

# Development of Computational Resources For Improving Healthcare

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**Raghava's** group focuses on development of *in silico* tools in the field of Bioinformatics, Cheminformatics, Pharmainformatics & Medicalinformatics for improving healthcare. In contrast to traditional research groups where a group contributes to a particular problem or field; his group contributed to multiple problems/fields important for translational medicine. Group is working on diverse areas of research, including diseases like HIV, cancer, tuberculosis, viral infections, etc. Group has contributed significantly in the development of subunit vaccine designing and developed of many web servers and databases. Recently, group has taken lead into the development of *in silico* tools for the prediction and designing of different classes of therapeutic peptides e.g, cell penetrating, tumor homing, anticancer peptides. Group have published more than 150 research papers in reputed journals with cumulative impact factor more than 600. Raghava's group is strong supporter of open source resources, all software, web servers, databases & dataset developed at group are

- 1986 Raghava joined IMTECH as a computer scientist.
- 1991 First paper on analysis of ELISA Data.
- 1992-95 Ph.D on proteins secondary structure prediction.
- 1996-98 Postdoctoral Fellow at Oxford University, UK.
- 1999 First student joined group for PhD
- 1999 Vaccine, protein & gene informatics initiated.
- 2004 *In silico* Annotation of Genomes and Proteomes.
- 2008 Computer Resources for Drug Discovery under OSDD.
- 2010 Pipelines for Assembling of genomes from NGS data.

- 2011 Model for Human body
- 2011 Experimental validation of therapeutics peptides
- 2011 Model for System Biology
- 2012 Genome-based Therapeutics against diseases
- 2012 Tissue level Modelling
- 2013 Pattern of gene expression
- 2013 OSDDlinux: An Operating System for Drug Discovery.
- Understand tissue

## Modelling of Cell activity

- Movement of protein in cell
- Interaction of proteins

## Gene, Protein and Pathways

- Modelling a genome, gene, promoters repeats
- Protein Modelling and simulations

Home | OSDD | Raghava | News | Rewards | Challenges | OSDDpub | Forum | Indipedia | Drugpedia | FAQ | License | Register.

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

### Computational Resources for Drug Discovery

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

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

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

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

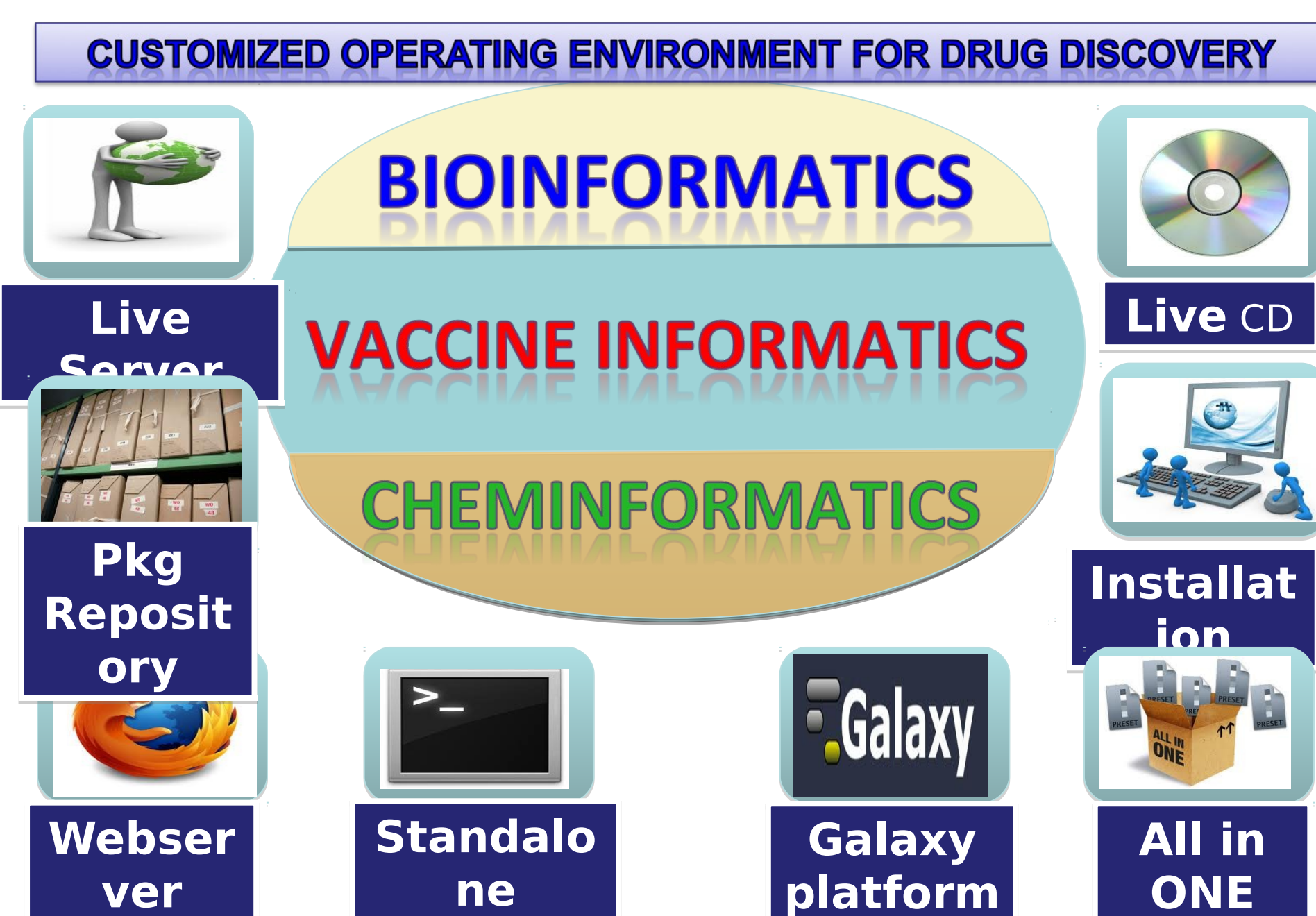
Target Identification: Genome Annotation, Protein Annotation, Potential Targets, Protein Structure

Virtual Screening: QSAR Techniques, Docking & QSAR, Cheminformatics, SINA/AmRNA

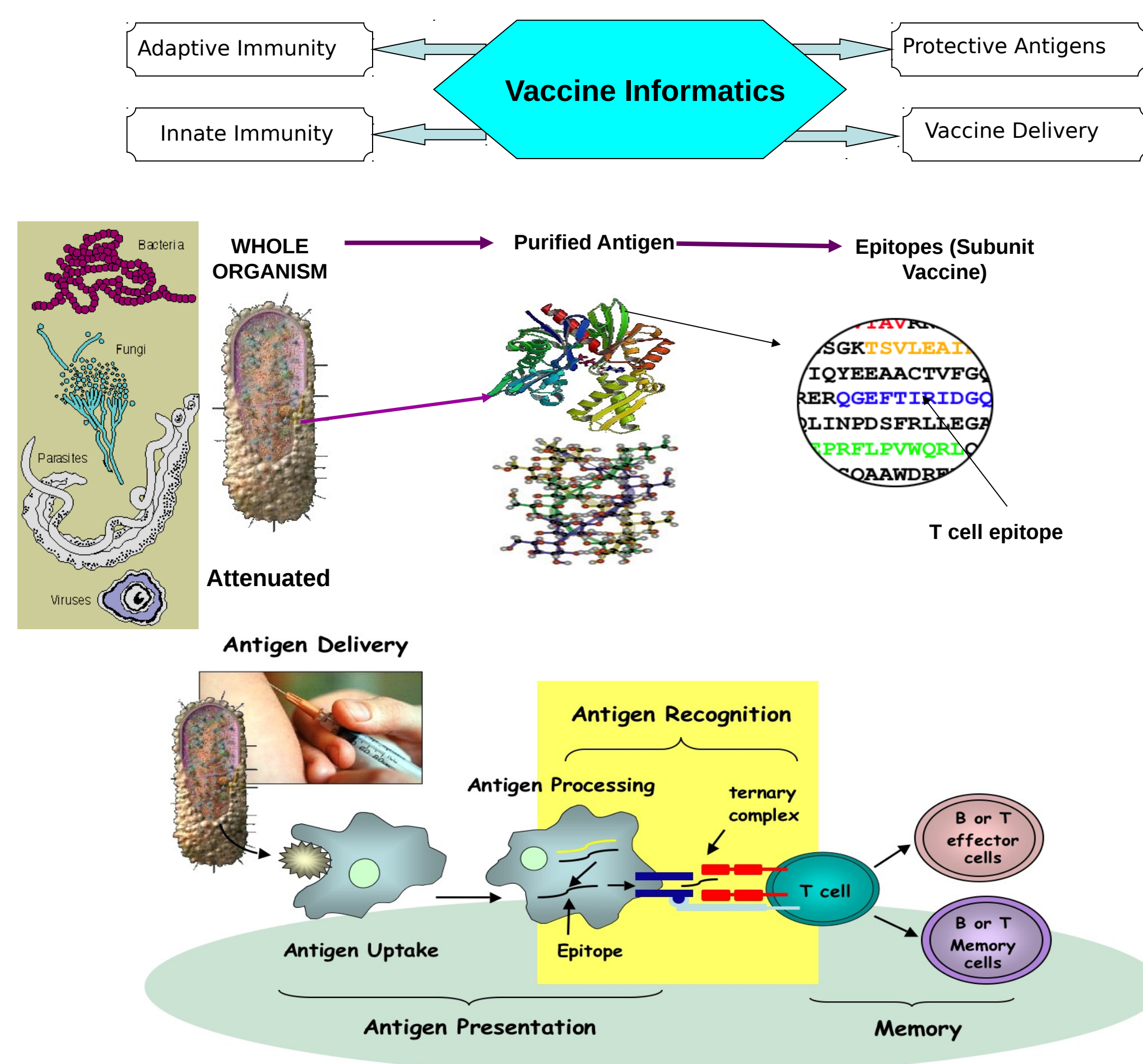
Drug Design: Lead Optimization, Pharminformatics, ADMET, Clinical Informatics

How to Contribute?: Experimentalists, Virtual Trainers/Jobs, Software Developers

Computational Resources: Library Interfaces, Help Services, Publishing Document, Link us, etc.

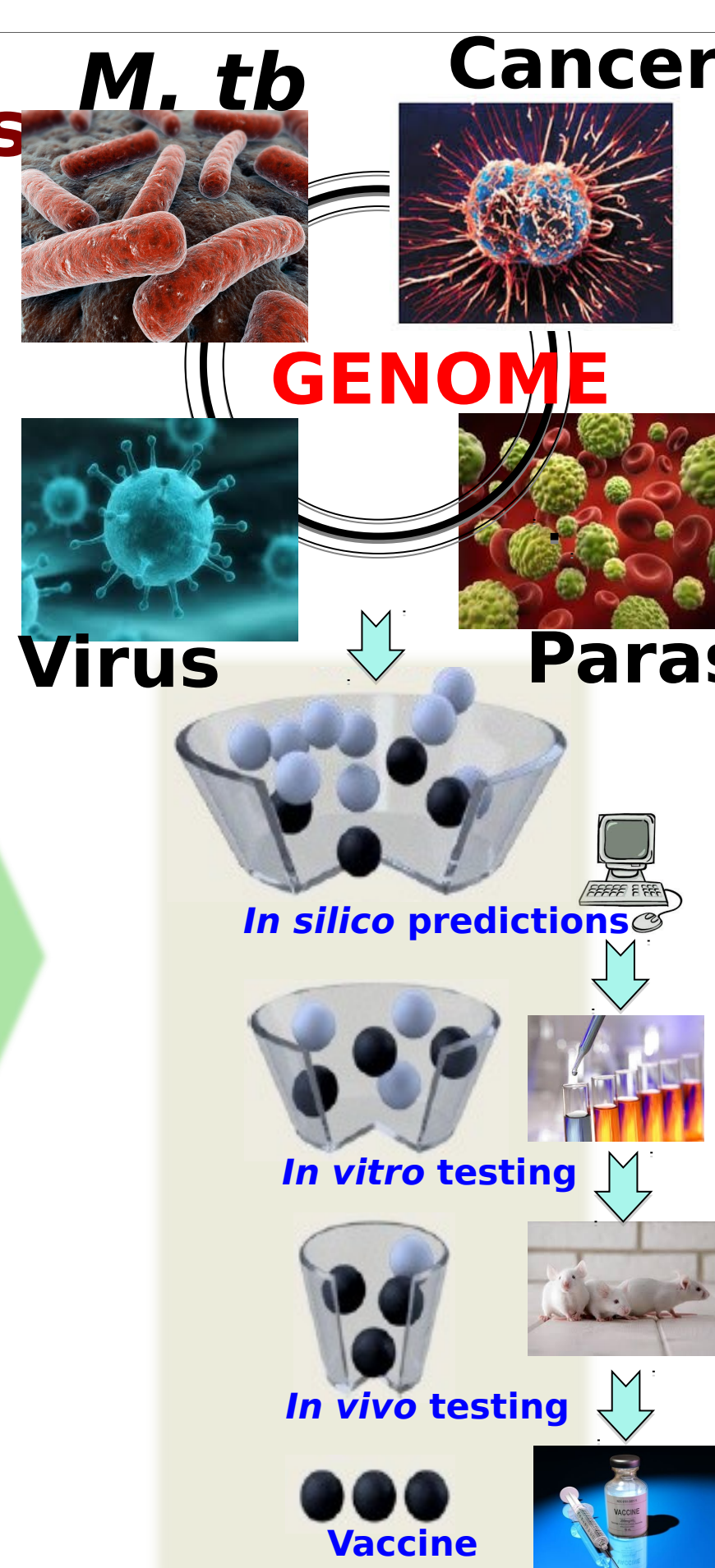


**A customize linux operating system for drug discovery that integrates most of freely available computational tools required for drug discovery. It is an *in silico* platform for providing ambient environment for computer-aided drug design.**



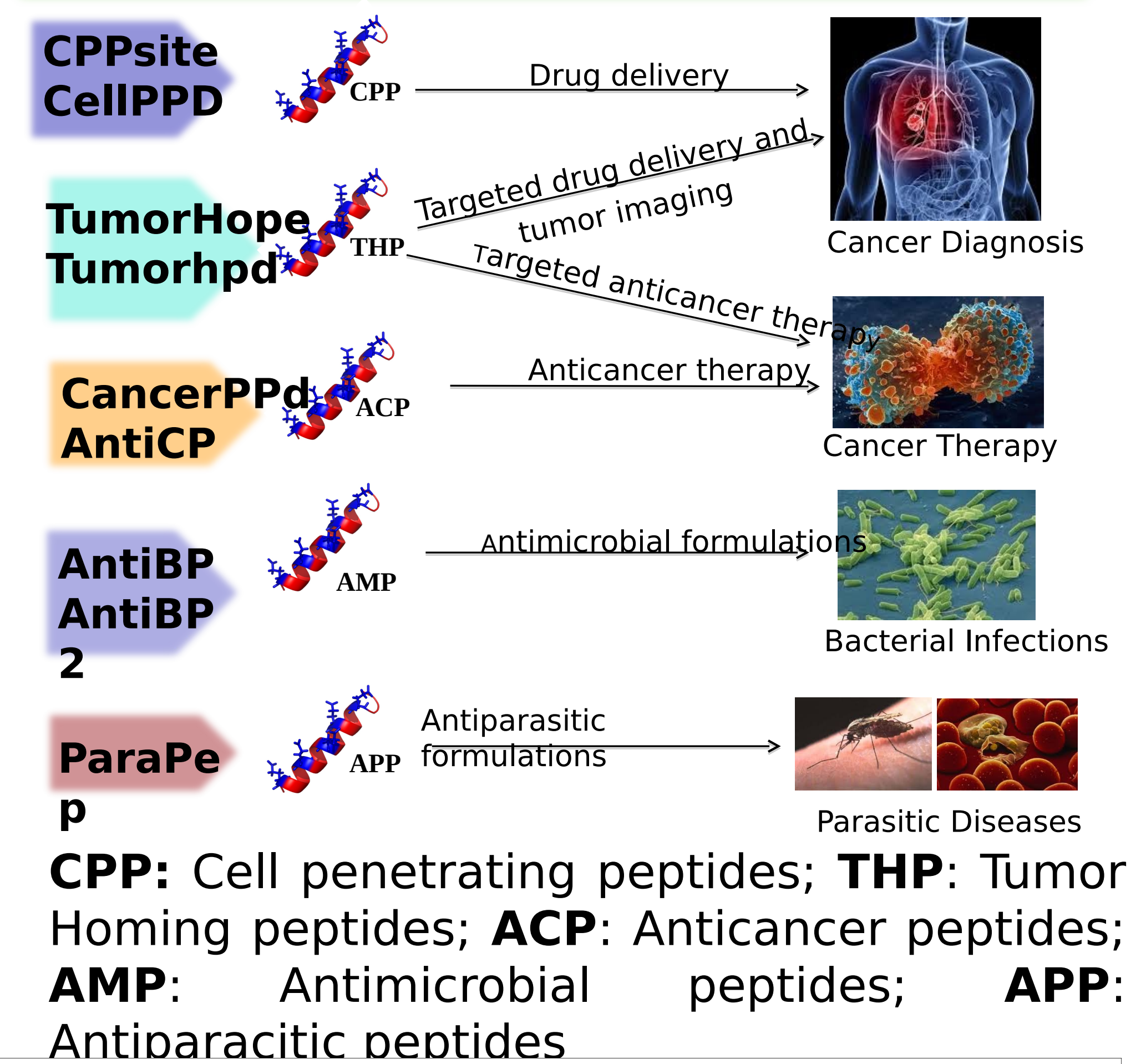
## T-Cell Epitopes Prediction

MHCBN  
Propred  
Propred1  
CTLpred  
nHLApred  
Pcleavage  
IFNepitope  
s  
MHCbench  
TAPpred  
IL4pred  
FDR4



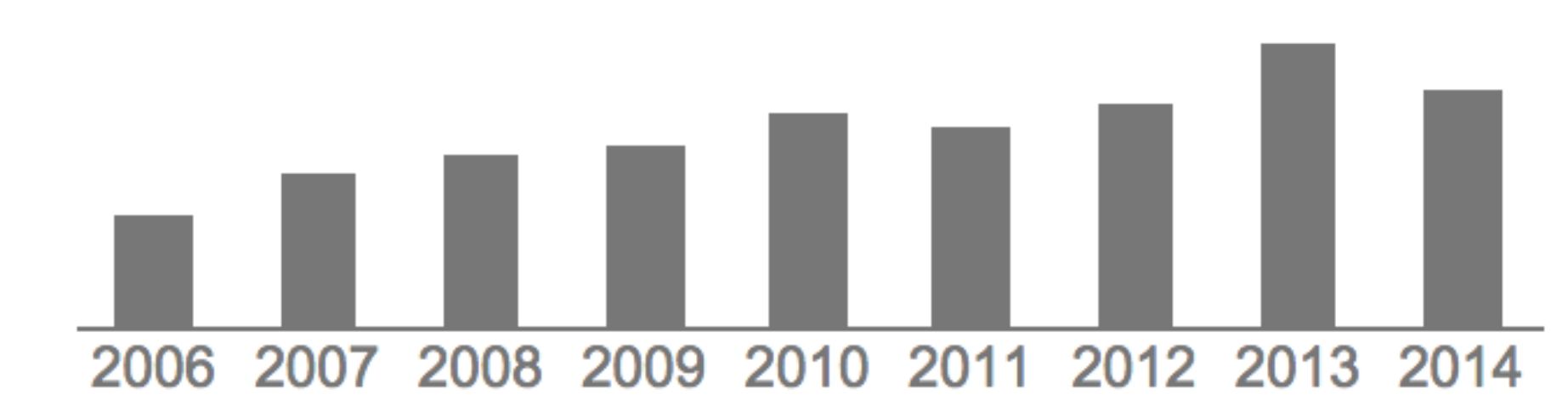
B-cell epitopes/ Innate Immunity  
BCIpep  
LBtope  
IgPred  
BCEpred  
AntigenDB  
VaccineDA  
HaptenDB  
ABCpred  
ALGpred  
PRRDB  
CBtope

## In Silico Tools Therapeutic peptide class Applications



**Group is providing science-based service to community. Most of the papers published from group are highly cited (Google Scholar).**

Citation indices	All	Since 2009
Citations	6099	4207
h-index	43	37
i10-index	101	95



## Home Page:

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

**CRDD Page:** <http://crdd.osdd.net/>

**OSDDlinux page:** <http://osddlinux.osdd.net/>

**OSCAR Page:** <http://crdd.osdd.net/oscar/>



Highly Cited Researchers 2014 :  
Raghava has been listed in "The World's Most Influential Scientific Minds" by Thompson Reuters.

- National young Leadership award 2011 (LS-IIM Lucknow)
- Prestigious JC Bose National Fellowship 2010.
- Fellow of National Academy of Sciences, India.
- Fellow of Indian Academy of Sciences, Bangalore.
- India Research Front Awards 2009 by Thompson Reuters.
- NASI-Reliance Industries Platinum Jubilee Award

