Computational Resources for Cancer

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

Cancer : Patient Management

Old Age, Fatigue, Pain, Lumps, Severe weight loss etc.

Screening and Diagnosis

CT scan, MRI, PET, Biopsy, X-Ray, Tumor Markers

Risk assessment/Prognosis

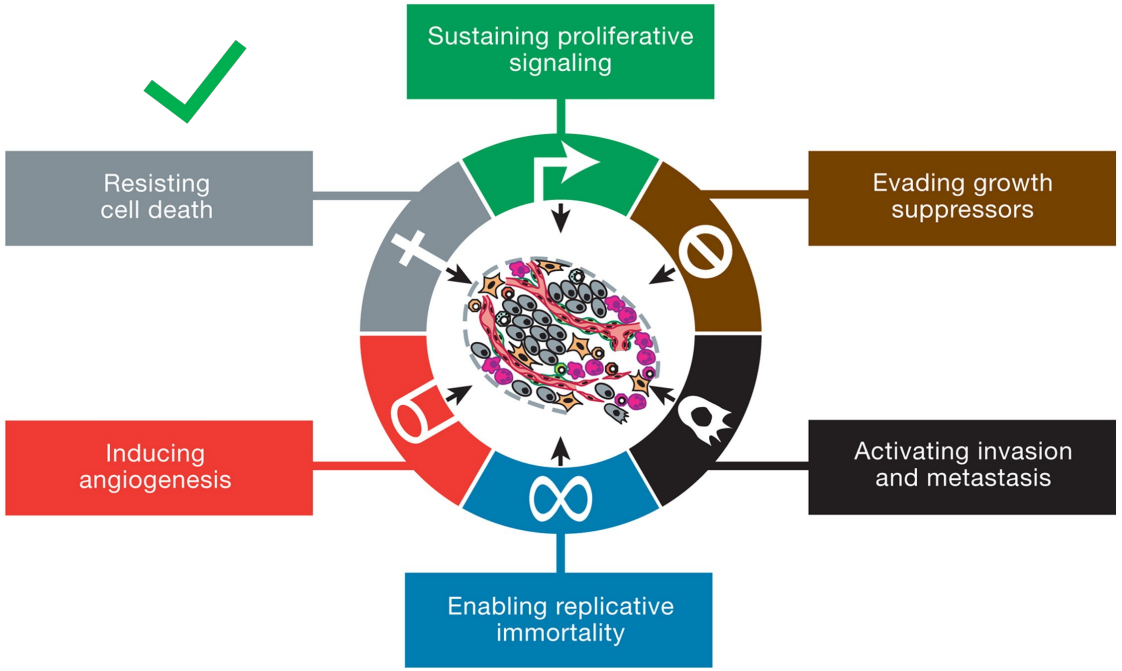
Cancer Staging, Cancer Biomarkers

Treatment

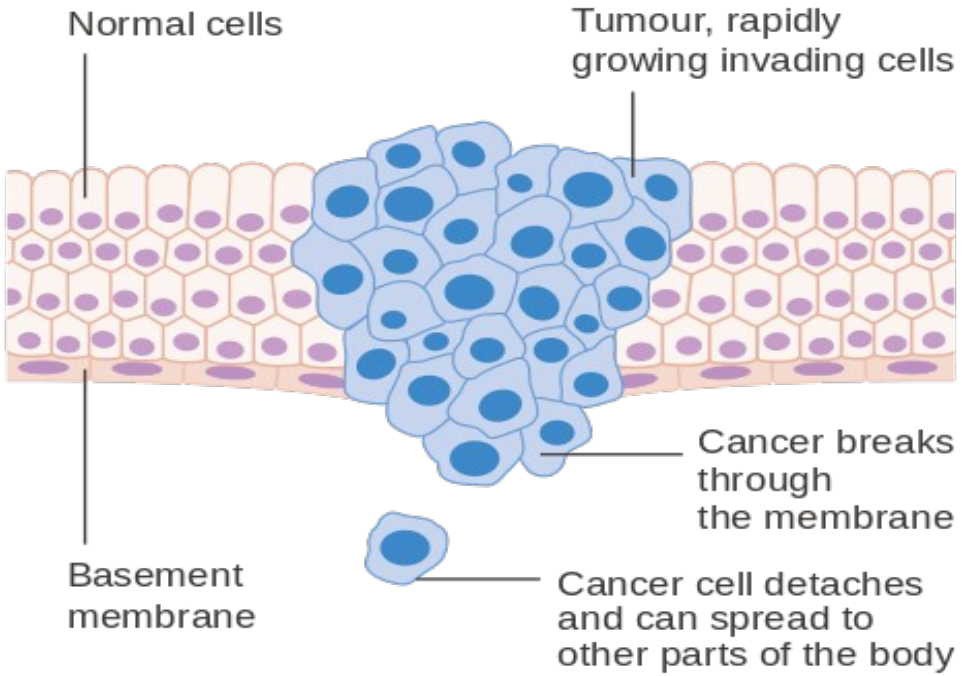
Surgery **if possible** and/or Chemo, Radio, Immuno-therapy etc.

Cancer : Hallmarks

Primary tumor : initial mass (surgical removal, treatment)



Hanahan *et al*, 2011

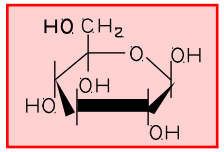


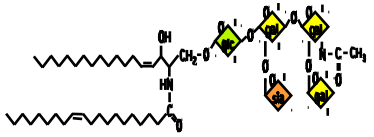
Singular agenda: Make more and more copies!!

Benign : localized, don't expand
Malignant: aggressive, invade surrounding areas

Metastatic tumor : spread to other parts (very difficult to treat, treatment to reduce growth, Alleviate pain and symptoms)

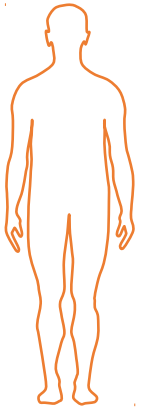
Glycomics (Sugars)

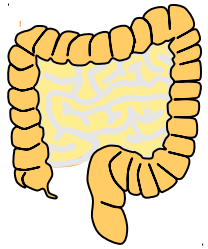




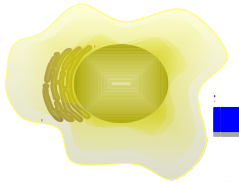
Lipidomics (Lipids)

Metabolomics

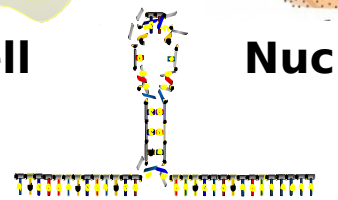




Organ, Tissue

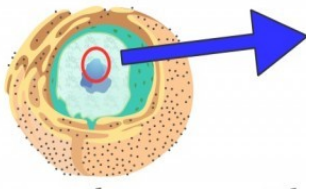


Cell



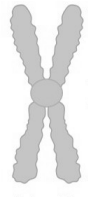
miRNA

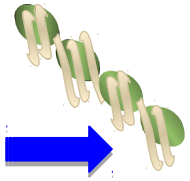
Non-coding RNA



Nucleus

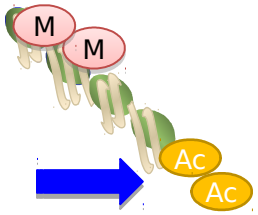
Chromosome (23 pair)



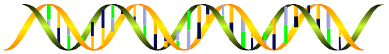


Chromatin

Epigenomics



Genomics (3×10⁹)

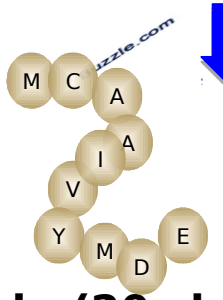


DNA (4 chemicals: A, T, G, C)

World of OMICs

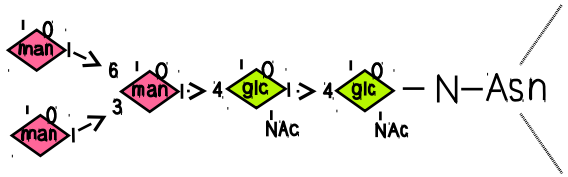
mRNA

Transcriptomics (copies)



Proteomics

Protein (20 chemicals:



Glycomics (Sugars

Computation Resources for Cancer Research

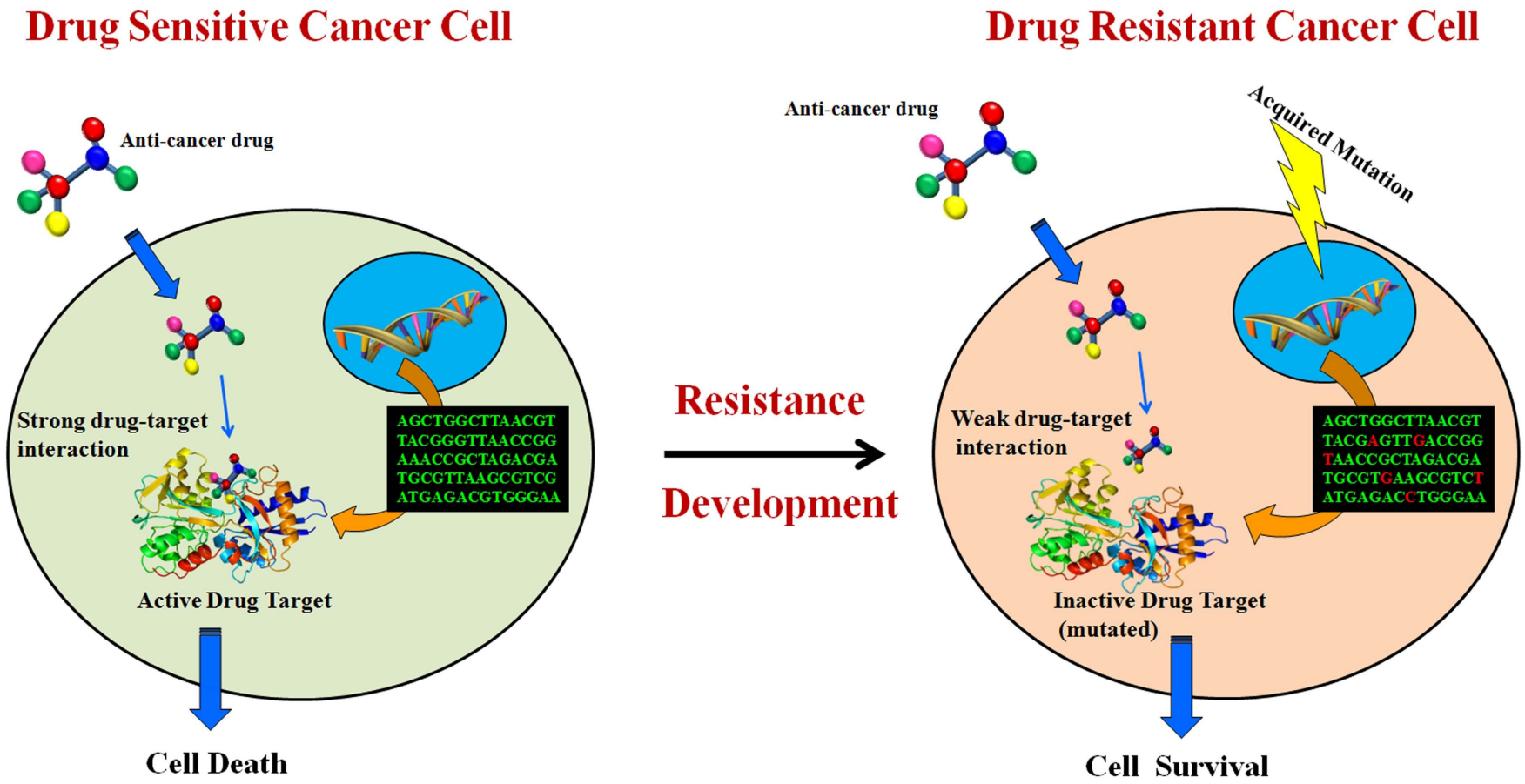
- Drug resistance
  - CancerDR (http://webs.iiitd.edu.in/raghava/cancerdr/)
  - HercepitinR (http://webs.iiitd.edu.in/raghava/heceptinr/)
- Gene databases
  - PCMdb (http://webs.iiitd.edu.in/raghava/pcmdb/)
  - dbEM (http://webs.iiitd.edu.in/raghava/dbem/)
  - ApoCanD (http://webs.iiitd.edu.in/raghava/apocand/)
- Drug delivery
  - OvirusTDB (http://webs.iiitd.edu.in/raghava/ovirustdb/)
  - TumorHope (http://webs.iiitd.edu.in/raghava/pcmdb/)
- Cancer Biomarkers
  - CancerLiver (http://webs.iiitd.edu.in/raghava/cancerliver/)

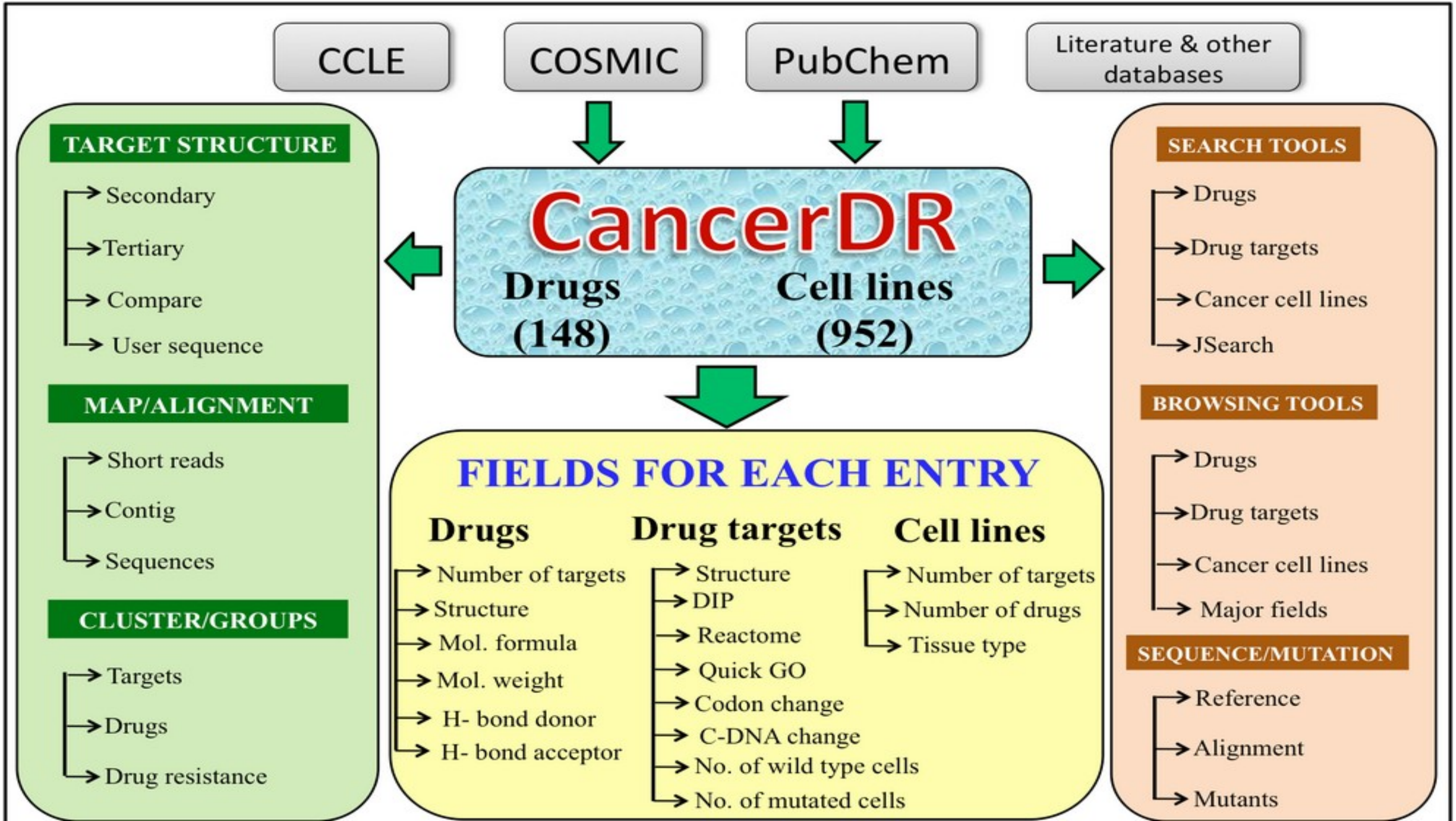
CancerDR: Cancer Drug Resistance Database

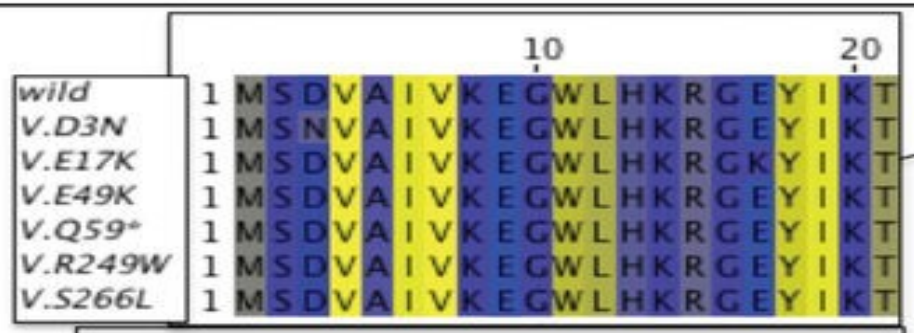
CSIR - Institute of Microbial Technology, India

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

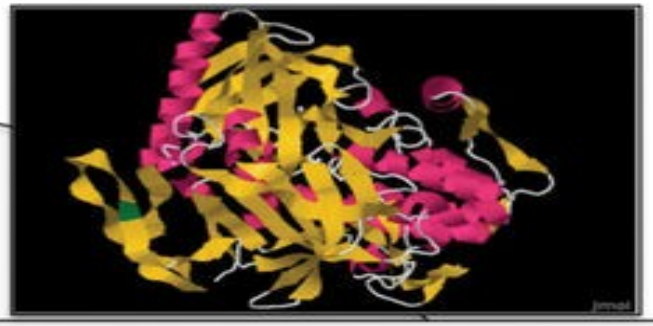
Search
Browse
Alignment/Mutation
Target Structure
Map/Alignment
Clusters/Groups
Downloads



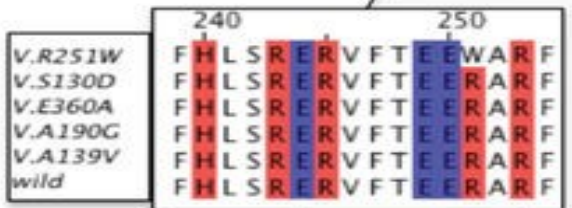

CCLE
COSMIC
PubChem
Literature & other databases
CancerDR
Drugs (148)
Cell lines (952)
TARGET STRUCTURE
Secondary
Tertiary
Compare
User sequence
MAP/ALIGNMENT
Short reads
Contig
Sequences
CLUSTER/GROUPS
Targets
Drugs
Drug resistance
FIELDS FOR EACH ENTRY
Drugs
Number of targets
Structure
Mol. formula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



Multiple Sequence Alignment of Targets

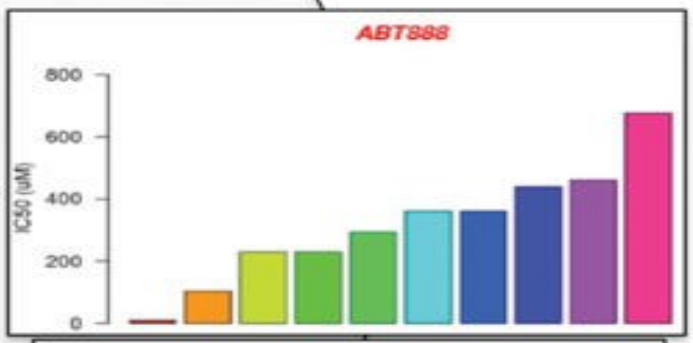


Tertiary structure prediction of targets and their Mutants

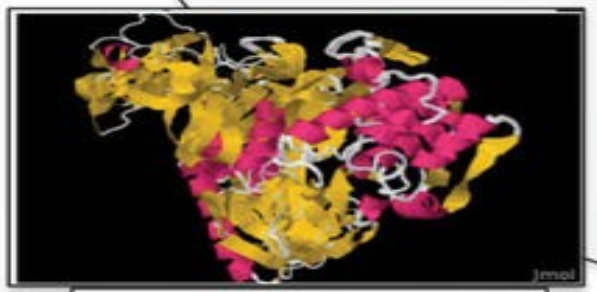


Sequence Alignment on the basis of Structure

CancerDR



Pharmacological Drug Profiling



Structure Comparison

Short read alignments with CancerDR Targets

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.

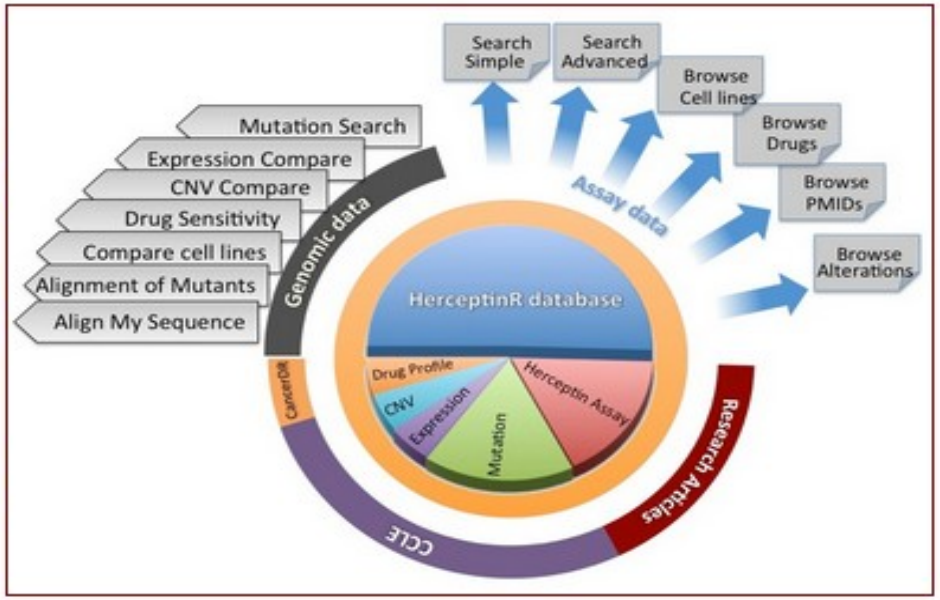
Major features of HerceptinR

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).

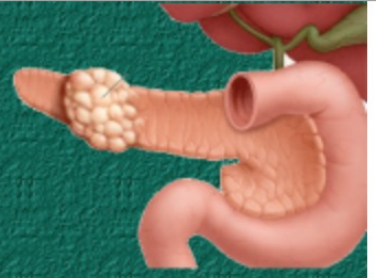
Cell Line Data: This database also provides comprehensive information about breast cancer cell lines (e.g., mutation, copy number variation, expression of genes), in order to facilitate user to design herceptin biomarkers.

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

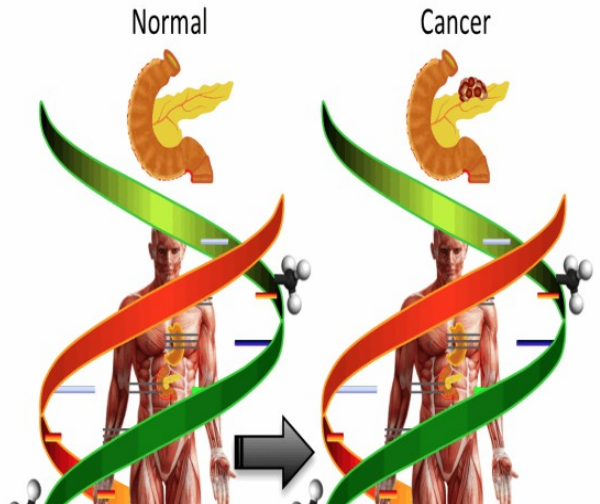


PCMdb | SEARCH | BROWSE | SUMMARY | DRUG RESISTANCE | TOOLS | GUIDE/HELP | CONTACT

Welcome to Home Page of PCMdb

arma, M.; Kumar, S.; Chaudhary, K.; Gupta, S.; Gautam, A. and Raghava, G.P.S. (2014) PCMdb: Pancreatic Cancer Methylation Database. Sci. Rep. 4:419

PCMdb is a database of methylated genes found in pancreatic cancer cell lines and tissues. In other words, it provides comprehensive information about methylation status of various genes in Pancreatic Cancer (PCa) and their comparison with transcriptomics and genomics landscape. It is a manually curated database where information is collected and compiled from literature/databases. This database will be very useful to discover novel biomakers for PCa as well as to understand the role of methylation in drug resistance.



Major Features of PCMdb

SEARCH/BROWSE:
Keyword and Advanced search options allow one to retrieve data from PCMdb. Browse facility facilitates users to categorize/classify PCMdb data on different fields (Cell Lines, Genes, Chromosome, Method and Methylation Category).

Integration of Tools:
A large number of web based tools have been integrated into PCMdb that include similarity search techniques like BLAST and SMITH-WATERMAN. It also facilitates users to process

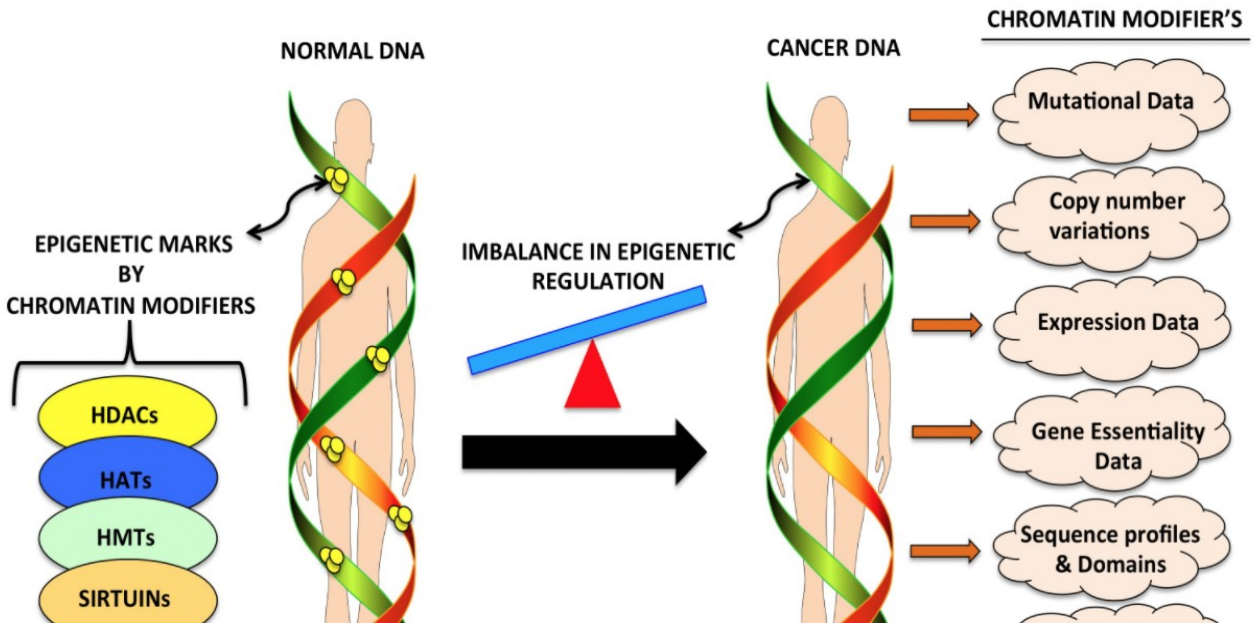
dbEM

A Database of Epigenetic Modifiers

Cite: Nanda JS, Kumar R, Raghava GP. (2016) dbEM: A database of epigenetic modifiers curated from cancerous and normal genomes. Sci Rep. 6:19340.

Welcome to dbEM

dbEM is a database of epigenetic modifiers curated from cancerous and normal genomes. It is created to study role of epigenetic proteins in oncogenesis and cancer drug resistance. This database maintain genomic information about each epigenetic modifier like mutations, copy number variation and gene expression in thousand of tumor samples, cancer cell lines and healthy individuals; obtained from COSMIC, CCLE and human thousand-genome project.

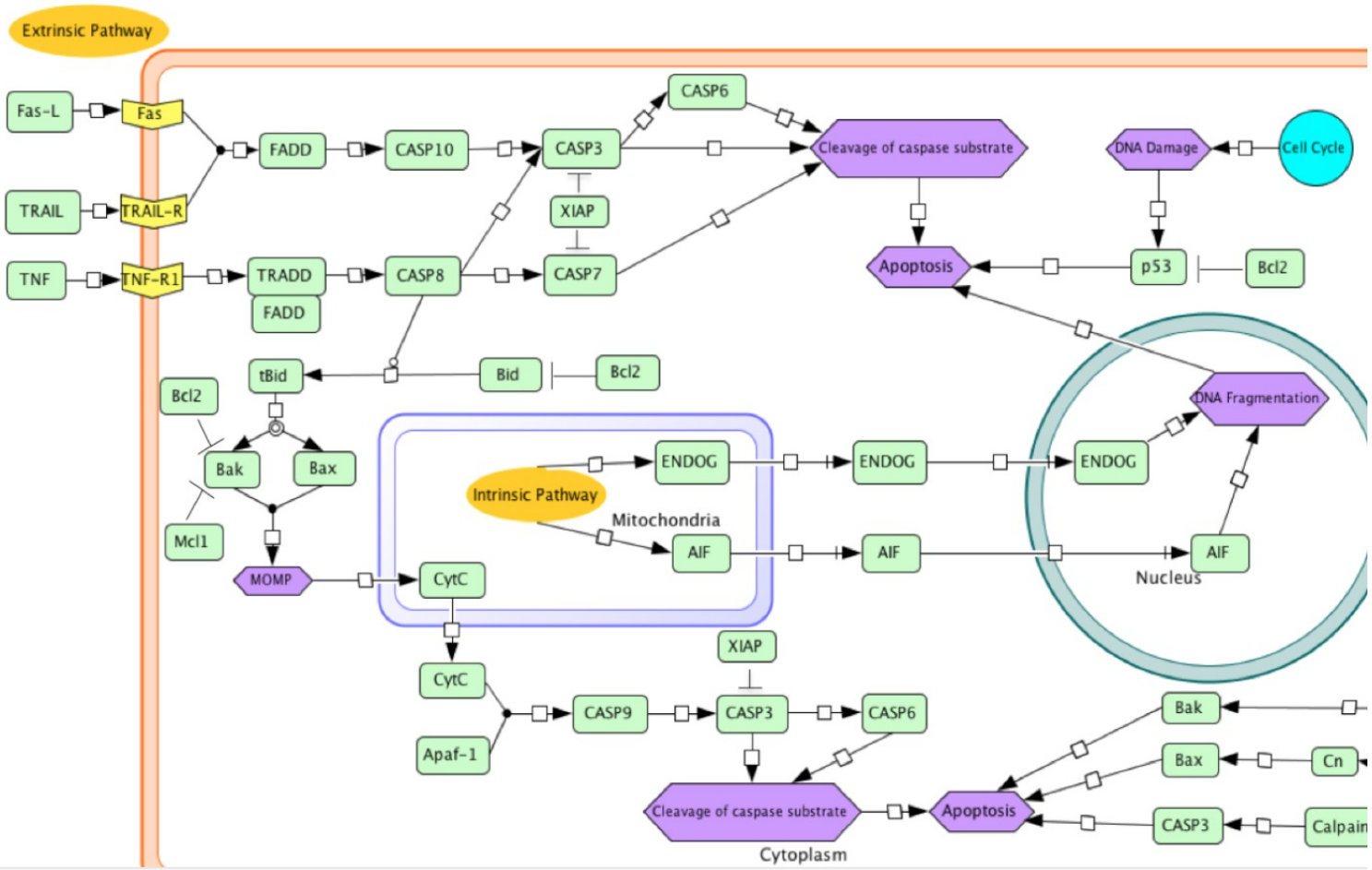


ApoCanD: Database of Human Apoptotic Proteins in the context of cancer

Ragh

Reference: Kumar, R. and Raghava, G.P. (2016) ApoCanD: Database of human apoptotic proteins in the context of cancer. Scientific Reports 6, 20797

Apoptosis is a crucial cellular process, which determines the ultimate cell fate and has its own significance both in normal and diseased condition. Cancer understands the significance of apoptosis process very well and modifies it to ameliorate its survival. Apoptosis process is inhibited in cancer cells, so that it can prolong its life without any regulatory check. To keep in mind the importance of this process, we have dedicated this database called "**ApoCanD**" for the better understanding of role of apoptosis process in cancer. This database contains 82 proteins involved in various stages of apoptosis. Here, we included **mutation status, expression level and copy number variation** of these proteins across the thousands of cancer cell lines and tumour samples. Along with this crucial genomic information, this database also contains **gene essentiality data**. From sequence point of view, this database imparts with the **sequence alignments** of these proteins with mutated sequences and their homologus proteins. **Structures** were predicted for those proteins, whose structures are not available in protein databank (PDB). In structural information, this database also provides the **PFAM and Superfamily domains** present in these proteins. This database contains the crucial information and help users to understand the apoptosis process from



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

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

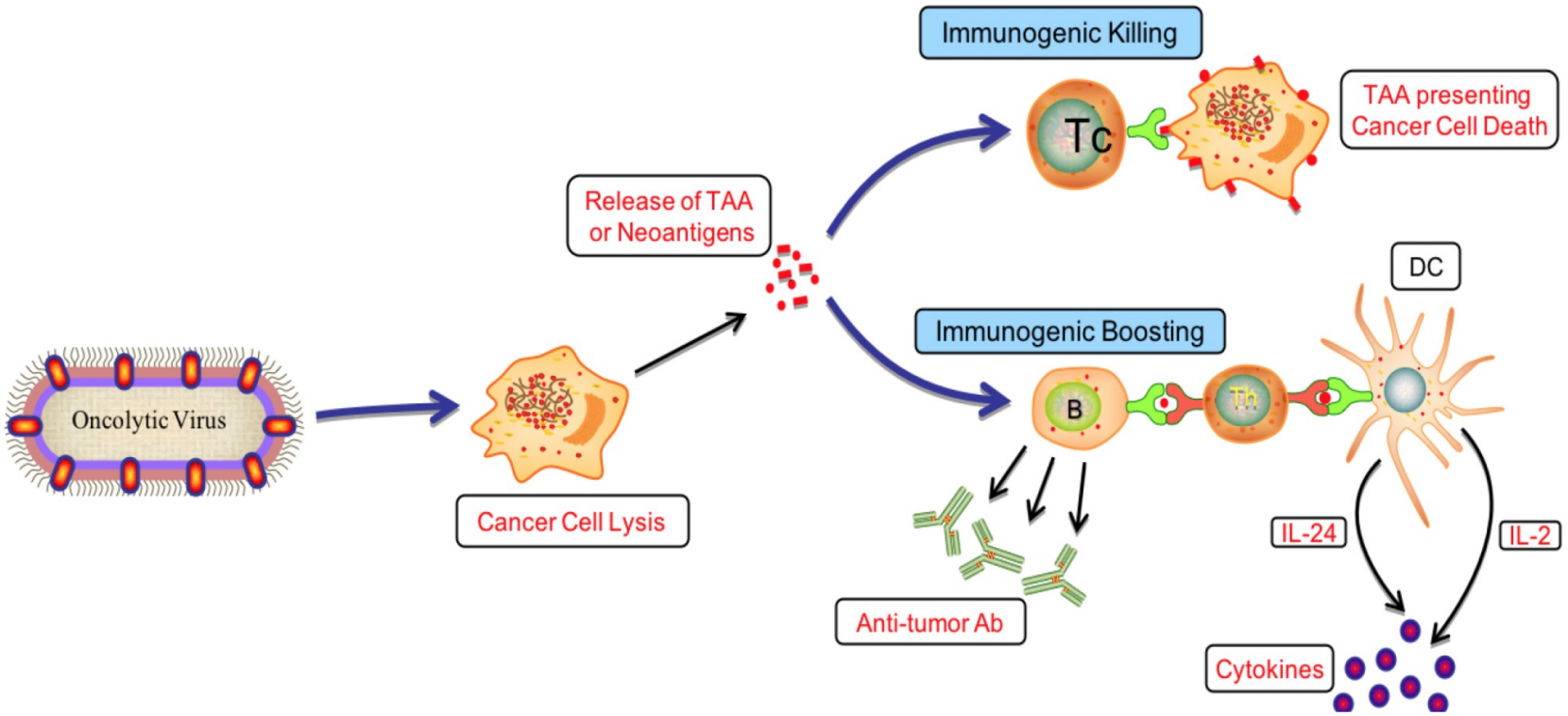
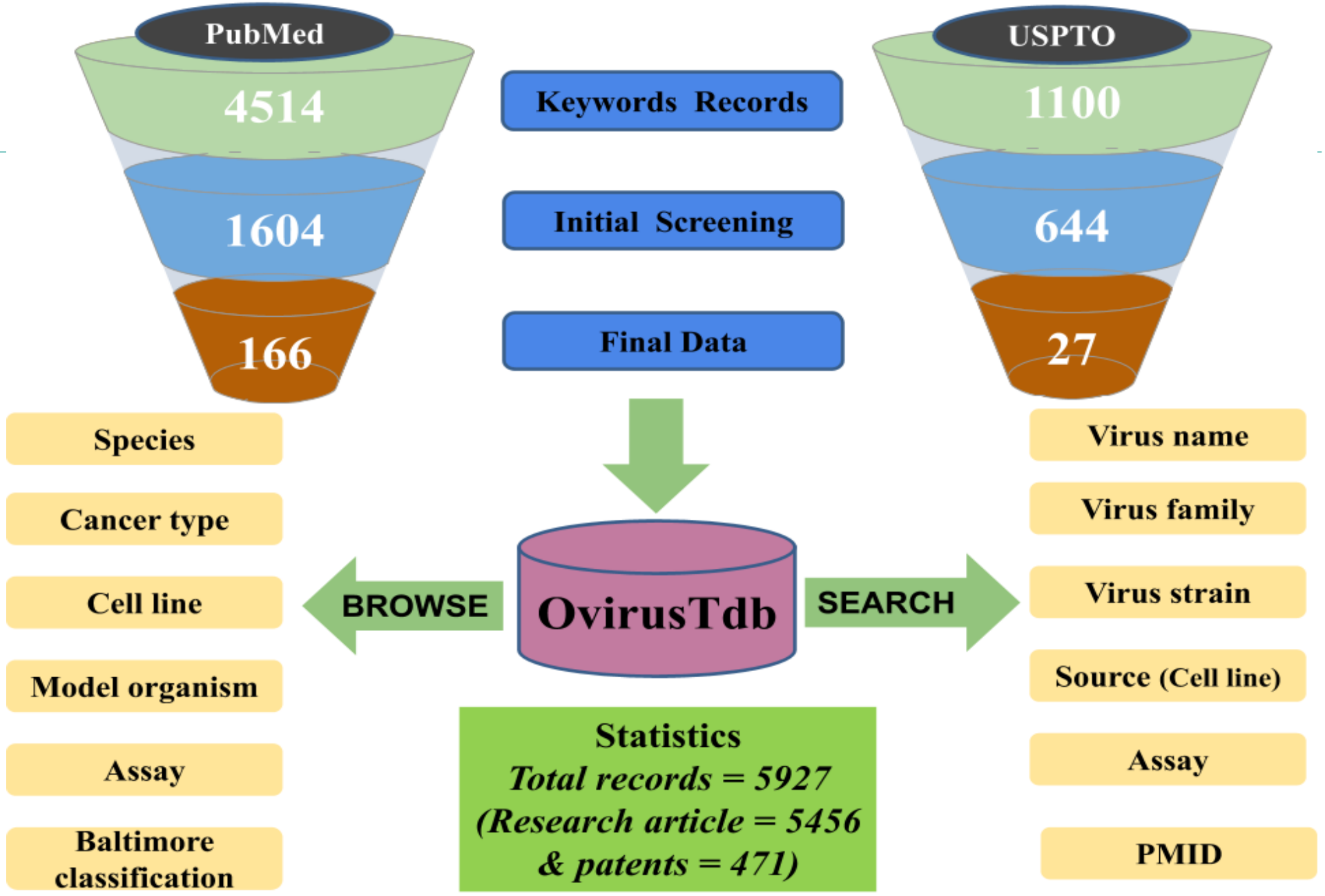


Figure illustrating mechanism of oncolysis and immunogenic effect induced by Oncolytic virus

Database organisation and architecture



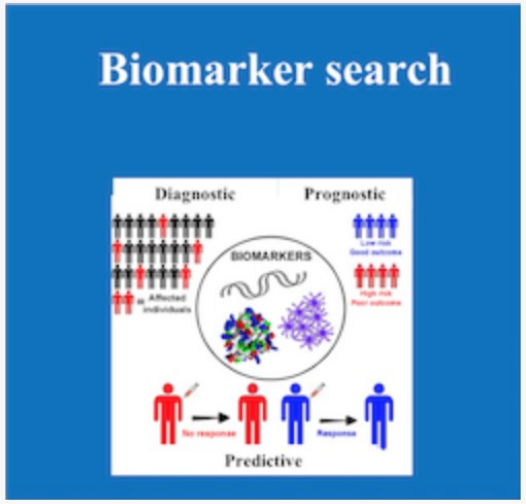
Web server: https://webs.iiitd.edu.in/raghava/ovirustdb/

, Gajendra PS Raghava, CancerLivER: a database of liver cancer gene expression resources and biomarkers, Database, Volume 20

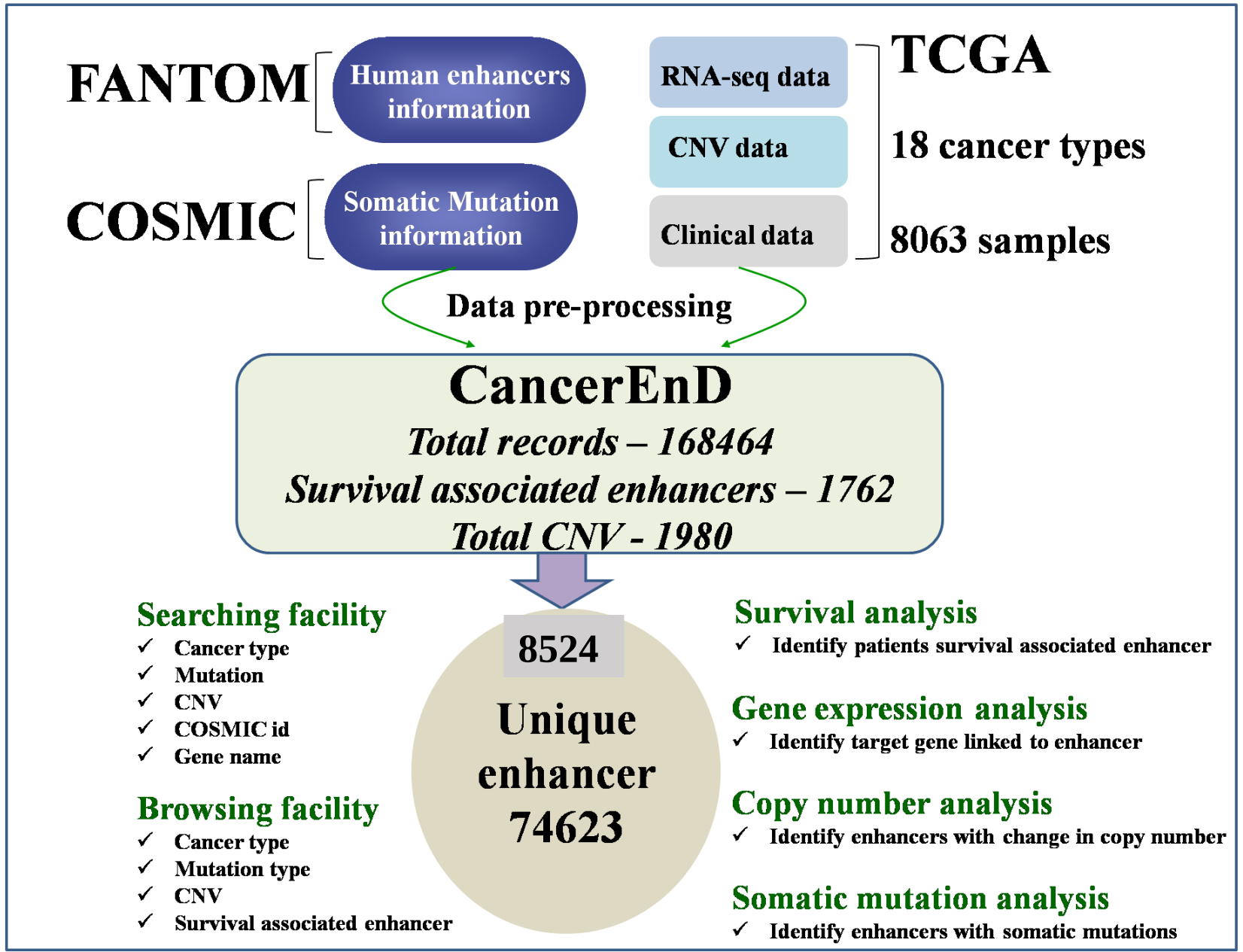
CancerLivER: A Database of Gene expression and Biomarker data of Liver Cancer

CancerLivER (Liver Cancer Expression Resource) is a database of liver cancer that maintains gene expression datasets and biomarkers curated from public repositories and literature respectively. It contains the following three modules for extracting and analyzing data.

Major Modules of CancerLivER

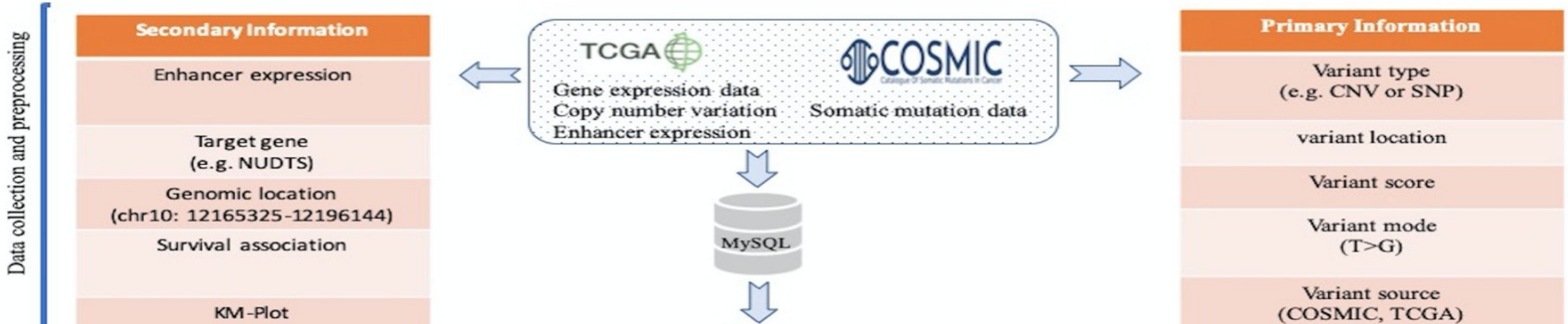


CancerEnD: a database of cancer associated enhancers



CancerEnD - A Comprehensive Resource On Enhancer Information For TCGA Cancer Types

CancerEnD Genome-wide association studies have successfully identified thousands of genomic loci potentially associated with hundreds of complex traits in the past decade. Nevertheless, the fact that more than 90% of such disease-associated variants lie in non-coding DNA with unknown functional implications has been appealing for advanced analysis of plenty of genetic variants. Toward this goal, recent studies focusing on individual non-coding variants have revealed that complex diseases are often the consequences of erroneous interactions between enhancers and their target genes. CancerEnD is a database of Enhancers expression, their somatic mutation & CNV in 18 cancer types by extracting data from various large repositoies This database provides a user-friendly interface for browsing and searching, and it also allows users to download data freely. CancerEnD has the potential to become a helpful and important resource for researchers who aim to understand the molecular mechanisms of enhancers involved in complex diseases.



Web Services for Predicting Biomarkers and Therapeutics

- Personalized vaccines and drugs
  - CancerTope (http://webs.iiitd.edu.in/raghava/cancertope/)
  - CancerDP (http://webs.iiitd.edu.in/raghava/cancerdp/)
- Promiscuous Cancer Drugs
  - DiPCell (http://webs.iiitd.edu.in/raghava/cancerdp/)
- Cancer Biomarkers (Stage, Progression, Prognostic)
  - CancerLSP (http://webs.iiitd.edu.in/raghava/cancerlsp/) Stage prediction
  - CancerSSP (http://webs.iiitd.edu.in/raghava/cancerend/) Progression
- Peptide-based solutions
  - CancerPDF (http://webs.iiitd.edu.in/raghava/cancerpdf/)
  - CancerPPD (http://webs.iiitd.edu.in/raghava/cancerpppd/)
  - AntiCP2 (http://webs.iiitd.edu.in/raghava/anticp2/)
  - TumorHPD (http://webs.iiitd.edu.in/raghava/tumorhpd/)

Cancertope

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

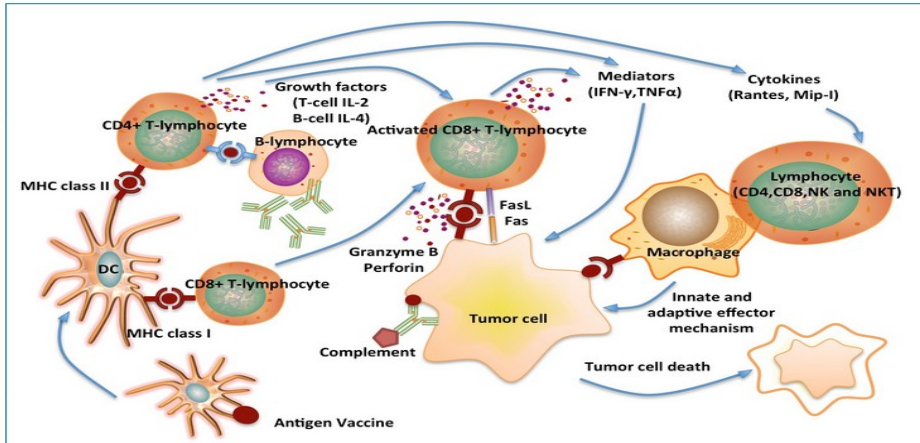
Welcome to Cancertope

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.

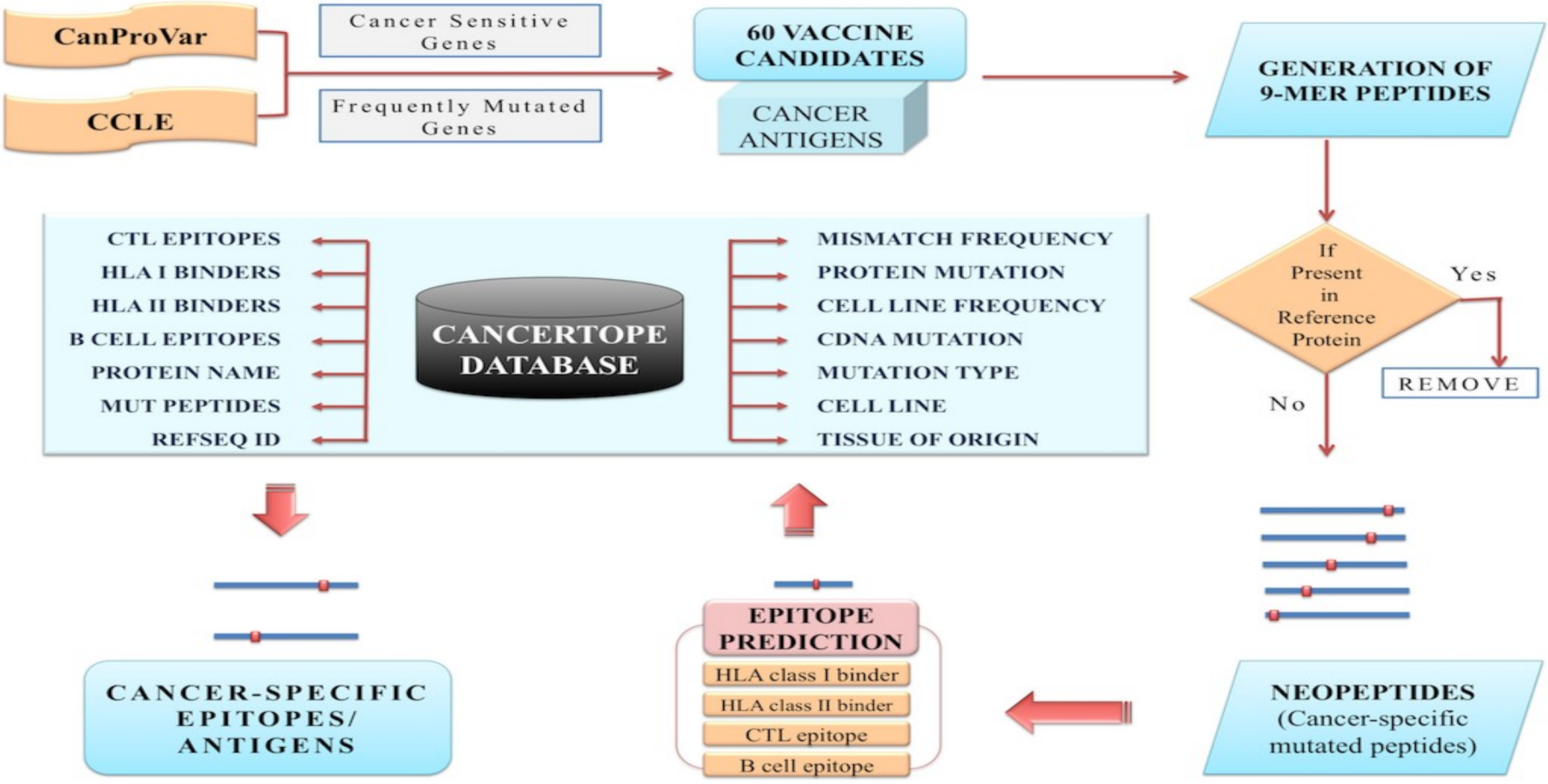
Advancement in Technology: In last two decades, there is a tremendous advancement in the field of genome sequencing, immunology and in immuno-informatics. Due to advancement in the field of genome sequencing, important genes of more than thousands of cancer cell-lines have been sequenced. Generation 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:

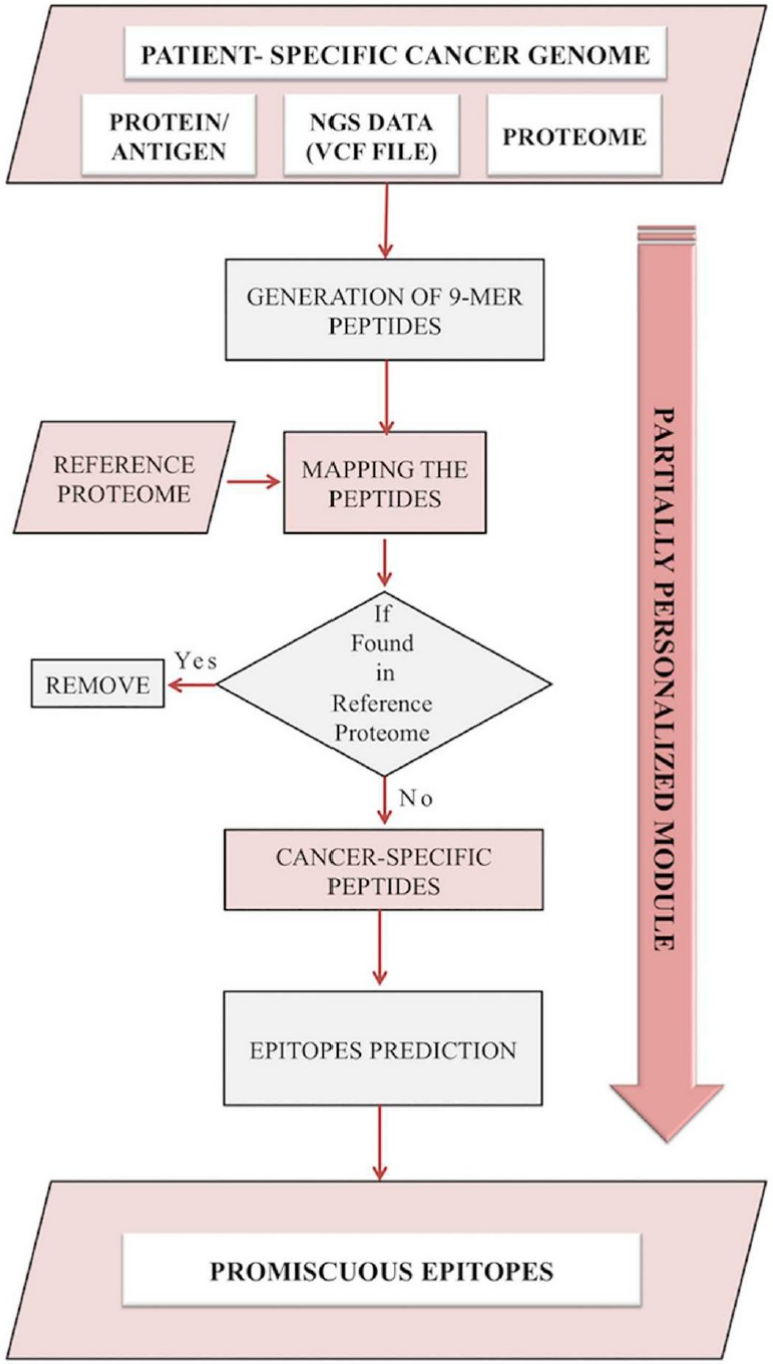
- **Cancer-Specific Epitopes:** This module is designed to identify "antigenic/epitopic" regions suitable to design vaccine against a specific type of cancer or cell line. Basically, it is a database of epitopes (B-cell, T-helper and CD8+) generated from around 60 cancer vaccine targets belonging to 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

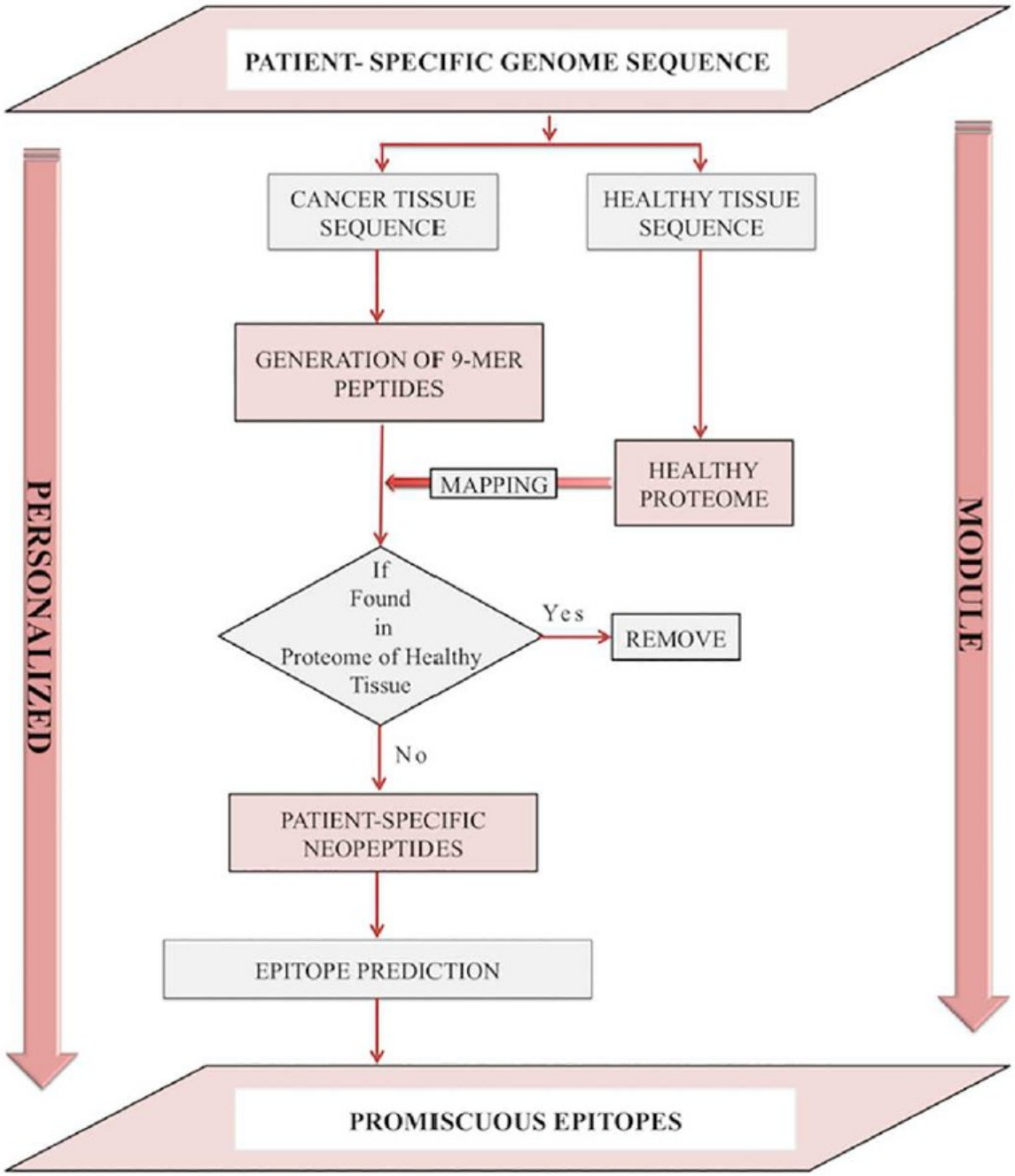


Architecture of CancerTope



Partially and Fully Personalized Modules of CancerTope





VLCvirus

A Web Resource For Designing Subunit Vacccine Candidates Against Lung Cancer Associated Viruses

Reference: Lathwal A, Kumar R and Raghava GPS (2021) In-silico Identification of Subunit Vaccine Candidates against Lung Cancer-associated Oncogenic Viruses. Computers in Biology and Medicine. doi 10.1016/j.compbiomed.2021.104215

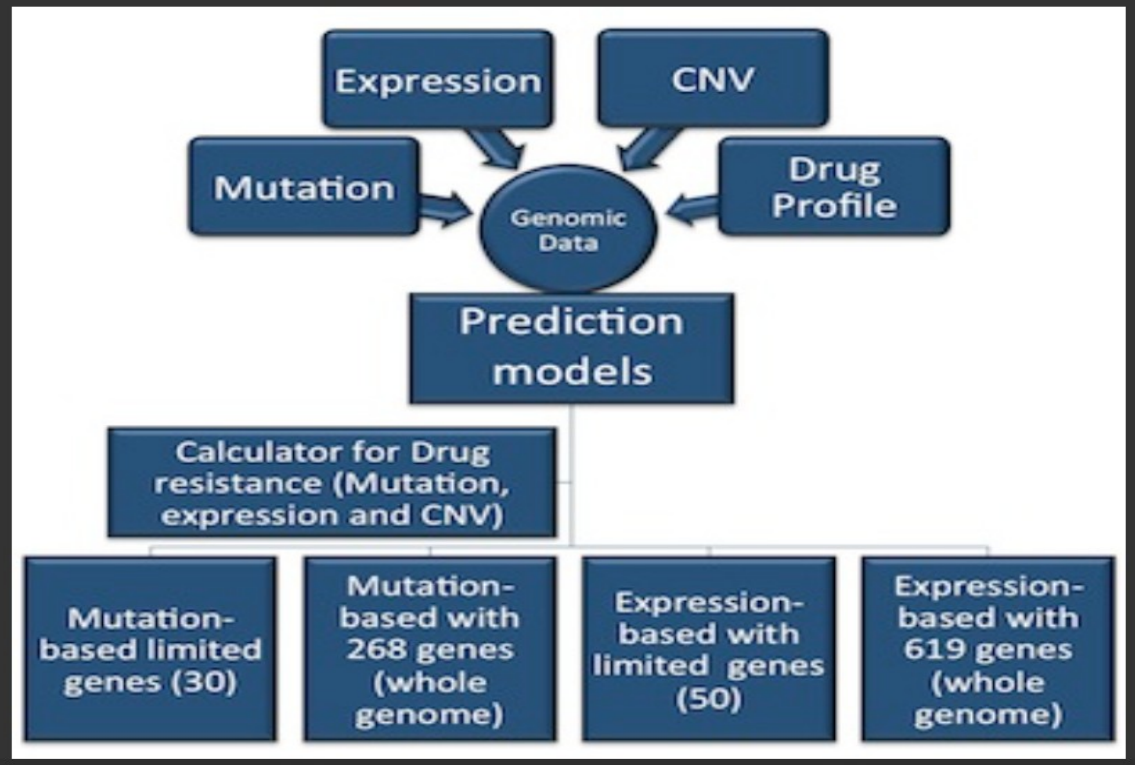
Antiviral vaccines have been the most successful biomedical intervention for preventing epidemic viral disease. Vaccination for smallpox in humans was the first successful example for the eradication of the disease. While early vaccines were developed empirically by passage in live animals or eggs, more recent vaccines have been developed because of the advent of new technologies, particularly cell culture and molecular biology. Technological advances in gene delivery and expression, nanoparticles, protein manufacturing, and adjuvants have created the potential for new vaccine platforms that may provide solutions for vaccines against viral pathogens for which no interventions currently exist. In recent years, use of In silico methods for designing and prioritizing vaccine candidates becomes the backbone of the pharmaceutical industries. This draws the attention of the researchers and scientists working in this field.

The present platform is designed to guide the vaccine designing process against major lung cancer causing oncogenic viruses. The genomic and proteomic information of **09** oncogenic lung cancer virus species, **100** reference proteome of virus strains as well as **945** target proteins information was taken into consideration. The identified vaccine candidates have the potential to stimulate adaptive immunity, thus helps in providing both protective and antiviral immunity. We hope the developed platform could best serves the need of scientific community for improving the cancer immunotherapy process.

CancerDP

Prioritization Of Anticancer Drugs

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



Drug Prioritization Prediction

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

Drug Calculator: Interactive calculation of drug resistar
probability.

Genome Submit: Prediction of anticancer drug based

Signatures: Browsing significant and correlated genes.

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

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

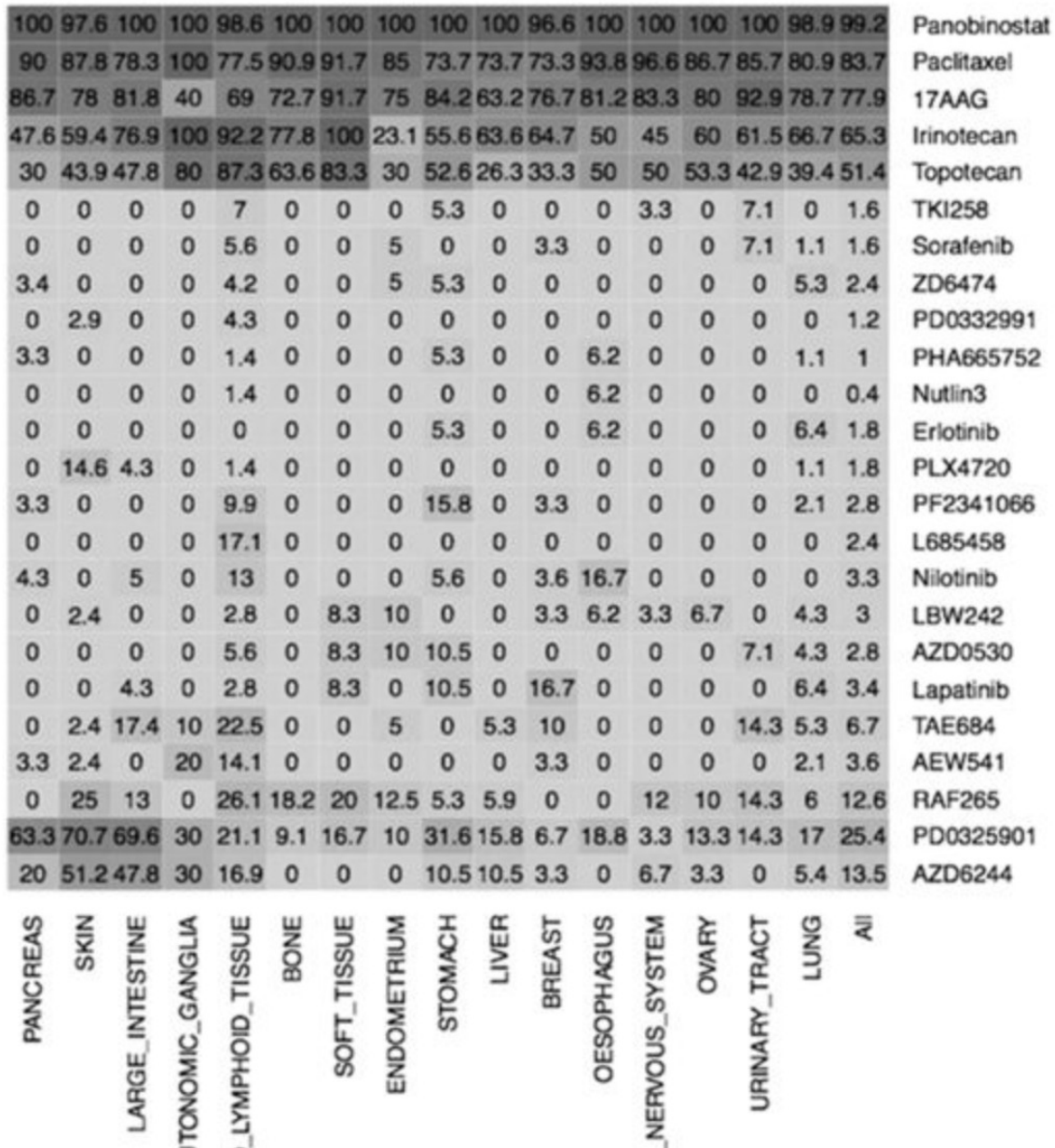


Table 3: The performance of SVM models developed using various genomic features that include mutant genes, variant genes, CNV, expression, hybrid.

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

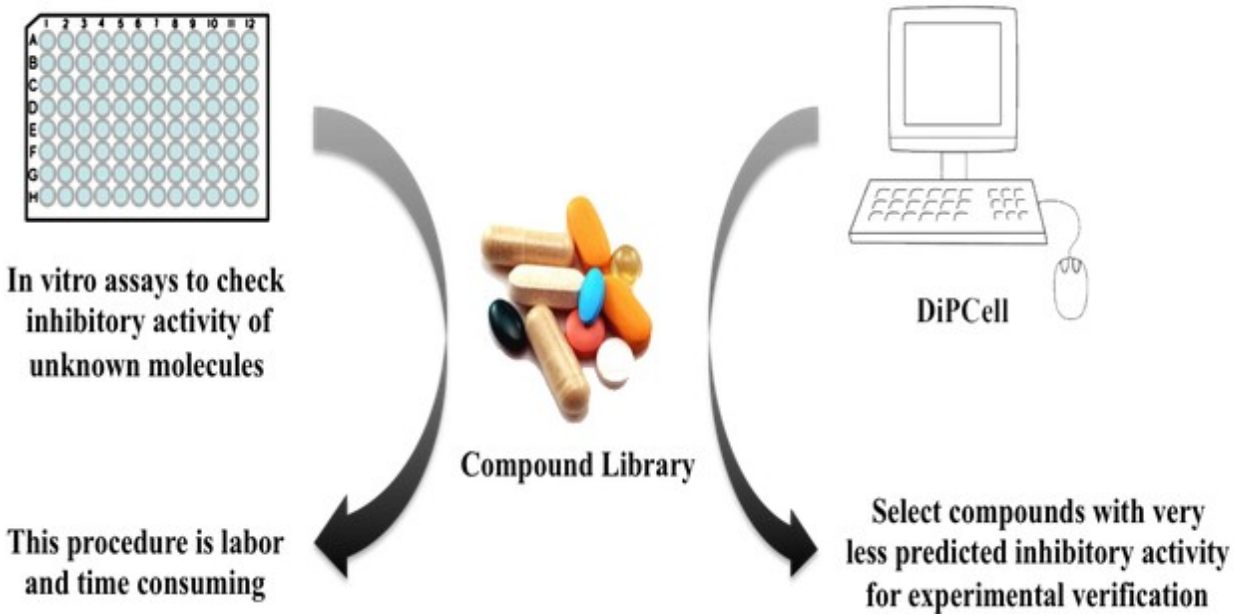
Drug	Mutation	Variation	Expression	CNV	Hybrid	CCLE*
17AAG	0.42	0.55	0.67	0.54	0.76	0.43
AEW541	0.25	0.54	0.69	0.54	0.75	0.33
AZD0530	0.41	0.45	0.65	0.56	0.71	0.19
AZD6244	0.52	0.51	0.81	0.56	0.82	0.59
Erlotinib	0.48	0.56	0.79	0.62	0.82	0.3
Irinotecan	0.58	0.65	0.84	0.56	0.87	0.68
L685458	0.44	0.63	0.82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

DiPCell: Designing of inhibitors of pancreatic cancer cell

CSIR – Institute of Microbial Technology, India

Welcome to DiPCell

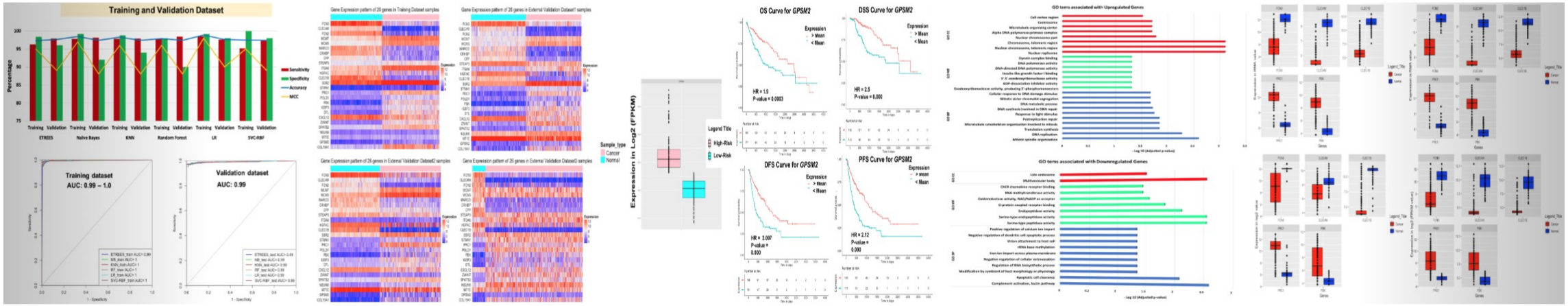
DiPCell is a webserver for the predicting inhibitory activity of unknown molecules and designing their analogs against pancreatic cancer cell lines. DiPCell implements the QSAR models, which were developed by using SMOreg machine learning algorithm on high throughput drug screening data. This high throughput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



HCCpred

R and Raghava GPS (2020) Identification of Platform-Independent Diagnostic Biomarker Panel for Hepatocellular Carcinoma Using Large-Scale Transcriptomics Data. Front. Genet. 10:1306. doi: 10.33

A webserver to predict Hepatocellular carcinoma (HCC)



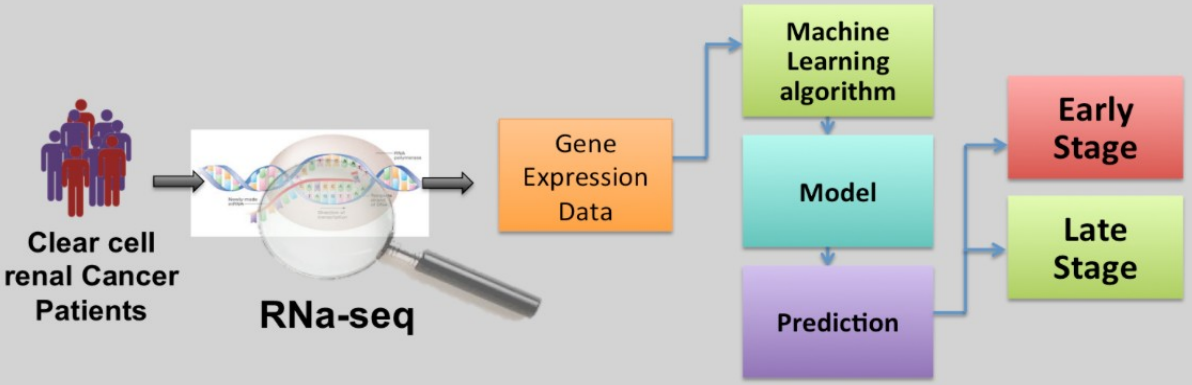
MAJOR WORKS

HCCpred is a web-bench for the prediction of tumorous and non-tumorous Hepatocellular Carcinoma (HCC) patients. Our major prediction modules based on the robust biomarkers such as 3-Gene HCC Biomarker, 4-Gene HCC Biomarker, 5-Gene HCC Biomarker. These HCC biomarkers identified using gene expression profiles of a total of 3,961 samples include 2,306 HCC and 1,655 non-tumorous samples. The datasets derived from various profiling platforms such as Affymatrix, Illumina, High-througput and Agilent.

eference: Bhalla et. al. (2017) Gene expression-based biomarkers for discriminating early and late stage of clear cell renal cancer. Scientific Reports, , 44996

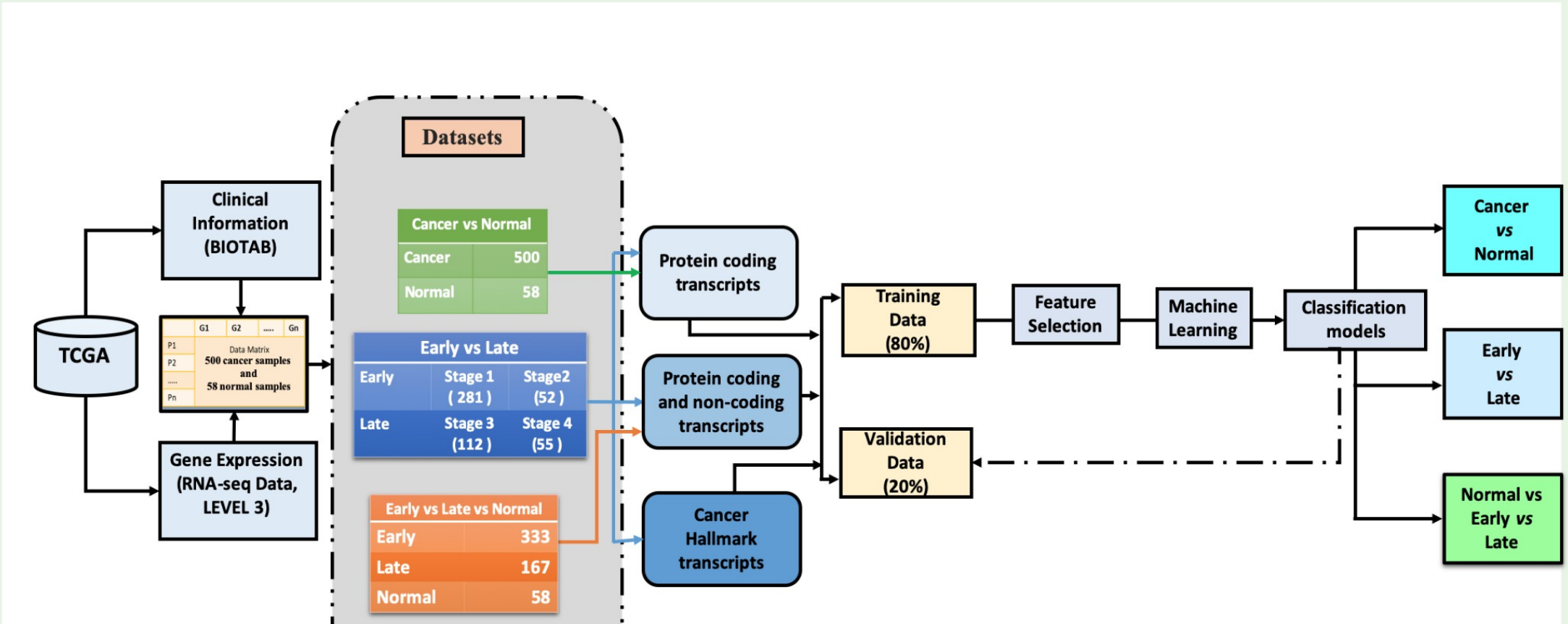
Home Page of cancerCSP

CancerCSP (clear cell renal cancer stage prediction) is a web-bench developed for predicting Early and Late stage of clear cell renal cell carcinoma (ccRCC) patients using gene expression data derived from RNA-seq experiments in the form of RNA-Seq by Expectation Maximization (RSEM) values. The user can also analyze data regarding expression of a gene in early and late stage of ccRCC for any gene among 20,531 genes included in TCGA analysis. The models used in this study were trained on TCGA genomics Level 3 data for cancer patients of 519 cancer patients. We are able to discriminate early and late stage patients with accuracy of 72.64% with ROC of 0.78 on validation dataset.



CancerTSP

CancerTSP is a web-bench designed for stage prediction of Papillary Thyroid Carcinoma (PTC) using RNA expression data (derived from RNA-seq experiments in the form of RNA-Seq FPKM values). Primarily Early v/s Late stage prediction module predicts stage of PTC tissue sample. Further Cancer v/s Normal prediction module predicts whether tissue sample is cancerous or normal. Analysis module allows the user to analyze data regarding expression of an RNA transcript in Early or Late stage of PTC.



CancerLSP

Liver Heptacellular Carcinoma Stage Prediction

Reference: Kaur H et. al., (2019) Classification of early and late stage liver hepatocellular carcino patients from their genomics and epigenomics profiles. PLoS One. 14(9):e0221476.

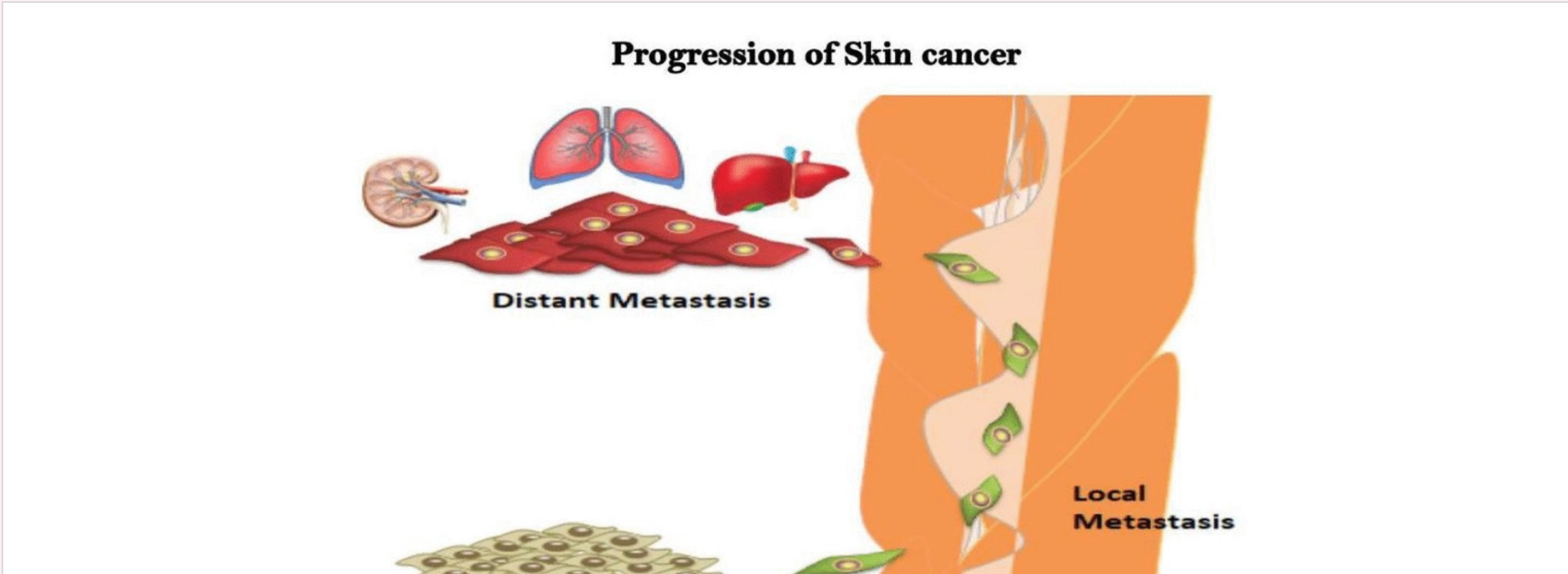
CancerLSP

CancerLSP is a web-bench Liver cancer stage prediction Server. It is developed to predict whether liver tissue samples is cancerous or normal and it also predict whether sample belong to Early (Stage-I) and Late stage of LIHC patients using gene expression data (derived from RNA-seq experiments in the form of RNA-Seq FPKM values) and Methylation Data (The methylation profiles acquired with the Illumina Human- Methylation450K DNA Analysis BeadChip assay, which is based on genotyping of bisulfite-converted genomic DNA at individual CpG-sites to provide a quantitative measure of DNA methylation in terms of Beta values). The user can also analyze data regarding expression of a gene in cancer or Normal and Early or late stage of LIHC for any gene among RNA transcripts included in this analysis.

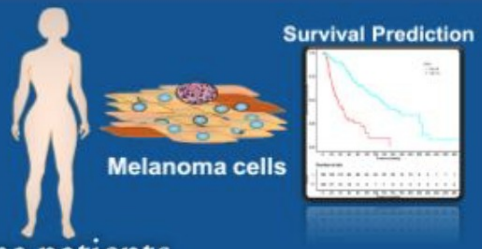
Dhall, A., Raghava, GPS. Prediction and Analysis of Skin Cancer Progression using Genomics Profiles of Patients. Sci Rep 9, 1

Welcome to CancerSPP

CancerSPP is a web-bench for skin cutaneous melanoma (SKCM) progression prediction. It is established for the prediction and analysis of primary and metastatic tumor of SKCM using signature genes expression data (derived from RNA-seq, miRNA and methylation RSEM expression quantification values) . Further, prediction module is used to predict multiple states of metastatic samples from primary tumor samples. Analysis module allow the user to analyze RNA-seq expression profiles data in primary and metastatic states of SKCM.



SKCMhrp

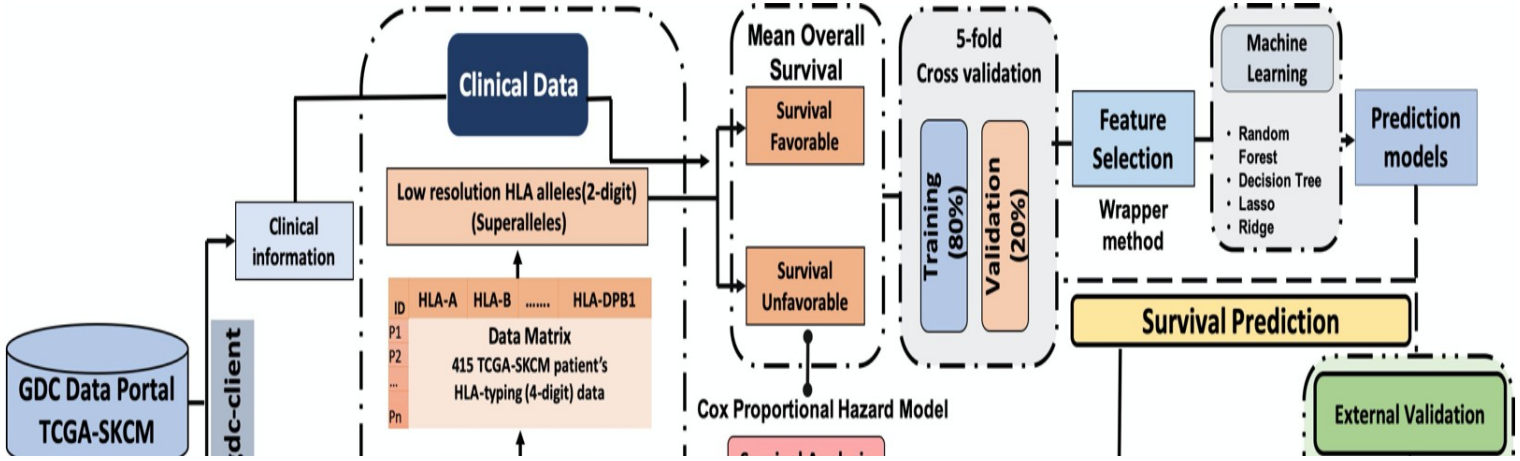


Web-server for risk prediction in Skin Cutaneous Melanoma patients

Computing Skin Cutaneous Melanoma Outcome From the HLA-Alleles and Clinical Characteristics. Front Genet. 2020;11:221. Published 2020 Mar 26. doi:10.3389/fgene.2020.

Welcome to SKCMhrp

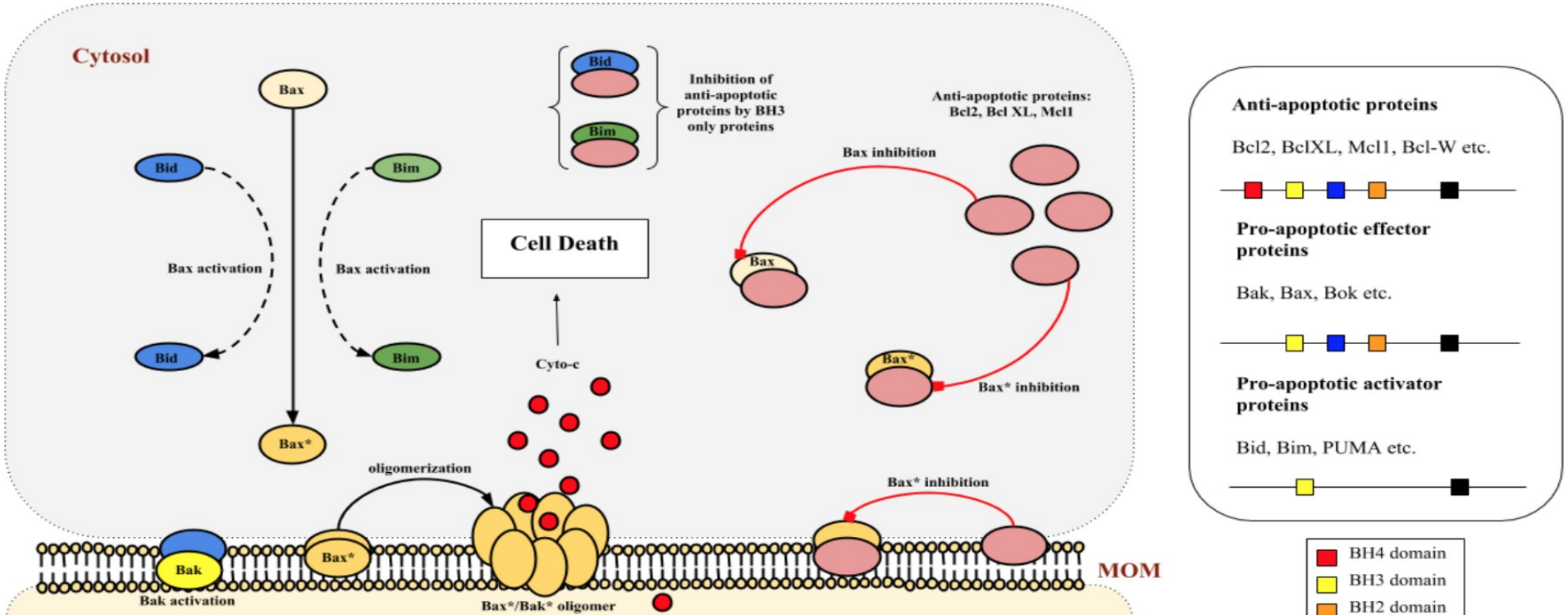
Skin Cutaneous Melanoma High-Risk Prediction(SKCMhrp) webserver can be used to distinguish high risk SKCM patients from low risk SKCM patients from their HLA-superallele and clinical characterstics. The risk estimation is based on statistical and survival analysis on recent SKCM datasets. See general section for more information.



Welcome to CRCRpred

*** **Reference:** Lathwal A, Arora C, Raghava GPS (2019) Prediction of risk scores for colorectal cancer patients from the concentration of proteins involved in mitochondrial apoptotic pathway. PLoS One 14(9):e0217527.***

Colo-Rectal Cancer Risk Prediction (CRCRpred) webserver can be used to distinguish high risk CRC patients from low risk CRC patients given the protein concentration of one or more apoptotic proteins (Bak, Bax, Bcl2, BclXL or Mcl1) involved in the process of Mitochondrial Outer Membrane Permeabilization (MOMP), which is defunct in the case of cancer. The risk estimation is based on statistical and survival analysis on recent CRC datasets. See supplement section for more information.



CRCRpred

Web-server for risk prediction in Colorectal Cancer patients

HOME | PREDICT | SUPPLEMENT | HELP | DEVELOPERS | CONTAC

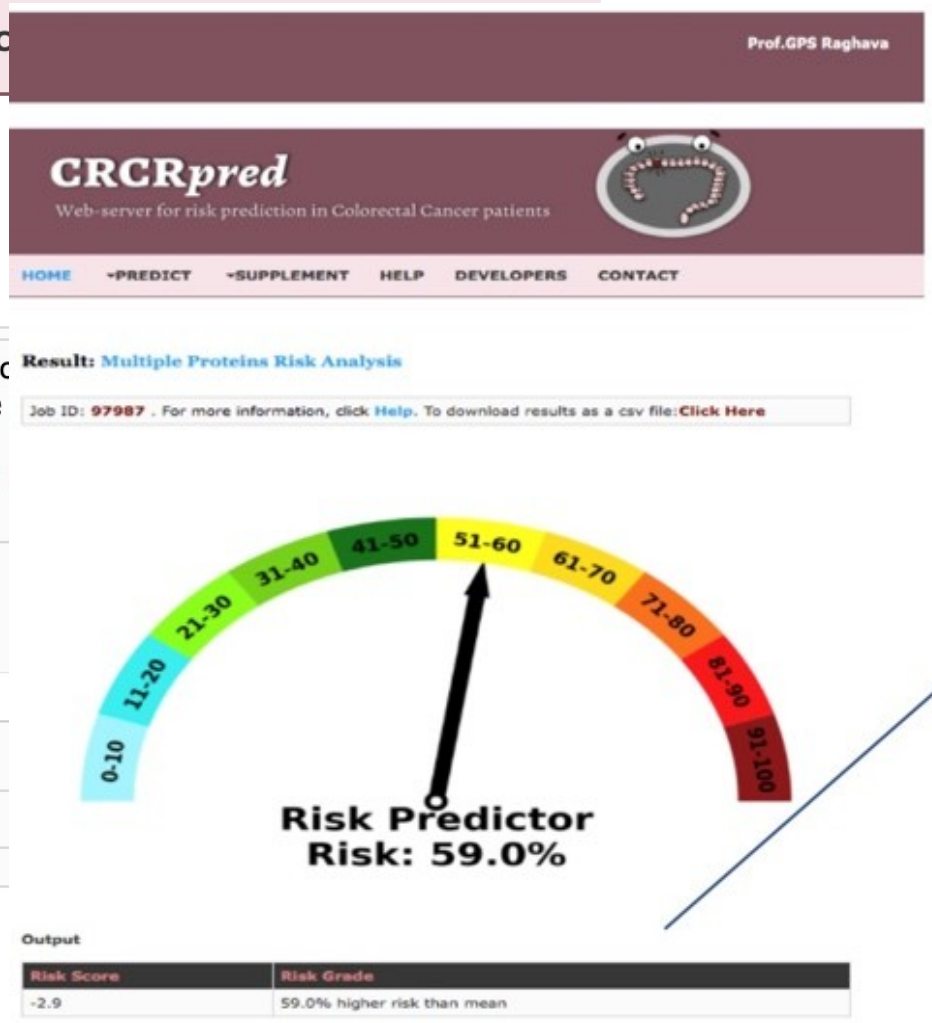
Multiple Proteins Prediction

This module computes the risk score in colorectal patient with the given cc
Estimation is done on the basis of all the proteins. If no value is provided, the
nM. For more information, refer to **Algorithm** and **HELP** pages.
NOTE: All entry box must have some value greater than equal to 0, otherwise

Select the protein and enter concentration (nM):

BAX 5 **BAK** 30 **BCL2** 70 **BCL-XL** 80

Clear All | Submit



Risk Score and percent

raghava@iiitd.ac.in

IIITD

Raghava's group

CMcrpred

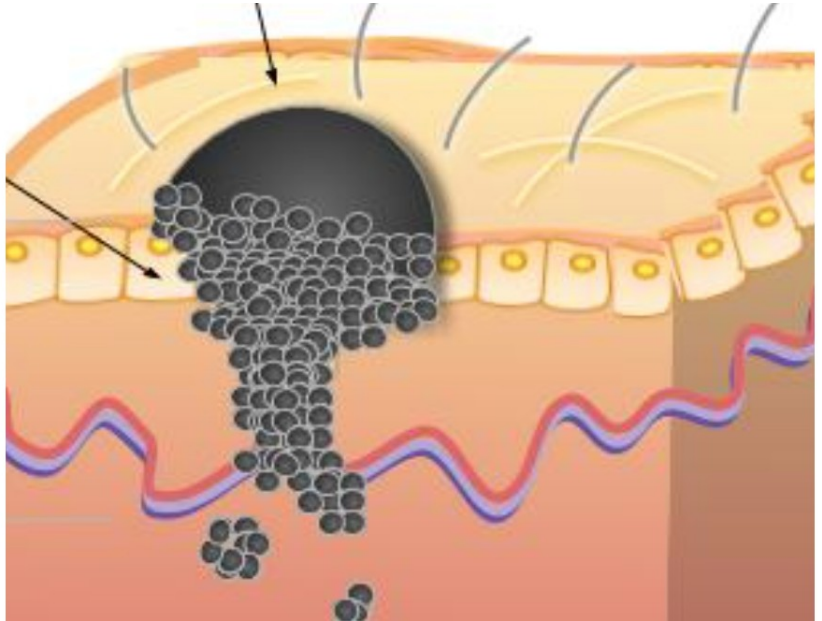
Research article

Risk prediction in cutaneous melanoma patients from their clinico-pathological features: superiority of clinical data over gene expression data

Chakit Arora, Dilraj Kaur, Anjali Lathwal, Gajendra P.S. Raghava *

Department of Computational Biology, IIIT- Delhi, New-Delhi, India

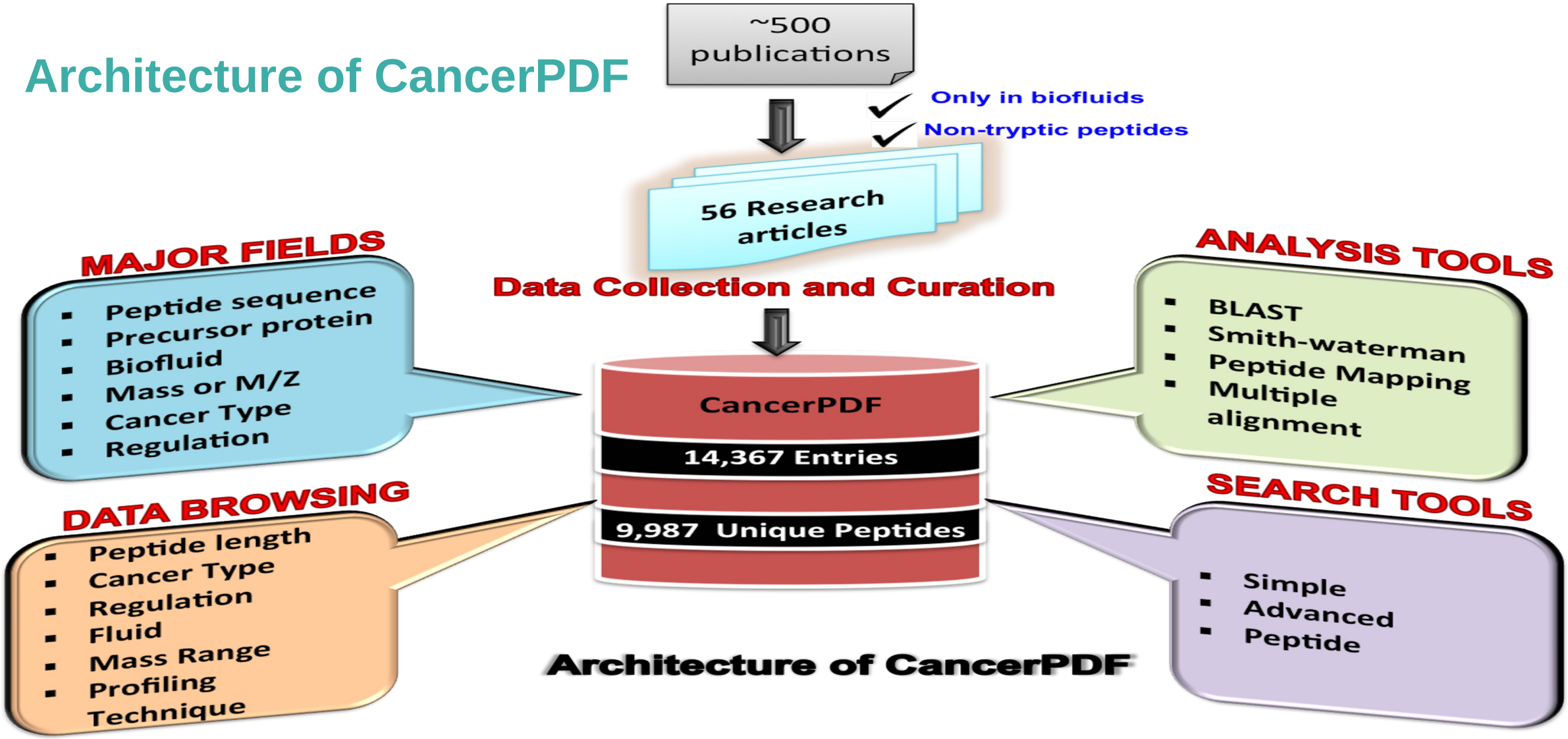
CMcrpred web-server can be used to estimate survival risk in cutaneous melanoma patients based on the clinically measured (AJCC approved) features for a given patient viz. N stage, M stage, Breslow Thickness and Ulceration status. These clinical features have been widely used in the past to stratify patients in different risk categories and consequently for decision-making regarding therapy regimens. Here, the risk estimation is based on an ensemble model that integrates all these features by



Peptide as Diagnostics

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

Architecture of CancerPDF



Peptide based Inhibitors

CancerPPD
Database of Anticancer Peptides & Proteins

Home | Information | Data Submission | Developers | Contact | Assistance | Related Databases

The Mobile Version of CancerPPD

Search
- Basic
- Conditional
- Peptide
- SMILES

Browse
- Protein wise
- Peptides wise
- Tissue wise
- Cell Line wise
- Year-wise
- Assay Type
- Length
- Modifications

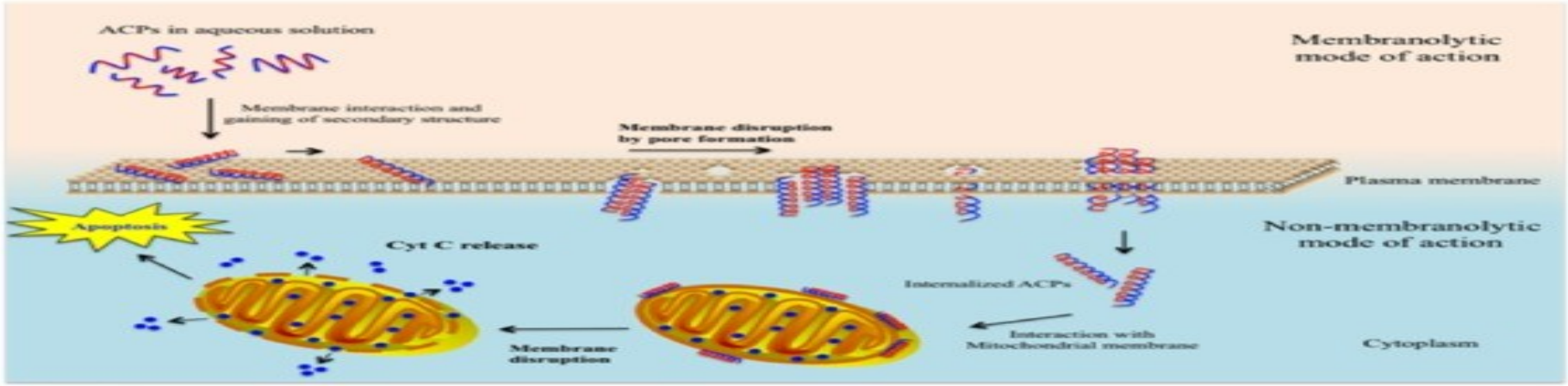
Tools
- BLAST
- Smith-Waterman
- Mapping
- Sequence Alignment
- Structure Alignment

Download
- Sequence
- Structure
- Reference
- Acknowledgement

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



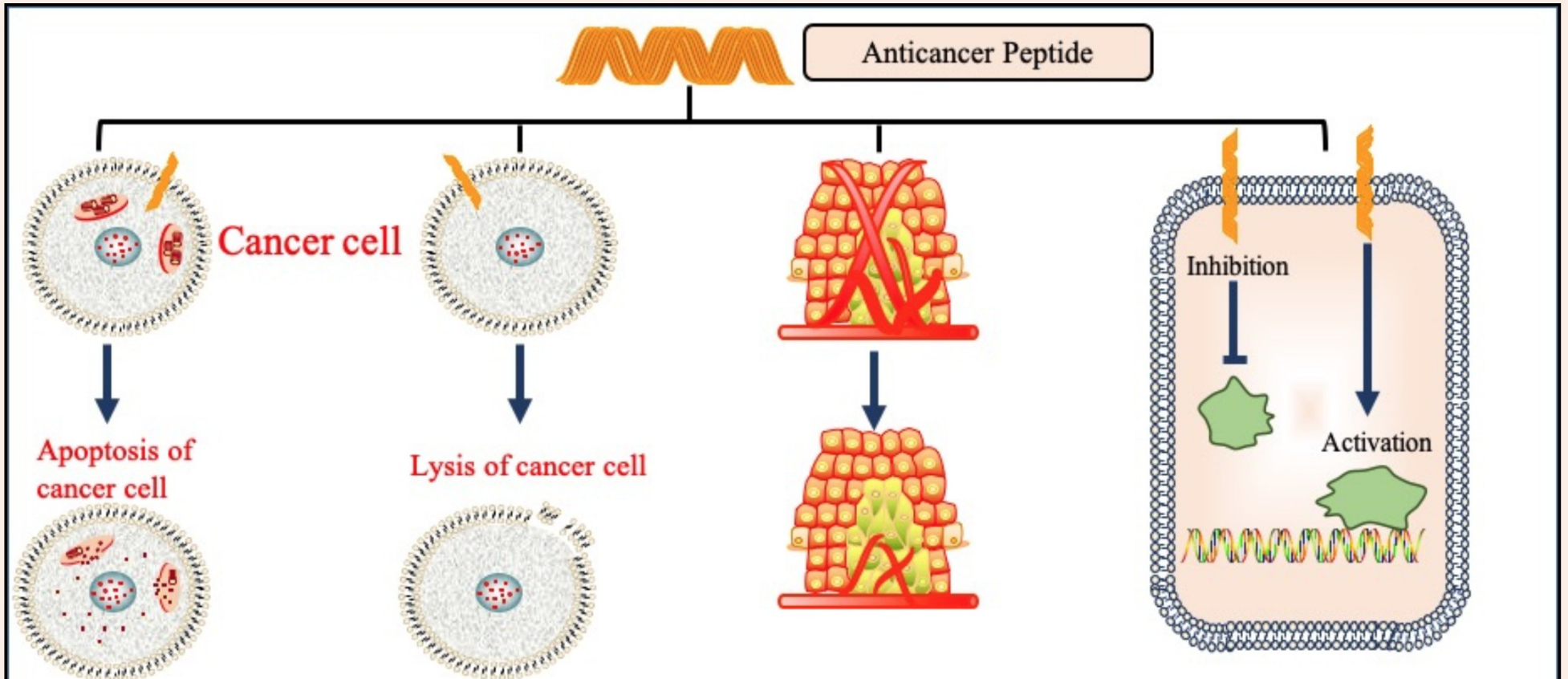
Key Features

(1) **Data Retrieval:** Tools for data fetching like simple, and advanced search were integrated. In addition, to search peptides, peptide search and SMILES search options are also provided.
(2) **Data Analysis:** BLAST, Smith-waterman, sequence and structure mapping tools are incorporated, which facilitate the similarity-based search.
(3) **Browsing:** Various browsing fields have been provided, which facilitate the data browsing in a very convenient way.
(4) **SMILES and Structures:** An important feature of CancerPPD is that it contains information of ACPs in SMILES format. In addition, predicted tertiary structures of all ACPs are available which makes it comprehensive resource.

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).



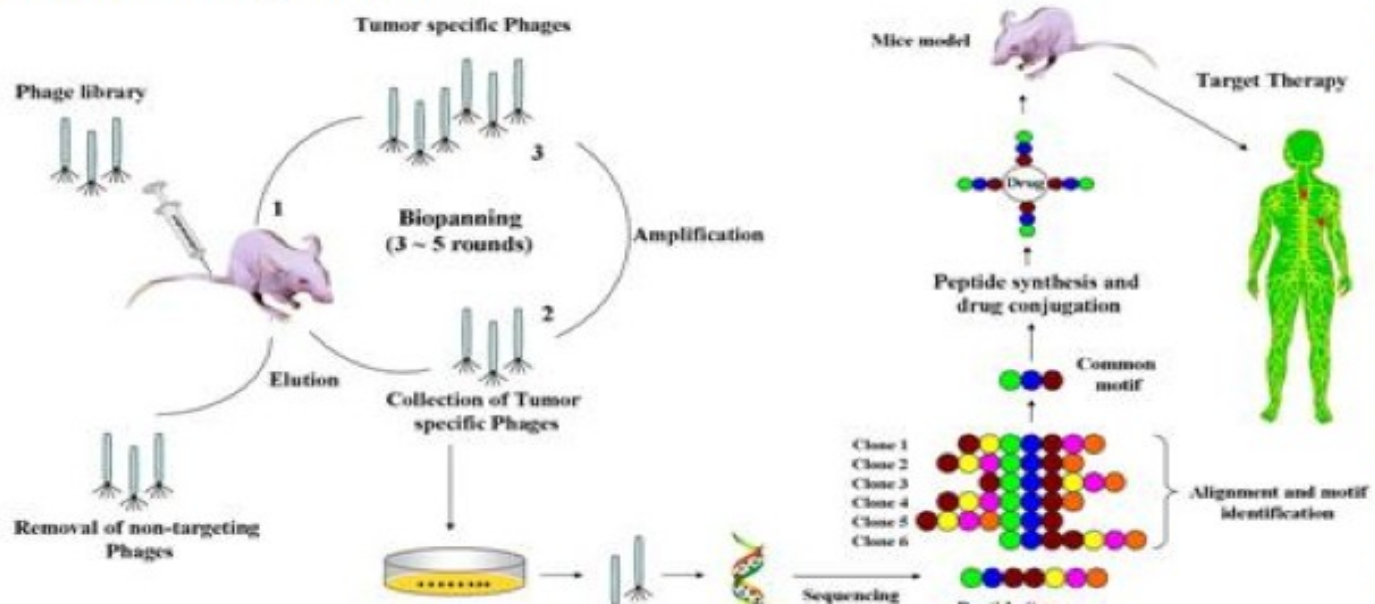
Drug Delivery

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*

Drug Delivery

crdd.osdd.net/raghava/tumorhpd/

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

TumorHPD: Designing of Tumor Homing Peptides

(Institute of Microbial Technology, Chandigarh, India)

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

Welcome to TumorHPD

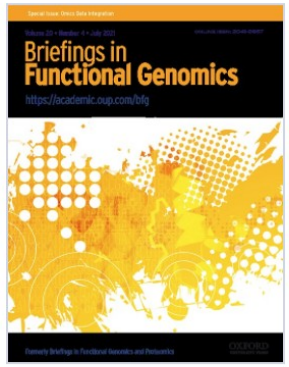
Tumor homing peptides are the short peptides having average length between 7 to 12 residues. These peptides h
bind to tumor cells or tissues. These peptides can be used to deliver target specific drugs and as imaging agents for t
Thus prediction of tumor homing peptide is important for managing cancer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

Briefings in Functional Genomics



Volume 20, Issue 4
July 2021

Article Contents

EDITOR'S CHOICE

Computational resources for identification of cancer biomarkers from omics data FREE

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

Briefings in Functional Genomics, Volume 20, Issue 4, July 2021, Pages 213–222,
https://doi.org/10.1093/bfgp/elab021
Published: 01 April 2021 **Article history** ▾

Abstract

Cancer is one of the most prevailing, deadly and challenging diseases worldwide. The advancement in technology led to the generation of different types of omics data at each genome level that may potentially improve the current status of cancer patients. These data have tremendous applications in managing cancer effectively with improved outcome in patients. This

Thank You