

Recent Trends in Computational Proteomics

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Bioinformatics | Drug Informatics | Chemoinformatics |

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<http://crdd.osdd.net/>

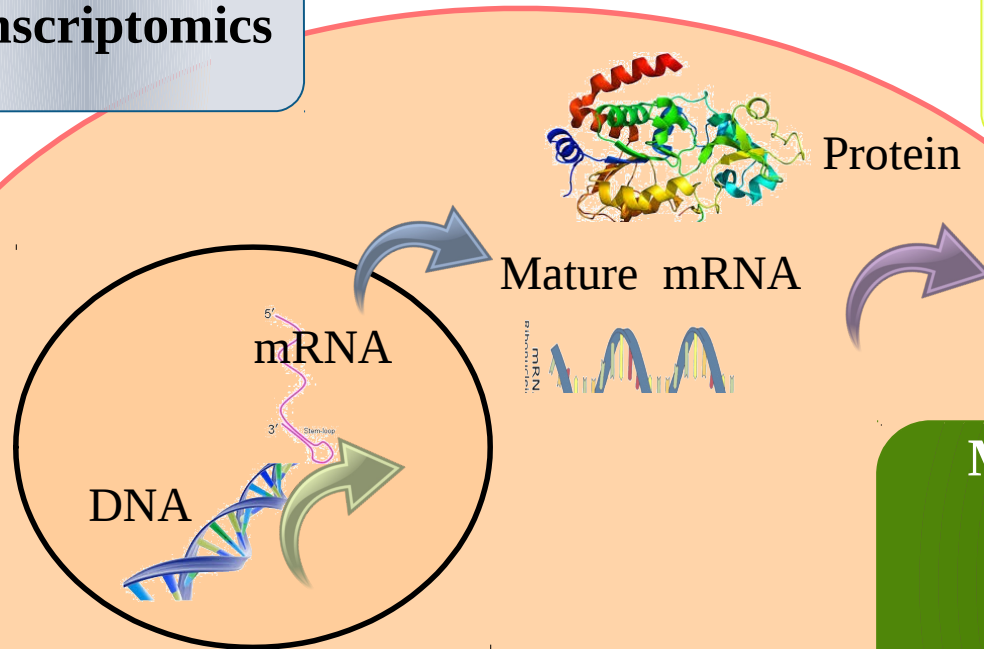
<http://www.imtech.res.in/raghava/>

Studying Central Dogma with “Omis”

Transcriptomics

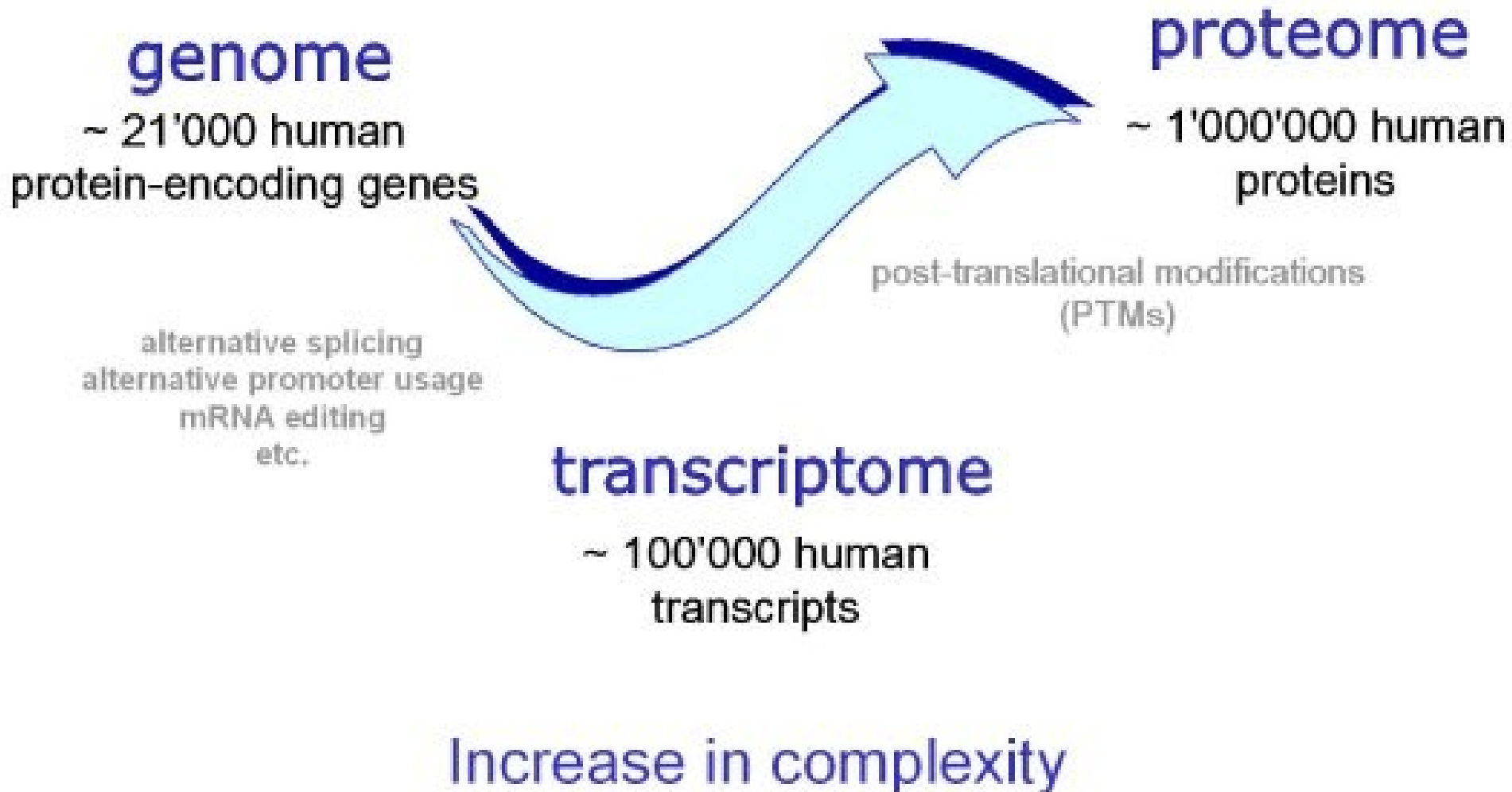
Proteomics

Genomics



Metabolomics
(all the
endogenous
metabolites
produced)

Complexity of the system



NEXT GENERATION SEQUENCING

- Sequence full genome of an organism in a few days at a very low cost.
- Produce high throughput data in form of short reads.



Illumina
a



ABI's
Solid



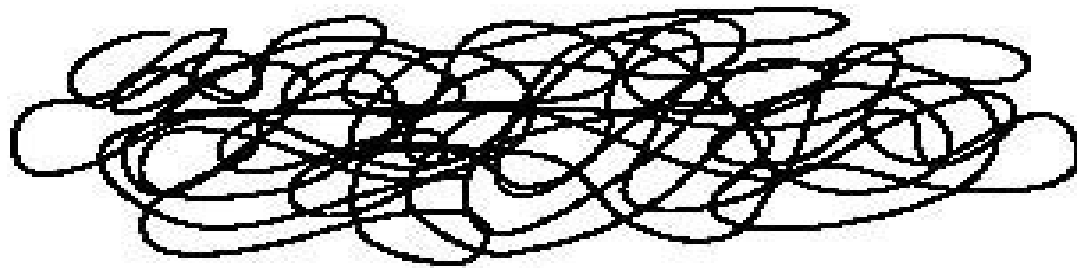
Roche's
454 FLX



Ion
torrent

Hierarchical shotgun sequencing

Genomic DNA



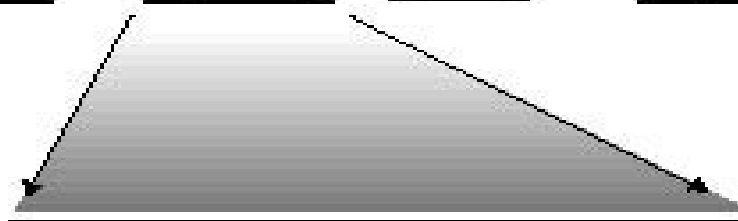
BAC library



Organized mapped large clone contigs



BAC to be sequenced



Shotgun clones



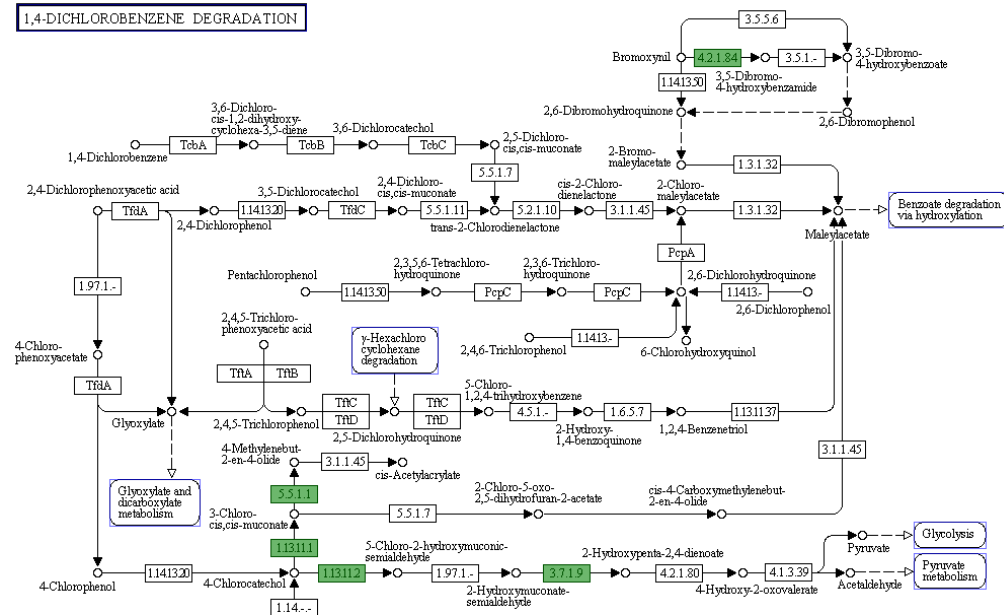
Shotgun sequence

...ACCGTAAATGGGCTGATCATGCTTAAA
TGATCATGCTTAAACCCTGTGCATCCTACTG...

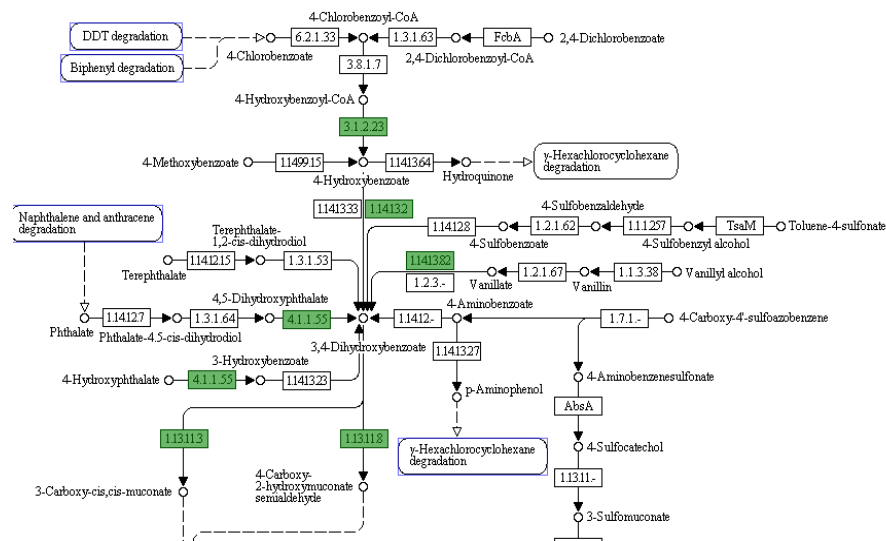
Assembly

...ACCGTAAATGGGCTGATCATGCTTAAACCCTGTGCATCCTACTG...

1,4-DICHLOROBENZENE DEGRADATION



2,4-DICHLOROBENZOATE DEGRADATION



Journal of
Bacteriology

Genome Sequence of the Nitroaromatic Compound-Degrading Bacterium *Burkholderia* sp. Strain SJ98

Shailesh Kumar, Surendra Vikram and Gajendra Pal Singh Raghava
J. Bacteriol. 2012, 194(12):3286. DOI: 10.1128/JB.00497-12.

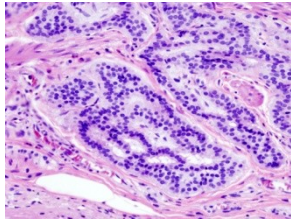
Genome assembly and annotation done at IMTECH

- ***Burkholderia* sp. SJ98 (Kumar et al. 2012).**
- ***Debaryomyces hansenii* MTCC 234 (Kumar et al. 2012).**
- ***Intechella halotolerans* K1^T (Kumar et al. 2012).**
- ***Marinilabilia salmonicolor* JCM 21150^T (Kumar et al. 2012).**
- ***Rhodococcus intechensis* sp. RKJ300 (Vikram et al. 2012).**
- ***Rhodospiridium toruloides* MTCC 457 (Kumar et al. 2012).**

RNA sequencing

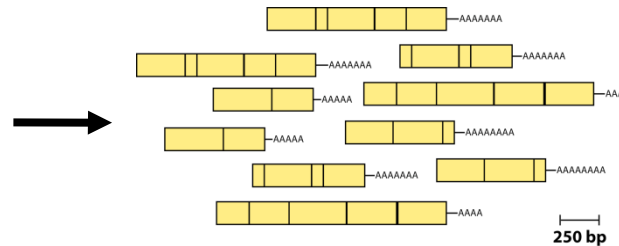
RNA-Seq is a recently developed approach to transcriptome profiling that uses deep-sequencing technologies to measure levels of transcripts and their isoforms.

Samples of interest

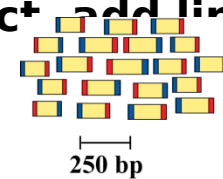


Condition
(colon tumor)

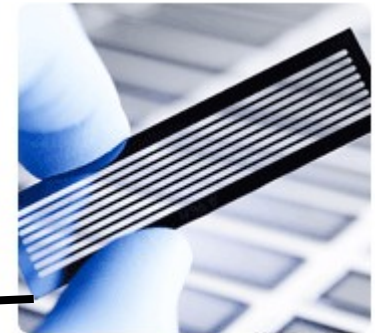
Isolate RNAs



Generate cDNA, fragment, size select, and add linkers

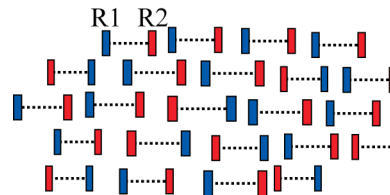


Sequence ends



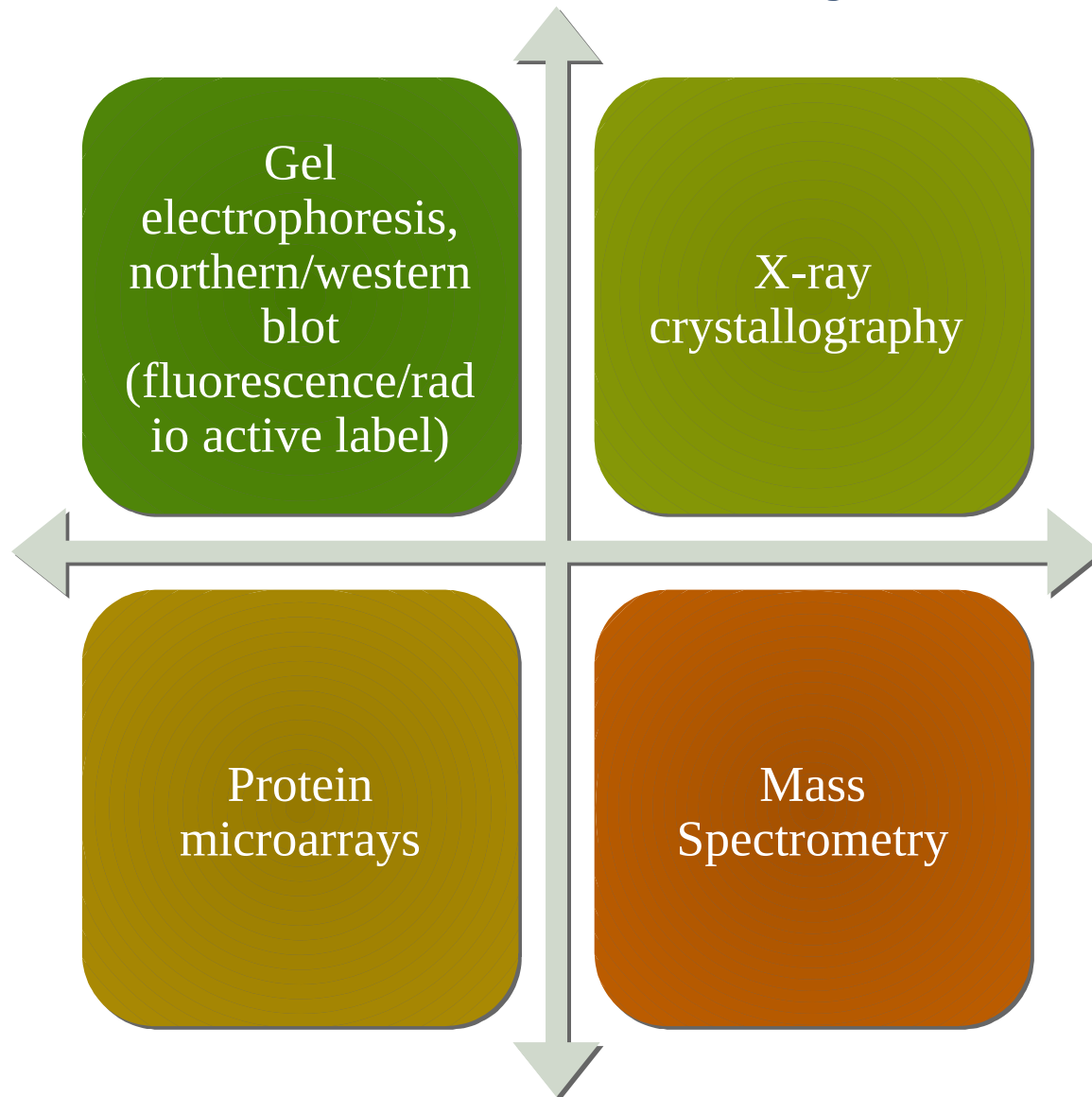
Map to
genome,
transcriptome,
, and
predicted
exon
junctions

Downstream analysis



100s of millions of paired reads
10s of billions bases of sequence

Methods for Protein Analysis



Protein arrays

High throughput analysis of hundreds of thousands of proteins.

Proteins are immobilized on glass chip.

Various probes (protein, lipids, DNA, peptides, etc) are used.

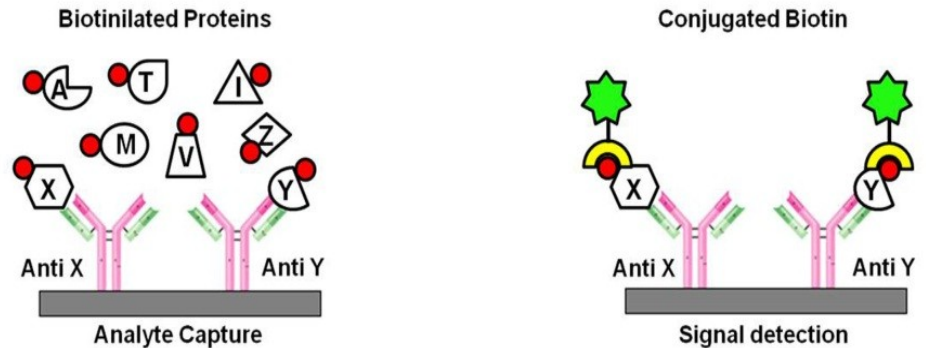
Cons

Require a priori knowledge of the proteins of interest.

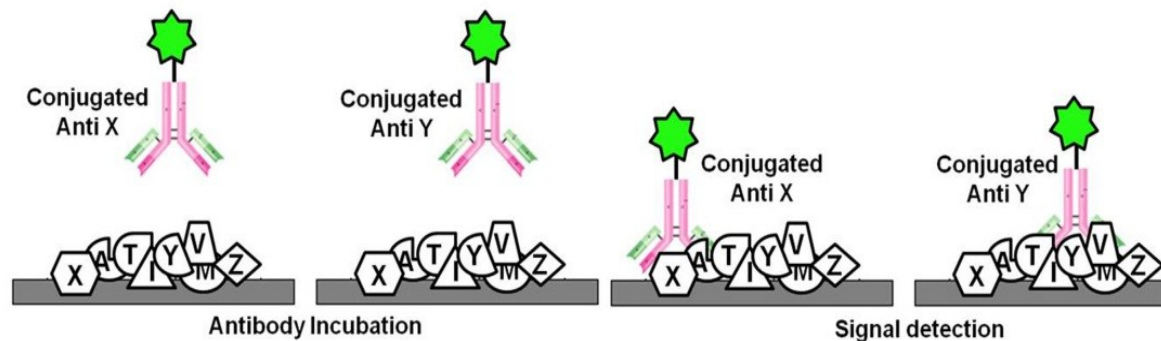
Availability of suitable antibodies.

Measure only a small fraction of the proteome

Forward Phase Protein Array



Reverse Phase Protein Array



Mass Spectrometry

Find a way to “charge” an atom or molecule (**ionization**).

Place charged atom or molecule in a **magnetic field or electric field** and measure its speed or radius of curvature relative to its mass-to-charge ratio (**mass analyzer**).

Detect ions using microchannel plate or photomultiplier tube (**Detection**).

Sample



Ion source:
makes ions

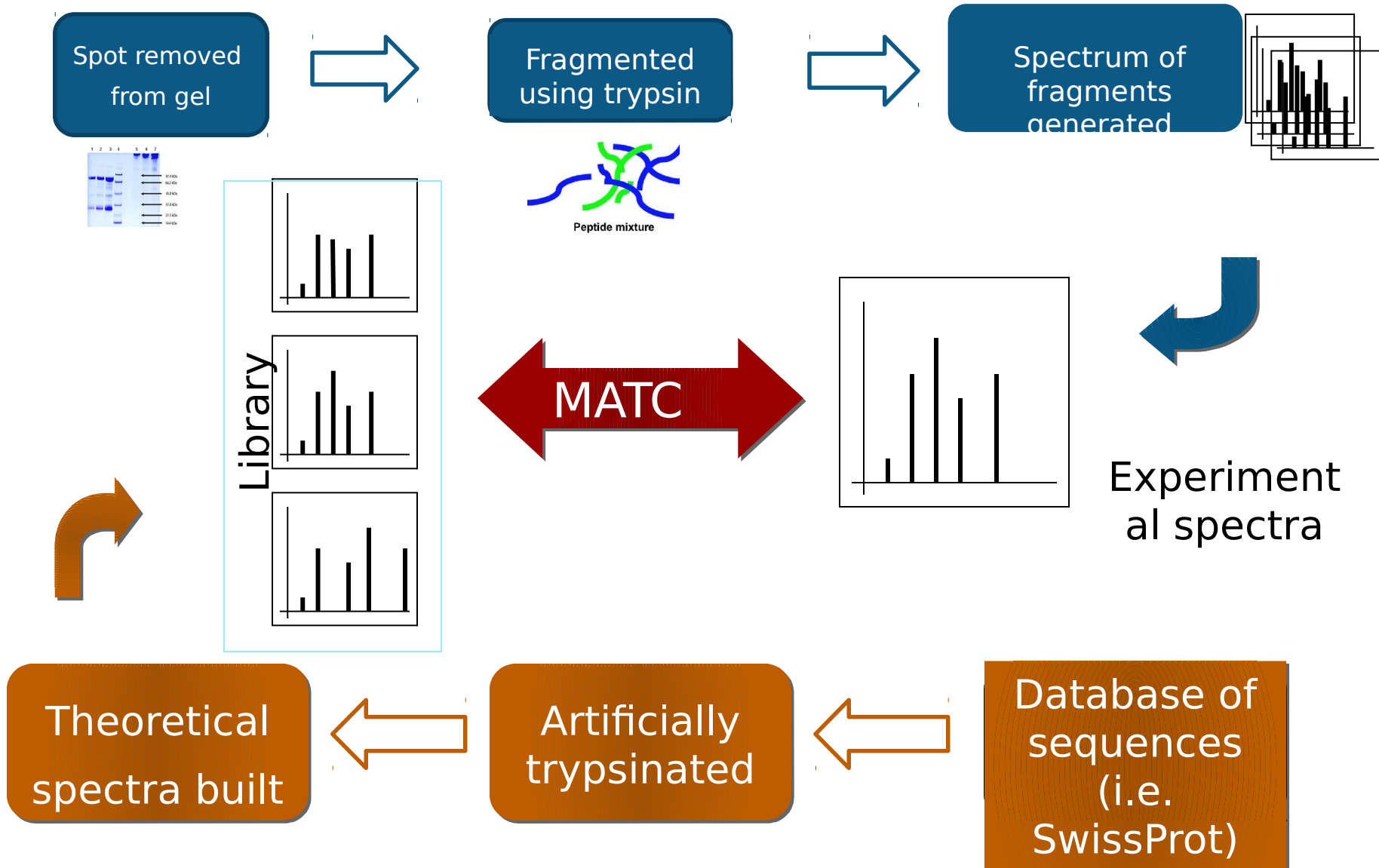


**Mass
analyzer:**
separates
ions

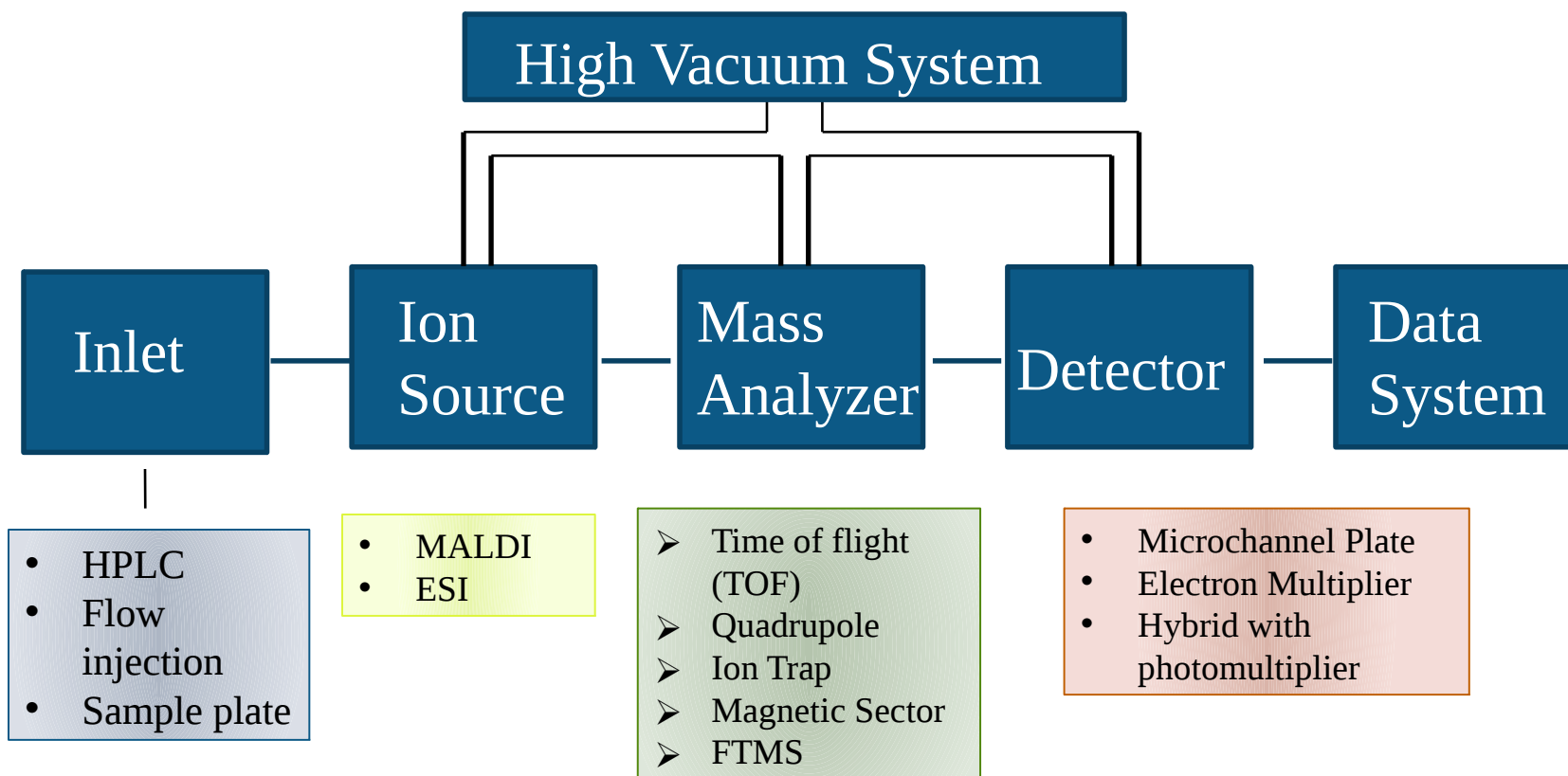


Mass spectrum
Presents
information

Protein Identification by MS



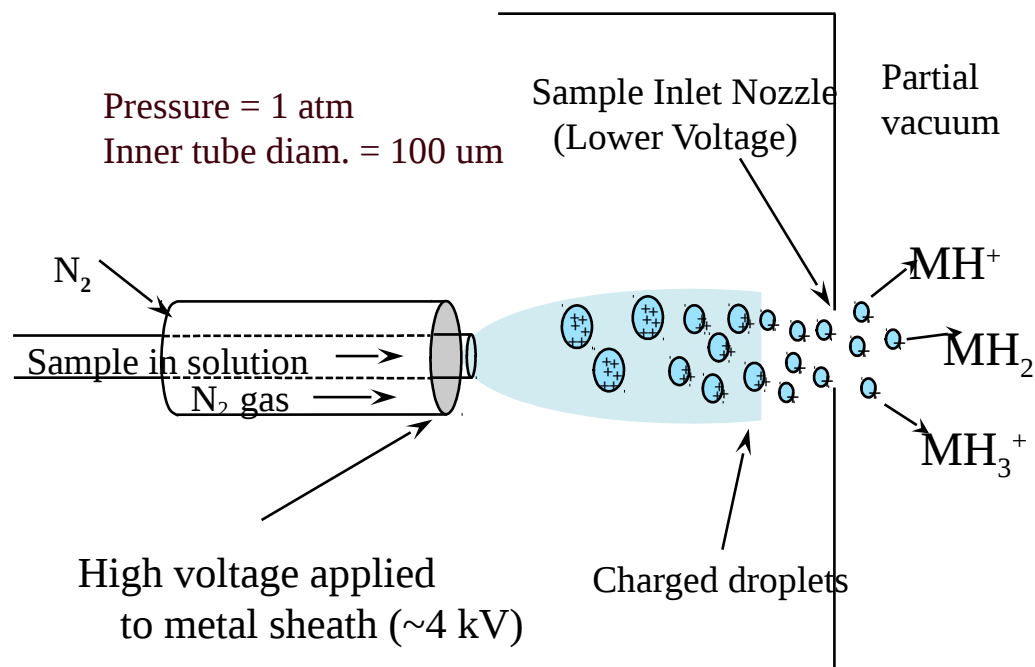
Instrumentation



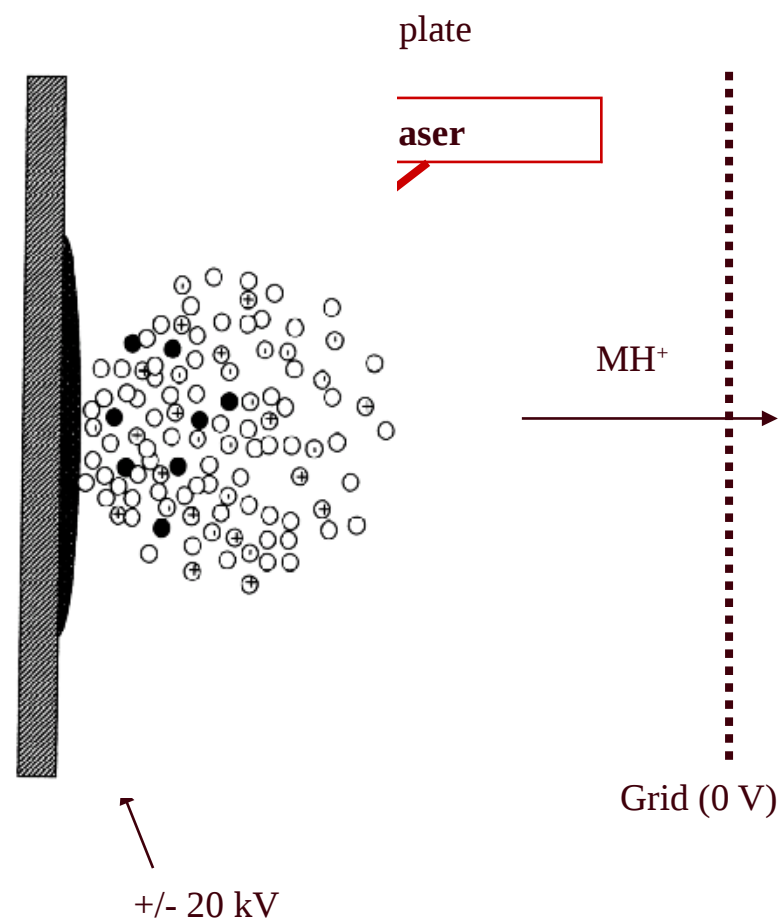
Ion Sources make ions from sample molecules

(Ions are easier to detect than neutral molecules.)

Electrospray ionization



MALDI



Mass analyzers separate ions based on their mass-to-charge ratio (m/z)

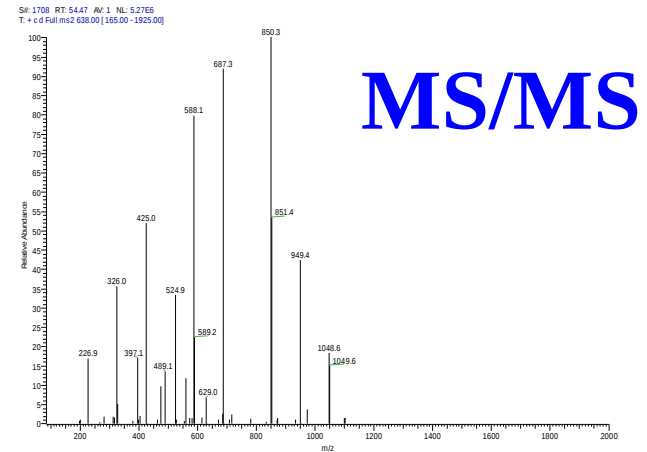
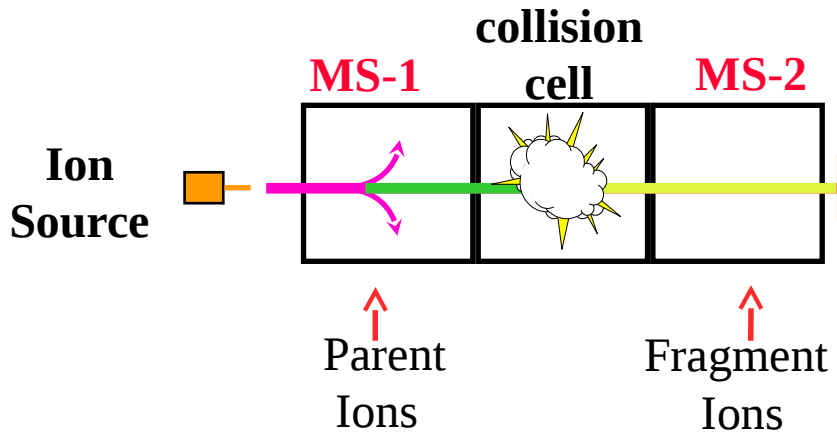
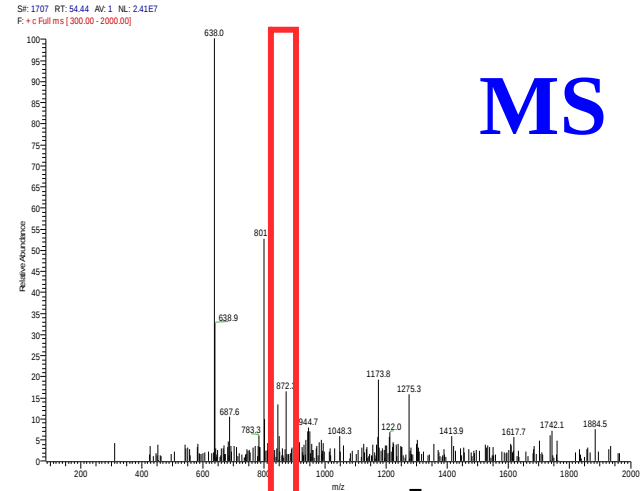
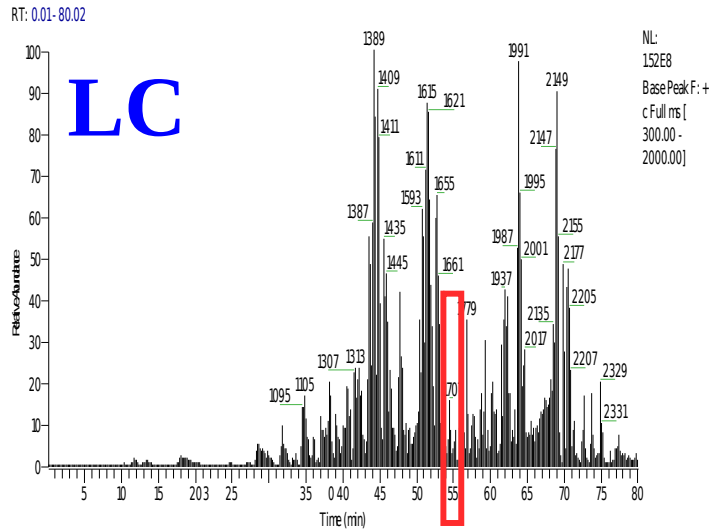
Operate under high vacuum (keeps ions from bumping into gas molecules)

Actually measure mass-to-charge ratio of ions (m/z)

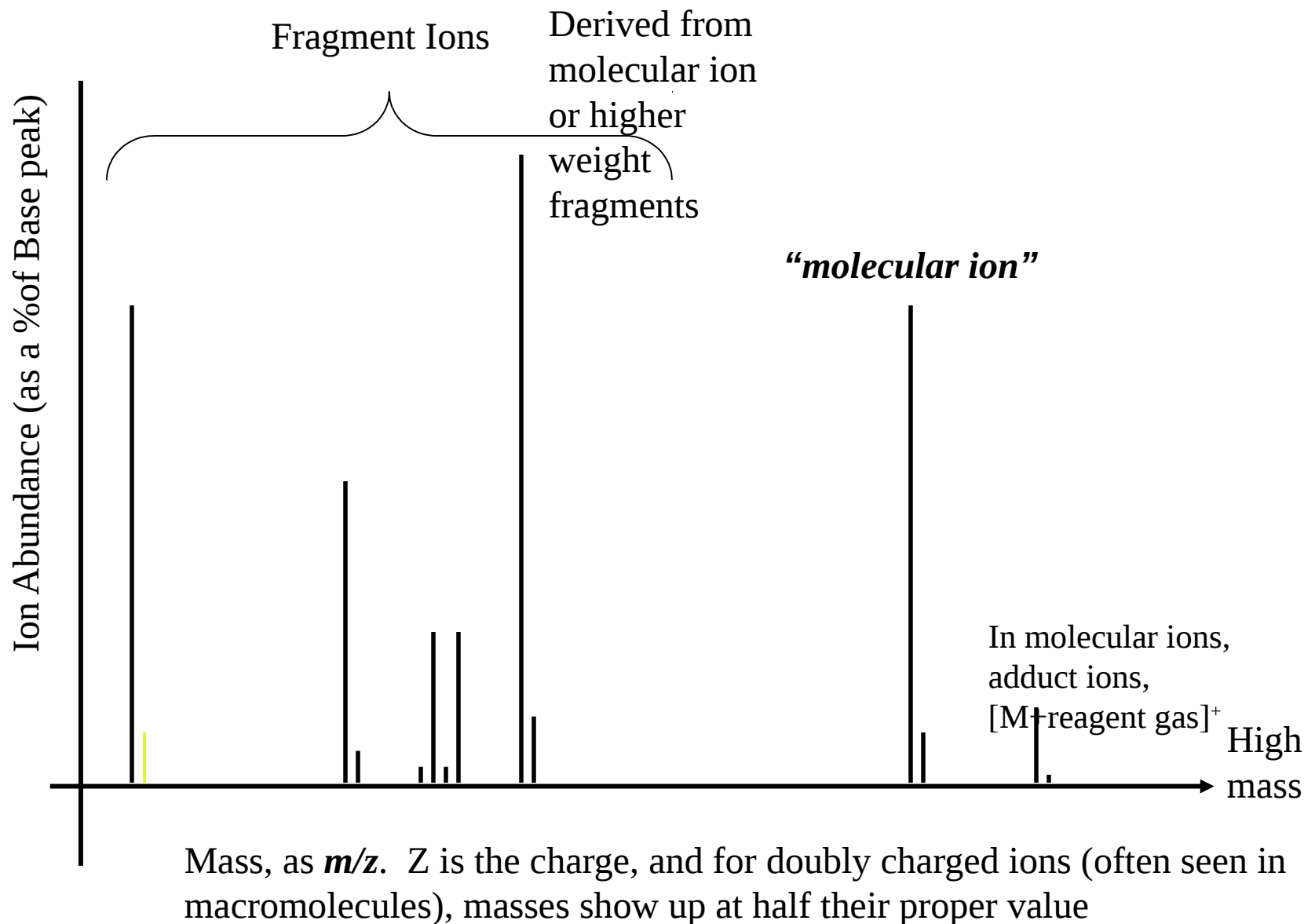
Key specifications are resolution, mass measurement accuracy, and sensitivity.

Several kinds exist: for bioanalysis, quadrupole, time-of-flight and ion traps are most used.

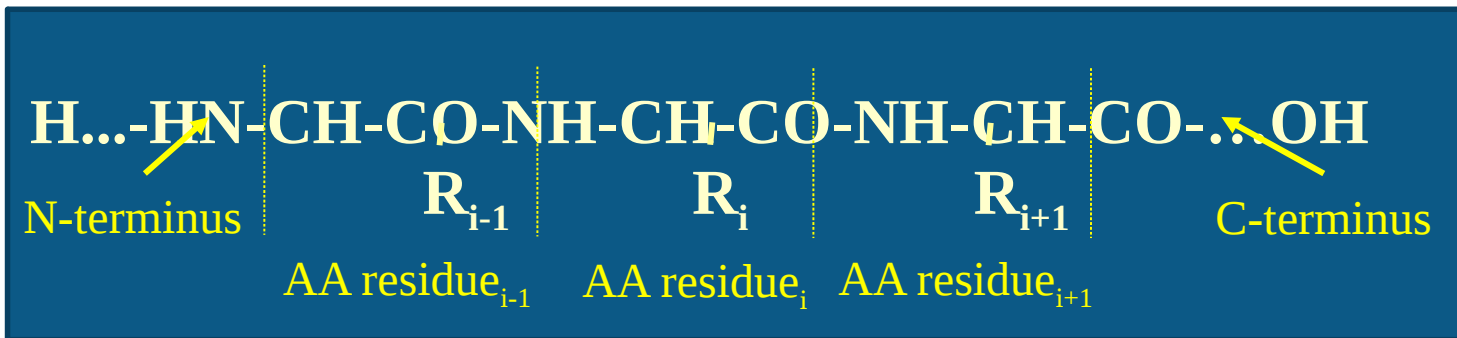
Tandem Mass Spectrometry



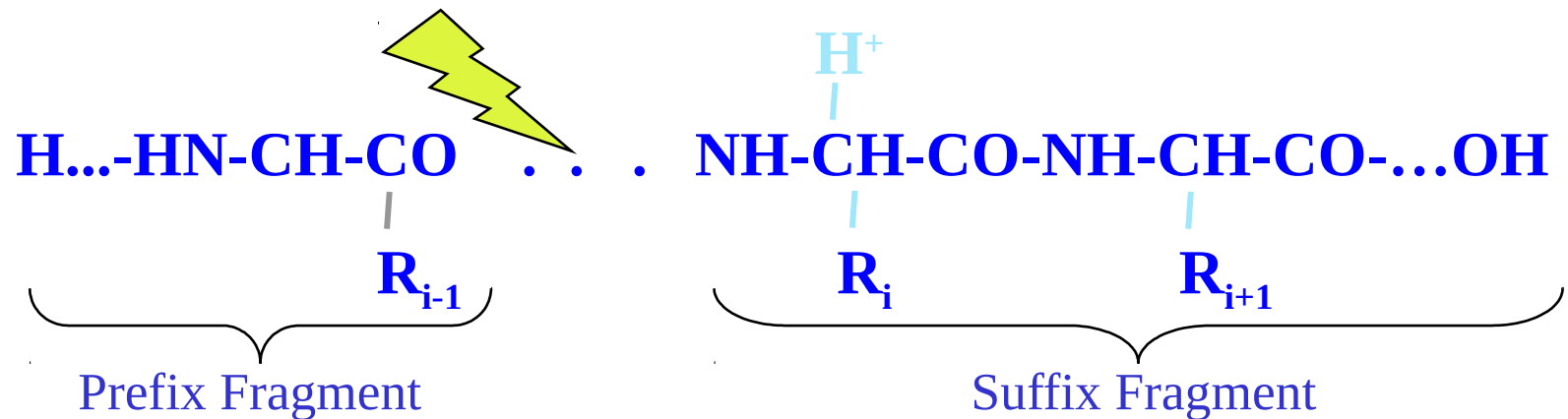
What's in a Mass Spectrum?



Peptide Fragmentation

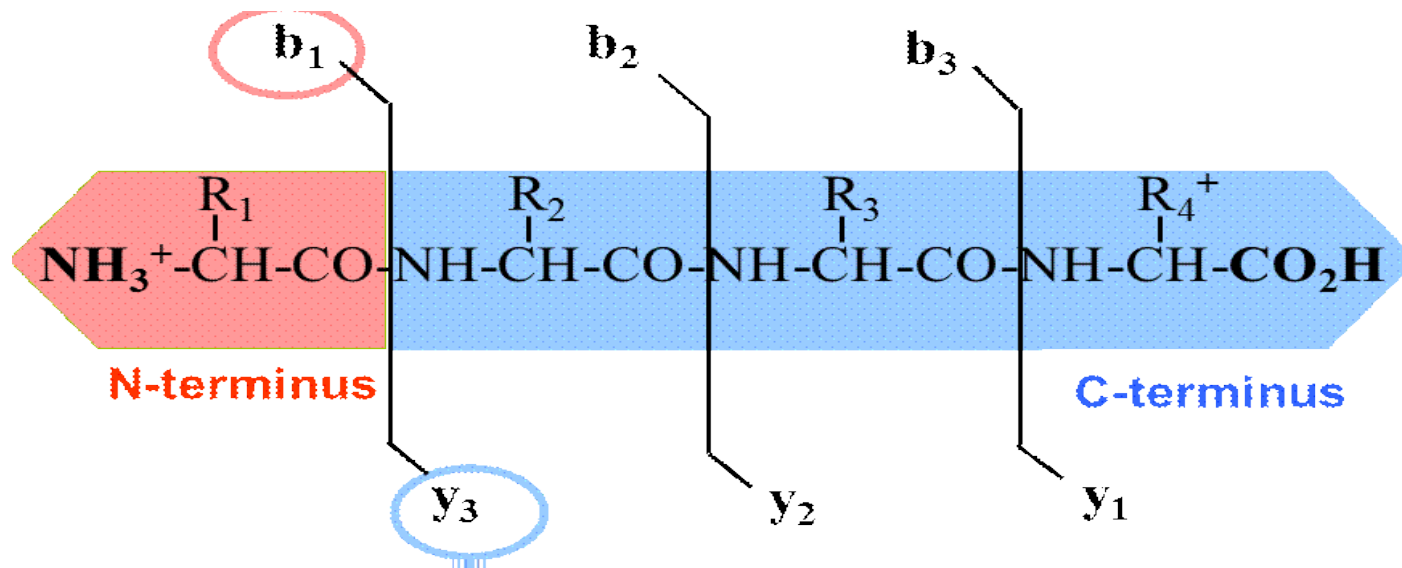


Collision Induced Dissociation



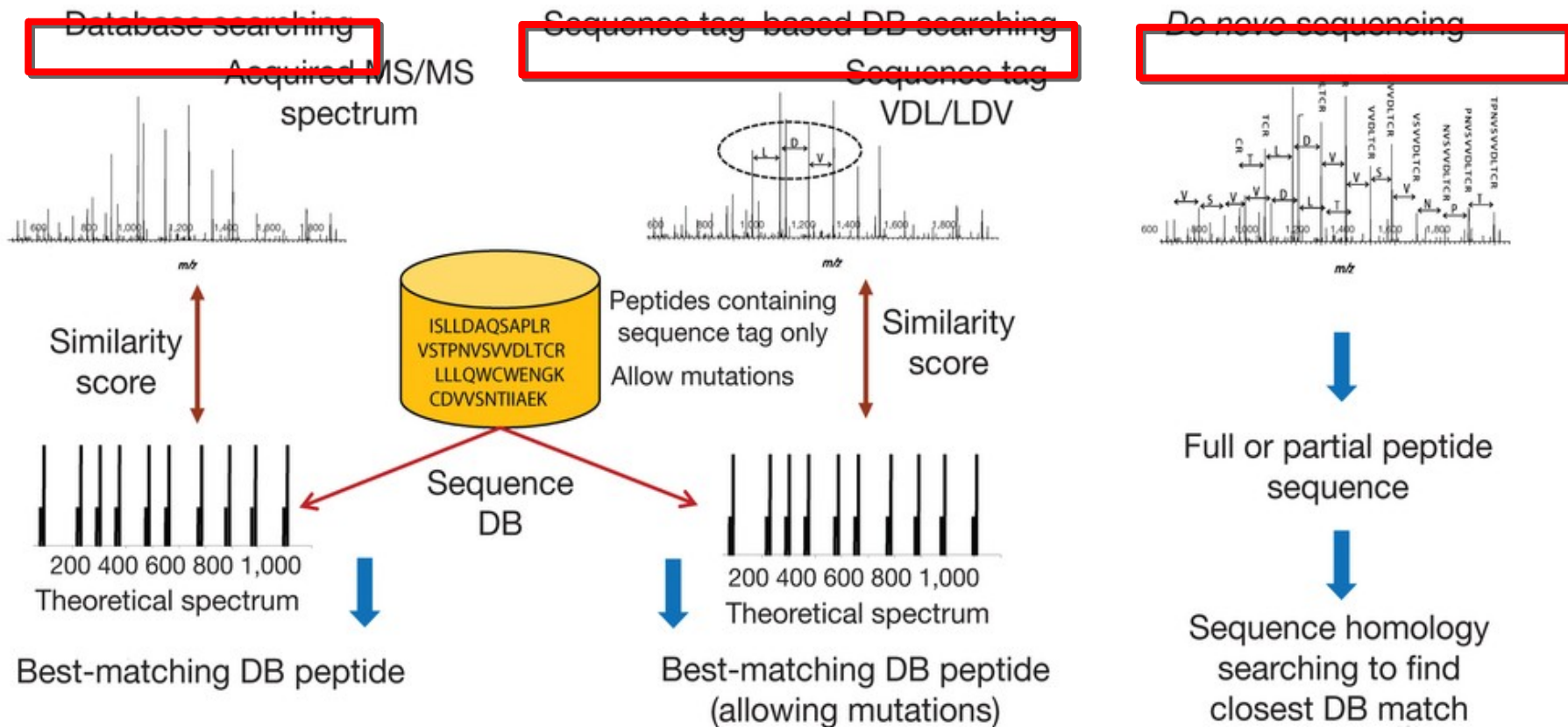
-
-

B ions and Y ions



Mass spectra searching techniques

b Peptide identification using MS/MS spectra



Commercial Software

SEQUEST (Yates et al., 1995)

MASCOT (Perkins, Pappin, Creasy, & Cottrell, 1999)

Open Database search tools

Myrimatch

X!Tandem

MSGF

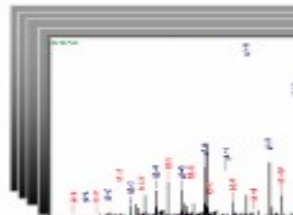
OMSSA

More accurate than Mascot and sequest (Kim & Pevzner, 2014)

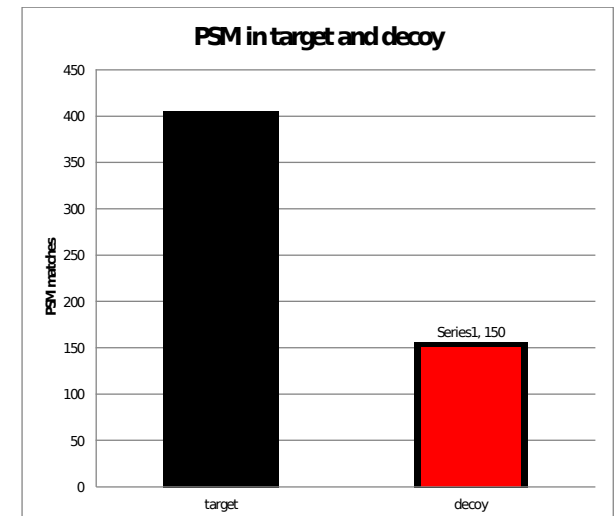
Target-Decoy Search Strategy for Mass Spectrometry-Based Proteomics

- incorrect “decoy” sequences added to the search space will correspond with incorrect search results that might otherwise be deemed to be correct.

Mass spectrum



Target and reversed Decoy database

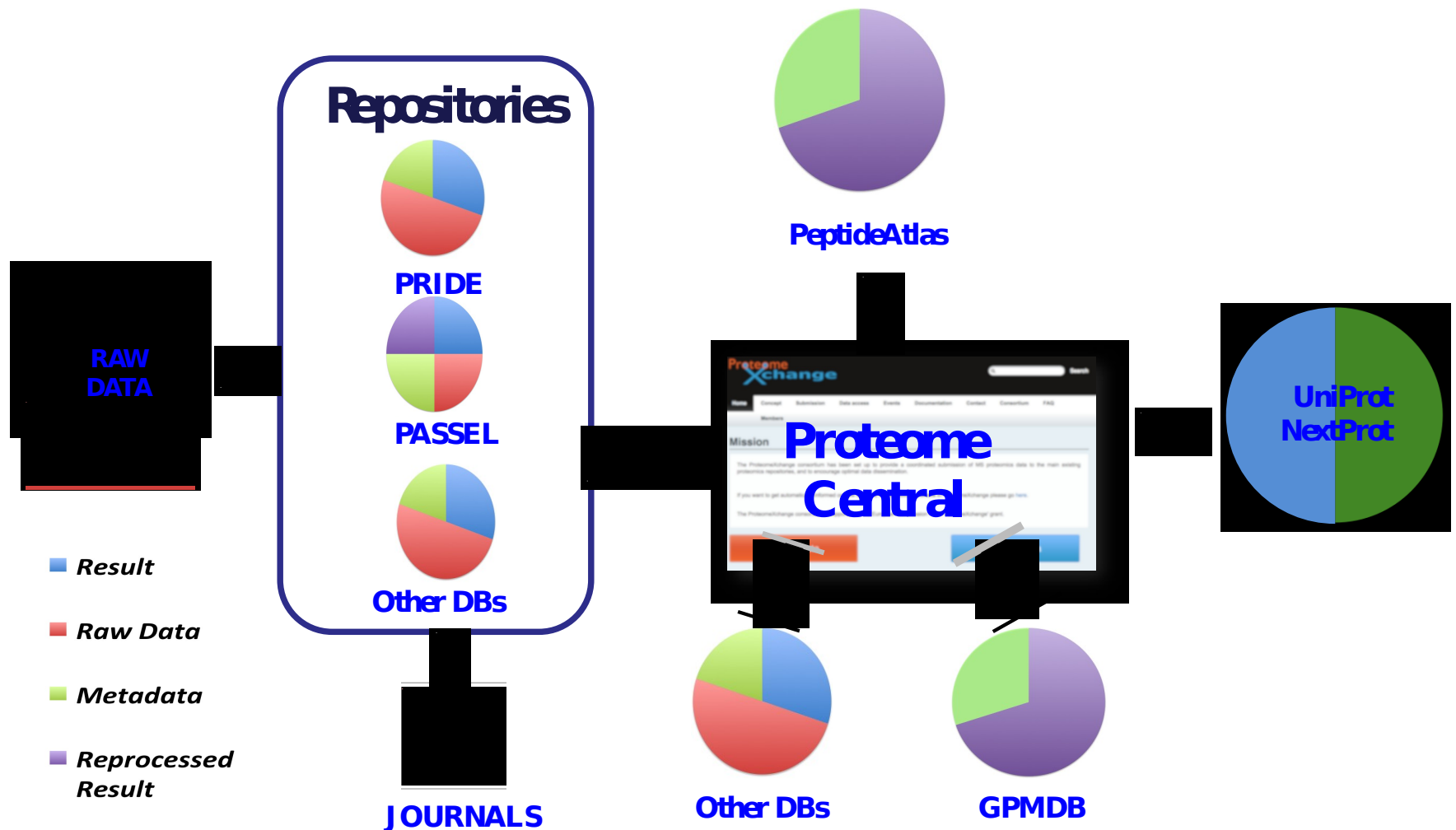


Proportion of matches in decoy database represent false matches

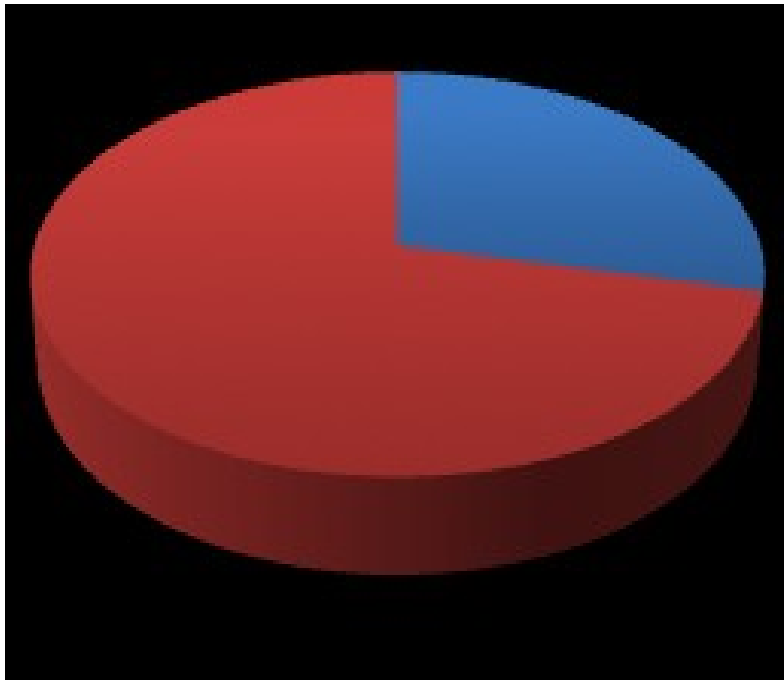
Applications

- **Analyzing Protein Modifications**
 - Finding all modifications on a single protein
 - Proteome wide scanning of modifications
- **Protein Profiling**
 - Generate large scale proteome maps
 - Annotate and correct genomic sequences
 - Analyze protein expression as a function of cellular state
- **Detection of amino acid substitutions**
- **Protein sample identification/confirmation**
- **Protein sample purity determination**

Major Proteomics Repositories



Major Challenge



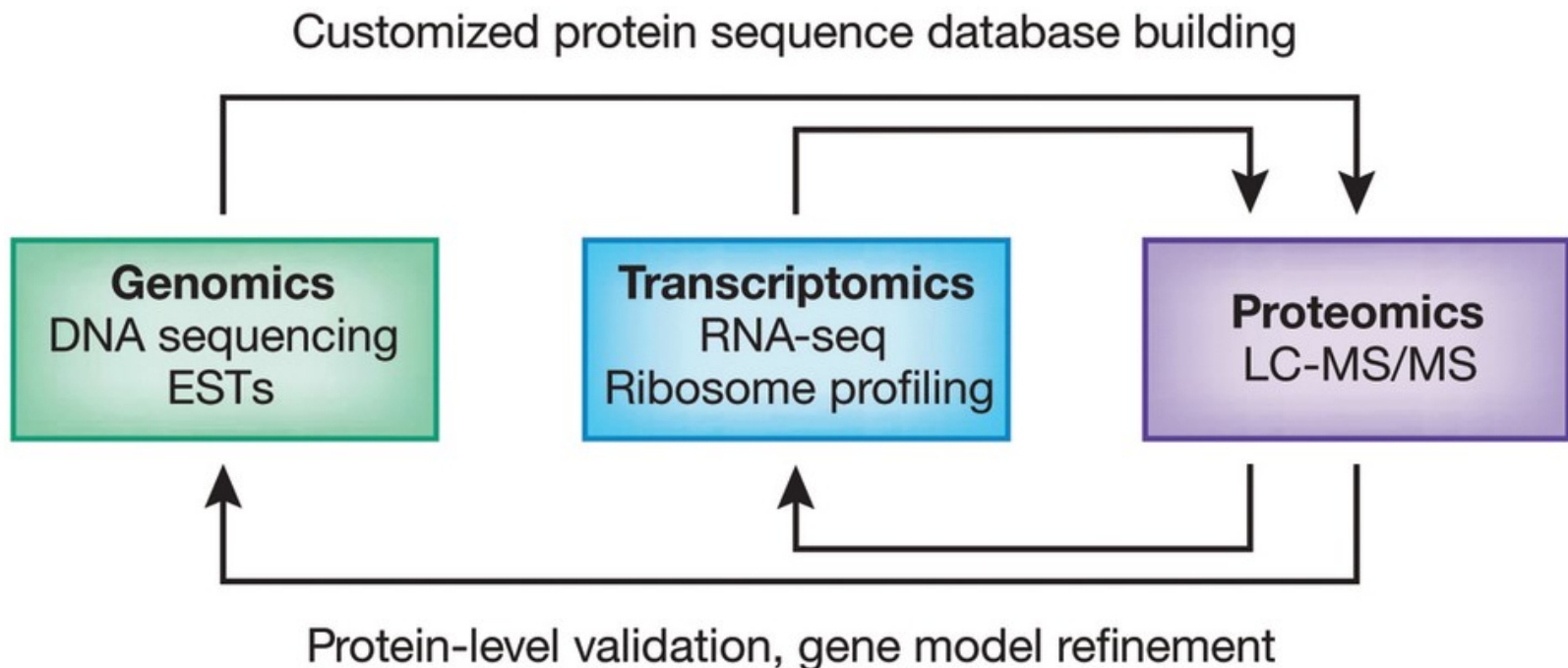
identified
unidentified

**Large number of
unidentified spectra**

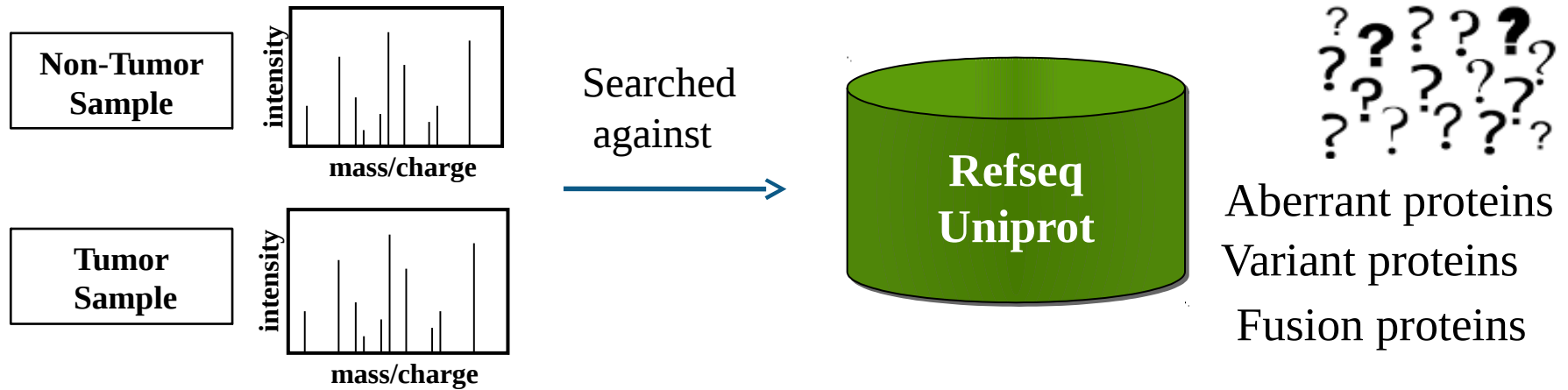
**May be peptides are missing in the database searched.....
Are all the reference databases complete ???**

Proteogenomics

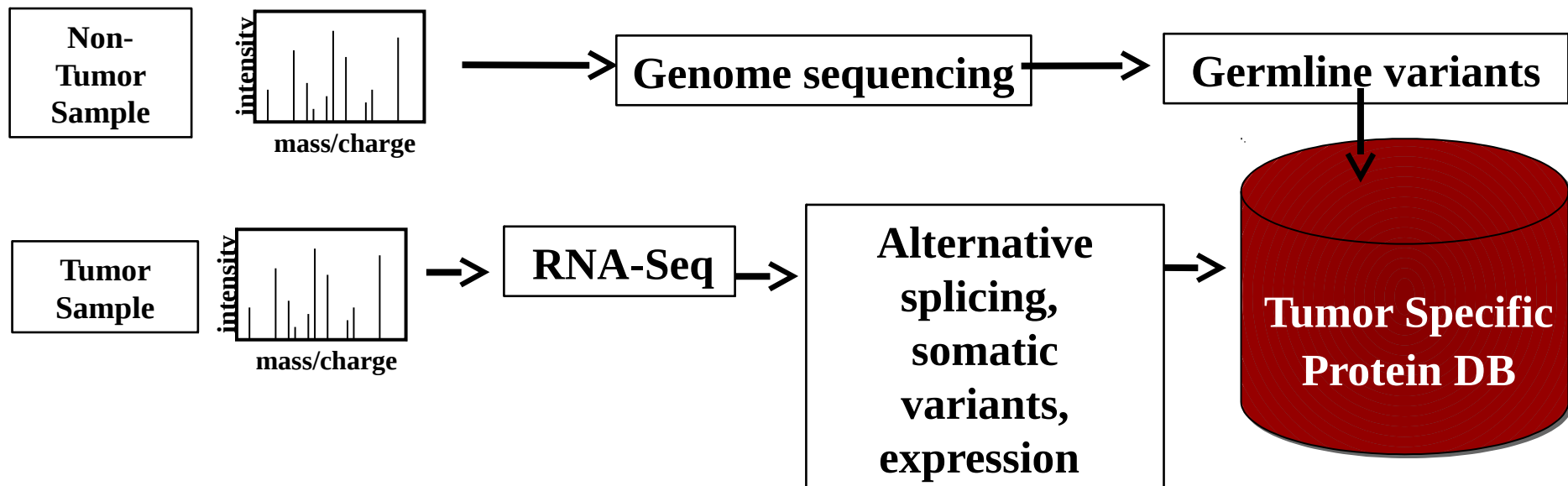
- **Term coined in the literature in 2004.**
- **Genomic for generating customized databases.**
- **Identify novel peptides.**
- **Disease biomarkers based on novel mutation**



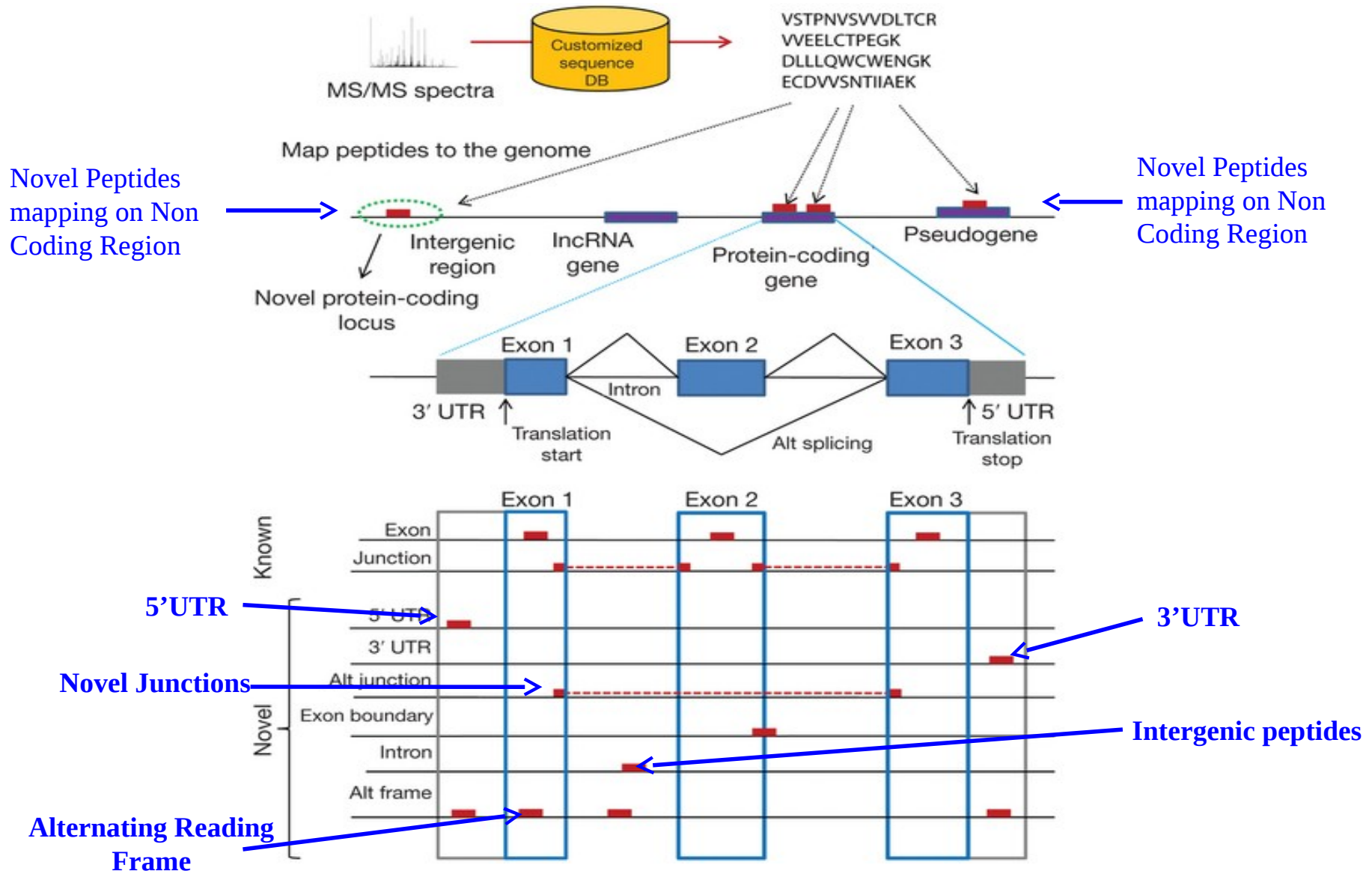
Proteomics



Proteogenomics



TYPES OF PEPTIDES IDENTIFIED IN PROTEOGENOMICS



Methods of generation of customized databases

6 Frame Translation of Reference Database

- Perl or python scripts

Ab initio gene prediction.

- Perl and python scripts

RNA-seq data

- CustomProdb, Galaxy-P system, sapFinder

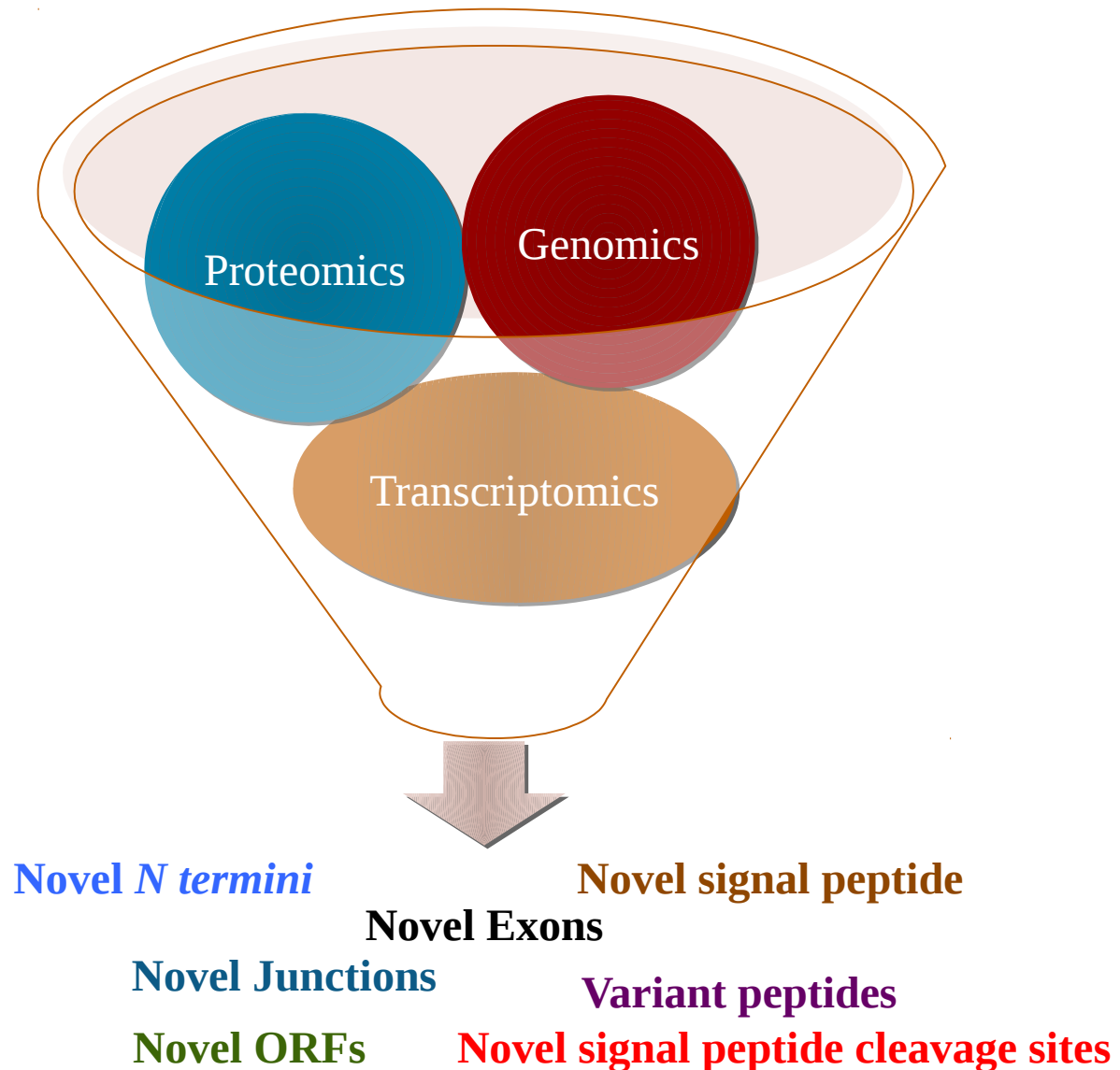
Whole genome Sequencing

- Peppy

Other Databases

- OMIM, neXtProt, Ecgene, ChimerDB, COSMIC

What does proteogenomics offer?



[illegible]

- Home Page
- Web Services
- Research
- Services Offered
- Group Members
- Miscellaneous
- Contact Us

- | | | | | | | |
|-------------------|------------------|----------------|-------------------|---------------------|----------------------|-----------------------|
| Protein Structure | Protein Function | Vaccine Design | Genome Annotation | Biological Database | Therapeutic Peptides | Molecular Interaction |
|-------------------|------------------|----------------|-------------------|---------------------|----------------------|-----------------------|

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

Chemoinformatics and Pharmacoinformatics

Web Server	Description
DrugMint	A Server for Identification of Drug-like Molecules
ABMPred	Prediction of AntiBacterial Compounds against MurA Enzyme
MDRIpred	Prediction of Inhibitor against Drug Resistant M.Tuberculosis
DMKpred	Prediction of Drug molecules for kinase protein
KiDoQ	Prediction of inhibition constant of a molecule against Dihydrodipicolinate synthase enzyme
TOXIpred	Prediction of aqueous toxicity of small chemical molecules in T. pyriformis.
MetaPred	Prediction of cytochrome P450 isoform responsible for metabolizing a drug molecule.
GDoQ	Model for prediction of GLMU inhibitors using QSAR and docking approach.
KetoDrug	Binding affinity prediction of ketoxazole derivatives against fatty acid amide hydrolase.
WebCDK	Web Interface for CDK libraries
TLR4HI	SVM based model for computing inhbitors against human TLR4 (Toll like receptor).
DMKPred	A webserver for the prediction of binding of chemical molecules with specific kinases.
ntEGFR	Predicting and designing imidazothiazoles/pyrazolopyrimidines based inhibitors against wild/mutant EGFR.
CancerIn	Classification and designing of anti-cancer inhibitors.
EGFRpred	Prediction of inhibitor of anti-EGFR molecules of diverse class.
DiPCell	Designing of inhibitors against pancreatic cancer cell lines.
HIVfin	Prediction of fusion protein inhibitors against HIV.

Molecular Interactions

Software name	Description
ADPint	Prediction of ADP interacting residues in a protein.
ATPint	Identification of ATP binding sites in ATP-binding proteins.
DOMprint	SVM based model for predicting domain-domain interaction (DDI).
GlycoEP	Prediction of C-, N- and O-glycosylation site in eukaryotic proteins.
GlycoPP	Prediction of potential N-and O-glycosites in prokaryotic proteins.
GTPbinder	Identification of GTP binding residue in protein sequences.
MYCOprint	A tool fort exploration of the interactome of Mycobacterium tuberculosis.
NADbinder	Prediction of NAD binding proteins and their interacting residues.
Pprint	ANN based method for identification of RNA-interacting residues in a protein.
PreMieR	Identification of mannose interacting residues (MIRs) in protein sequences.
PROprint	Prediction of physical/functional interaction between two protein molecules.
RNApin	A server for the prediction of protein interacting nucleotides in RNA sequences.
tRNAmoD	Prediction of post transcriptional modifications in transfer-RNA (tRNA) sequence.
VitaPred	Identification of different class of vitamin interacting residues in a protein.

Biological Databases

Database name	Description
MHCBN	A curated database of MHC-binding, Non-binding peptides and T-cell epitopes.
Bcipep	A database of B-cell epitopes.
HaptenDB	A database of hapten molecules that can not activate immune system.
PolysacDB	Compilation of antigenic polysaccharides found on surface of microbial organism.
TumorHope	A database of experimentally characterized tumor homing peptides.
AntigenDB	Information about a wide range of experimentally-validated antigens.
OXDBase	Compilation of oxygenases involved in the biodegradation on xenobiotic compounds.
HMRBase	A manually curated database of hormones and their Receptors.
CPPsite	Compilation of experimentally validated Cell Penetrating Peptides (10-30 amino acids).
BIAdb	Information about Benzylisoquinoline Alkaloid molecules
HIVsir	A manually curated database of anti-HIV siRNAs.
CCDB	Catalog of genes involved in the different stages of cervical carcinogenesis.
ProGlycProt	Repository of experimentally characterized eubacterial and archaeal glycoproteins.
NPACT	A database of plant derived natural compounds that exhibit anti-cancerous activity.
CancerDR	Compilation of anticancer drugs and their effectiveness against various cancer cell lines.
ccPDB	Compilation and creation of datasets from PDB for structural/functional annoation of proteins.
ParaPep	HIPdb is a manually curated database of experimentally validated antiparasite peptides.
EGFRindb	Collection of EGFR inhibitors from literature.
CancerPPD	Collection and compilation of experimentally validated anticancer peptides
PCMdb	Pancreatic cancer methylation database provides large scale collection of metylated genes.
HerceptinR	Information about assays performend to test sensitivity/resistance of Herceptin Antibody.
HemolytiK	A resource of experimentally tested hemolytic peptides.
CancerTope	A database of epitopes found in protein involved in cancer.
AHTPDB	AHTPDB is an ideal platform for complete & relevant information for large number of antihypertensive peptides

Genome Annotations

Server Name	Description
FTG	Locating probable protein coding region in nucleotide sequence using FFT based algorithm.
GWBLAST	Genome wide similarity search using BLAST
GWFASTA	Genome Wide Sequence Similarity Search using FASTA.
EGPred	Prediction of gene (protein coding regions) in eukaryote genomes that includes introns/exons.
SVMgene	SVM based approach to identify the protein coding regions in human genomic DNA.
SRF	Find repeats through an analysis of the power spectrum of a given DNA sequence.
MyPattern	A program for detection of a 'motif' in DNA sequence using an exact search method.
GeneBench	A suite of datasets and tools for evaluating gene prediction methods.
FTGPred	A web server for predicting genes in a DNA sequence.
PHDcleav	Prediction of Human Dicer cleavage sites.
PolyApred	Prediction of polyadenylation signal (PAS) in human DNA sequence.
siRNAPred	Predicting actual efficacy of both 21mer and 19mer siRNAs with high accuracy.
ECGPred	Analysis of expression data and correlation between gene expression and nucleotides composition of genes.
desiRam	Designing of highly efficient siRNA with minimum mutation approach
MARSpred	Discriminating between Mitochondrial and Cytosolic Aminoacyl tRNA Synthetases
Icaars	Identification & Classification of Aminoacyl tRNA Synthetases.
LGEpred	Prediction of correlation between amino acid residue and gene expression level.

Immunoinformatics or Vaccine Informatics

Software name	Description
T-Helper Epitopes or MHC/HLA Class II binders (Adaptive Immunity, Exogenous Antigen)	
MHCBN	A database of MHC-Binding, Non-binding peptides and T-cell epitopes.
ProPred	Identification of promiscuous MHC Class-II binding regions in an antigen sequence
HLA-DR4Pred	Identification of HLA-DRB1*0401(MHC class II alleles) binding peptides.
MHC	Matrix Optimization Technique for identification of binding core in MHC II binding peptides
MHC2pred	The MHC2Pred is an SVM based method for prediction of promiscuous MHC class II binding peptides.
MHCBENCH	Benchmarking of MHC binding peptide prediction algorithms.
FDR4	Prediction of binding affinity of HLA-DRB*0401 binders in an antigenic sequence.
IL4pred	In silico platform for designing and discovering of interleukin-4 inducing peptides.
IFnepitope	Designing of interferon-gamma inducing epitopes.
CTL Epitopes or MHC/HLA Class I binders (Adaptive Immunity, Endogenous Antigens)	
PROPPRED1	Prediction of promiscuous binders for 47 MHC/HLA class I alleles using quantitative matrices;
Pcleavage	Identification of proteasomal cleavage sites in a protein sequence.
TPPred	Prediction of TAP binding peptides for understanding of peptide internalization to endoplasmic reticulum
CTLPred	A direct method for prediction of CTL epitopes.
nHLAPred	This is a comprehensive method for prediction of MHC binding peptides or CTL epitopes of 67 MHC class alleles.
MMBPred	Prediction of mutated MHC class I binders in an antigen, having high affinity and promiscuousity.
HLAPRED	The method can identify and predict HLA (both class I & II) binding regions in an antigen sequence.
Linear & Conformational B-cell Epitopes	
BCIPEP	Collection & compilation of B-cell epitopes from literature
BCEPRED	Prediction of linear B-cell epitopes, using Physico-chemical properties
ABCPred	Mapping of B-cell epitope(s) in an antigen sequence, using artificial neural network.

Functional Annotation of Proteins

Server name	Description
NRpred	Prediction and classification of nuclear receptors, SVM models based on composition.
GPCRpred	Prediction of families and superfamilies of G-protein coupled receptors (GPCR)
ESLPred	Subcellular localization of the eukaryotic proteins using dipeptide composton and PSI-BLAST.
PSLPred	Prediction of subcellular localization of bacterial proteins
BTXPred	It predicts bacterial toxins and their function from primary amino acid sequence.
GPCRsclass	This webserver predicts amine type of G-protein coupled receptors
Mitpred	Specifically trained to predict mitochondrial proteins with high accuracy
Oxypred	Classification and prediction of oxygen binding proteins.
VGIchann	Classification and prediction of proteins involved in voltage gated ion channels.
HSLpred	Subcellular localization of human proteins with high accuracy
DNAsize	Compute length of DNA or protein fragments from gel using a graphical method.
GSTpred	SVM-based method for predicting Glutathione S-transferase protein.
Mango	A server for predicting functional class of a protein.
LGEpred	Calculate correlation coefficient between amino acid residue and gene expression level.
NTXPred	Identification of neurotoxins their source and function from primary amino acid sequence.
VICMpred	Classification of bacterila proteins particularly virulent proteins
ALGPred	Prediction of allergenic proteins and mapping of IgE epitopes in antigens.
PseaPred	Prediction of proteins secreted by Malarial Parasite P. falciparum into infected-erythrocyte.
RSLPred	SVM based method for subcellular localizaton of rice proteins.
COPid	Composition based identification and classification of proteins.
ESLPred2	Advanced method for subcellular localization of eukaryotic proteins.
ISSpred	Identification of Inteins hiding in their protein sequences.
CyclinPred	CyclinPred is a SVM based prediction method to identify novel cyclins.

Proteins Structure Prediction

Web Server	Description
AlphaPred	A neural network based method for predicting alpha-turn in a protein.
APSSP2	Prediction of secondary structure of proteins from their amino acid sequence.
AR_NHPred	Identification of aromatic-backbone NH interaction in protein residues.
BetatPred	Statistical-based method for predicting Beta Turns in a protein.
Betatpred2	Prediction of Beta-turns with high accuracy using multiple sequence alignment.
BetaTurns	It predict different types of beta-turns (e.g., Types I/II/IV/VIII) in a protein.
BhairPred	Prediction of beta hairpins in proteins using ANN and SVM techniques.
CHpredicts	Prediction of CH-O, CH-PI interactions in backbone residues of a protein
GammaPred	Identification of gamma-turn containing residues in a given protein sequence.
PEPstr	Prediction of tertiary structure of small peptides (7 to 25 residues).
Proclass	Classification of proteins based on secondary structure contents.
PSA	Analyze the amino acid sequence and multiple sequence alignment of proteins.
RPFOLD	A fold recognition server for searching protein fold in PDB.
SARpred	ANN-model for redicting real-value of surface acessibility of protein residues.
TBBpred	This server predict Transmembrane Beta Barrel regions in a protein.
PEP2D	This server allows you to predict secondary structure of peptides.



Search

Target Identification

[Genome Annotation](#)
[Proteome Annotation](#)
[Potential Targets](#)
[Protein Structure](#)

Virtual Screening

[QSAR Techniques](#)
[Docking & QSAR](#)
[Chemoinformatics](#)
[siRNA/miRNA](#)

Drug Design

[Lead Optimization](#)
[Pharmainformatics](#)
[ADMET](#)
[Clinical Informatics](#)

How to Contribute?

[Experimentalists](#)
[Virtual Trainees/Jobs](#)
[Software Developers](#)

Computational Resources

[Library Interfaces](#)
[Meta Servers](#)
[Publishing Document](#)
[Data on M.tb.](#)

Who Are We??

[Core Team](#)
[Contact Address](#)
[History of CRDD](#)

[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.



CSIR-Informatics Portal

Web services & software developed and maintained by CSIR, India

[Home](#)[BioInformatics](#) ▾[Therapeutics](#) ▾[Resources](#) ▾[Sites](#)[Contact](#)[g+1](#) 2[✓ Like](#)[Share](#)

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India specific Genomes Sequenced, Assembled and Annotated

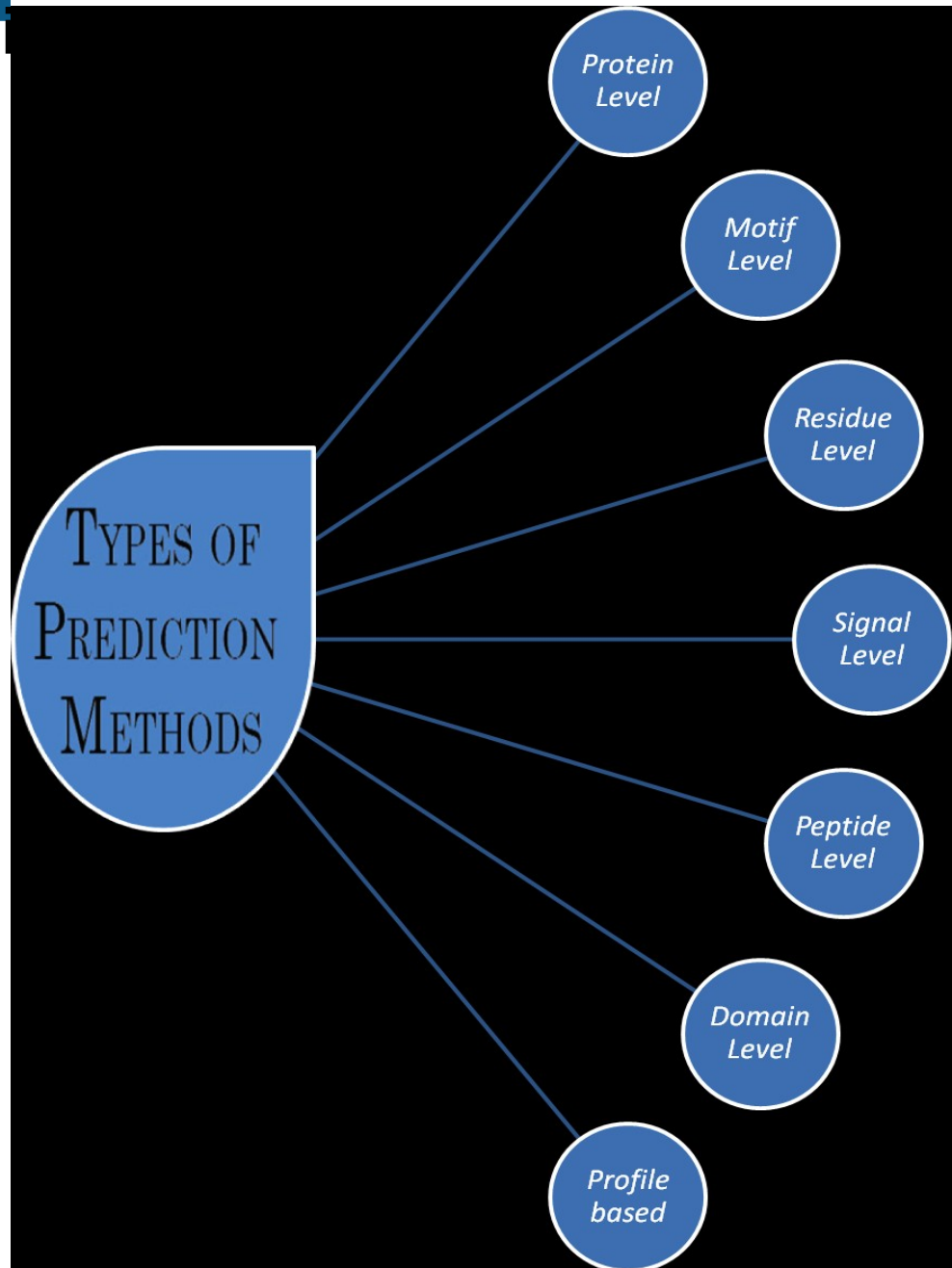
Genomes sequence/assemble/annotate at CSIR Institutes

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 gancidicus Strain BKS 13-15	Isolated from mangrove sediment samples collected from the Bhitari Kanika Mangrove Reserve Forest, Odisha, India.	CSIR-IMTECH	23599292
Serratia fonticola Strain AU-AP2C	Isolated from the Pea Rhizosphere	CSIR-IMTECH	24309742
Pantoea sp. Strain AS-PWVM4	Isolated from the rhizosphere of Punica granatum, exhibits phosphate solubilization	CSIR-IMTECH	24309733

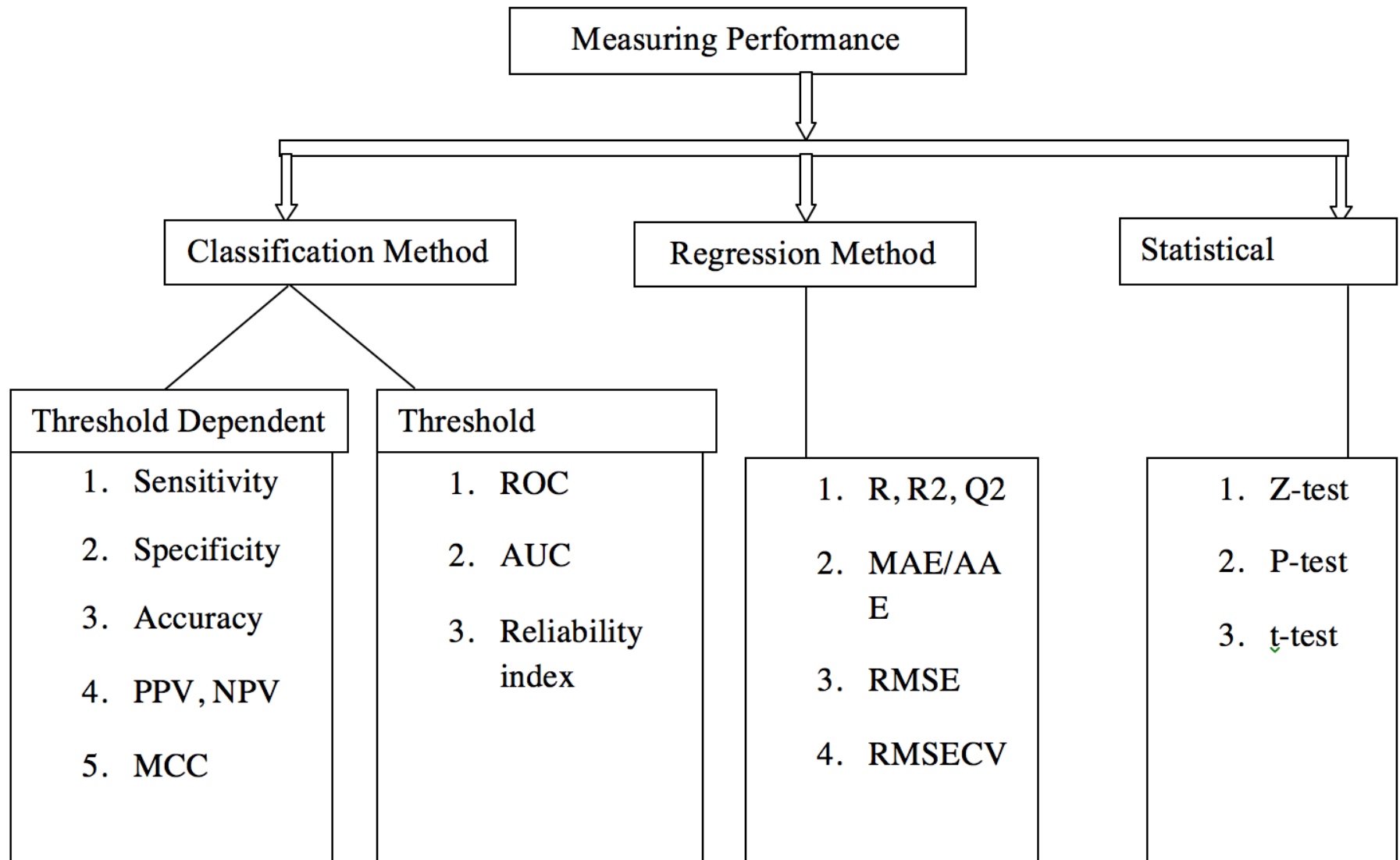
GPSR: A Resource for Genomics Proteomics and Systems Biology

- **A journey from simple computer programs to drug/vaccine informatics**
- **Limitations of existing web services**
 - History repeats (Web to Standalone)
 - Graphics vs command mode
- **General purpose programs**
 - Small programs as building unit
- **Integration of methods in GPSR**

Types of Prediction



Measuring Performance



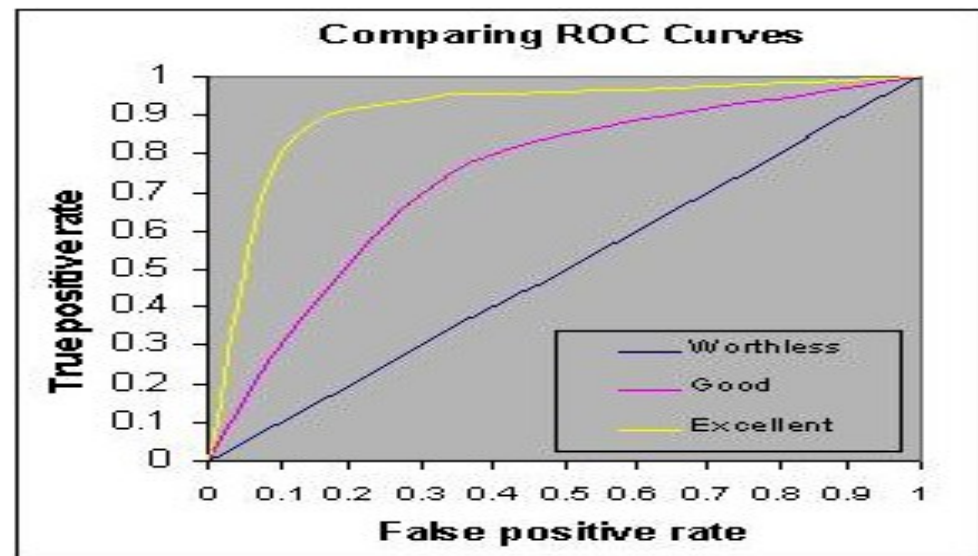
$$\text{Sensitivity} = \frac{TP}{TP + FN} \times 100$$

$$\text{Specificity} = \frac{TN}{TN + FP} \times 100$$

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN} \times 100$$

$$\text{MCC} = \frac{(TP \times TN) - (FP \times FN)}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}} \times 100$$

Predicted	Actual			
		Positive	Negative	
	Positive	TP	FP	PPV
	Negative	FN	TN	NPV
		Sensitivity	Specificity	



GPSR

A resource for genomics, proteomics and systems biology

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Manual Contents

- [1 Message to users](#)
- [2 Disclaimer and copyright](#)
- [3 Types of prediction methods](#)
- [4 Evaluation of bioinformatics methods](#)
- [5 Commonly used bioinformatics tools](#)
 - [Support Vector Machine](#)
 - [Artificial Neural Network](#)
 - [Hidden Markov Model](#)
 - [k-Nearest Neighbor](#)
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- [7 Stand-alone programs](#)
 - [Installation of GPSR 1.0 package](#)
 - [ESLPred](#)
 - [HSLPred](#)
 - [PSLPred](#)

Integration of Computer Programs Developed at



GPS Raghava's Group

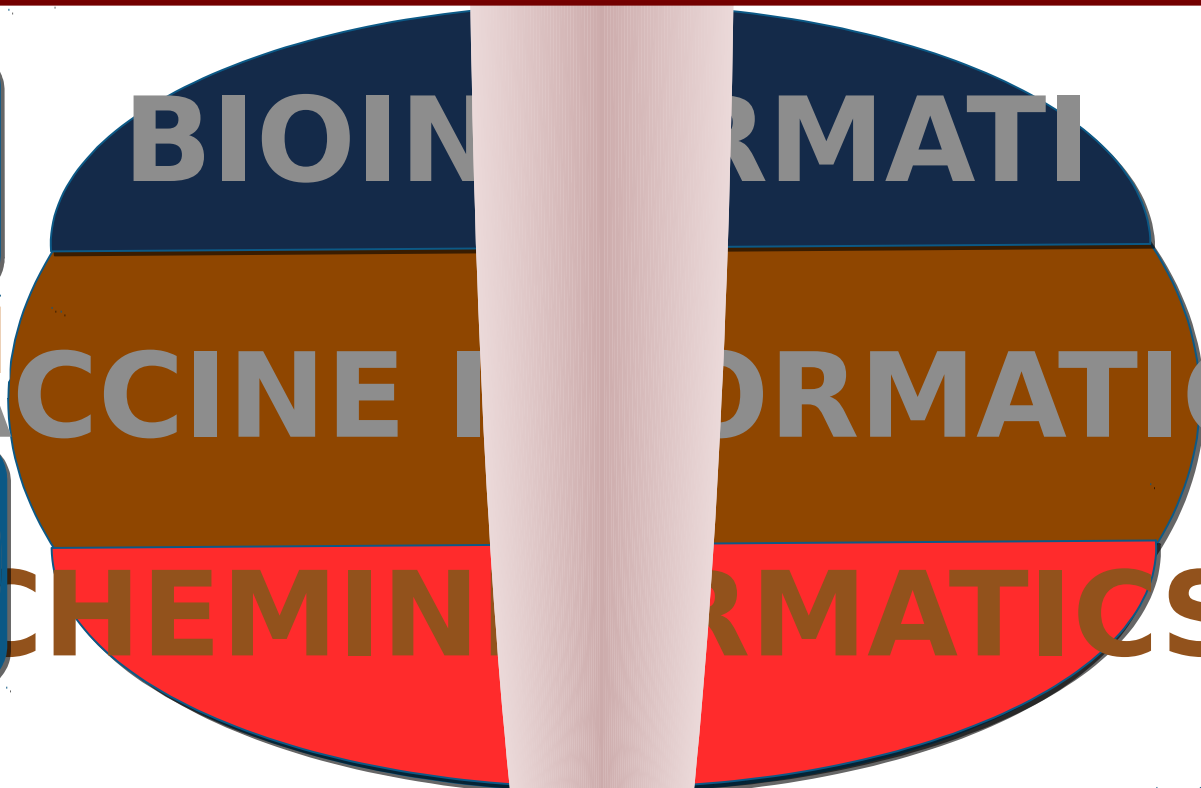
Bioinformatics Centre,
Institute of Microbial Technology, Chandigarh



OSDD LINUX



Customized operating environment for drug discovery pipeline



Live Server



Live CD



Pkg
Repository



Installation



Webserver



Standalone



Galaxy
platform



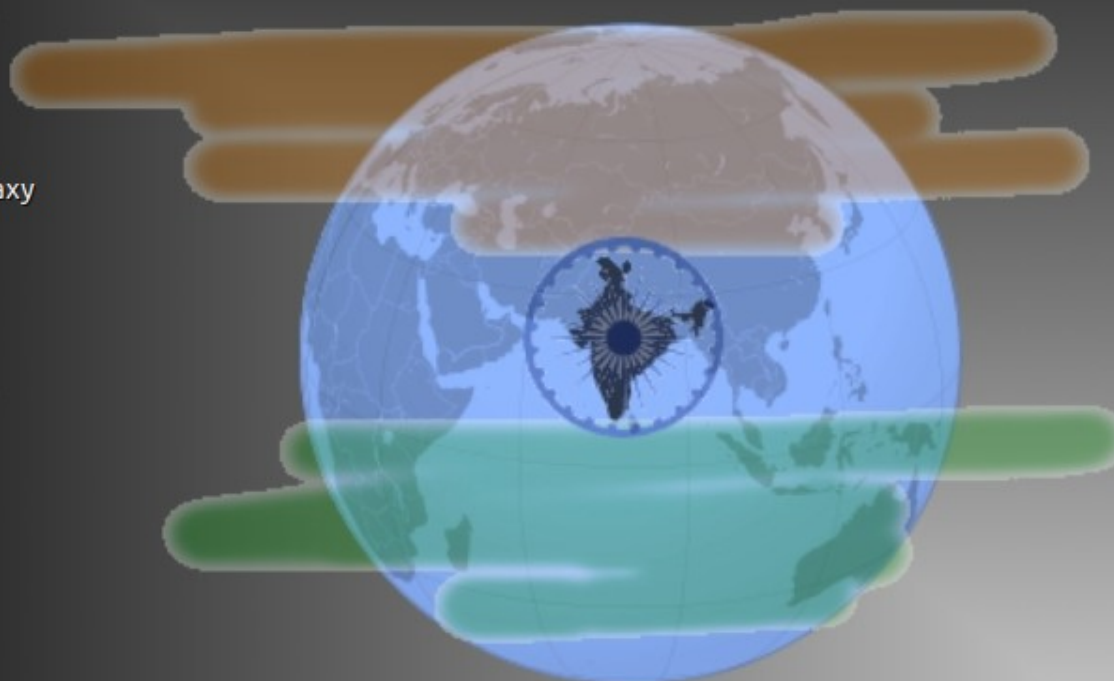
All in ONE

OSDDLinux_
StandaloneOSDDLinux_
Webserver

OSDDLinux_Galaxy

OSDDLinux_
WebServers

Osddlinux desktop
is ready for use.



Password for sudo : osddlinux root : osddlinux



A Customized Operating System For Drug Discovery
OSDDLinux
<http://osddlinux.osdd.net/>



Osddlinux installation on system hard drive

OSDD



LINUX

CONNECT

Next

A Custom
f

Operating System for Drug Discovery

General Information +

Software Packages +

Install/Download +

Service to Community +

OSDDLinux Online +

Important Resources +

Open Source Drug Discovery (OSDD), a mission to provide affordable drugs for poors, is in the process of creating an in silico platform for designing, discovering and simulating drugs. OSDD have initiate number of projects to support in silico drug discovery, including OSDD-Linux and computational resources for drug discovery (CRDD).

OSDD-Linux (a customize linux operating system for drug discovery) intergtate open source software, libraries, workflows and web service in linux for creating environment for drug discovery. First time an attempt have been made to customize linux to provide service to community working in the field of drug discovery. OSDD-Linux may bring down the cost of drug discovery as well as it may increase speed of drug discovery.

Install/Download -

Live DVD/USB

Full Installation

Virtual Box

On existing machine

Package Repository

Upgrade/New Packages

General Information -

Major Features

Installation Guide

Users Guide

Drug Discovery manual

GPSR manual

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List of Packages

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Command Mode

Web Services

Galaxy Portal

GUI-based Software

Software Packages -

Bioinformatics

Vaccine Informatics

Drug Informatics

Biotherapeutics

Analysis of NGS data

Education & Research

Basic Scripts



Gajendra PS Raghava

Head Bioinformatics Centre, CSIR Institute of Microbial Technology, Chandigarh, India

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](#), [Shailesh](#)

Title	1-20	Cited by	Year
ProPred: prediction of HLA-DR binding sites	H Singh, GPS Raghava Bioinformatics 17 (12), 1236-1237	500	2001
Prediction of continuous B-cell epitopes in an antigen using recurrent neural network	S Saha, GPS Raghava Proteins: Structure, Function, and Bioinformatics 65 (1), 40-48	305	2006
ESLpred: SVM-based method for subcellular localization of eukaryotic proteins using dipeptide composition and PSI-BLAST	M Bhasin, GPS Raghava Nucleic acids research 32 (suppl 2), W414-W419	257	2004
Support vector machine-based method for subcellular localization of human proteins using amino acid compositions, their order, and similarity search	A Garg, M Bhasin, GPS Raghava Journal of Biological Chemistry 280 (15), 14427-14432	213	2005
MHCBN: A Comprehensive Database of MHC Binding and Non-Binding Peptides	M Bhasin, H Singh, G Raghava Bioinformatics 19 (5) 665	192	2003



Gajendra Pal Singh Raghava

M.Tech, PhD

Project Investigator (PI, OSDD)

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Dr Raghava is a scientist working at Bioinformatics Centre, Institute of Microbial Technology (IMTECH), Chandigarh, India. For more information see web sites
<http://www.imtech.res.in/raghava/>
<http://crdd.osdd.net/>

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Shailesh Kumar

22.41 · 39.11 · (23)

Institute of Microbial Technology



Manoj Bhasin

A word cloud featuring the phrase "Thank you" in numerous languages and colors. The central and largest text is "thank you" in red. Other prominent words include "gracias" in green, "danke" in blue, "merci" in orange, and "obrigado" in green. Smaller words include "спасибо" (Russian), "dziękuję" (Polish), "sukriya" (Hindi), "kop khun krap" (Thai), "arigato" (Japanese), "takk" (Norwegian), "dank je" (Dutch), "ngiyabonga" (Xhosa), "tesekkür ederim" (Turkish), "tapadh leat" (Irish), "mochchakkeram" (Tamil), "go raibh maith agat" (Irish), "dakujem" (Slovak), "merci" (French), "terima kasih" (Indonesian), "감사합니다" (Korean), "ευχαριστώ" (Greek), "sagolun" (Hebrew), "hvala" (Slovene), "maururu" (Māori), "bedankt" (Dutch), and "moachhakkeram" (Tamil). The words are arranged in a circular pattern around the central "thank you".