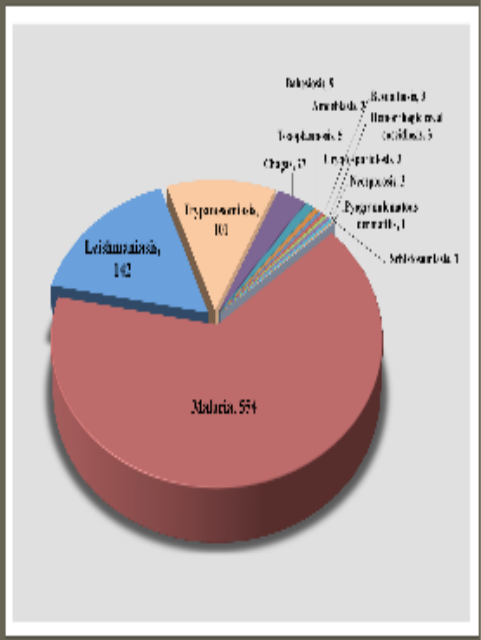
ParaPep: It is a manually curated repository of experientially validated anti-parasitic peptides and their structures. Data have been collected from research papers, published patents and other databases.

Peptide sequences: The current release of ParaPep contains 863 anti-parasite peptide entries, which have been tested against 12 different types of parasites. Most of the entries have been compiled for Malaria followed by Leishmaniasis and Trypanosomiasis.

Type of Peptides: ParaPep consists of various types of peptides, which includes linear peptides, cyclic peptides and peptides having L-amino acids, non-natural amino acids (e.g., D-amino acid, ornithine, etc.) and chemically modified residues.

Structure of Peptides: We determined secondary and tertiary structure of each peptide in ParaPep. using PepStr software. First, we scan PDB to identify all identical peptides to assign their tertiary structure. Structure of remaining peptides were predicted using PEPstr. Secondary structure of peptides were assigned using DSSP from their tertiary structure.

Parasitic Disease Covered



Quick View of ParaPep

Peptide Web Servers

AntiBP2 : Server for antibacterial peptide prediction

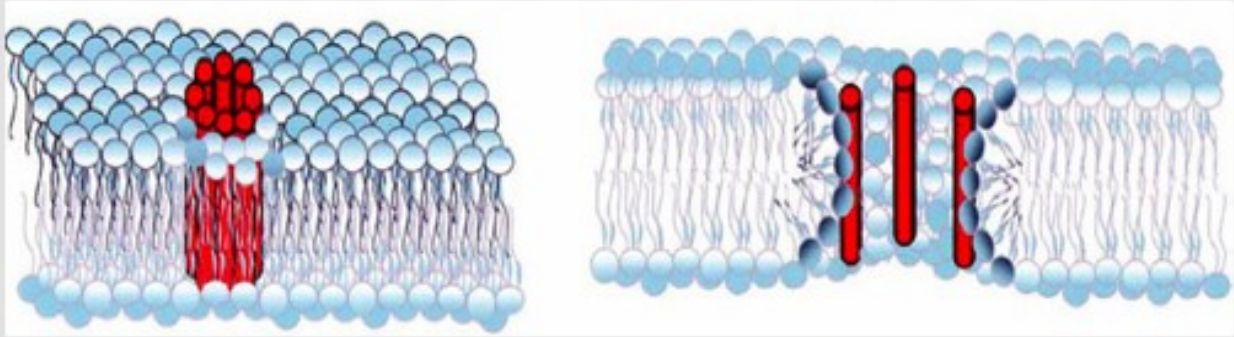
- Home
- Algorithm
- Submission
- Help
- Team
- Contact

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 Web Servers

PEPstr: PEPTIDE TERTIARY STRUCTURE PREDICTION SERVER

Bioinformatics Centre, Institute of Microbial Technology, Chandigarh

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

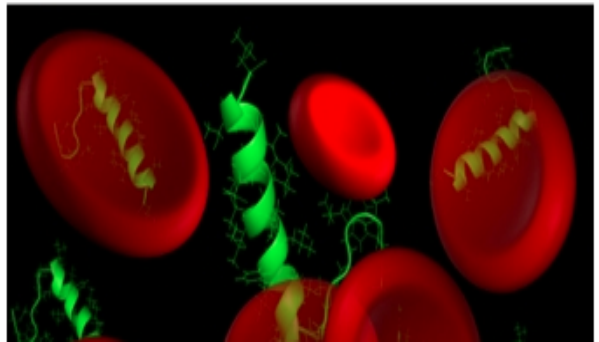
HEMOLYTIK: A Database of Hemolytic and Non-hemolytic Peptides

Welcome to Homepage

Hemolytik is a manually curated database of experimentally validated Hemolytic and Non-hemolytic peptides. In this database, peptides have been collected from both published articles as well as from other repositories like CAMP, DAMPD, APD2 and Swiss-Prot. In addition, tertiary structure of peptides have been predicted using PEPstr and secondary structure states are assigned using DSSP. First time, structure of modified peptides (containing Non-natural, D-amino acids, Modified-amino acid like Ornithine, Terminal modifications like Acetylation/Amidation) have also been predicted. In order to provide comprehensive information, peptides were searched and linked with important peptide and protein databases such as IEDB, PDB, Swiss-Prot and TrEMBL.

Major Features

(1) **Resource:** It provides comprehensive information about hemolytic peptides that include their Sequence, Name, Origin, Type (Linear/Cyclic), Chirality, End modification, Chemical modification, Source of RBCs, Hemolytic activity and Function. Data is collected from wide sources like literature and various other databases. Basic and Conditional Search facility enables the users to search a specific peptide/query in Hemolytik database.



DESTAMP: Designing of stable antibacterial mutant peptides

S.No.	Peptides	Prediction	Mutation Position	Half-life(s)	Antibacterial Activity (%)	HPLC parameter	Hydrophobicity (KJ/mol)	pKa	pKb	Residue volume	Molecular weight
Original peptide sequence											
0	DKADSFGPLMNCERT	Antibacterial Peptide	NO	0.393	71.329	45.100	193.000	31.720	141.480	1953.500	1936.060
Mutant peptide sequences predicted to be antibacterial. Mutant residues are colored RED.											
Sorting											
1	AKADSFGPLMNCERT	Antibacterial Peptide	1	0.316	74.192	37.200	258.000	32.180	141.570	1931.000	1892.050
2	CKADSFGPLMNCERT	Antibacterial Peptide	1	0.345	73.814	36.500	263.000	31.800	142.160	1955.100	1924.110
3	EKADSFGPLMNCERT	Antibacterial Peptide	1	0.322	71.539	42.900	219.000	32.030	141.010	1983.200	1950.090
4	FKADSFGPLMNCERT	Antibacterial Peptide	1	0.383	81.156	25.900	303.000	31.670	141.010	2031.700	1968.150
5	GKADSFGPLMNCERT	Antibacterial Peptide	1	0.698	83.114	40.800	211.000	32.180	141.480	1902.700	1878.030
6	HKADSFGPLMNCERT	Antibacterial Peptide	1	0.327	73.580	37.200	169.000	31.660	141.050	1995.300	1958.120
7	IKADSFGPLMNCERT	Antibacterial Peptide	1	0.463	71.569	27.100	311.000	32.200	141.480	2011.200	1934.130
8	KKADSFGPLMNCERT	Antibacterial Peptide								2018.300	1949.150
9	LKADSFGPLMNCERT	Antibacterial Peptide								2011.200	1934.130
10	MKADSFGPLMNCERT	Antibacterial Peptide								2004.900	1952.170

Designing of antibacterial stable peptides

Scanning of peptides in a protein

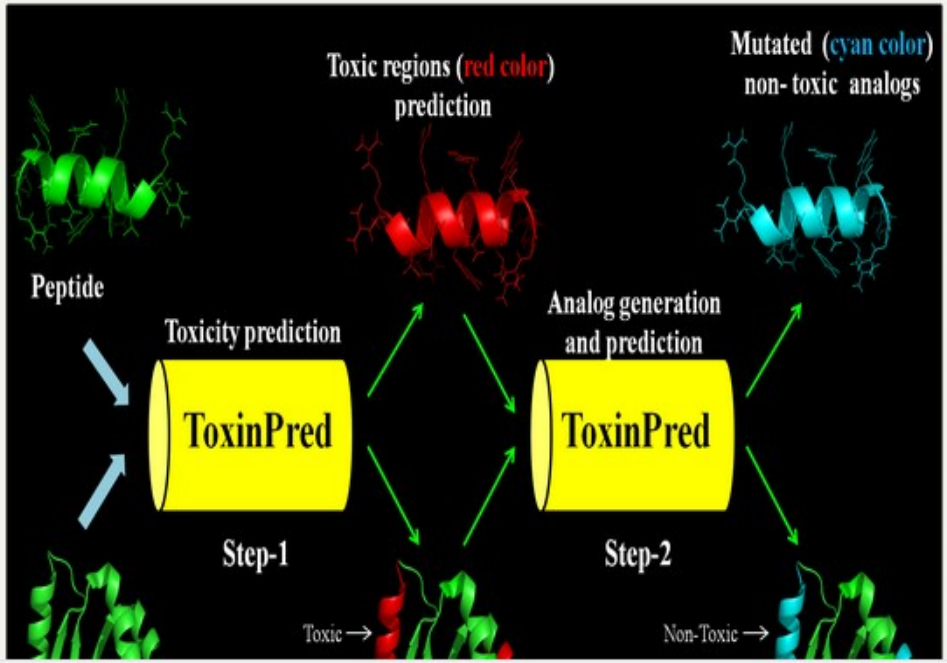
Submition of multiple peptides

ToxinPred

Designing and prediction of toxic peptides

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).

HerceptinR: Herceptin Resistance Database

Bioinformatics Centre, CSIR-Institute of Microbial Technology, India

- **Home**
- **Search Assays**
  - Simple Search
  - Advance Search
- **Browse Assays on**
  - Cell lines
  - Suppl. Drugs
  - Alterations in Cells
  - Publications
- **Cell Line Data**
- **Data Retrieval**
  - Mutaion Search
  - Summary of Cell lines
  - Browse on Cell Lines
  - Relative gene function
- **Web Tools**
  - Compare Genes
  - Alignment of Mutants
  - Align My Sequence
- **General Information**
  - Resistant Genes
  - Guide/Help/FAQ
  - Data downloads
  - Acknowledgement
  - Who are we?

Welcome to Home Page of HerceptinR

HerceptinR is a database of assays performed to test sensitivity or resistance of Herceptin Antibodies towards breast cancer cell lines. This database provides comprehensive information about experimental data perform to understanding factors behind herceptin resistance aas well as assays peformed for improving Herceptin sensitivity with the help of supplementary drugs. Best of our knowledge this is the first database developed to understand herceptin resistance, which can be used for designing herceptin sensitive biomarkers.

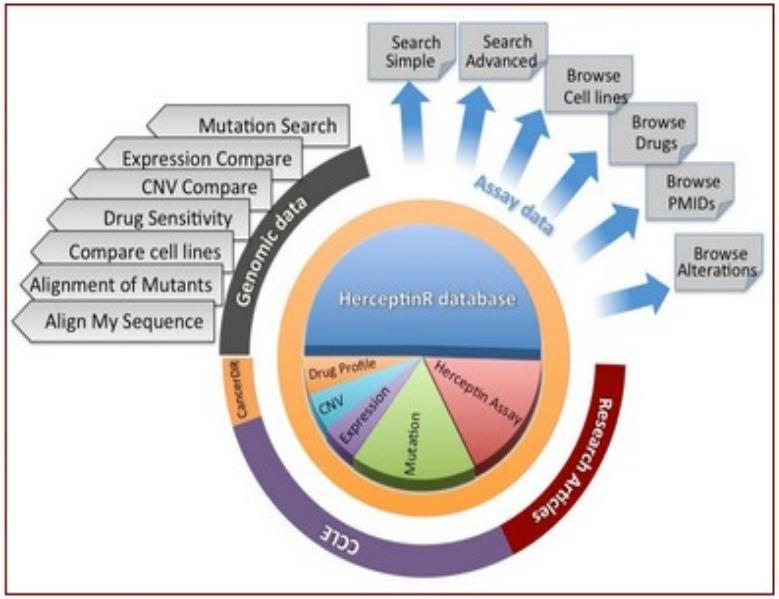
Major features of HerceptinR

Herceptin Assays: It provides information about 2500 herceptin assays performed to test efficacy of herceptin on various breast cell lines (~ 30 unique cell lines) with and without supplementary drugs (~100 unique drugs).

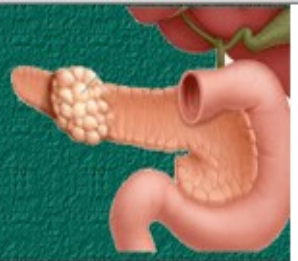
Cell Line Data: This database also provides comprehensive information about breast cancer cell lines (e.g., mutation, copy number variation, expression of genes), in order to facilitate user to design herceptin biomarkers.

Important Genes: Comprehensive information about herceptin resistant genes (due to their mutation or altered expression), reported in literature.

Web Tools: Number of tools have been integrated that include comparison of gene functions (expression, CNVs, mutations) of sensitive and resistant cell lines.



PCMDB: Pancreatic Cancer Methylation Database



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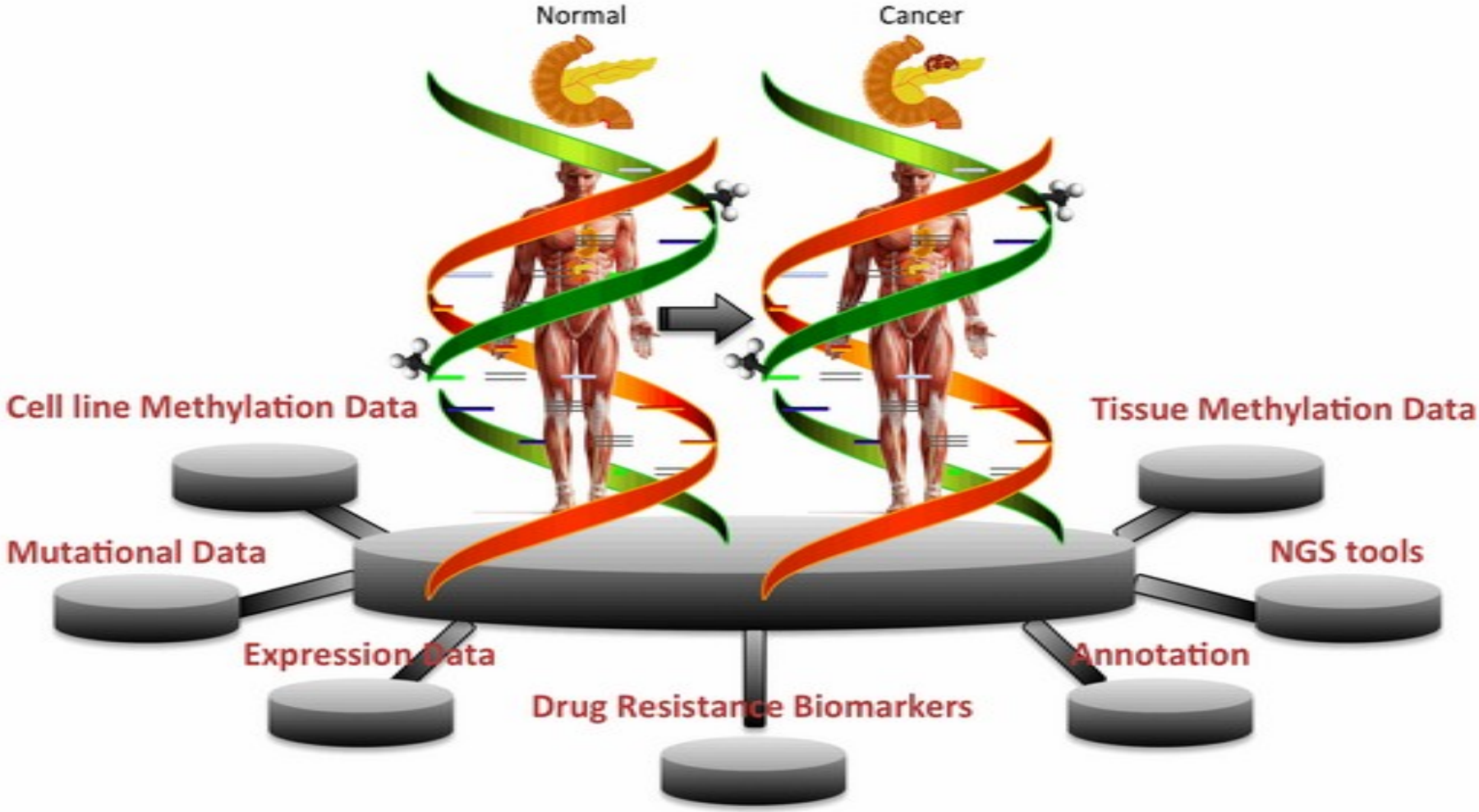

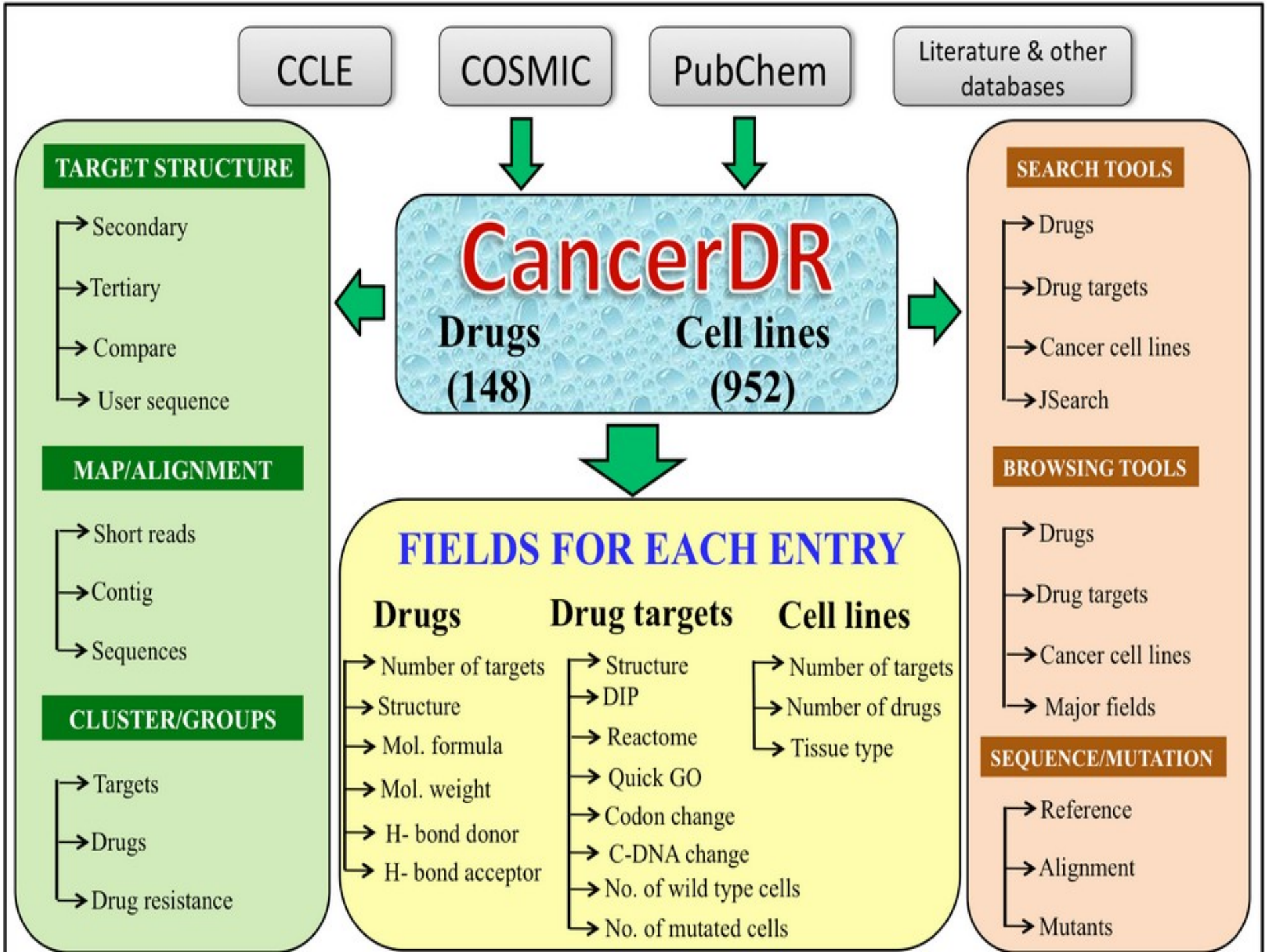
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Literature & other databases
TARGET STRUCTURE
Secondary
Tertiary
Compare
User sequence
MAP/ALIGNMENT
Short reads
Contig
Sequences
CLUSTER/GROUPS
Targets
Drugs
Drug resistance
CancerDR
Drugs (148)
Cell lines (952)
FIELDS FOR EACH ENTRY
Drugs
Number 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

DrugMint

A SERVER FOR IDENTIFICATION OF DRUG-LIKE MOLECULE

Home OSCADD

Inhibitor Prediction

KiDoQ (Mtb target)

GDoQ (Mtb target)

ABMpred (Mtb target)

eBooster (Mtb target)

MDRIpred (Mtb cell)

CancerIN (Cancer)

ntEGFR (Cancer EGFR)

EGFRpred (Cancer EGFR)

DiPCell (Pancreatic Cancer)

Welcome to Design Analogs Module

Lead optimization is a time consuming process in drug discovery. This tool generate all the possible analogs c
user-defined or identified R groups. Finally, the server will generate the virtual chemical library, which wo
properties. After screening, the results will be displayed in tabular format with the facility to sort them as per u
click help.

Paste Scaffold structure:
Use Scaffold Example

Paste Building Blocks structure:
Use Building Blocks Example

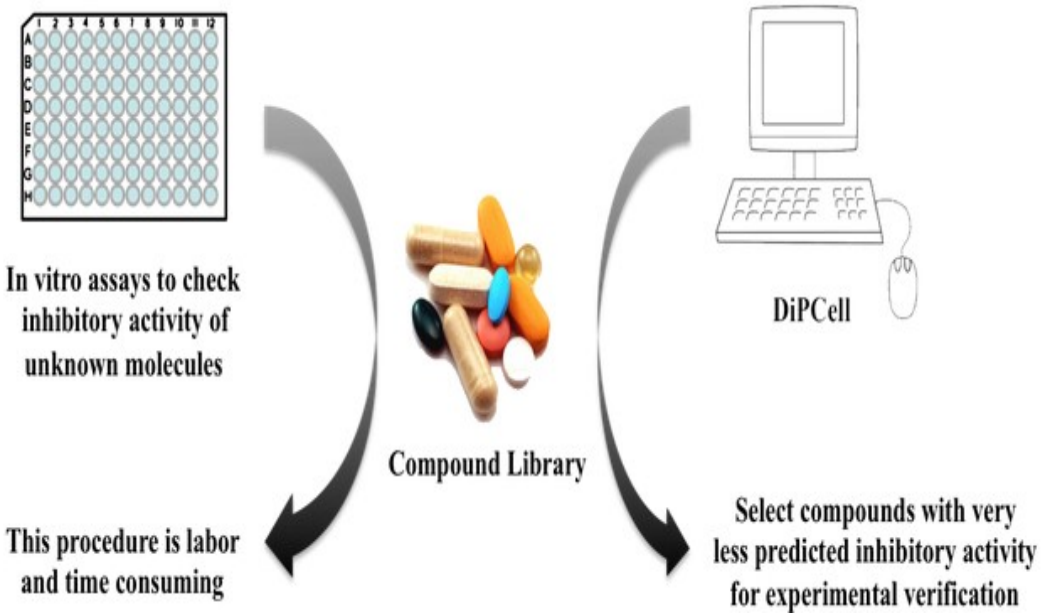
Paste linkers :
Use Linker Example

DiPCell: Designing of inhibitors of pancreatic cancer cell

CSIR – Institute of Microbial Technology, India

Welcome to DiPCell

DiPCell is a webserver for the predicting inhibitory activity of unknown molecules and designing their analogs against pancreatic cancer cell lines. DiPCell implements the QSAR models, which were developed by using SMOreg machine learning algorithm on high throughput drug screening data. This high throughput screening data is obtained from the Genomics of Drug Sensitivity in Cancer (GDSC) database.



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

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

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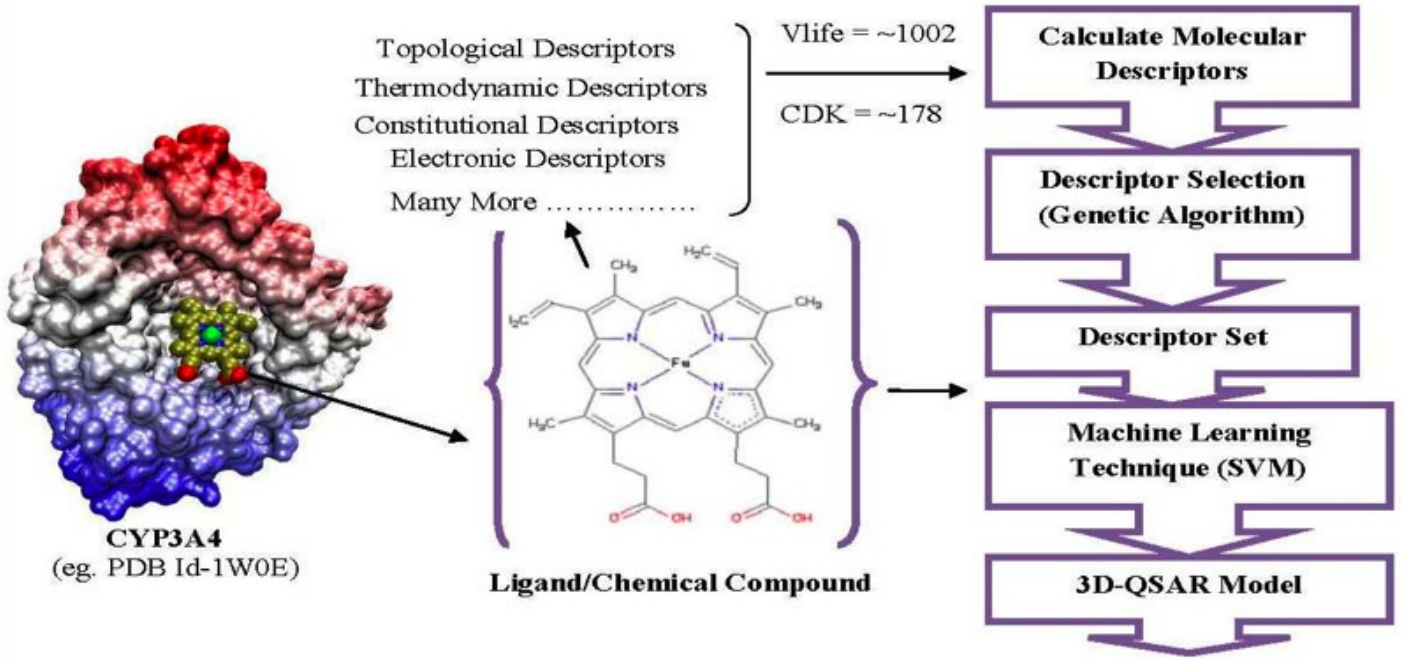
Cytochrome P450 enzymes (CYPs) are a multi gene family of heme-containing isoenzymes that are involved in oxidative metabolism of drug, steroids and carcinogens. About sixty CYPs are reported in human genome, but more than 90% of all therapeutic drugs are metabolized by five isoforms i.e. CYP1A2, CYP2C9,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

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



ToxiPred: A server for prediction of aqueous toxicity of small chemical molecules in T. pyriformis

Home OSCADD

Inhibitor Prediction

KiDoQ (Mtb target)

GDoQ (Mtb target)

ABMpred (Mtb target)

eBooster (Mtb target)

MDRIpred (Mtb cell)

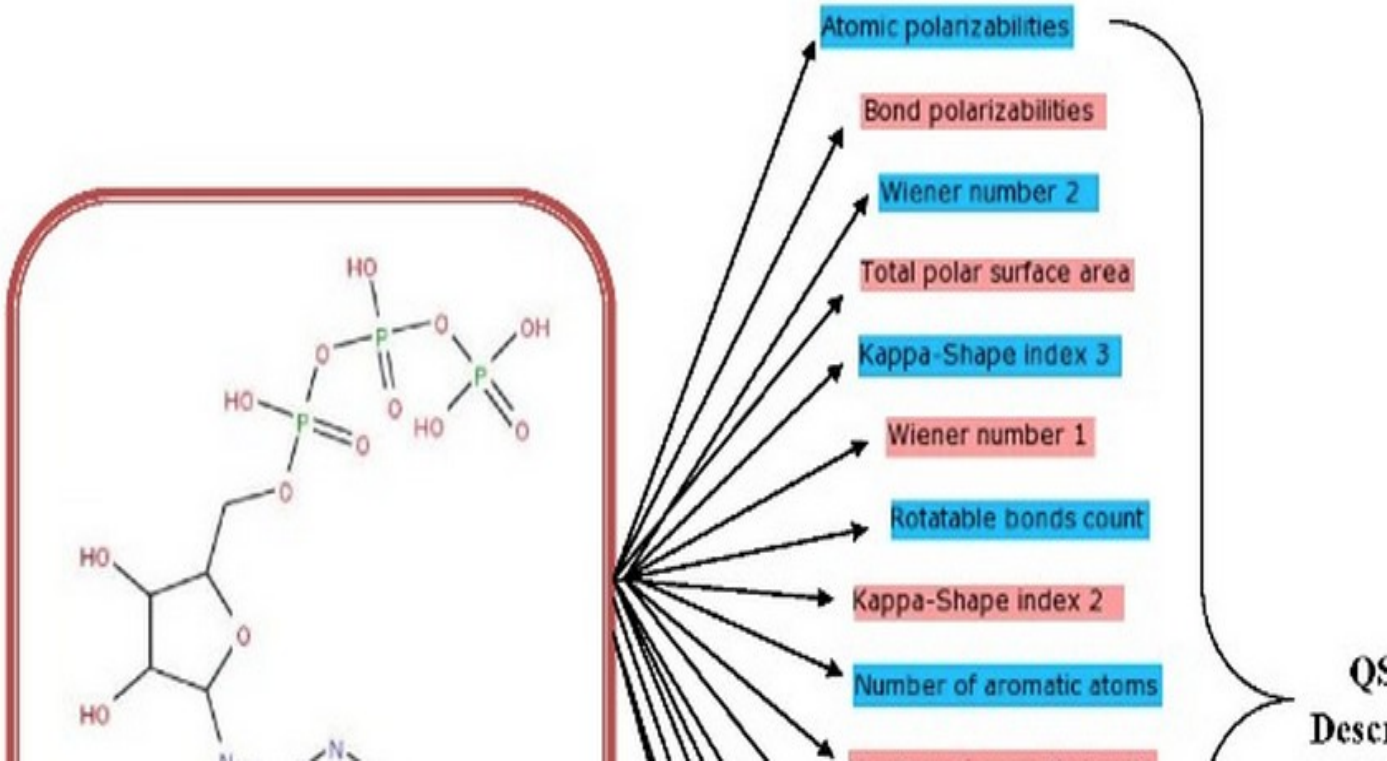
CancerIN (Cancer)

ntEGFR (Cancer EGFR)

EGFRpred (Cancer EGFR)

DiPCell (Pancreatic Cancer)

Identification of non-toxic drug design is a major challenge in the field of drug design, most of th
development or even in clinical trials. Thus the use of predictive toxicology is called for. Keeping this
employed previously but we have started this study with latest dataset and apply different machin
implemented in WEKA and linear method (Multiple linear regressions (MLR)) using R-package. To
molecules in the commonly used format (mol/SMILE/sdf) and after descriptors calculation our server w
hope that present model will aid in the area of drug designing.



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Bioinformatics, genomics, Computational biology, chemoinformatics, immunoinformatics
Verified email at imtech.res.in - Homepage

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Co-authors View all...

Manoj K. Bhasin, Sudipto Saha, Manish Kumar, Harpreet Singh, s

Title 1–20	Cited by	Year
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Thank You

http://www.imtech.res.in/raghava/