

Bioinformatics & Biostatistics

Lecture 1 – Introduction to Bioinformatics

AGTCCGCGAATACAGGCTCGGT AGTCCGCGAATACAGGCTCGGT

Petrus Tang, Ph.D. (鄧致剛)

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and

Bioinformatics Center, Chang Gung University.

petang@mail.cgu.edu.tw

EXT: 5136



Molecular Regulation and Bioinformatics Laboratory

Home

MRBLab

Research

CV

Publications

Parasitology

Bioinformatics

The Molecular Regulation & Bioinformatics Laboratory (MRBLab) use bioinformatics approaches to integrate multi-omic (including genomics, proteomics, transcriptomics, metabolomics, etc.) analysis techniques to study parasite-host interaction and to develop pipelines/visualization methods that makes computational biology accessible to research scientists with no programming experience



Molecular Regulation & Bioinformatics Laboratory

Dept. Parasitology, College of Medicine, Chang Gung University, TAIWAN



Prof. Petrus Tang, Ph.D.

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Taoyuan 333. Taiwan.

Phone number:

+886-3-2118800#5136

Fax:

+886-3-2118122

E-mail:

petang@mail.cgu.edu.tw

LATEST NEWS

[Announcements]

● [Trichomonas videos](#)

1. [Trichomoniasis: Why is It the Neglected STD?](#) by M. Hobbs

2. [A Trich-y parasite: genomics, population genetics and evolution of Trichomonas vaginalis](#) by Jane Carlton

[Lectures]

● [Applications of Bioinformatics and Computational Techniques in Biomedical Research](#)



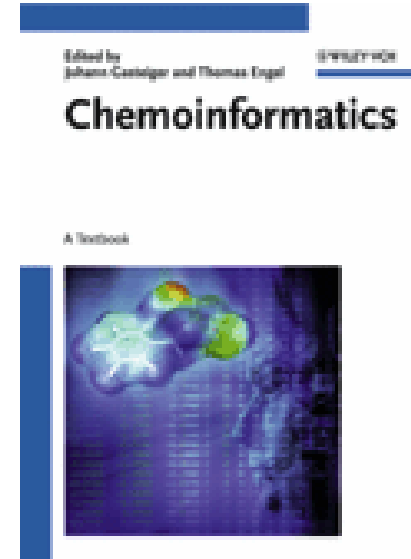
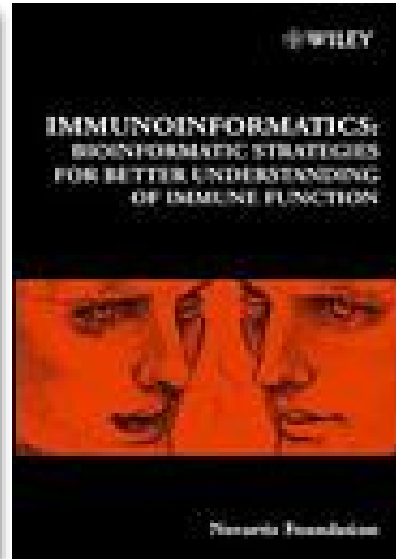
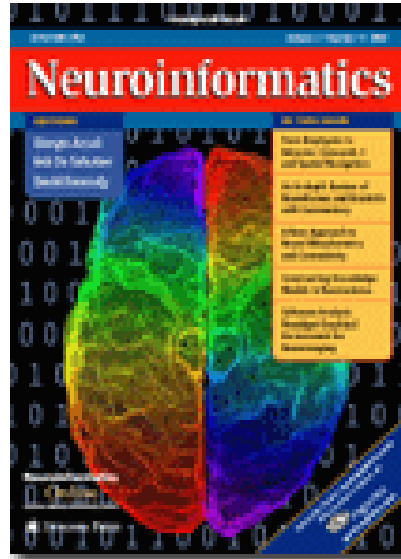
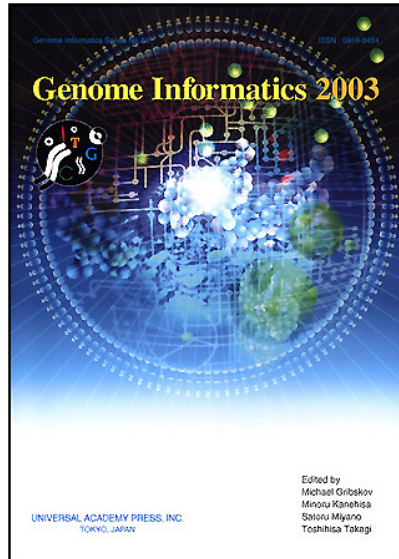
Bioinformatics & Biostatistics

Time: Thursday 13:10~15:00

Classroom: 8th Floor Medical Building, Room 0860-1

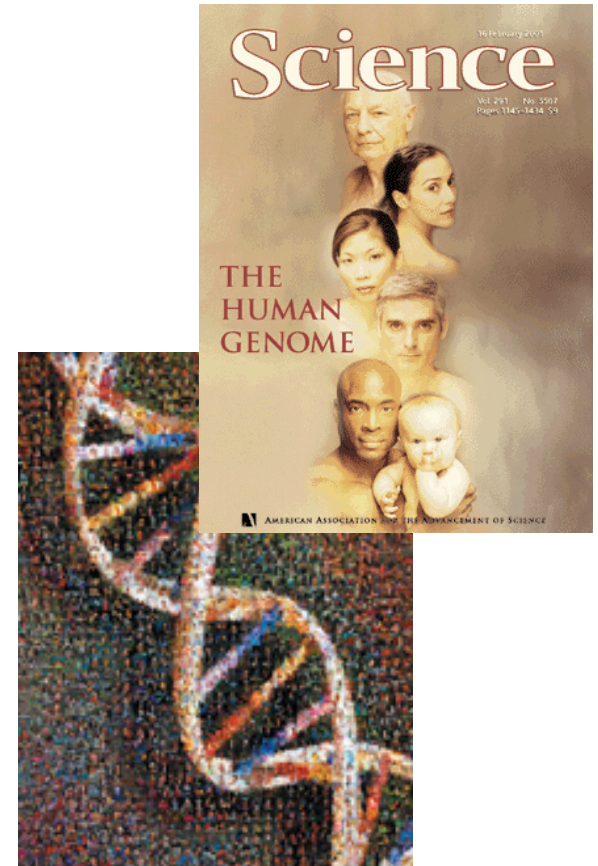
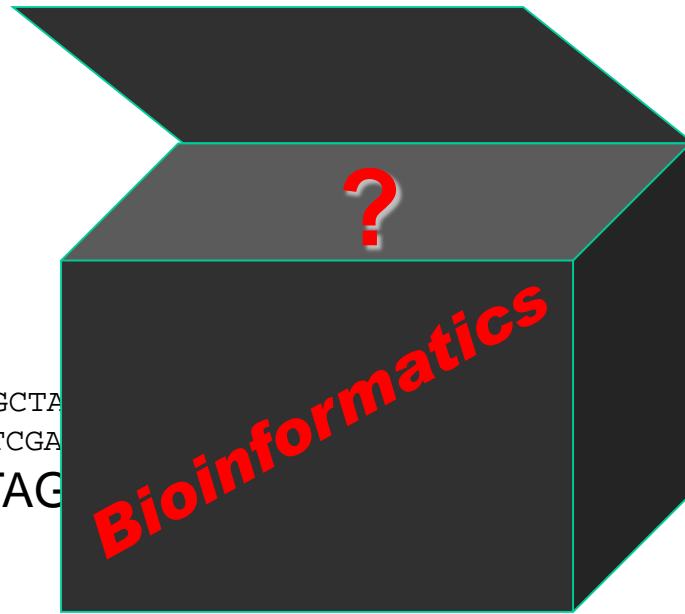
Week	Date	Topic	Lecturer	Lecture Notes
1	2017-09-21	IBiostatistics Basics	Lai-Chu SEE	
2	2017-09-28	Introduction to Biostatistics	Lai-Chu SEE	
3	2017-10-25	Hypothesis testing	Lai-Chu SEE	
4	2017-10-12	Fundamental statistics: probability and descriptive statistics	Lai-Chu SEE	
5	2017-10-19	Hypothesis testing	Lai-Chu SEE	
6	2017-10-26	Comparison between 2 or more means (2-sample t-test, 1-way ANOVA and nonparametric approaches)	Lai-Chu SEE	
7	2017-11-02	General linear model(1)	Lai-Chu SEE	
8	2017-11-09	General linear model(2)	Lai-Chu SEE	
9	2017-11-16	Logistic regression	Lai-Chu SEE	
10	2017-11-23	Introduction to Bioinformatics	<u>Petrus TANG</u>	
11	2017-11-30	Introduction to Bioinformatics	<u>Petrus TANG</u>	PDF
12	2017-12-07	Bio-Databases	<u>Petrus TANG</u>	PDF
13	2017-12-14	Gene Expression Analysis	<u>Ting-Wen Chen</u>	PDF
14	2017-12-21	Nucleic Sequence Analysis	<u>Petrus TANG</u>	PPT ZIP
15	2017-12-28	Protein Sequence Analysis	<u>Petrus TANG</u>	PDF
16	2018-01-04	New Generation Sequencing: Technologies	<u>Petrus TANG</u>	PDF MOVIE
17	2018-01-11	Applications New Generation Sequencing: Technologies	<u>Petrus TANG</u>	
18	2018-01-128	Final Examination	<u>Petrus TANG</u>	

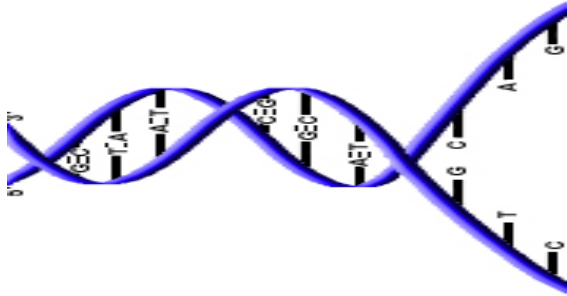
Bio informatics



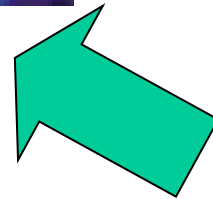
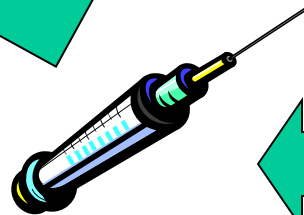
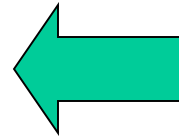
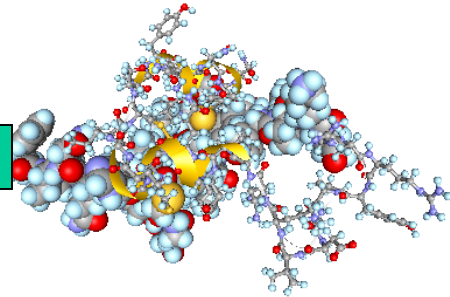
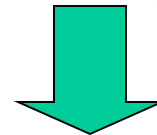
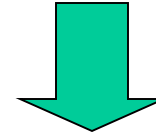
-Omics Mania *biome, cellomics, chronomics, clinomics, complexome, crystallomics, cytomics, degradomics, diagnomics, enzymome, epigenome, expressome, fluxome, foldome, secretome, functome, functomics, genomics, glycomics, immunome, transcriptomics, integromics, interactome, kinome, ligandomics, lipoproteomics, localizome, phenomics, metabolome, pharmacometabonomics, methylome, microbiome, morphome, neurogenomics, nucleome, secretome, oncogenomics, operome, transcriptomics, ORFeome, parasitome, pathome, peptidome, pharmacogenome, pharmacomethylomics, phenomics, phylome, physiogenomics, postgenomics, predictome, promoterome, proteomics, pseudogenome, secretome, regulome, resistome, ribonome, ribonomics, riboproteomics, saccharomics, secretome, somatonome, systeome, toxicomics, transcriptome, translome, secretome, unknome, vaccinome, variomics...*

WHAT IS BIOINFORMATICS?





AATGGCCAATTGATGACCAGAGATTTAGGCCAATTA
AATGTGAAATGGCCAATTGATGACCAGAGA



What is Bioinformatics?

- Development of methods & algorithms to organize, integrate, analyze and interpret biological and biomedical data
- Study of the inherent structure & flow of biological information
- Goals of bioinformatics:
 - Identify patterns
 - Classify
 - Make predictions
 - Create models
 - Better utilize existing knowledge

February 2001: Completion of the Draft Human Genome

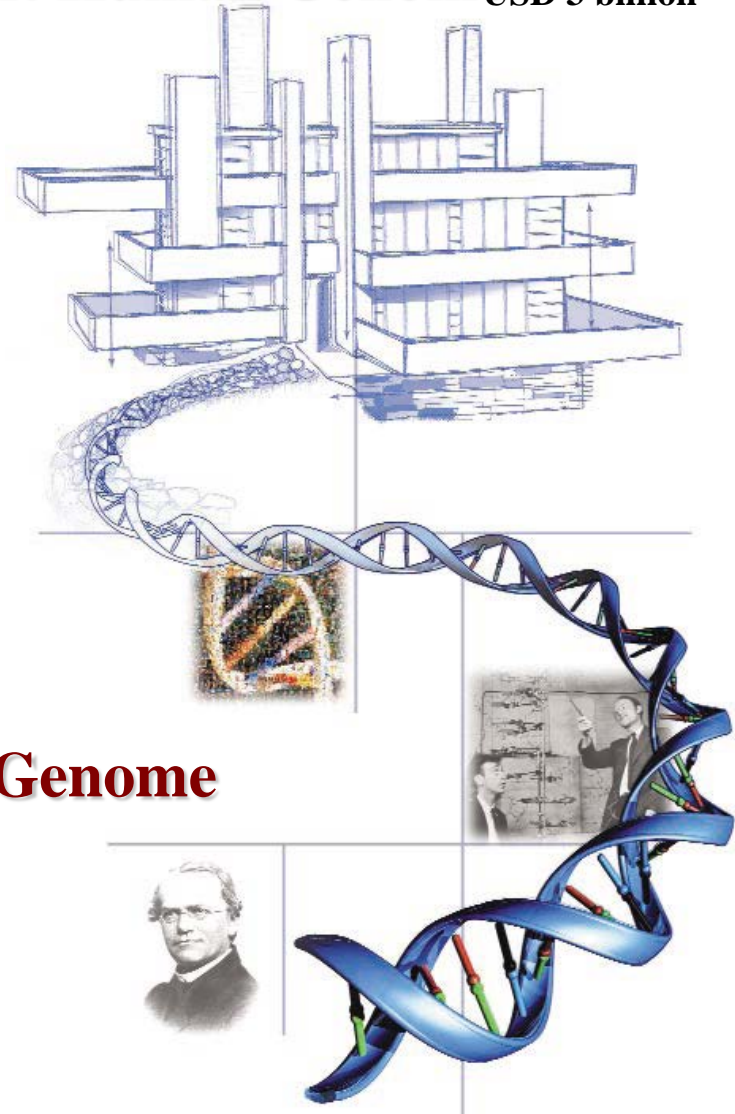
>10 years to finish
USD 3 billion



Science, 16 February 2001
Vol. 291, Pages 1145-1434



Nature, 15 February 2001
Vol. 409, Pages 813-960



April 2003: High-Resolution Human Genome

A vision for the future of genomics research

A blueprint for the genomic era.

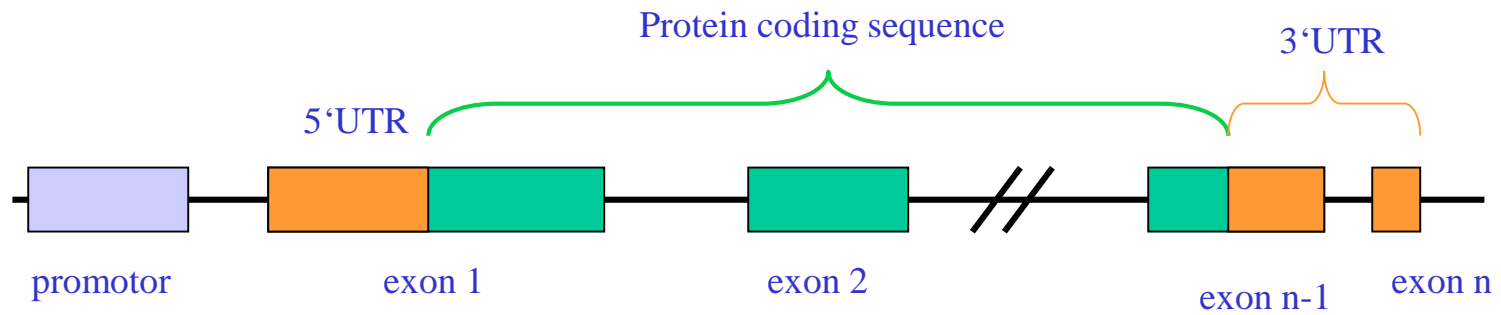
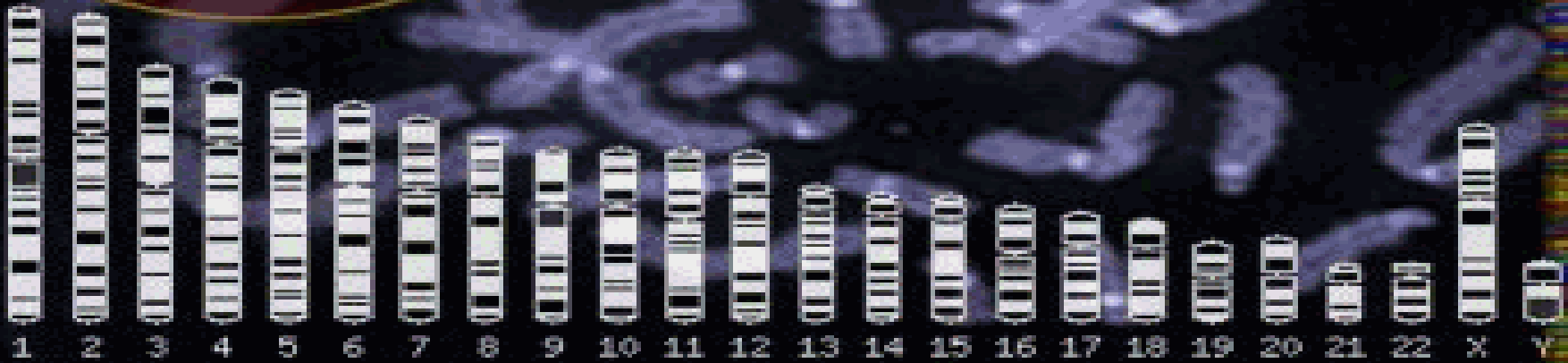
Francis S. Collins, Eric D. Green,
Alan E. Guttmacher and Mark S.
Guyer on behalf of the US National
Human Genome Research Institute*

50 Years of DNA: From Double Helix to Health
A Celebration of the Genome

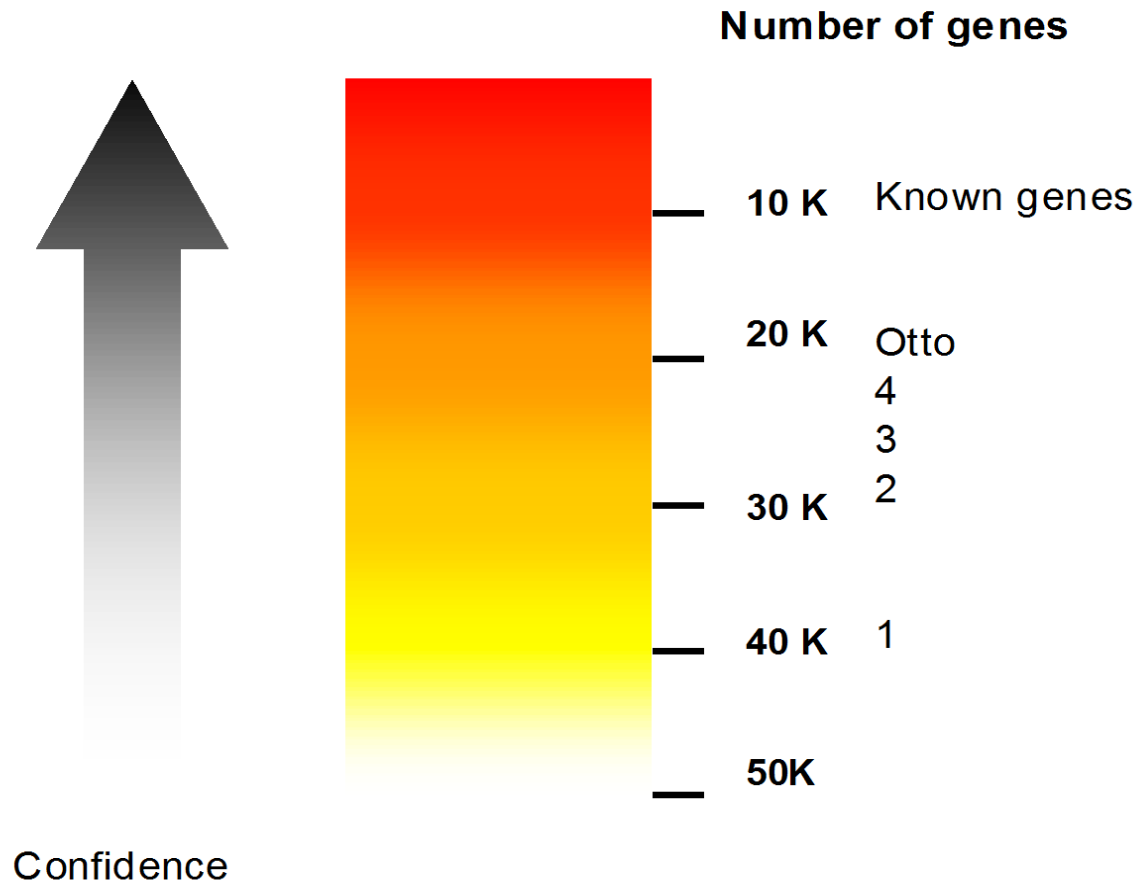
Nature, 23 April 2003
Vol. 422, Pages 1-13

Human Genome Project

3 billion basepairs

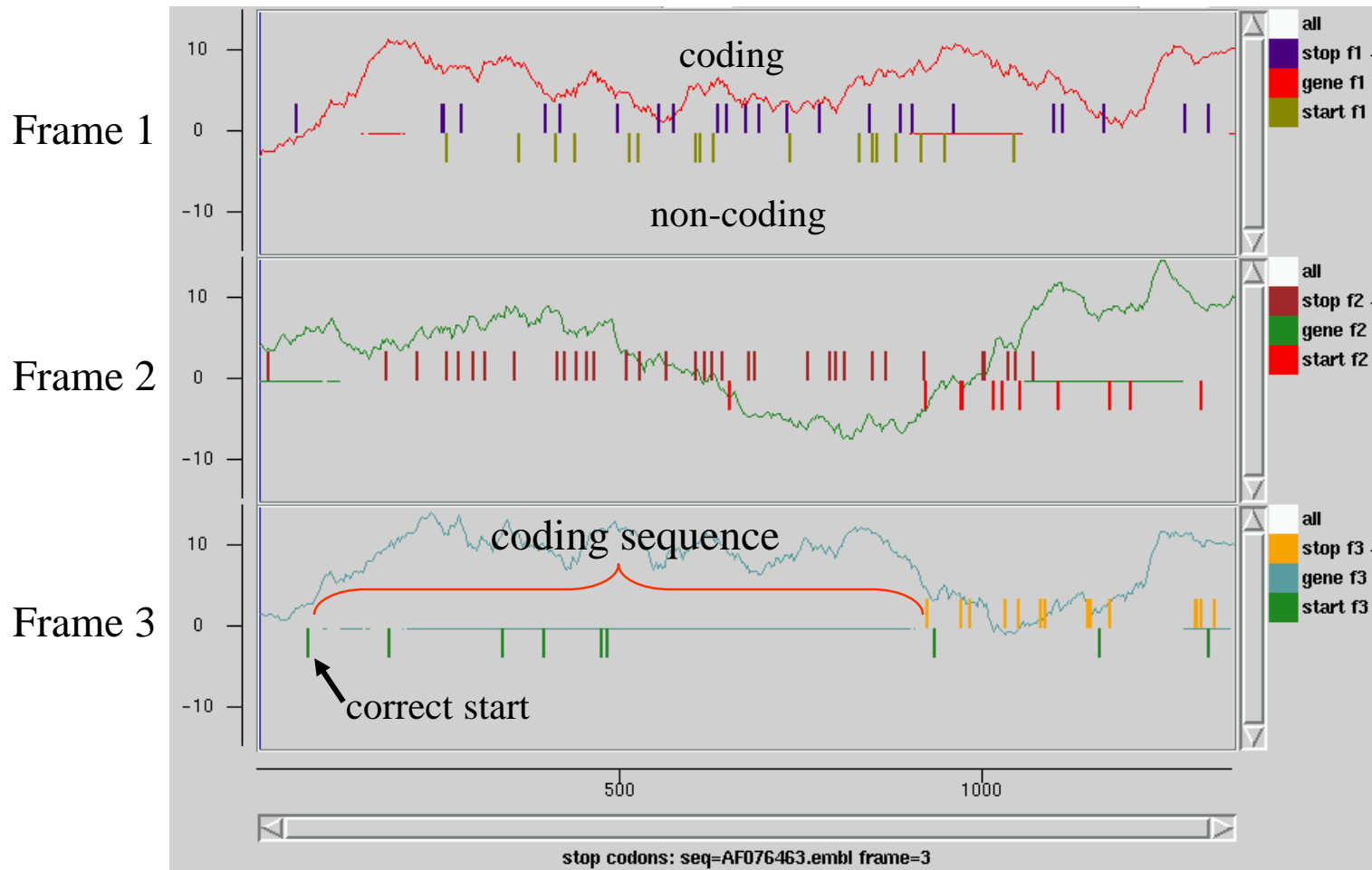


Gene Number in the Human Genome



Gene prediction

Codon usage (single exon)

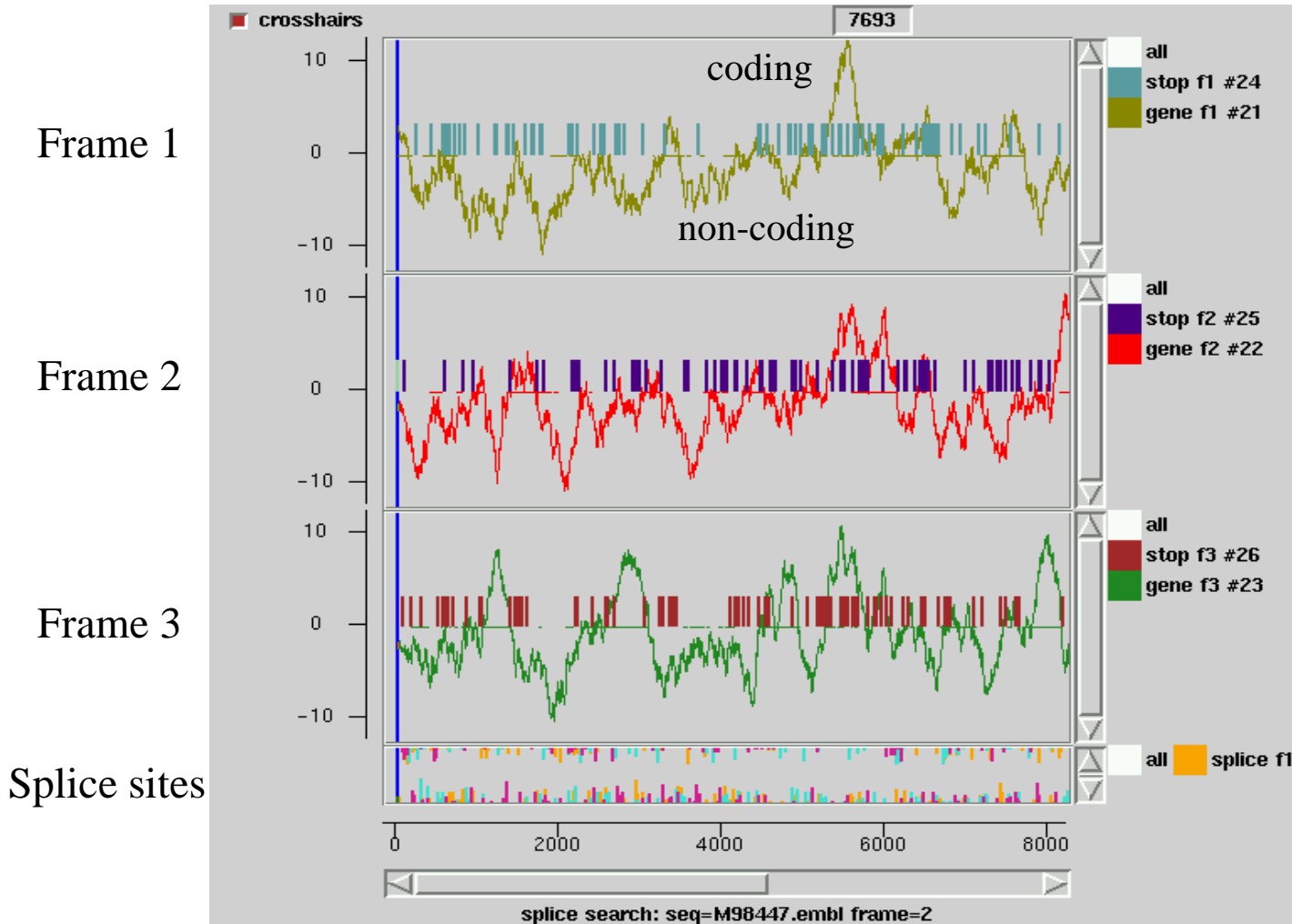


Gene prediction

Codon usage (multiple exons)

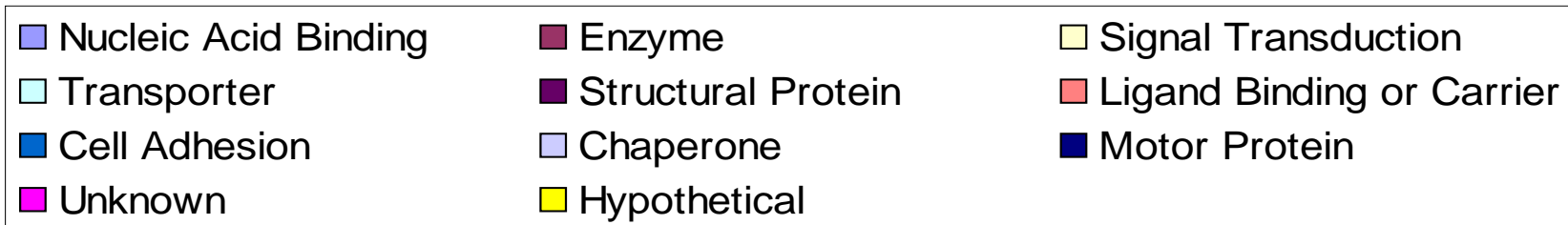
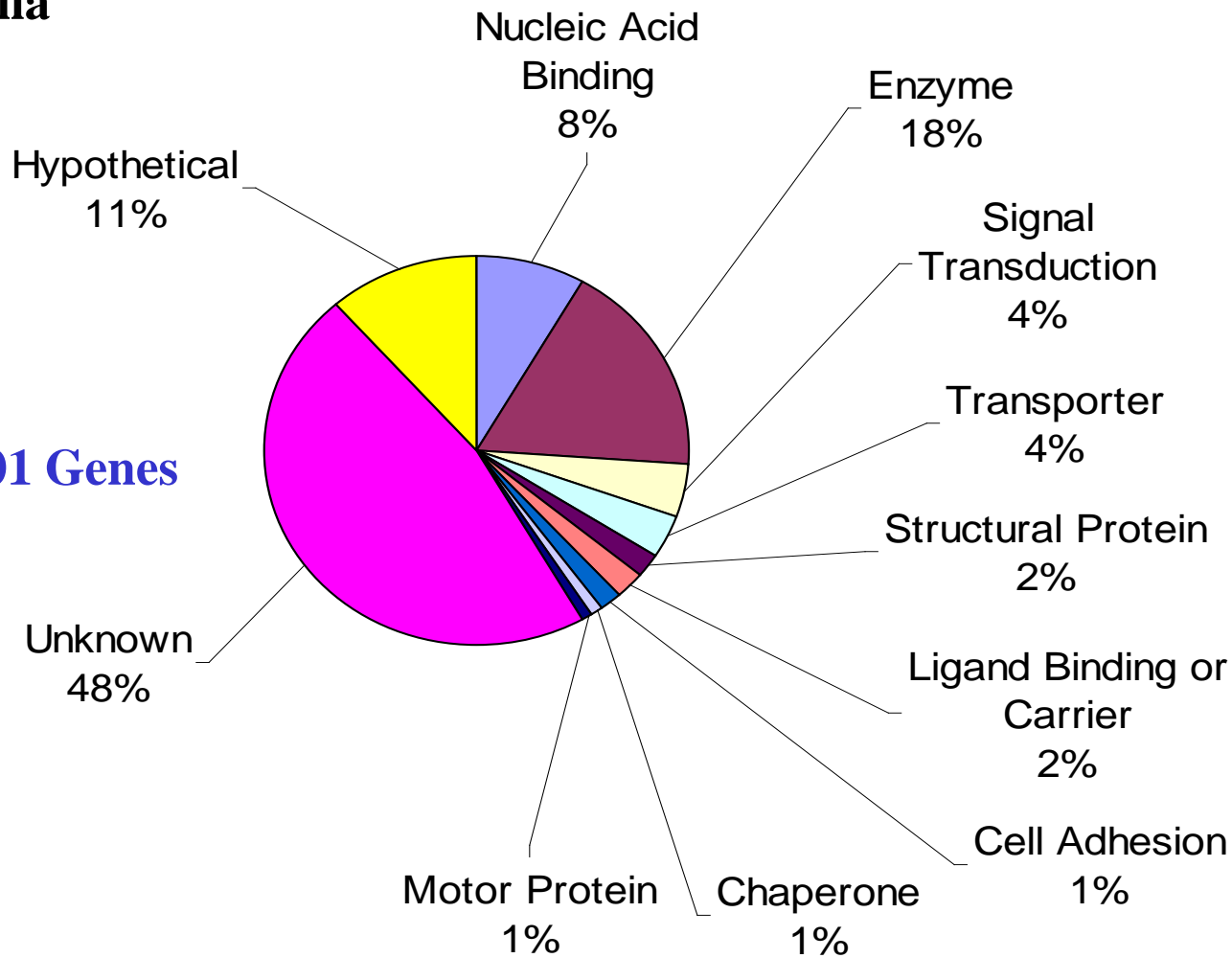
Exons:

208. .295
1029. .1349
1500. .1688
2686. .2934
3326. .3444
3573. .3680
4135. .4309
4708. .4846
4993. .5096
7301. .7389
7860. .8013
8124. .8405
8553. .8713
9089. .9225
13841. .14244

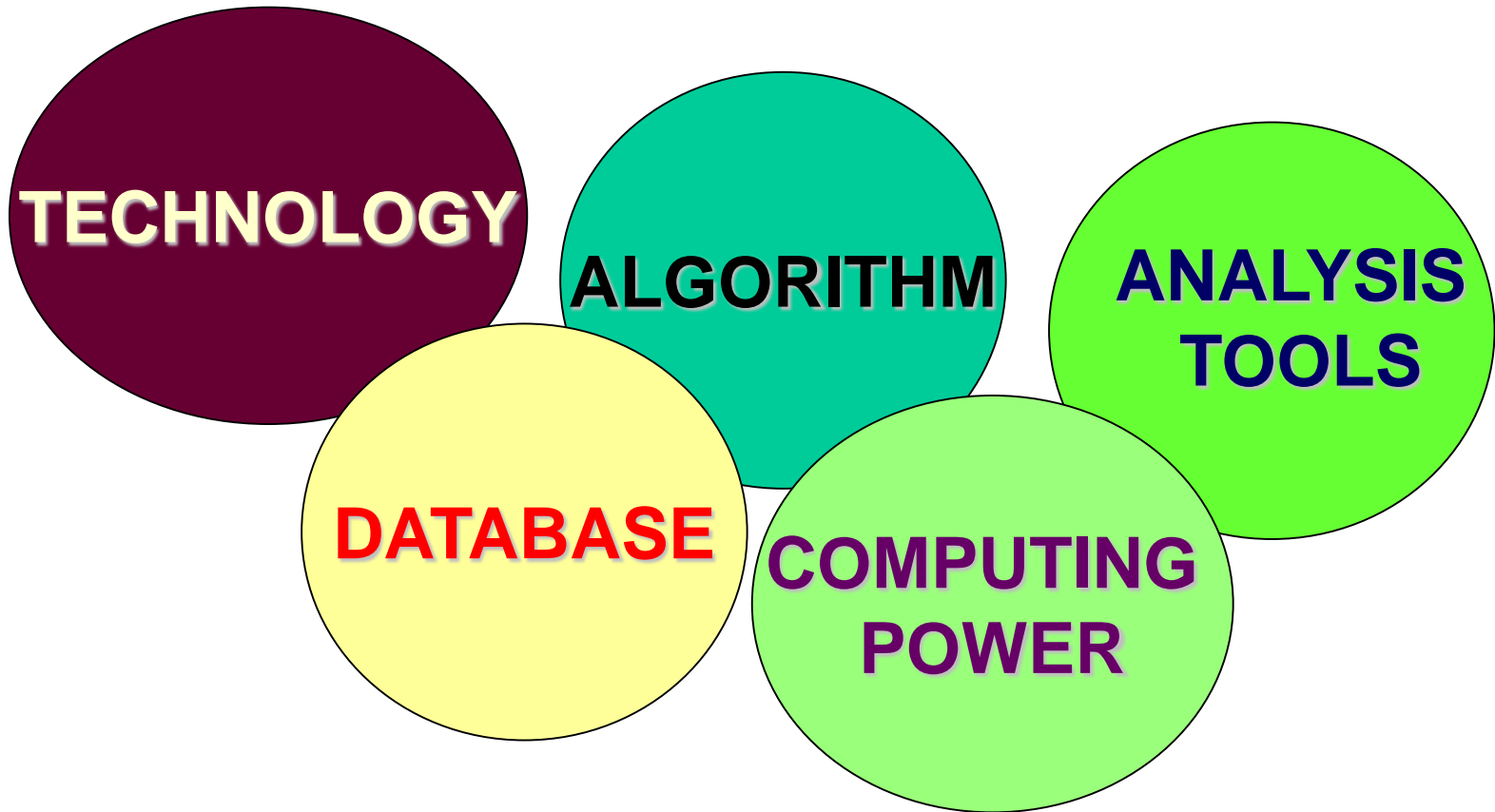


Drosophila

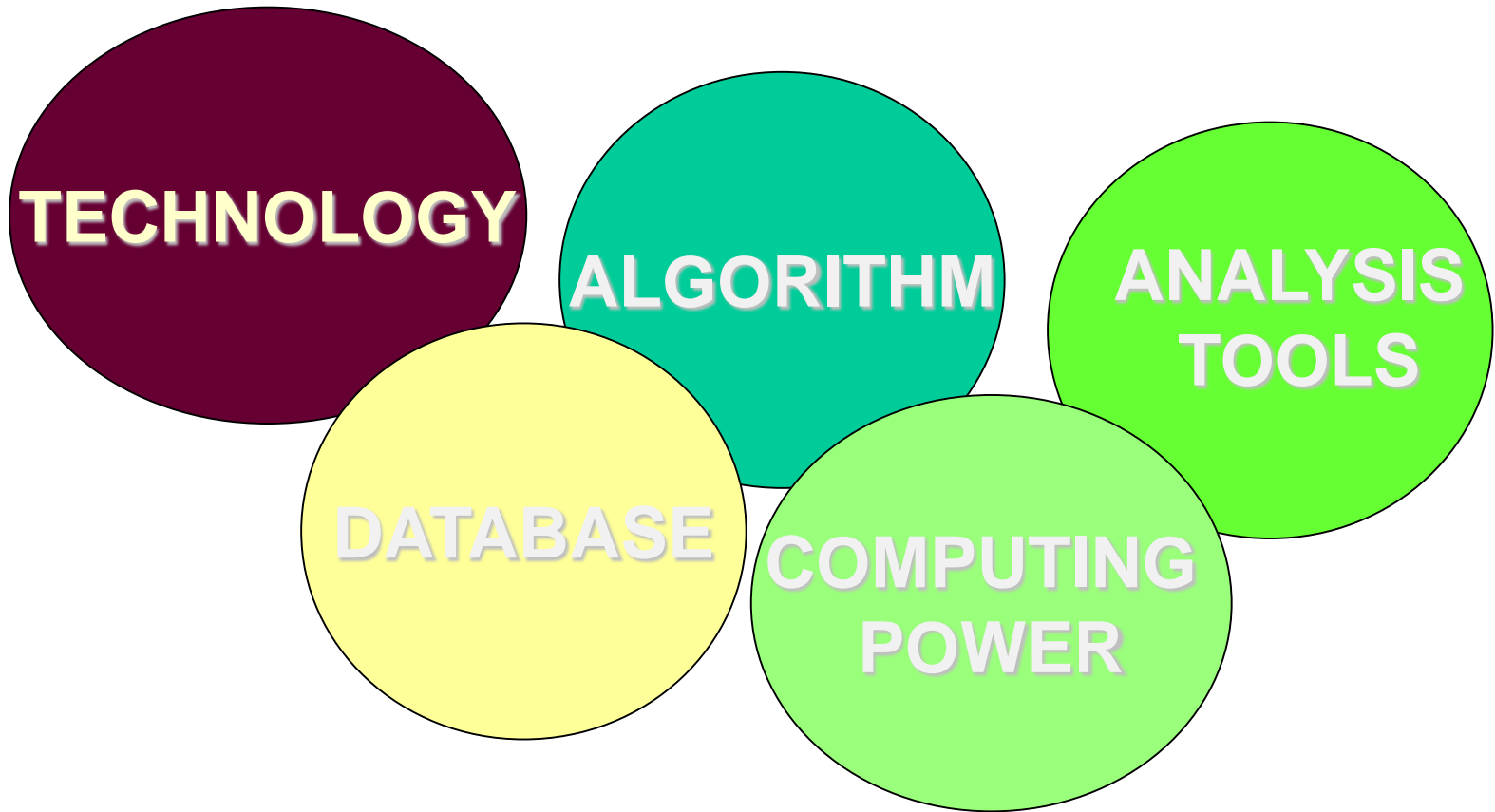
13,601 Genes



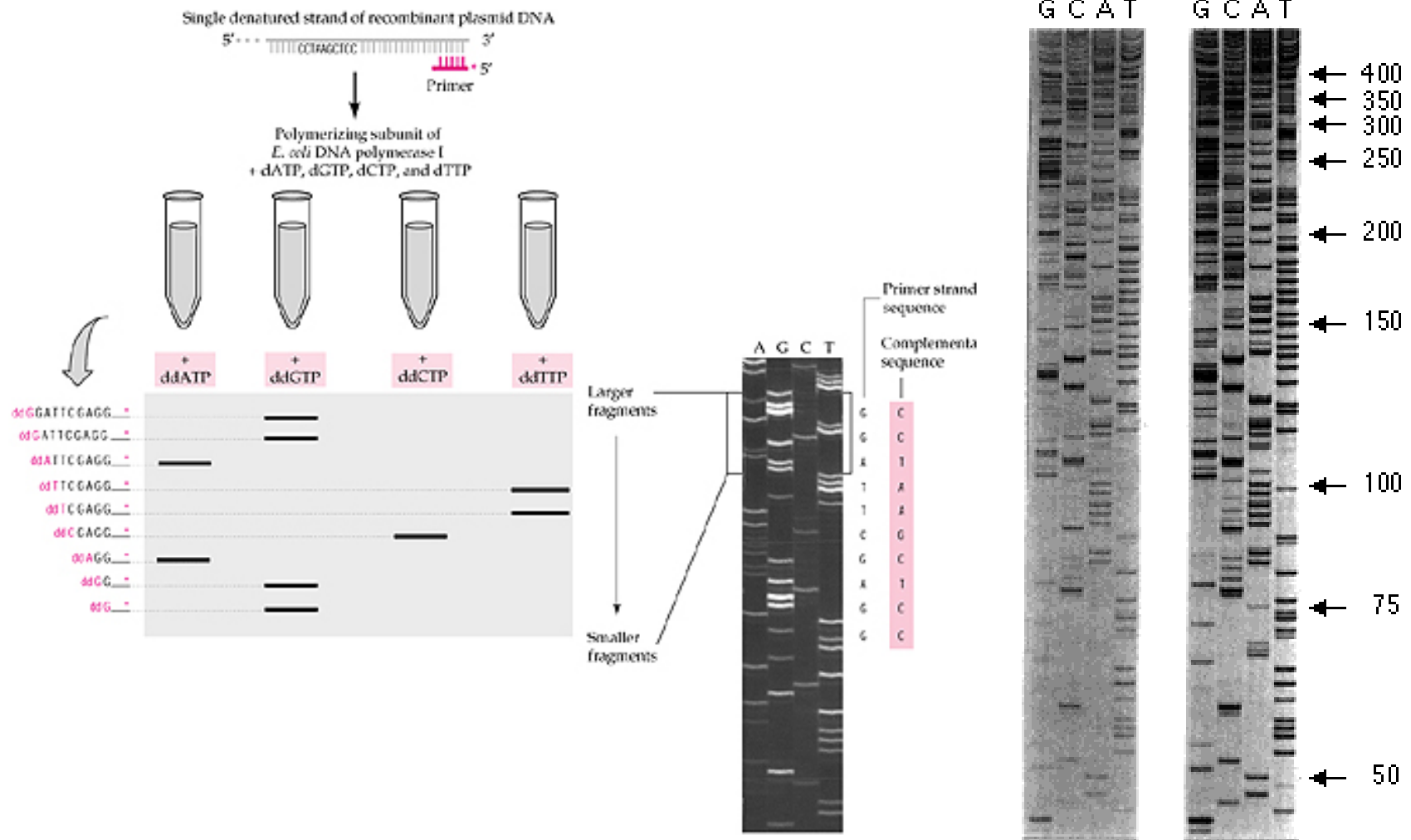
THE COMPONENTS OF BIOINFORMATICS



THE COMPONENTS OF BIOINFORMATICS

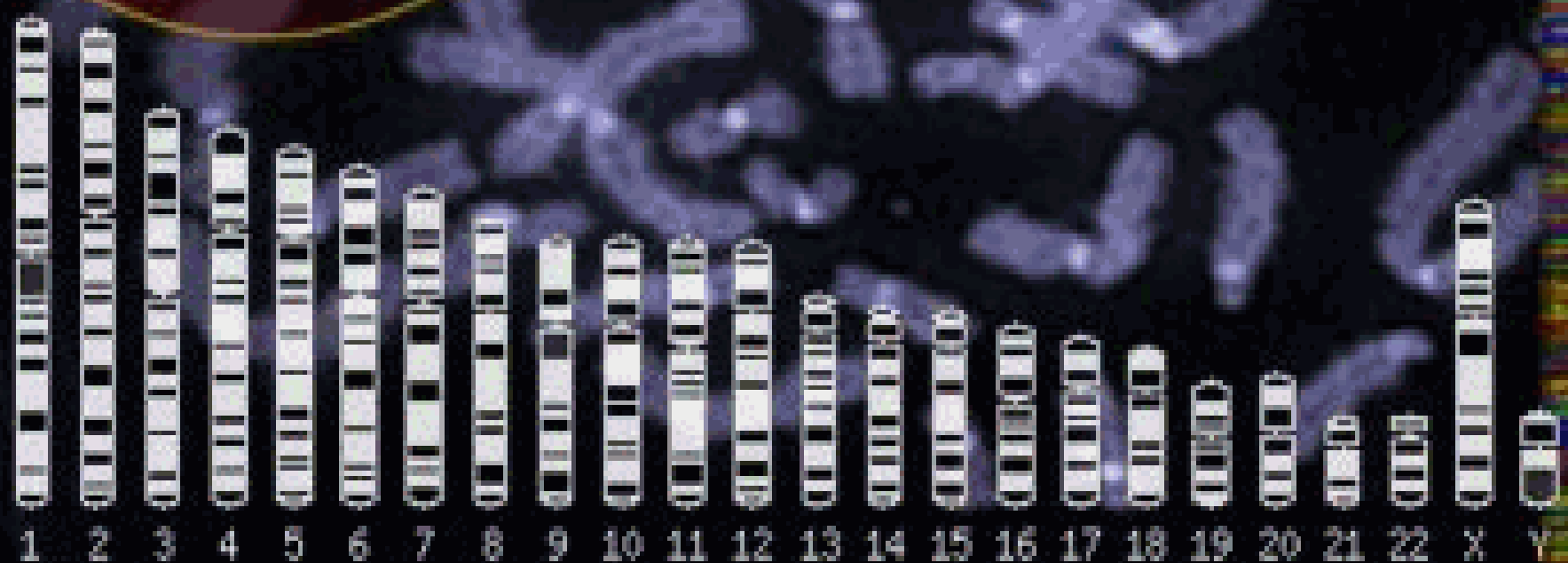


Sanger Dideoxy Sequencing

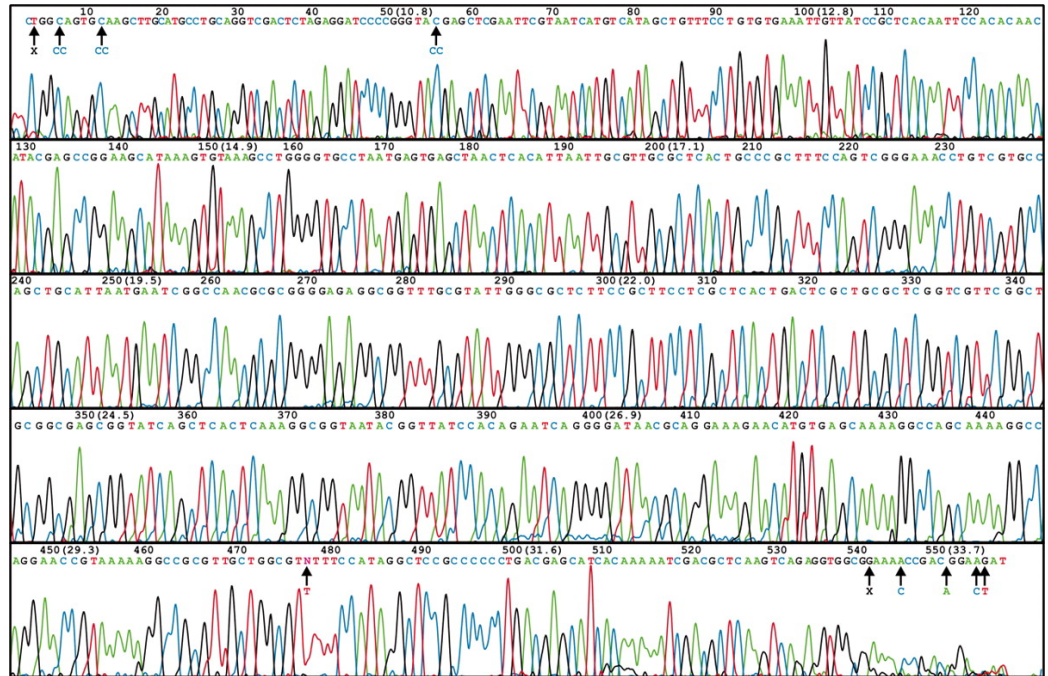


Human Genome Project

3 billion basepairs



ABI 3730 XL DNA Sequencer



96/384 DNA sequencing in 2 hrs, approximately 600-1000 readable bps per run.

1-4 MB bps/day

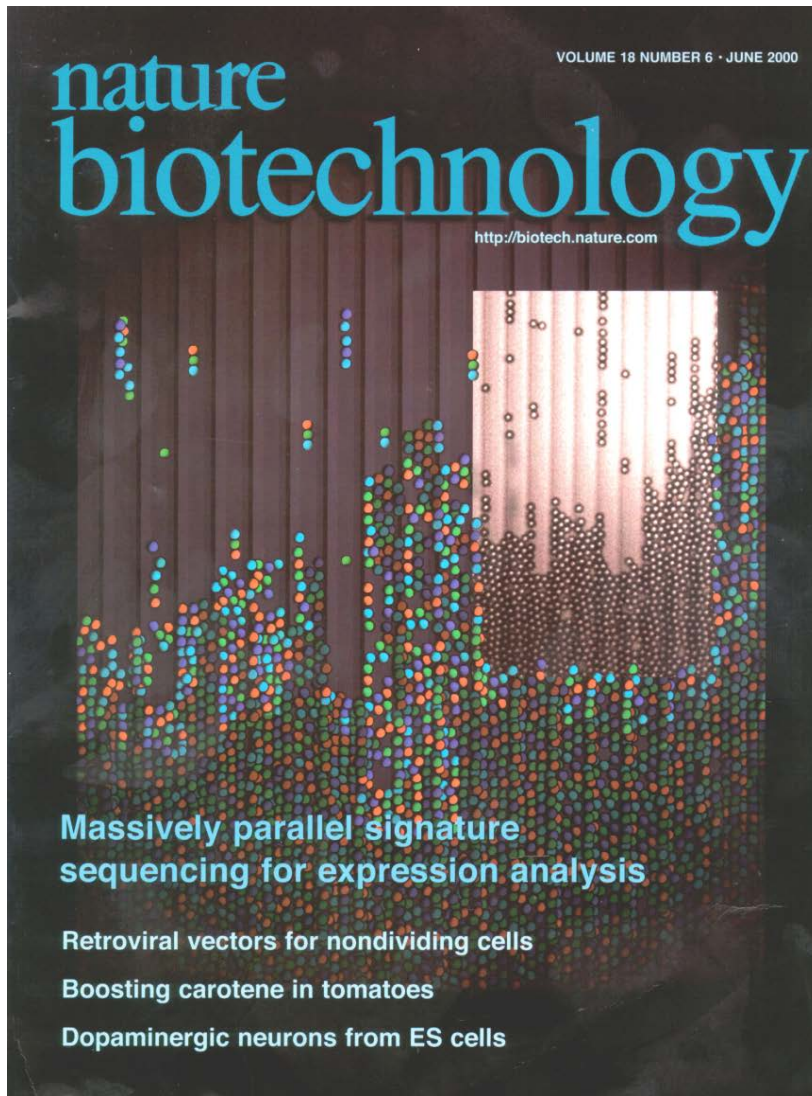
A human genome of 3GB need 750 days to finish

Next Generation Sequencing (NGS) Technology

nature
biotechnology

VOLUME 18 NUMBER 6 • JUNE 2000

http://biotech.nature.com



Massively parallel signature sequencing for expression analysis

Retroviral vectors for nondividing cells

Boosting carotene in tomatoes

Dopaminergic neurons from ES cells

ISSN 1088-9051

September 2008

GENOME
RESEARCH

Volume 18 Number 9



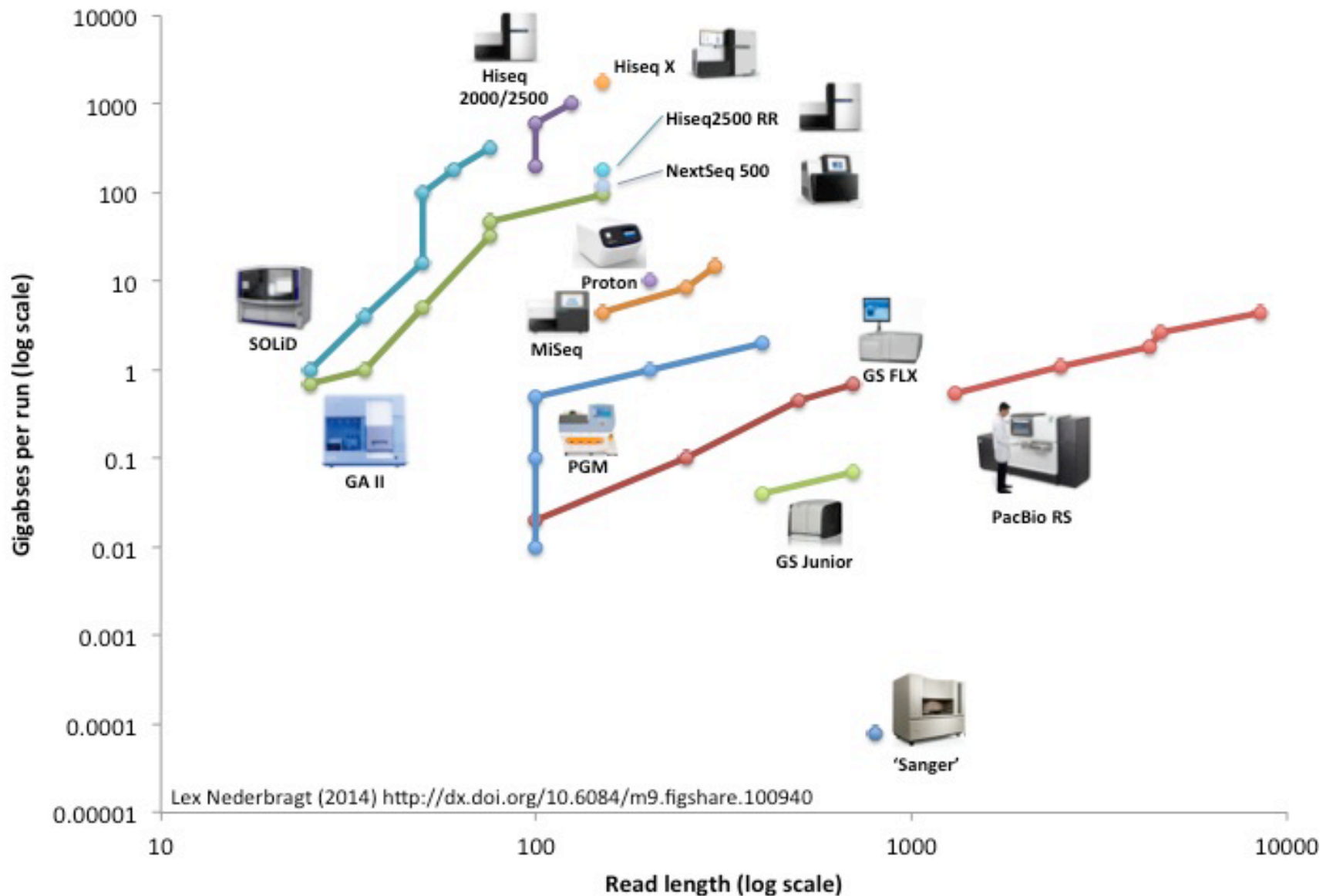
5095/15024 5050/5049 5075/5074 5190/5099 5129/15124

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AA TTTGATTACATTTTTTATTGGCGGTAGCTATT
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AAAAAT

Non-coding RNA in Stem Cell Differentiation • Human Tissue-Specific Differentially Methylated Regions • Very Small Mobile Elements • Dachshund Cone-Rod Dystrophy • EagleView Genome Assembly Viewer

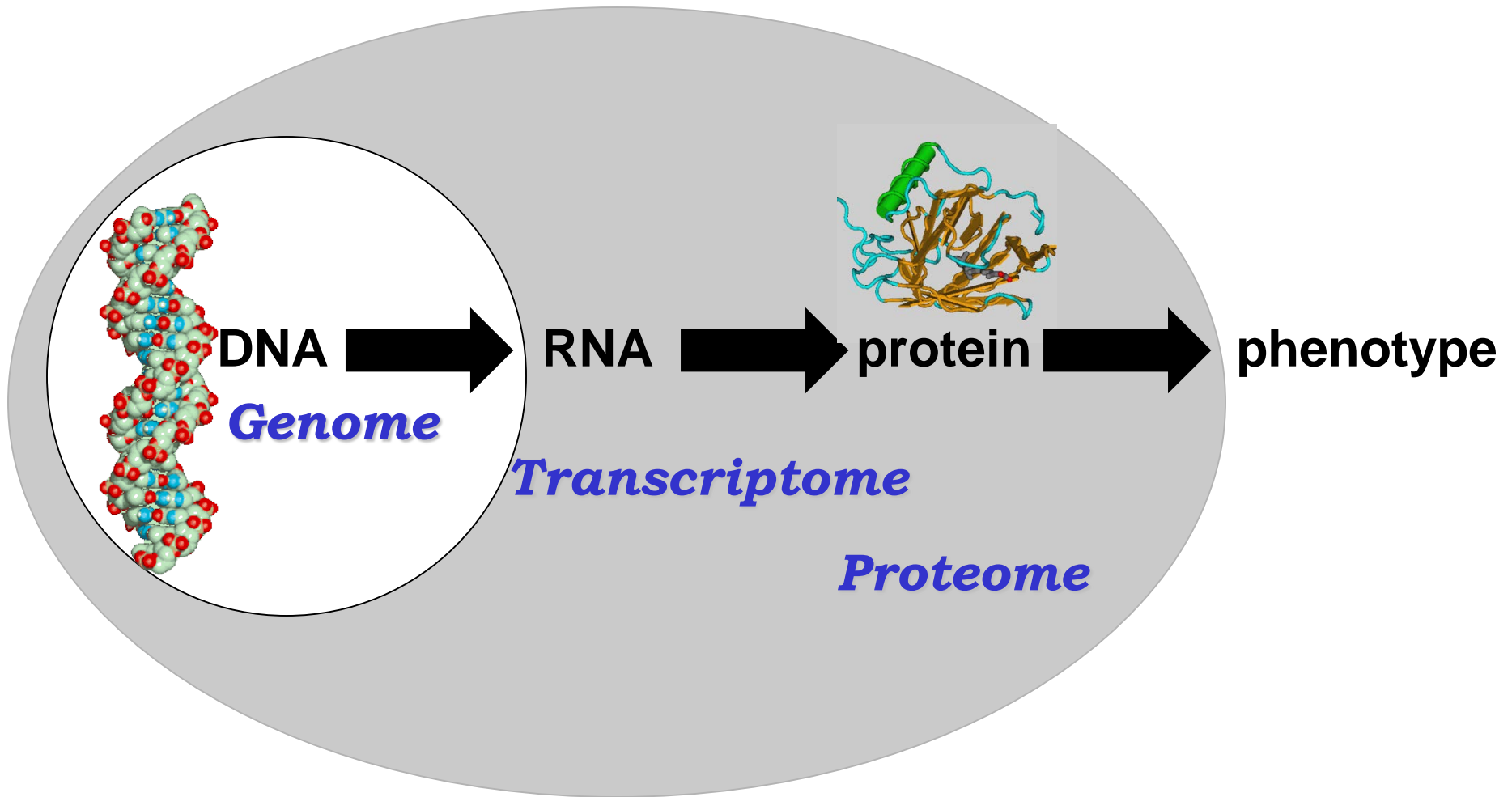
Cold Spring Harbor Laboratory Press

Throughput of NGS machines (2014)

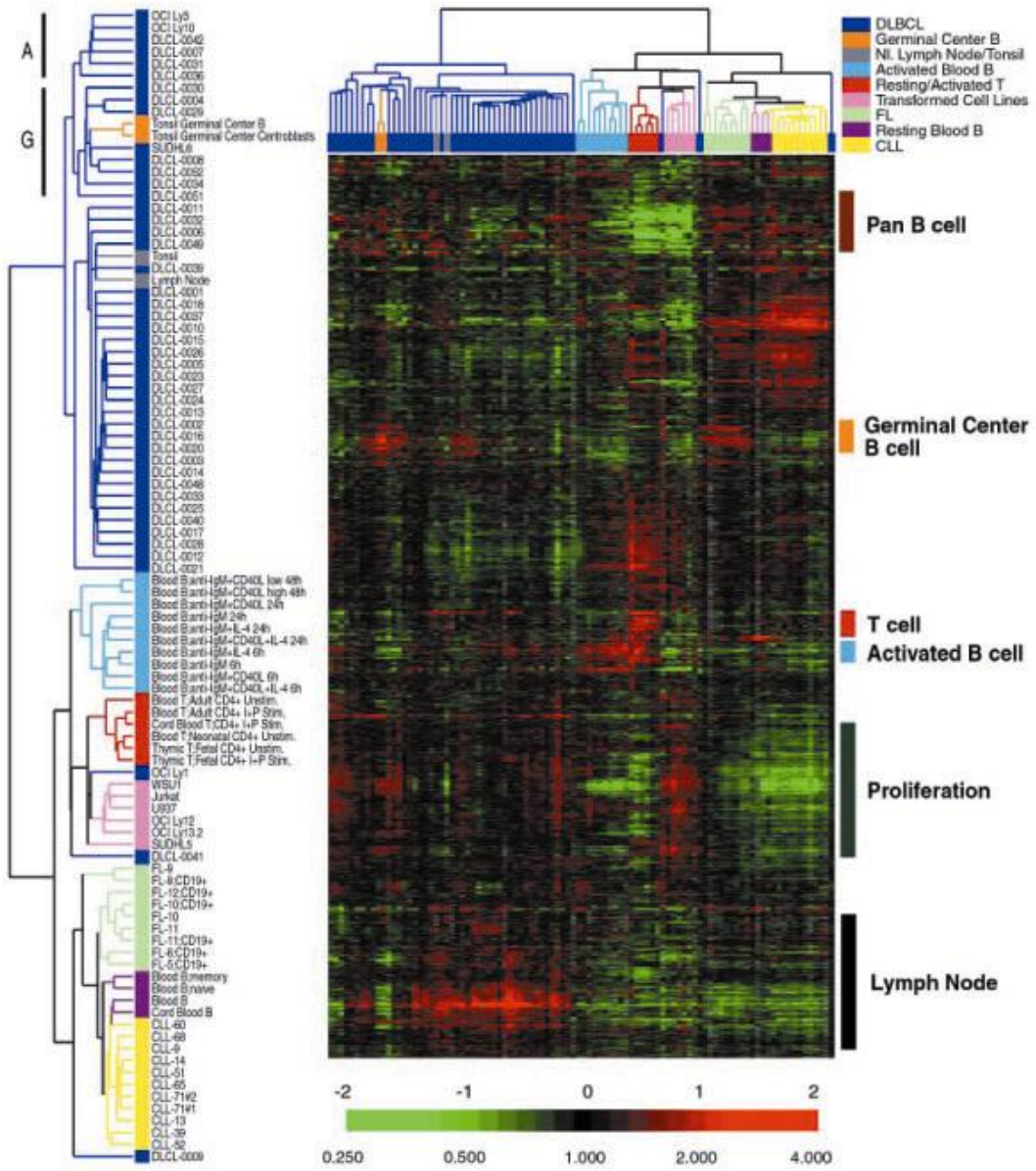


Applications on Biomedical Sciences

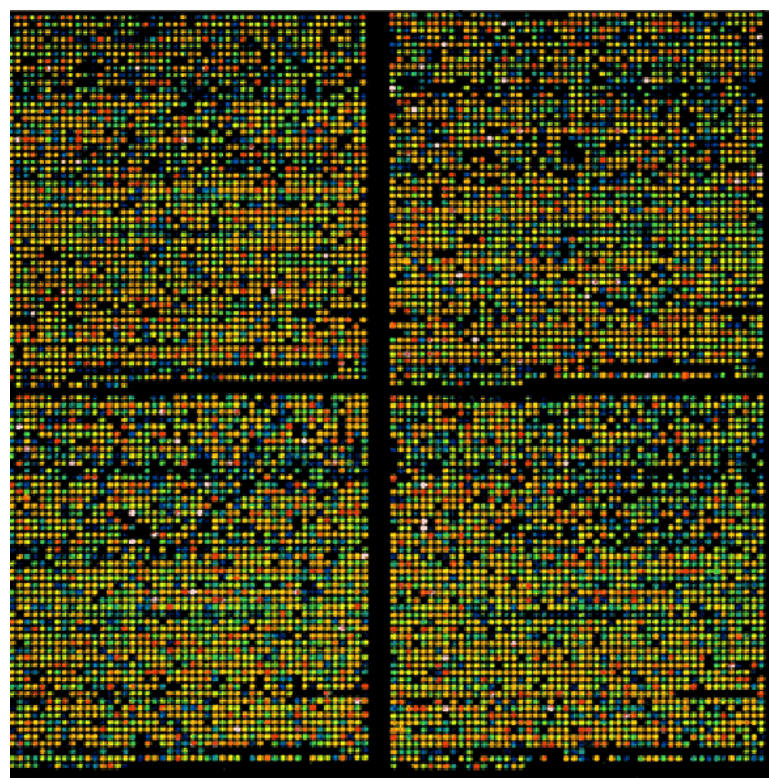
Category	Examples of applications
Complete genome resequencing	Comprehensive polymorphism and mutation discovery in individual human genomes
Reduced representation sequencing	Large-scale polymorphism discovery
Targeted genomic resequencing	Targeted polymorphism and mutation discovery
Paired end sequencing	Discovery of inherited and acquired structural variation
Metagenomic sequencing	Discovery of infectious and commensal flora
Transcriptome sequencing	Quantification of gene expression and alternative splicing; transcript annotation; discovery of transcribed SNPs or somatic mutations
Small RNA sequencing	microRNA profiling
Sequencing of bisulfite-treated DNA	Determining patterns of cytosine methylation in genomic DNA
Chromatin immunoprecipitation–sequencing (ChIP-Seq)	Genome-wide mapping of protein-DNA interactions
Nuclease fragmentation and sequencing	Nucleosome positioning
Molecular barcoding	Multiplex sequencing of samples from multiple individuals



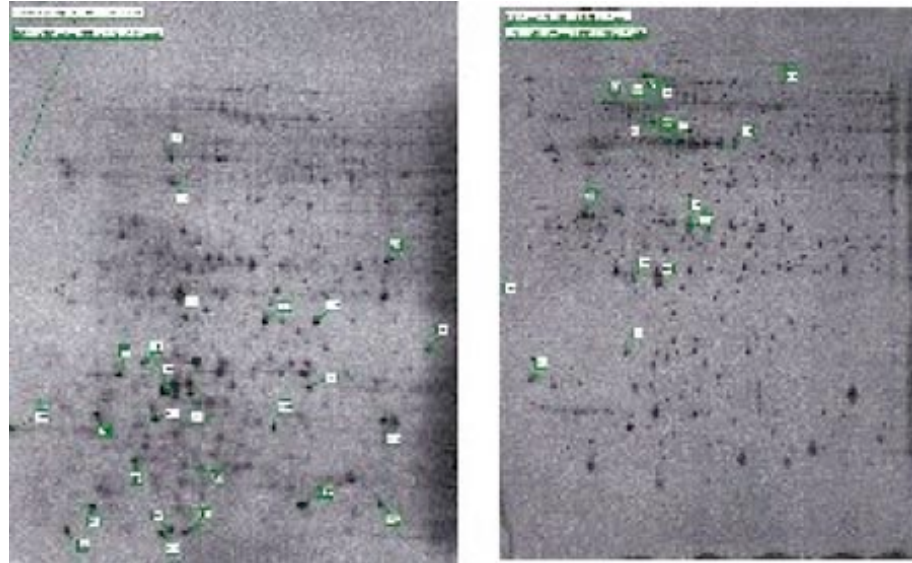
Microarray



20,000-40,000
Clones
per
slide



Proteomics

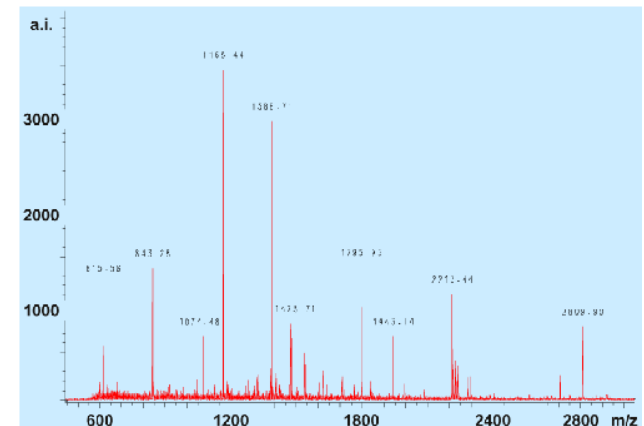


2 Dimensional Electrophoresis gels, differences that are characteristics of the individual starting states recognized by comparison of two protein pattern

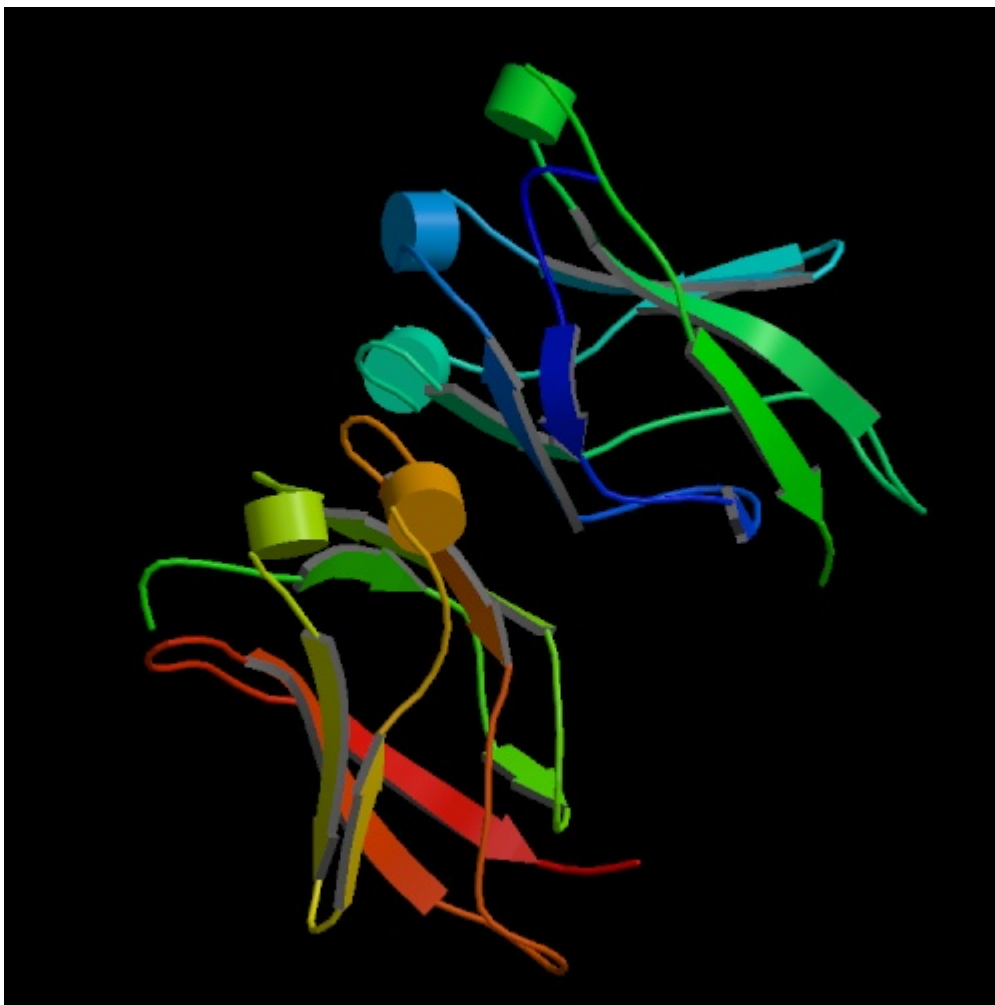
6,000
protein spots
per gel



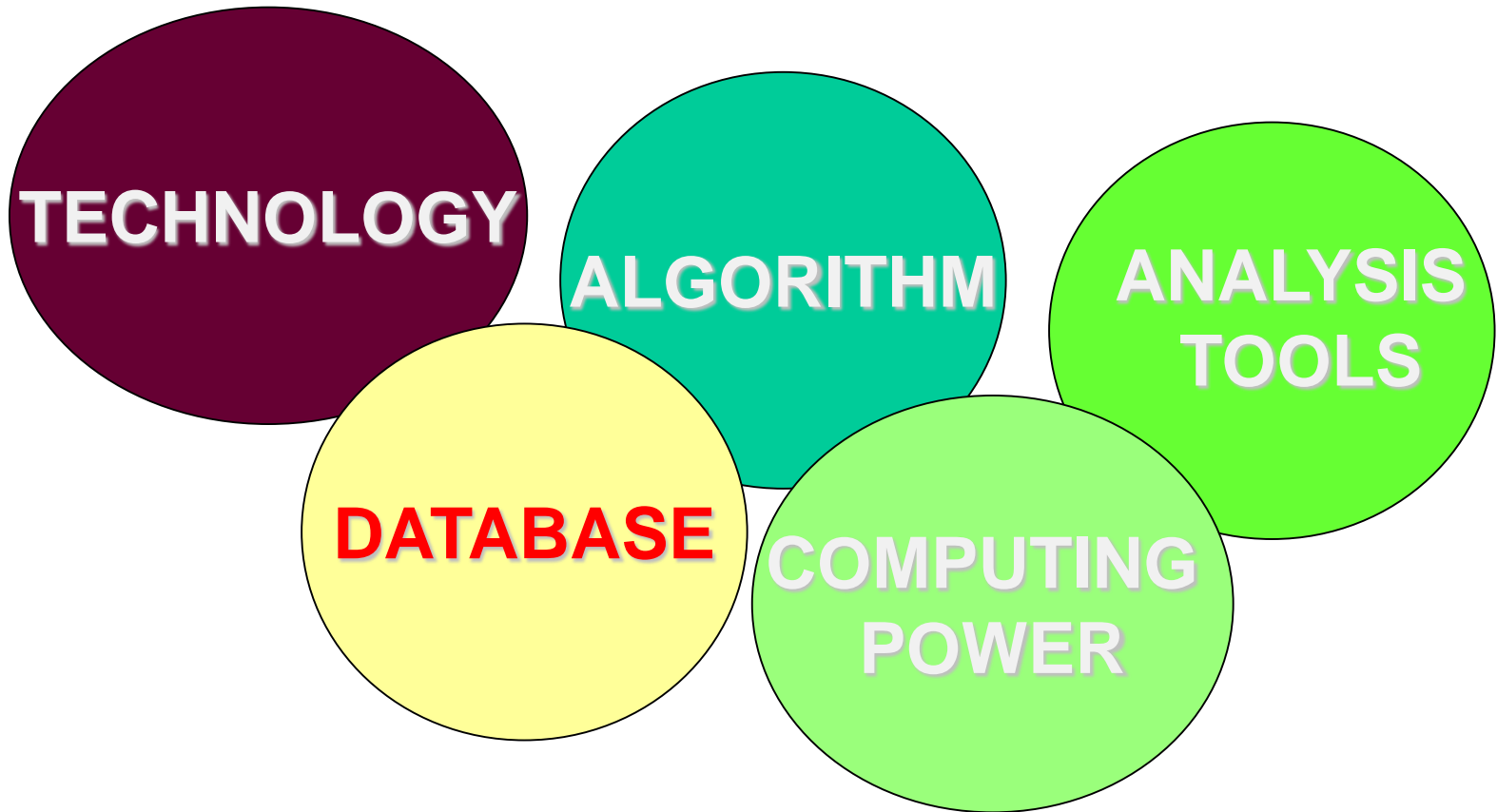
MALDI-MS peptide mass fingerprint, for identification of proteins separated by 2D electrophoresis



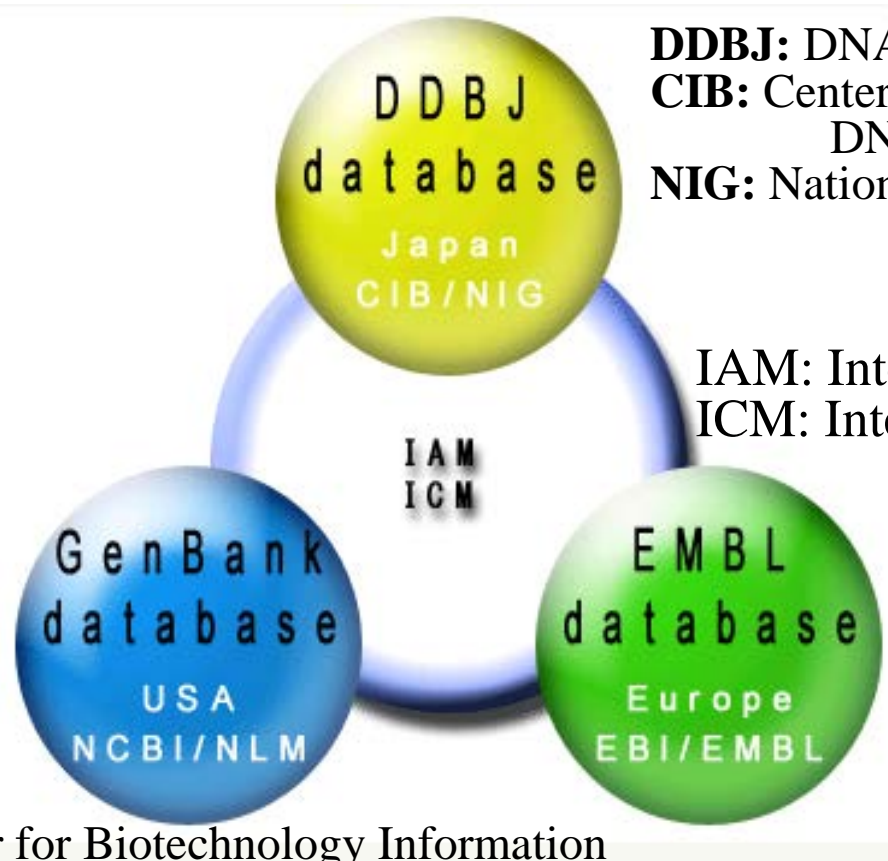
3D Modeling



THE COMPONENTS OF BIOINFORMATICS



GenBank/EMBL/DDBJ International Nucleotide Sequence Database



DDBJ: DNA Data Bank of Japan

CIB: Center for Information Biology and
DNA Data Bank of Japan

NIG: National Institute of Genetics

IAM: International Advisory Meeting

ICM: International Collaborative Meeting

EMBL:

European Molecular Biology
Laboratory

EBI:

European Bioinformatics
Institute

NCBI:

National Center for Biotechnology Information

NLM:

National Library of Medicine

GenBank

Recent years have seen an explosive growth in biological data. Large sequencing projects are producing increasing quantities of nucleotide sequences. The contents of nucleotide databases are doubling in size approximately every 14 months. The latest release of GenBank exceeded 165 billion base pairs. Not only the size of sequence data is rapidly increasing, but also the number of characterized genes from many organisms and protein structures doubles about every two years. To cope with this great quantity of data, a new scientific discipline has emerged: **bioinformatics, biocomputing or computational biology**

ENTRIES

20614460
9724856
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744380
1332169
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SPECIES

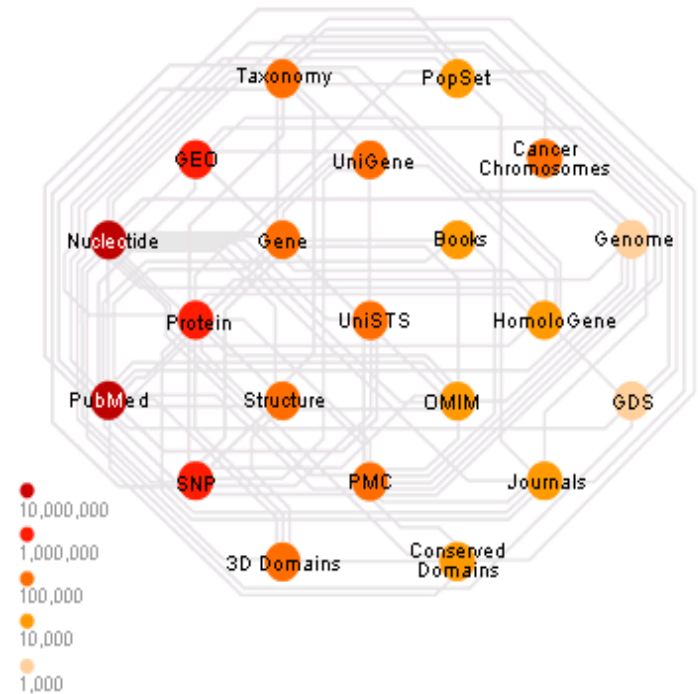
Homo sapiens
Mus musculus
Rattus norvegicus
Bos taurus
Zea mays
Sus scrofa
Danio rerio
Triticum aestivum
Solanum lycopersicum
Hordeum vulgare subsp. vulgare
Strongylocentrotus purpuratus
Macaca mulatta
Oryza sativa Japonica Group
Xenopus (Silurana) tropicalis
Nicotiana tabacum
Arabidopsis thaliana
Drosophila melanogaster
Vitis vinifera
Glycine max
Pan troglodytes

Genetic Sequence Data Bank

Aug 15 2014,

Release 203.0

165,722,980,375 bases, from
174,108,750 reported sequence



SITE MAP

 Alphabetical List
 Resource Guide

About NCBI

 An introduction to
 NCBI

GenBank

 Sequence
 submission support
 and software

**Literature
 databases**

 PubMed, OMIM,
 Books, and PubMed
 Central

**Molecular
 databases**

 Sequences,
 structures, and
 taxonomy

Genomic biology

 The human genome,
 whole genomes,
 and related
 resources

Tools

Data mining

**Research at
 NCBI**

 People, projects,
 and seminars

**Software
 engineering**
What does NCBI do?

Established in 1988 as a national resource for molecular biology information, NCBI creates public databases, conducts research in computational biology, develops software tools for analyzing genome data, and disseminates biomedical information - all for the better understanding of molecular processes affecting human health and disease. [More about NCBI...](#)

NLM/NCBI H1N1 Flu Resources

- [Newest H1N1 influenza sequences](#)
- [Submit flu sequences to GenBank](#)
- [Latest H1N1 citations in PubMed](#)
- [MedlinePlus \(consumer health information\)](#)
- [Enviro-Health links](#)

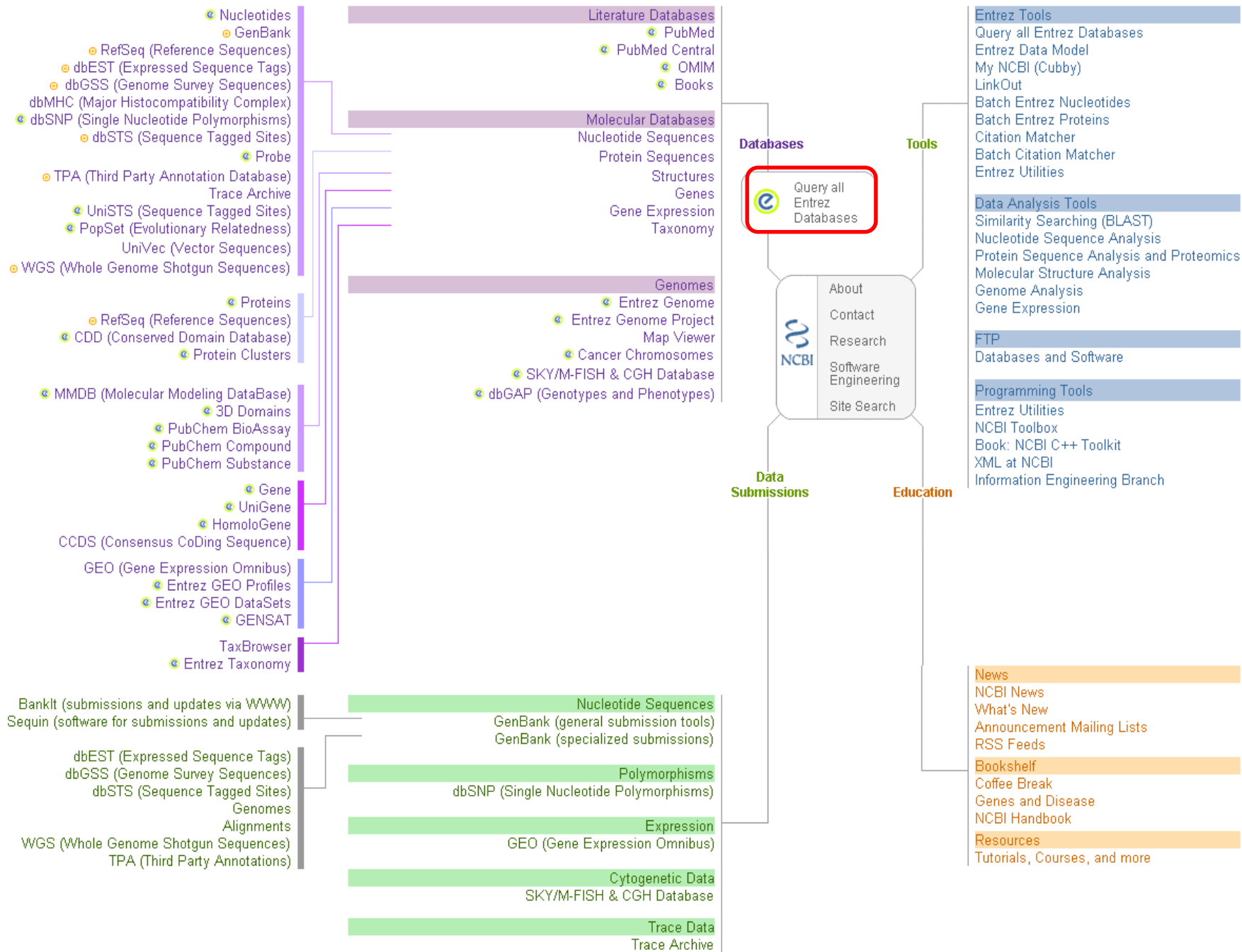

Peptidome

The new [Peptidome](#) database archives and distributes tandem mass spectrometry peptide and protein identification data. Read [more](#) about Peptidome data, browsing, and submissions.

Hot Spots

- ▶ Clusters of orthologous groups
- ▶ Coffee Break, Genes & Disease, NCBI Handbook
- ▶ Electronic PCR
- ▶ Entrez Home
- ▶ Entrez Tools
- ▶ Gene expression omnibus (GEO)
- ▶ Human genome resources
- ▶ Influenza Virus Resource
- ▶ Map Viewer
- ▶ dbMHC
- ▶ Mouse genome resources
- ▶ My NCBI
- ▶ ORF finder
- ▶ Rat genome resources
- ▶ Reference sequence project






















Search across databases

[Help](#)

Welcome to the Entrez cross-database search page

 PubMed: biomedical literature citations and abstracts 	 Books: online books 
 PubMed Central: free, full text journal articles 	 OMIM: online Mendelian Inheritance in Man 
 Site Search: NCBI web and FTP sites 	 OMIA: online Mendelian Inheritance in Animals 

 CoreNucleotide: Core subset of nucleotide sequence records 	 dbGaP: genotype and phenotype 
 EST: Expressed Sequence Tag records 	 UniGene: gene-oriented clusters of transcript sequences 
 GSS: Genome Survey Sequence records 	 CDD: conserved protein domain database 
 Protein: sequence database 	 3D Domains: domains from Entrez Structure 
 Genome: whole genome sequences 	 UniSTS: markers and mapping data 
 Structure: three-dimensional macromolecular structures 	 PopSet: population study data sets 
 Taxonomy: organisms in GenBank 	 GEO Profiles: expression and molecular abundance profiles 
 SNP: single nucleotide polymorphism 	 GEO DataSets: experimental sets of GEO data 
 Gene: gene-centered information 	 Cancer Chromosomes: cytogenetic databases 
 HomoloGene: eukaryotic homology groups 	 PubChem BioAssay: bioactivity screens of chemical substances 
 GENSAT: gene expression atlas of mouse central nervous system 	 PubChem Compound: unique small molecule chemical structures 
 Probe: sequence-specific reagents 	 PubChem Substance: deposited chemical substance records 
 Genome Project: genome project information 	 Protein Clusters: a collection of related protein sequences 

 Journals: detailed information about the journals indexed in PubMed and other Entrez databases 	 MeSH: detailed information about NLM's controlled vocabulary 
 NLM Catalog: catalog of books, journals, and audiovisuals in the NLM collections 	

Search across databases [Help](#)

- Result counts displayed in gray indicate one or more terms not found

50967		PubMed: biomedical literature citations and abstracts		820		Books: online books	
26807		PubMed Central: free, full text journal articles		450		OMIM: online Mendelian Inheritance in Man	
16		Site Search: NCBI web and FTP sites		1		OMIA: online Mendelian Inheritance in Animals	
10064		Nucleotide: Core subset of nucleotide sequence records		none		dbGaP: genotype and phenotype	
760		EST: Expressed Sequence Tag records		410		UniGene: gene-oriented clusters of transcript sequences	
35		GSS: Genome Survey Sequence records		40		CDD: conserved protein domain database	
5655		Protein: sequence database		618		3D Domains: domains from Entrez Structure	
229		Genome: whole genome sequences		587		UniSTS: markers and mapping data	
168		Structure: three-dimensional macromolecular structures		46		PopSet: population study data sets	
none		Taxonomy: organisms in GenBank		366385		GEO Profiles: expression and molecular abundance profiles	
750		SNP: single nucleotide polymorphism		250		GEO DataSets: experimental sets of GEO data	
2301		Gene: gene-centered information		302		Cancer Chromosomes: cytogenetic databases	
none		SRA: Short Read Archive		29		PubChem BioAssay: bioactivity screens of chemical substances	
352		BioSystems: Pathways and systems of interacting molecules		4		PubChem Compound: unique small molecule chemical structures	
32		HomoloGene: eukaryotic homology groups		156		PubChem Substance: deposited chemical substance records	
13		GENSAT: gene expression atlas of mouse central nervous system		23		Protein Clusters: a collection of related protein sequences	
2357		Probe: sequence-specific reagents		none		Peptidome: MS/MS proteomic experiments	
none		Genome Project: genome project information					
none		Journals: detailed information about the journals indexed in PubMed and other Entrez databases		142		MeSH: detailed information about NLM's controlled vocabulary	
65		NLM Catalog: catalog of books, journals, and audiovisuals in the NLM collections					



Data Resources & Tools

- **EMBL-BANK**
- **UniProt**
- **Gene Expression**
- **Ensembl**
- **InterPro**
- **PDBe**
- Genomes
- Nucleotide Sequences
- Protein Sequences
- Macromolecular Structures
- Small Molecules
- Gene Expression
- Molecular Interactions
- Reactions & Pathways
- Protein Families
- Enzymes
- Literature
- Taxonomy
- Ontologies
- Patent Resources
- Sequence Similarity & Analysis
- Pattern & Motif Searches
- Structure Analysis
- Text Mining
- Downloads
- Web Services



European Bioinformatics Institute

About the EBI

- **Research**
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- **Industry Support**
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- **EBI Funders**
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- People
- Events at the EBI
- Genome Campus Events
- How to Find us

EBI Hosted Project Websites

- 1000 Genomes
- BioCatalogue
- BioSapiens
- E-MeP
- EGA
- ELIXIR
- EMBRACE
- EMERALD
- ENFIN
- FELICS
- IMPACT
- INSDC
- LRG
- SPINE
- SYMBIOmatics

Latest News



UK leads European research programme with £10M investment in bioscience data handling capacity

25 August 2009

The UK has made its first substantial commitment to a major emerging pan-European science project with a £10M investment by the Biotechnology and Biological Sciences Research Council (BBSRC). BBSRC has awarded funding to the European Molecular Biology Laboratory's European Bioinformatics Institute to permit a dramatic increase in the institute's data storage and handling capacity... more

Events

- Next Open Day: 3 November 2009
Registration deadline: 12 October 2009
- Small Molecule Bioactivity Resources At The EBI
Registration deadline: 6 November 2009

Research Highlights

MCSC Consortium determines thousandth protein structure

17 July 2009

For over a decade researchers at the consortium institutes, including the EBI, have been dissecting the structure of important proteins, including those of dangerous human pathogens. By understanding the structure of proteins, scientists can design drugs to prevent infection and treat disease. All protein structures are stored in the Protein Data Bank and today the MCSC will deposit its



Genomes 450	Molecular Interactions 347
Ensembl 370 <i>Selected eukaryotic genomes</i>	IntAct Experiments 180 <i>Experimental procedures used to characterise molecular interactions</i>
Ensembl Genomes 22 <i>Non-vertebrate genomes of high scientific interest</i>	IntAct Interactions 143 <i>Descriptions of molecular interactions</i>
Integr8 58 <i>Completed genomes and proteomes</i>	IntAct Interactors 24 <i>Proteins taking part in molecular interactions</i>
Nucleotide Sequences 7,117	Reactions & Pathways 32
ASTD 0 <i>Database of alternative splice events and transcripts of genes from human, mouse and rat.</i>	BioModels 9 <i>Databases of Mathematical models of biological interest</i>
EMBL Bank 6,436 <i>Europe's primary nucleotide sequence resource</i>	Reactome 23 <i>Database of core biochemical pathways and reactions</i>
EMBL Bank (Coding Sequence) 682 <i>Coding Sequences in EMBL-Bank</i>	Rhea 0 <i>Manually annotated database of chemical reactions created in collaboration with the Swiss Institute of Bioinformatics (SIB).</i>
Protein Sequences 1,733	Protein Families 79
PRIDE 24 <i>Proteomics Identification Database</i>	GPCRDB 0 <i>Database of G Protein-Coupled Receptors</i>
UniProtKB 772 <i>UniProt Knowledge Base of protein sequences</i>	InterPro 78 <i>Database of protein families, domains and functional sites</i>
UniRef 937 <i>UniProt Non-redundant Reference Databases</i>	MEROPS Peptidases 0 <i>MEROPS Id Peptidase Database</i>
UniParc 0 <i>Non-redundant archive of protein sequences</i>	MEROPS Peptidase Clans 0 <i>MEROPS Clan Peptidase Database</i>
Macromolecular Structures 222	MEROPS Peptidase Families 1 <i>MEROPS Family Peptidase Database</i>
PDB 222 <i>Macromolecular structures database</i>	Enzymes 1
Small molecules 1	Intenz 1 <i>Integrated relational Enzyme database</i>
ChEBI 0 <i>Chemical Entities of Biological Interest</i>	Literature 51,026
Ligands 0 <i>Library of ligands, small molecules and monomers</i>	Medline 49,663 <i>Citations and abstracts from many life-science journals</i>
RESID 1 <i>Protein residue modifications database</i>	Patents 1,363 <i>Biology-related abstracts of patent applications</i>
Gene Expression 176	Ontologies 16
ArrayExpress (Repository of Microarray data) 64 <i>ArrayExpress Repository is a MIAME compliant public database for microarray data.</i>	BioCatalogue 0 <i>BioCatalogue</i>
ArrayExpress (Warehouse of Microarray experiments) 4 <i>ArrayExpress Warehouse is an expert-curated database of gene expression profiles.</i>	GO 15 <i>Gene Ontology</i>
ArrayExpress (Warehouse of gene expression profiles) 108 <i>ArrayExpress Warehouse is an expert-curated database of gene expression profiles.</i>	SBO 0 <i>Systems Biology Ontology</i>
	Taxonomy 1 <i>NCBI Taxonomy database of Organism names</i>

Protein Databases

ExPASy Molecular Biology Server <http://tw.expasy.org>



The ExPASy (**Expert Protein Analysis System**) [proteomics](#) server of the [Swiss Institute of Bioinformatics](#) (SIB) is dedicated to the analysis of protein sequences and structures as well as 2-D PAGE

 Swiss Institute of Bioinformatics  **ExPASy Proteomics Server**

Databases Tools Services Mirrors Contact

You are here: ExPASy CH

The ExPASy (Expert Protein Analysis System) [proteomics](#) server of the [Swiss Institute of Bioinformatics](#) (SIB) is dedicated to the analysis of protein sequences and structures as well as 2-D PAGE ([Disclaimer](#) / [References](#) / [Linking to ExPASy](#)).

Databases

UniProtKB, ViralZone, PROSITE, SWISS-MODEL, SWISS-2DPAGE, World-2DPAGE Repository, MIAPEGelDB, ENZYME, GlycoSuiteDB,
[\[full list\]](#)

Education & services

Downloads, Popular Science (Protein Spotlight, Protéines à la «Une»), e-proxemis, Bioinformatics core facility for Proteomics
[\[full list\]](#)

Tools & Software

Proteomics tools, Blast, ScanProsite, Melanie, MSight, Make2D-DB, SWISS-MODEL, Swiss-PdbViewer
[\[full list\]](#)

Documentation

What's New?, E-mail alerts, UniProtKB documentation, How to link to ExPASy
[\[full list\]](#)

Latest News

ExPASy - Sep 11, 2009
We have redesigned the website according to the new SIB standards. We hope the new design also improves navigation and readability.

Protein Spotlight - Aug, 2009
paint my thoughts
Drawing is probably not a talent the layman would normally associate with Science...

[\[more news\]](#) [\[SIB news\]](#)

Protein Databases

Protein Data Bank <http://www.rcsb.org>

PDB
PROTEIN DATA BANK

The Protein Data Bank (PDB) is operated by Rutgers, The State University of New Jersey; the San Diego Supercomputer Center at the University of California, San Diego; and the National Institute of Standards and Technology -- three members of the [Research Collaboratory for Structural Bioinformatics \(RCSB\)](#). The PDB is supported by funds from the [National Science Foundation](#), the [Department of Energy](#), and two units of the National Institutes of Health: the [National Institute of General Medical Sciences](#) and the [National Library of Medicine](#).

RCSB PDB
PROTEIN DATA BANK

MyPDB Login A MEMBER OF THE PDB

An Information Portal to Biological Macromolecular Structures

As of Tuesday Sep 08, 2009 there are 60,046 Structures PDB Statistics

WHAT'S NEW | HELP | PRINT PDB ID or keyword Search Advanced Search

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Electron Microscopy
NMR
Validation Server
BioSync Beamline
Related Tools

Search

Advanced Search
Latest Releases
Latest Publications
Sequence Search
Ligand Search
Unreleased Entries
Browse Database
Histograms

Tools

File Downloads
File Formats
Services: RESTful | SOAP
Widgets
Compare Structures

Education

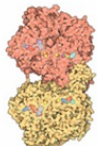
Looking at Structures
Molecule of the Month
Educational Resources

A Resource for Studying Biological Macromolecules

The PDB archive contains information about experimentally-determined structures of proteins, nucleic acids, and complex assemblies. As a member of the wwPDB, the RCSB PDB curates and annotates PDB data according to agreed upon standards.

The RCSB PDB also provides a variety of tools and resources. Users can perform simple and advanced searches based on annotations relating to sequence, structure and function. These molecules are visualized, downloaded, and analyzed by users who range from students to specialized scientists.


Molecule of the Month: Xanthine Oxidoreductase



Our diet includes a wide variety of different molecules. Many of these molecules are broken down completely and used to generate the metabolic energy that powers our cells. Others are disassembled piece-by-piece and recycled to build our own proteins and nucleic acids. The ones that are left over are broken down and discarded. Xanthine oxidoreductase, shown here from PDB entry 1fo4, is the last step for extra purine nucleotides (ATP and GTP) in our cells. Purines are broken down in several steps, ultimately yielding uric acid, which is excreted from the body.

Read more ... Previous Features

PSI Featured Molecule: Toxin-antitoxin VapBC-3



Tuberculosis bacteria, like many other bacteria, poison themselves with custom-made protein toxins. PSI researchers are exploring the structure of one of these toxins, and the antitoxin made by the bacterium to protect itself.

Read more from PSI SGB Previous Features

New user? Try the browser [compatibility check](#), information on [Getting Started](#), and a [narrated tutorial](#) about navigating the site.

News

- Complete News
- Newsletter
- Discussion Forum
- Job Listings

08-September-2009
Improved Navigation of the RCSB PDB Website

RCSB PDB web pages been reorganized to make navigating the website and search results easier and more intuitive.

The left-hand menu now groups frequently-used webpages into sections that can be moved up and down to create a left-hand menu ordered by user interest. This customized menu will then appear on every web page. Several enhancements have also been added to the **query result pages**.

More >>

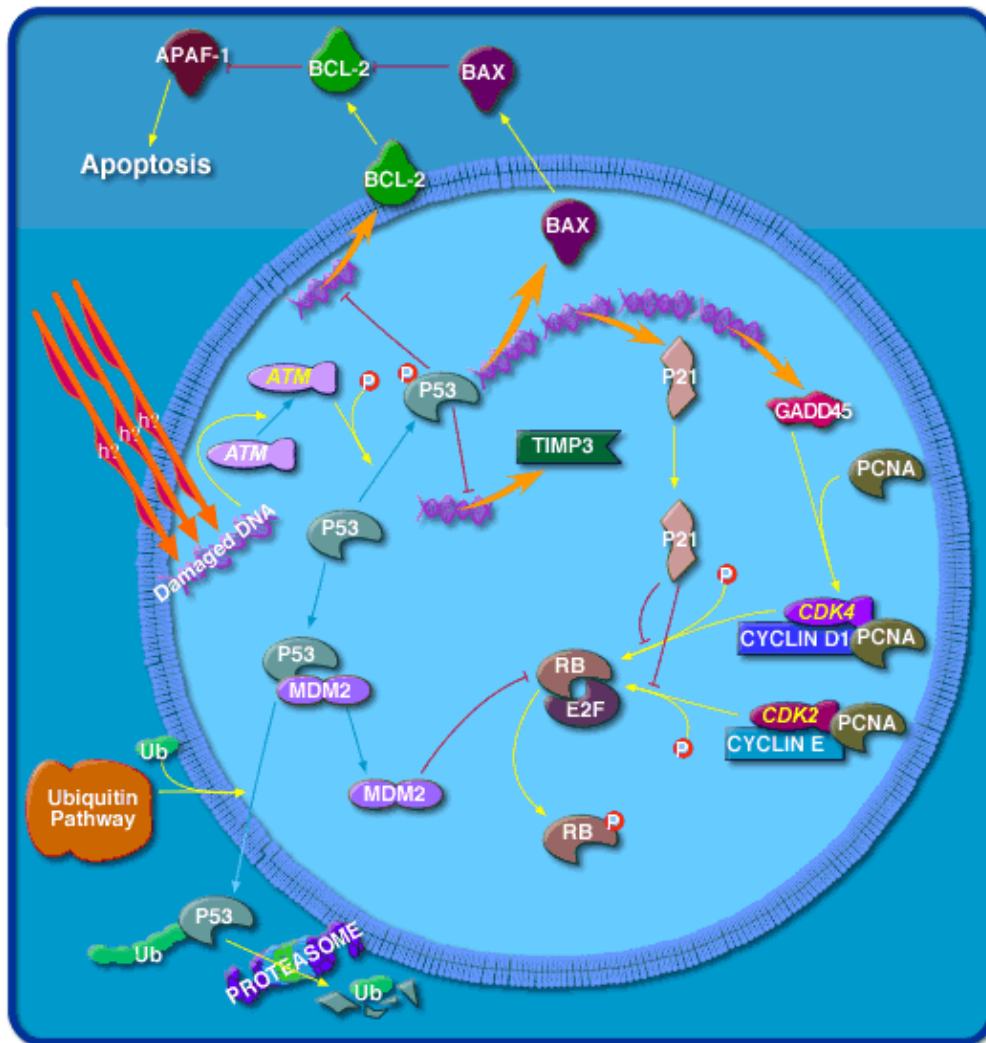
Data Snapshots

Time-stamped yearly snapshots of the PDB archive are available via FTP at:
<ftp://snapshots.wwpdb.org>
The snapshots provide readily identifiable data sets for research on the PDB archive.

The RCSB PDB is managed by two members of the RCSB: Rutgers and UCSD, and is funded by NSF, NIGMS, DOE, NLM, NCI, NINDS, and NIDDK.

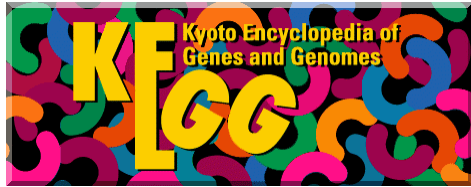
RCSB Protein Data Bank

Metabolic & Signalling Pathways



Biocarta
(<http://biocarta.com>)

Metabolic & Signalling Pathways



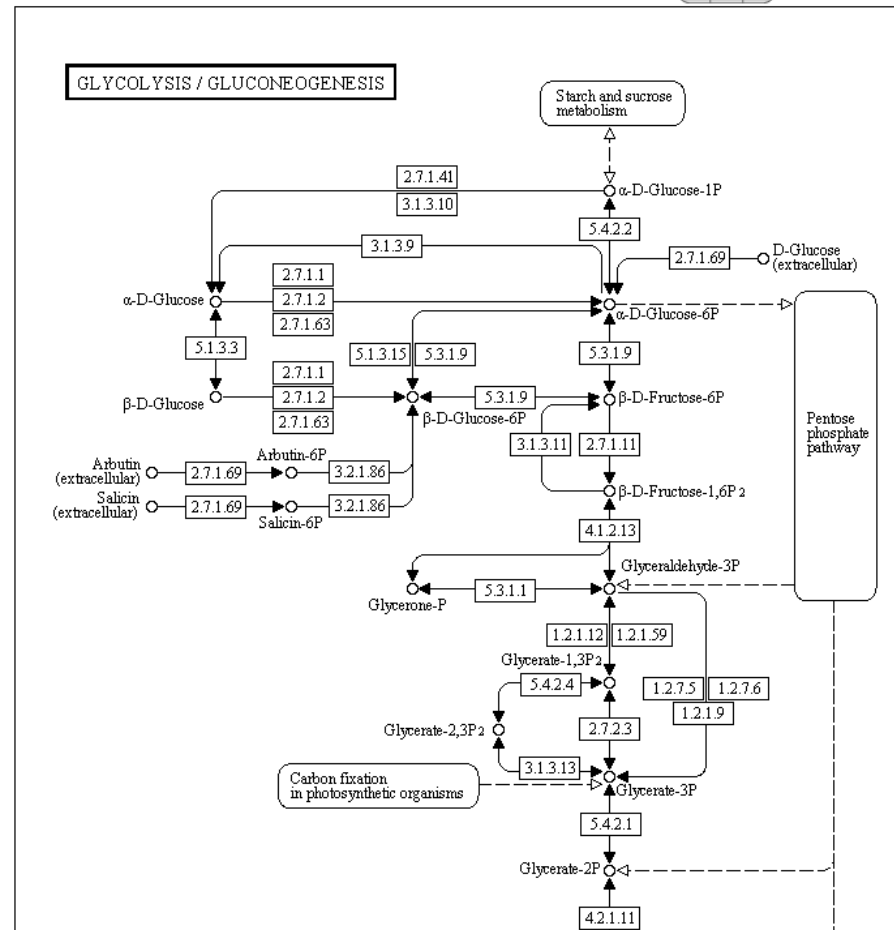
Kyoto Encyclopedia of Genes & Genomes
<http://www.genome.ad.jp/kegg/>

KEGG Glycolysis / Gluconeogenesis - Reference pathway

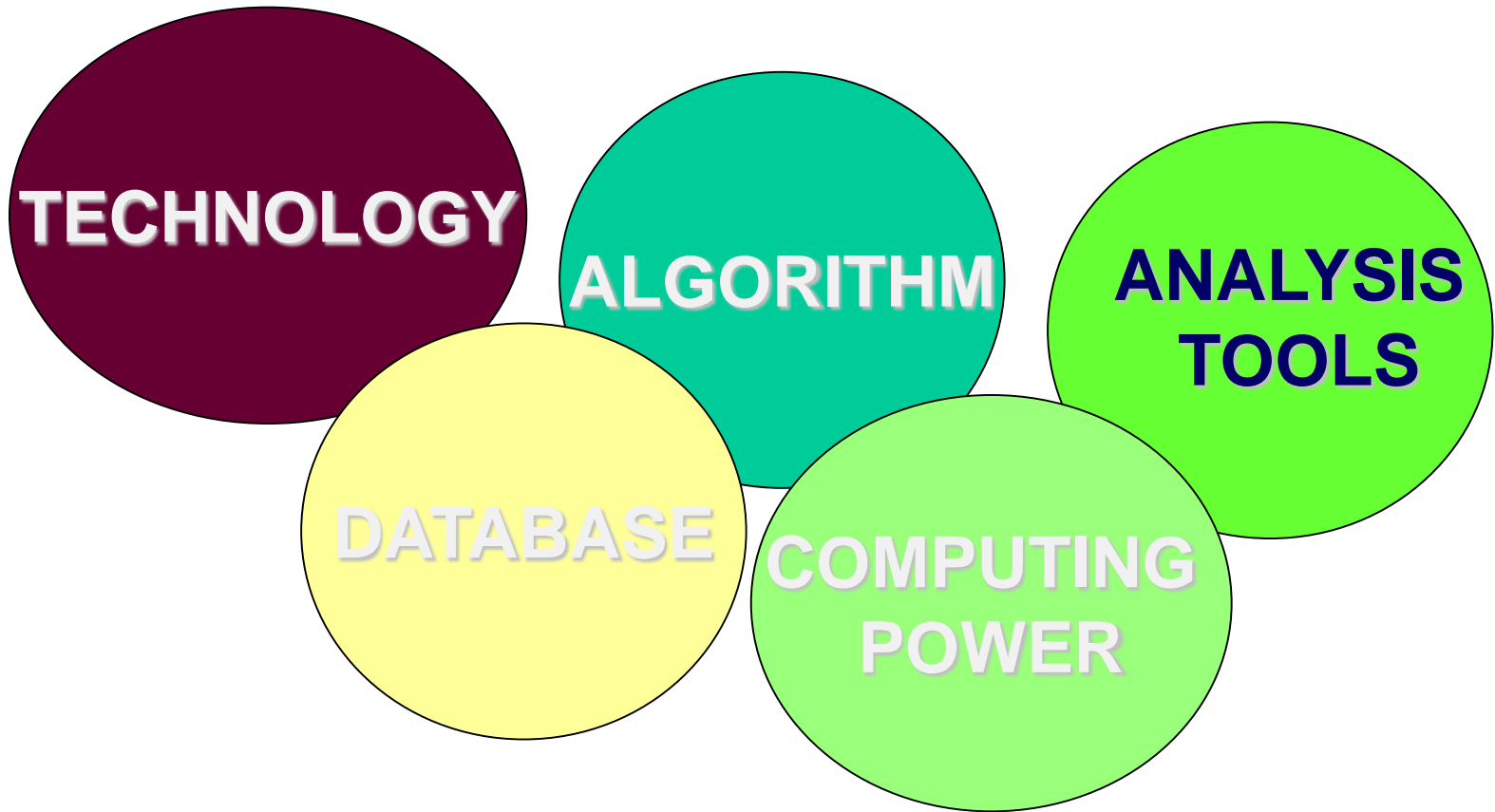
[Pathway menu | Pathway entry]

Reference pathway

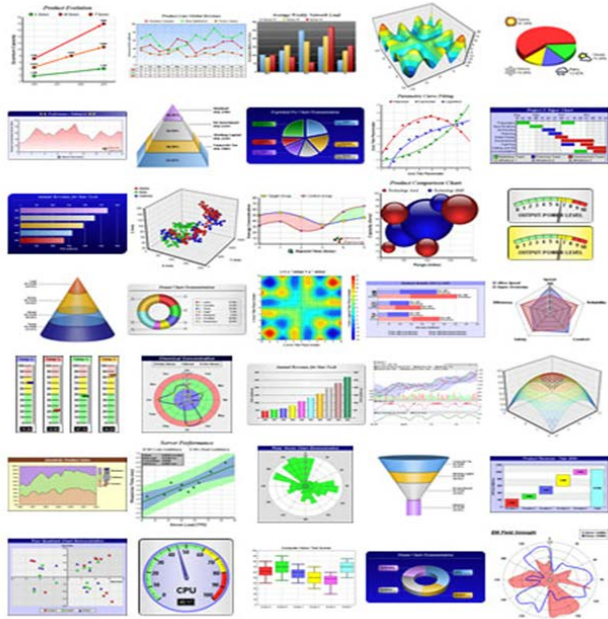
Go



THE COMPONENTS OF BIOINFORMATICS



BIOINFORMATICS ANALYSIS TOOLS



**CLC Genomics
Vector NTI suite
DNA Star**



**Staden Package
EMBOSS
BLAST
SMS....**

On line analysis tools

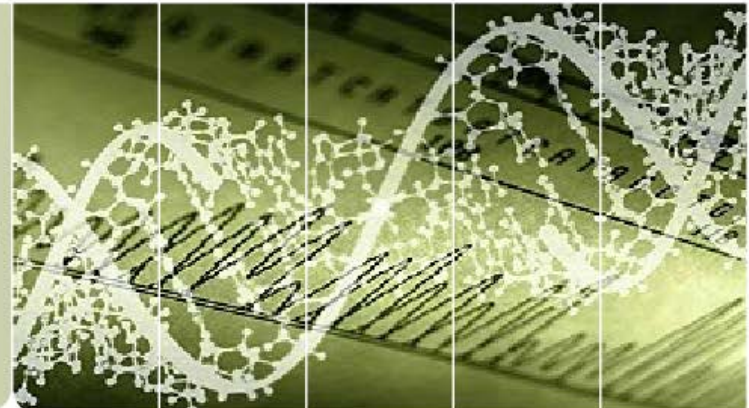


GMBD Bioinformatics Core



Bioinformatics Core for Genomic Medicine and Biotechnology Development (GMBD Bioinformatics Core) is a consortium formed by joint efforts of bioinformatics research groups in Taiwan, aiming at becoming bioinformatics infrastructure for our research community.

Welcome and enjoy your visit!



Unit 1

Unit 2

Unit 3

Unit 4

Unit 5



Coordination Unit

Since 1997, Department of Research Resources at NHRI has devoted considerable amount of resources in providing bioinformatics services in Taiwan. Coordination Unit will serve as the administration, education and service center of GMBD Bioinformatics Core.

Since 2002 Taiwan Bioinformatics Institute. All Rights Reserved.



❖ Databases

CPDB	Circular Permutation Database [NTHU]
dbPTM	Protein Post-Translational Modification Database [NCTU]
FlyDPI	Drosophila Database of Protein Interactomes [NHR1]
GPDB	Genome Profile Database [NTHU]
hp-DPI	H. pylori Database of protein interactomes [NHR1]
HPSG	Structural Genomics Databases of Helicobacter pylori [NTHU]
iGenome	A database index for the genome summarized information [NCTU]
KPSG	Structural Genomics Databases of Klebsiella pneumoniae [NTHU]
miRNAMap	Genomic Maps for microRNA [NCTU]
RegRNA	Regulatory RNA Motifs and Elements Database [NCTU]
RepeatMasker	Screening for low complexity DNA sequences and interspersed repeats [mirror at NCKU]
SM	Structural Genomics Databases of Stenotrophomonas maltophilia [NTHU]
SNP	SNP value-added database [NCKU]
SSDB	Disulfide Proteins Database [NCTU]
TAG	Tumor Associated Gene Database [NCKU]
The BEST	The Binding Element Searching Tool [NCKU]
TPMD	Taiwan Polymorphism Marker Database [NHR1]
XCC	Structural Genomics Databases of Xanthomonas campestris [NTHU]

❖ AnalysisTools Online

- Homology & Similarity

BLAST	BLAST Search at NCKU
PDB-BLAST	BLAST against PDB protein databank at NTHU
RPS-BLAST	BLAST against Motif/Domain database at NTHU
MyBLAST	BLAST against customized database (the databases built by yourself) [NHR1, Sinica]

- Sequence Analysis

Chameleon	Retrieve a small peptide fragment sequence from a collection of PDB sequences [NCTU]
Sequence Finder	Web-based Multiple Sequence Alignment [NTHU]
ClustalW	Identification and evolutionary analysis of novel exons and alternative splicing events [Sinica, NHR1]
ENACE System	A Web interface for visualizing ESTs [Sinica, NHR1]
ESTviewer	Web-based gene prediction service [NTHU]
GenePredict	Genetic Programming for RNA Motifs [NCTU]
GPRM	Predict phosphorylation sites within given protein sequences [NCTU]
KinasePhos	Multiple Sequence Alignment with Constraints [NCTU]
MuSiC	Primer Design Assistant [NHR1]
PDA	A Comparative Method for Identification of Gene Structures and Alternatively Spliced Variants [Sinica, NHR1]
PSEP System	RNA Motif Search Tool [NCTU]
RNAMST	An information repository for mRNA alternative splicing in human genome [NCTU]
SpliceInfo	Identify conserved sequence elements associated to mRNA splicing [NCTU]
SpliceMotif	Unique Probe Selector [Sinica, NHR1]

- Phylogenetic Analysis

Palm	Phylogenetic reconstruction by Automatic Likelihood Model selector [Sinica, NHR1]
POWER	Phylogenetic Web Repeater [NHR1]

- Topology Prediction

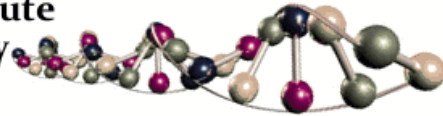
CELLO	Prediction of protein subcellular localization [NCTU]
pKNOT	pKNOT: the protein KNOT web server [NCTU]

- Structural Analysis

(PS)2	Protein Structure Prediction Server [NCTU]
3D-BLAST	Protein structure search [NCTU]
CPSARST	Circular Permutation Search Aided by Ramachandran Sequential Transformation [NTHU]
GEMDOCK	Generic Evolutionary Method for molecular DOCKing [NCTU]
PredictProtein	Sequence analysis and structure prediction [mirror at NTHU]
SARST	Structure Alignment by Ramachandran Search Tool [NTHU]
SDSE	Sequence Derived Structure Entropy [NCTU]
StEQ	Structural Entropy Query [NCTU]
Tm Predictor	Melting Temperature Prediction : Predict thermal stability of proteins [NTHU]

- Miscellaneous Tools

EMBOSS	European Molecular Biology Open Software Suite [NHR1]
EMBOSS GUI	EMBOSS Graphical User Interface: EMBOSS explorer [NHR1]
GCG	Wisconsin Sequence Analysis Package [NHR1]
Hubba-Hubba	Hub Objects Analyser, a web-based service designed to explore the essential nodes in a network [Sinica, NHR1]
JEMBOSS	Java user interface of EMBOSS [NHR1]
KPST	KEGG Pathway Search Tool [NTHU]
RMA	Reinforced Merging Algorithms [NTHU]
SeqWeb	Web-based GCG [NHR1]



[Home](#) / [Tools](#) / [GCG Application](#)

GCG, EMBOSS 序列分析工具帳號申請

■ 帳號申請

The Wisconsin Package (GCG/SeqWeb) 為商業軟體，經 Accelrys公司授權予國家衛生研究院，提供給非營利之醫療衛生與研究單位之實驗室主持人 (principal investigator, PI) 和博士後研究員 (Postdoc)申請使用。

非實驗室主持人申請時，需請實驗室主持人簽名 (或蓋職章) 作為確認。

※ 本院恕不提供帳號申請給營利性質之單位與公司。

本院提供申請表格式檔案，請自行下載使用。申請表內容請務必填寫正確，Email 欄位僅接受所屬機構之信箱。

填妥後，請以傳真方式：(037) 586410 或郵寄方式至：350 苗栗縣竹南鎮頂埔里科研路 35 號 生醫醫資料庫辦公室 收，我們將儘速為您處理！

下載申請表檔案



[bioinfo-form.doc](#)

(size: 49KB) Word 檔案格式

login: petang

Password:

Your password will expire in 10 days.

Last login: Tue Sep 12 13:50:57 from 163.25.92.192

Sun Microsystems Inc. SunOS 5.9 Generic May 2002

Welcome to GCG

Version 11.1-UNIX

Installed on solaris

Copyright (c) 1982 - 2006, Accelrys Inc.

All rights reserved.

Published research assisted by this software should cite:

GCG Version 11.1, Accelrys Inc., San Diego, CA

Databases available:

GenBank	Release	154.0	<06/2006>
GenPept	Release	154.0	<06/2006>
Refseq	Release	17.0	<05/2006>
UniProt	Release	8.2	<06/2006>
PROSITE	Release	19.30	<06/2006>
Pfam	Release	20.00	<05/2006>
Restriction Enzymes (REBASE)		607	<06/2006>

Technical support see: <http://www.accelrys.com/support/>

Online help: % genhelp or <http://www.accelrys.com/support/bio/genhelp/>

GCG System Support Environment Initialized.

v8803: petang [users/petang]> _



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EMBOSS is funded from May 2009 by BBSRC grant BBR/G02264X/1

Funded from May 2006 to April 2009 by BBSRC grant BB/D018358/1

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Help for biologists. EMBOSS tutorial. guides to major bioinformatics themes ... [more >](#)

生物資訊分析

上課時間：每週五上午 08:10~12:00 (08:10~09:00—授課，09:10~12:00—實習)

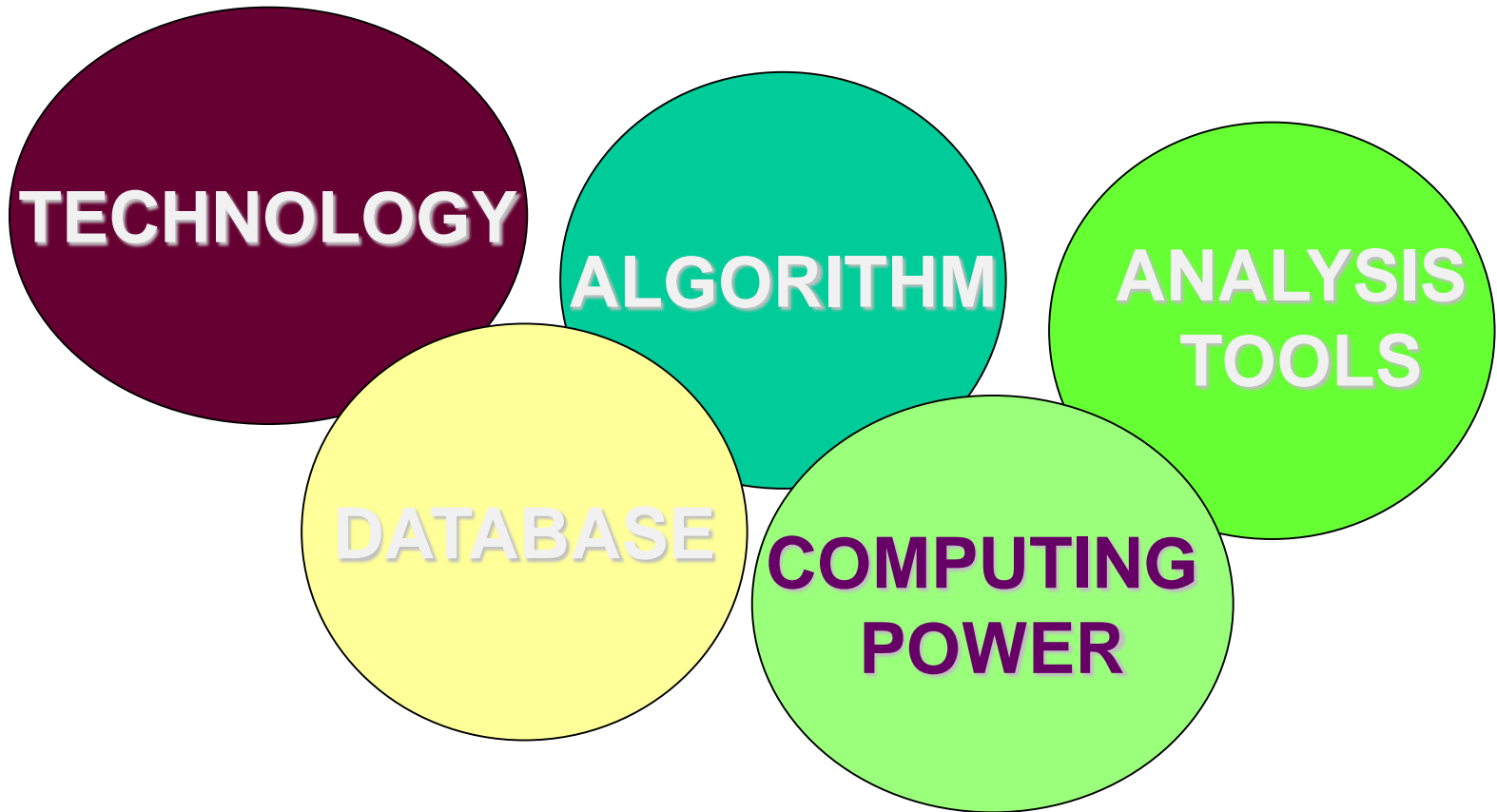
上課地點：醫學院 9F 生物資訊中心 電腦教室

助教：方怡凱(分機5690)，鄭尉弘(分機5690)

生物資訊中心：黃柏榕 老師 (分機3166)

進度	日期	課程進度	授課老師	講義下載
1	0926	Introduction to Bioinformatics	鄧致剛	PDF RAR Ex
2	1003	Bio-computing and Linux Basics	黃柏榕	PDF RAR Ex Unix cmd
3	1010	HOLIDAY		
4	1017	Bioinformatics Databases: searching & Management	鄧致剛	PDF RAR Ex
5	1024	Comparing Sequences and Multiple Sequence Alignment	鄧致剛	PDF RAR Ex
6	1031	DNA Sequence Analysis & Assembling	鄧致剛	PDF RAR Ex1 Ex2
7	1107	Phylogenetic Analysis	辛致煒	Phylip CLC Gen
8	1114	DNA Sequence Analysis (II)	林文昌	PPT RAR Ex
9	1121	Special Topic-Bioinformatics on the Internet	黃柏榕	PDF RAR Ex
10	1128	Protein Sequence Analysis	鄧致剛	PDF Ex ASS03
11	1205	Protein 3D Structure Modeling	呂平江	Rasmol2721 教學網
12	1212	Special Topic-Gene Chip Technology & Microarray Analysis	辛致煒	PDF MeV4 Dataset
13	1219	Special Topic-Integration of Omics (1) Metacore	鄧致剛	PDF RAR Ex
14	1226	Special Topic-Integration of Omics (2) David	鄧致剛	PDF RAR Ex
15	0102	Special Topic-Next Generation Sequencing Technology	劉軒	PDF RAR Ex
16	0109	Special Topic-microRNA analysis and databases	黃柏榕	PDF
17	0116	Student Project Presentation	鄧致剛	PDF RAR Ex
18	0123	Final Examination	鄧致剛	

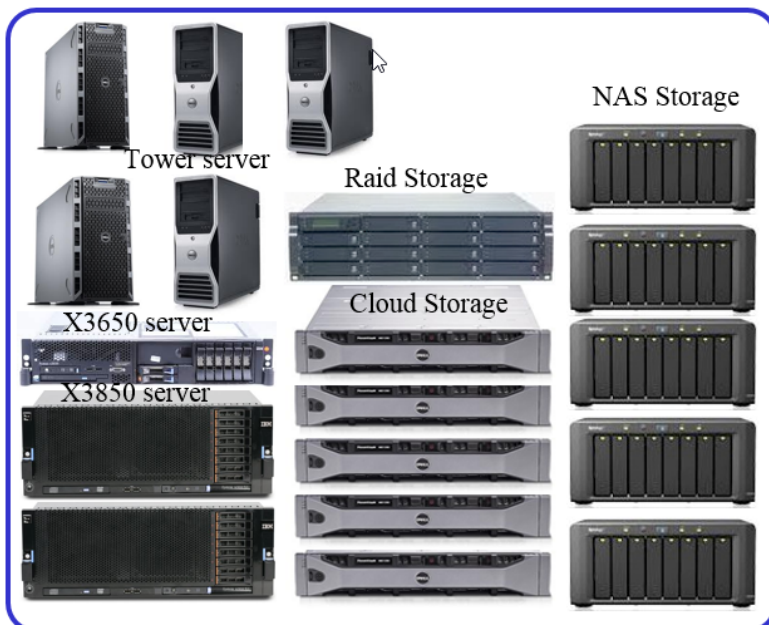
THE COMPONENTS OF BIOINFORMATICS



Chang Gung Bioinformatics Core

Server CPU/MEM: 436 Cores/3.04 TB
 Workstation GPU/MEM: 12 Cores/192 GB
 Workstation CPU/MEM: 66 Cores/ 512 GB
 Storage: 736 TB

NGS Core

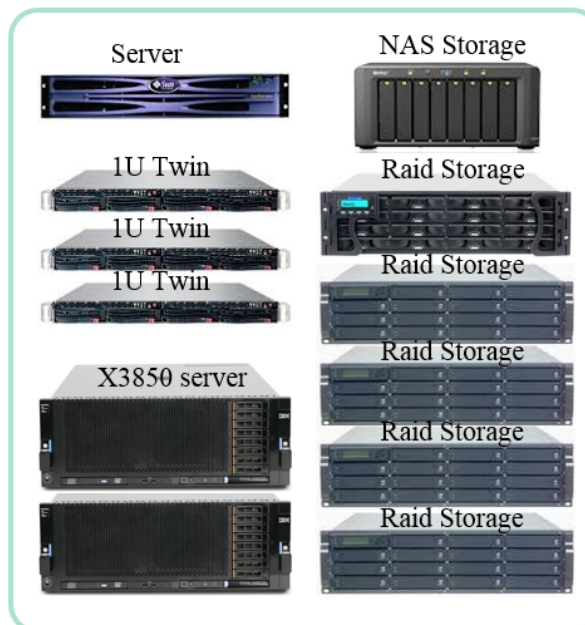


Tower Server	5
Server	3
Raid Storage	1
Cloud Storage	5
NAS Storage	5
Total	19

Software

Life Scope, Torrent Suite, Partek and Galaxy

Bioinformatics Core



Server	13
Raid Storage	5
NAS Storage	1
Total	19

Software

VectorNTI
 GeneGo (MetaCore)
 CLC Genomics Workbench
 CPAP, DSAP, FASTAnnotator & VIPDB
 VANNO, HMPD, CRSAP

Proteomics Core

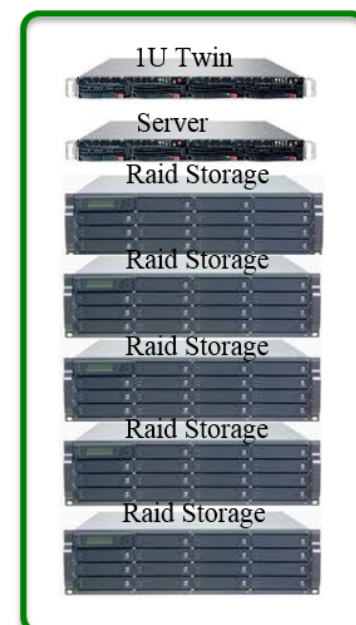


Image Center



Server	3
Raid	5
Server	2
Total	10

Small Genomes & Transcriptomes

24h購物

ASUS

4代i7四核
獨顯旗艦機

- Intel Core i7-4790K(3.4G)
- NV GTX750 1G 獨顯

USB3.0

i7-4790
GTX750



G10AJ

送LED燈+1TB雲端硬碟

華碩 4代i7四核Win8.1電玩旗艦機

最新第4代Core i處理器

- 處理器：Intel Core i7-4790(3.4GHz)
- 晶片：Intel H97
- 記憶體：16GB DDR3 (8G*2) → 64GB
- 硬碟：SATAIII 2TB+8G SSD(Hybrid) → 4TB
- 顯示介面：NVIDIA GTX750 1G GDDR5 獨立顯卡
- 光碟機：超薄Super Multi DVD燒錄機
- 作業系統：Windows 8.1 (64bit)
- 其他：USB3.0、HDMI
- 保固：三年保固(含零件、人工/三年到府收送)



An Example

Steps to Identify a Gene

- **Gene-Search**
- **Protein-Search**
- **Annotation**

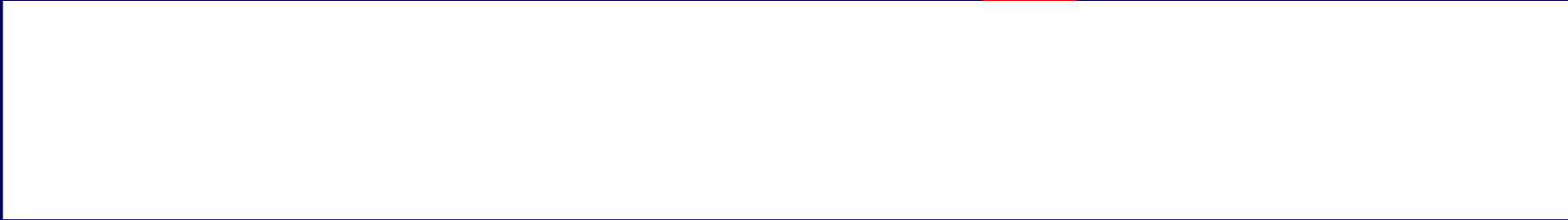
Full length ORF of *TvEST-14G2*

...AGATG

TGAAATAT ATTTTTATA TTATTTATTT
TTTTCTTTTT CTATCTGTAT ATTAAATGTA TTTCTATATT ATTAAAAAAA

Amino Acid Sequence Comparison

01B1
04E12
14G2
PFCK
Yeast
Human
Mouse
TcCK1.1
TcCK1.2





01B1
04E12
14G2
PFCK
Yeast
Human
Mouse
TcCK1.1
TcCK1.2



01B1
04E12
14G2
PFCK
Yeast
Human
Mouse
TcCK1.1
TcCK1.2



01B1
04E12
14G2
PFCK
Yeast
Human
Mouse
TcCK1.1
TcCK1.2

 : kinesin homology domain
 : casein kinase 1 specific motifs

PFCK : Plasmodium casein kinase 1
TcCK1.1: Trypanosoma cruzi casein kinase 1.1
TcCK1.2: Trypanosoma cruzi casein kinase 1.2

3-D Structure of TvEST-14G2 and other CK1s



1 MRKIYGN~~YIT~~ QKRLGSGSFG EVWEAVSHST GQKVALKLEP RNSSVPQLFF
51 EAKLYSMFQA SKSTNNSVEP CNNIPVVYAT GQTETTN~~YMA~~ MELLGKSLED
101 LVSSVPRFSQ KTILMLAGQM ISCVEFVHKH NFIHRDIKPD NFAMGVSENS
151 NKIYIIDFGL SKKYIDQNNR HIRNCTGKSL TGTARYSSIN ALEGKEQSIR
201 DDMESLVYVW VYLLHGRLPW MSLPTTGRKK YEAILMKKRS TKPEELCLGL
251 NSFFVNYLIA VRSLKFEEEP NYAMYRKMIY DAMIADQIPF DYRYD~~WV~~KTR
301 IVRPQRENQS QLSERQEGKC PNSAEFDGFS SIKGYSSHRQ VQSPVSSRDV
351 IKNSSSSPSK DILQSSTLDE SSQDKKPIKA VESNQPYPYTP PRTINTTETR
401 MRSKTTINTA RTTAKNSSAV KKESSATRTV KKETHPATTK TTKTVNRQLN
451 SSTTKPATTS SHKDSEPASS RRTSTLRSSR RQNDGIRPAK ERTALFTATA
501 SKPPVSYRTG MLPK~~WMM~~APL TSRR

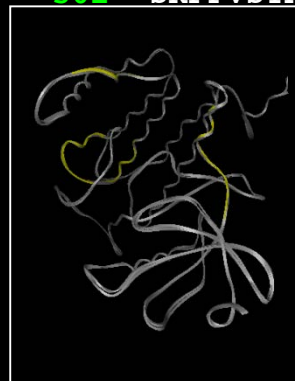
TVEST-14G2



TcCK1.1



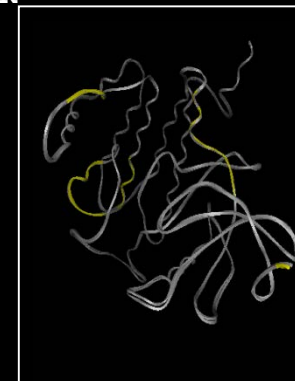
TcCK1.2



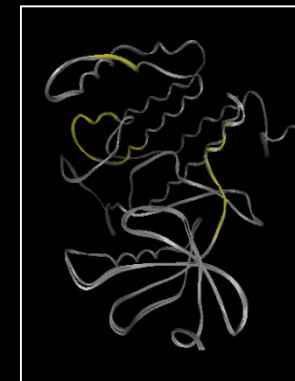
PfCK1



Yeast CK1



Mouse CK1



Human CK1-δ



**Experiment
Driven**

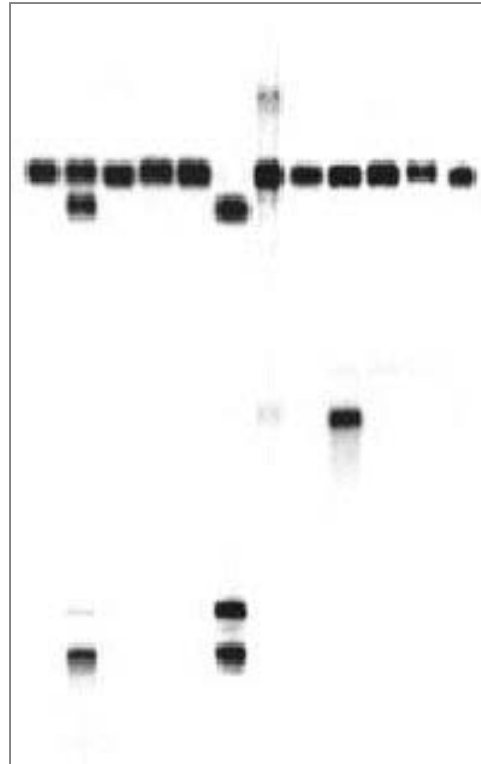
Hypothesis
↓
Experiments
↓
Results



**Information
Driven**

Experiments
↓
Hypothesis

The “old” biology



The most challenging task for a scientist is to get good data

The “new” biology



The most challenging task for a scientist is to make sense of lots of data

Old vs New – What's the difference? (1) Economics

- Miniaturize – less cost
- Multiplex – more data
- Parallelize – save time
- Automate – minimize human intervention
- Thus, you must be able to deal with large amounts of data and trust the process that generated it

What's the difference?

(2) Scale

- From gene sequencing (~ 1 KB) to genome sequencing (many MB, even GB)
- From picking several genes for expression studies to analyzing the expression patterns of all genes
- From a catalog of key genes in a few key species to a catalog of all genes in many species
- Analyzing your data in isolation makes less sense when you can make much more powerful statements by including data from others

What's the difference?

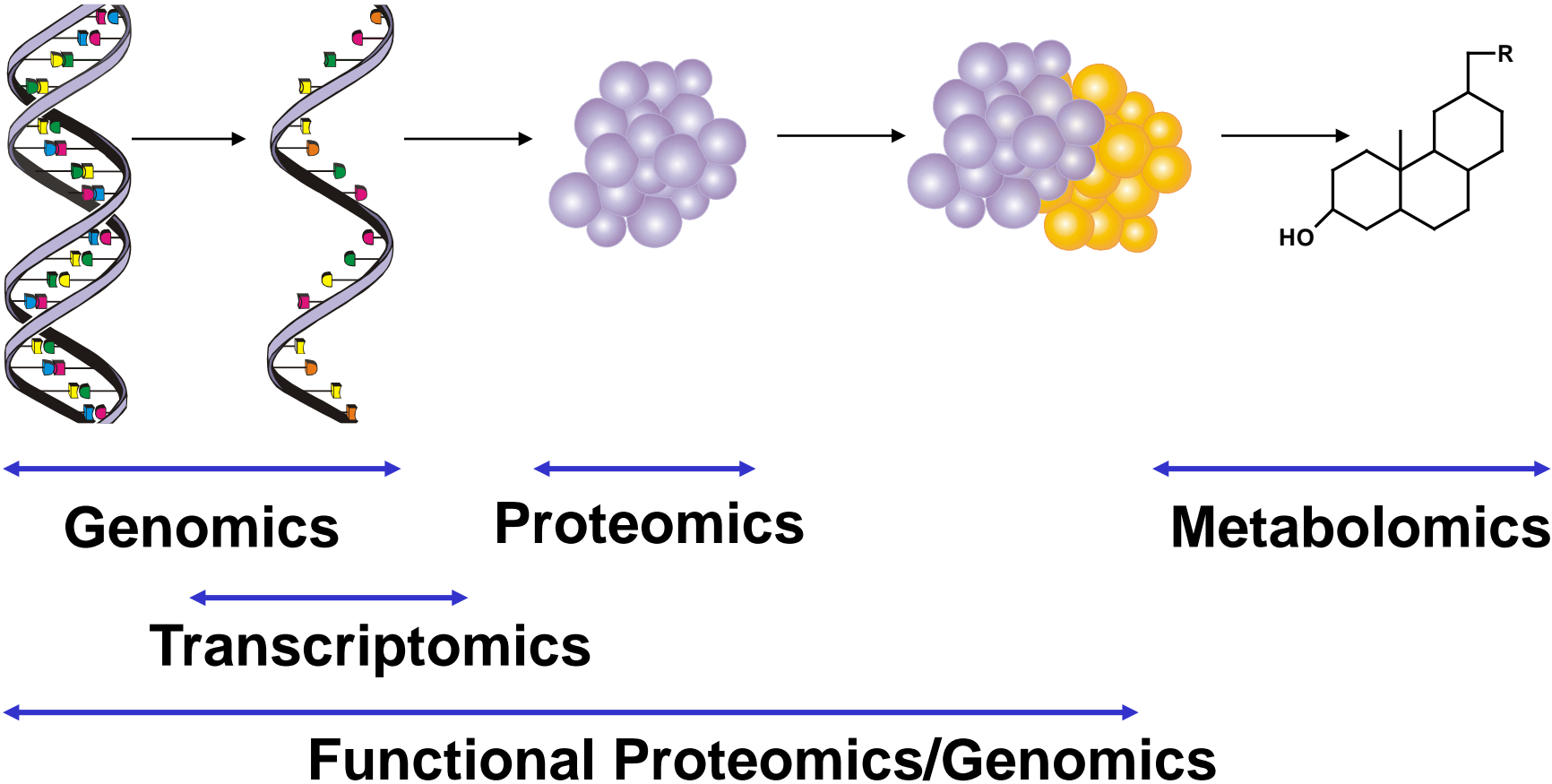
(3) Logic

- Hypothesis-driven research to data-driven research
- Expertise-driven approach versus information-driven approach
- Reductionist versus integrationist
- How to answer the question becomes how to question an answer
- Algorithmic approaches for filtering, normalizing, analyzing and interpreting become increasingly important

Data-driven Science Done Wrong

- Must have some hypothesis – data is not the end goal of science
- Finding patterns in the data is where analysis starts, not ends
- Must understand the limits of high-throughput technology (e.g. microarrays measure transcription only, one genome does not tell you about species variation, etc.)
- Must understand or explore the limits of your algorithm

Omics



SYSTEMS BIOLOGY



In 20 Jan 2015, President Obama called for a new initiative to fund precision medicine

THE PRECISION MEDICINE INITIATIVE



I want the country that eliminated polio and mapped the human genome to lead a new era of medicine—one that delivers the right treatment at the right time. In some patients with cystic fibrosis, this approach has reversed a disease once thought unstoppable. Tonight, I'm launching a new Precision Medicine Initiative to bring us closer to curing diseases like cancer and diabetes—and to give all of us access to the personalized information we need to keep ourselves and our families healthier.

高通量定序分析

上課時間：每週五上午 08:10~12:00 (08:10~09:00 – 授課 • 09:10~12:00 – 實習)

上課地點：醫學院 9F 生物資訊中心 電腦教室

助教：蔡智宇(分機5690)

進度	課程進度	授課老師	講義下載 L:lecture T:tutorial E:exercise
1	Introduction to New Generation Sequencing (NGS) Technologies	鄧致剛	Lecture
2	Databases and Tools for High Throughput Sequencing Analysis	黃柏榕	L T:FastQC Movie:FastQC T:FASTX T:SRA T:SRA2
3	Small RNA Analysis and Target Identification	黃柏榕	L T:CLC DSAP miRDEEP E
4	Gene Expression Analysis (I)	葉元鳴	
5	Gene Expression Analysis (II)	辛致煒	
6	Transcriptome Functional Profiling-1 (Metacore & DAVID)	鄧致剛/李正陽	
7	Transcriptome Functional Profiling-2 (GSEA & KEGG)	鄧致剛/李季青	
8	MID-TERM EXAMINATION	鄧致剛	
9	Bacteria Genome & Gene Expression Analysis	陳怡原	Lecture
10	Small Genome de novo Assembly	陳亭玟	Lecture Exercise I
11	Genome Annotation & Genome Browser	黃柏榕	
12	Chip Sequencing Analysis	陳亭玟	Lecture+Exercise
13	Metagenome Analysis	葉元鳴	Lecture+Exercise
14	Targeted Resequencing Analysis	黃柏榕	
15	Biological Big Data Visualization & Integration	鄧致剛/李季青	
16	HOLIDAY		
17	Student Presentation	鄧致剛	PDF
18	Final-Examination	鄧致剛	PDF

Q. As a biologist, what skills do I need to make the transition to bioinformatics?

The fact is that many of the jobs available CURRENTLY involve the design and implementation of programs and systems for the storage, management and analysis of vast amounts of DNA sequence data. Such positions require in-depth programming and relational database skills which very few biologists possess, and so it is largely the computational specialists who are filling these roles. This is not to say the computer-savvy biologist doesn't play an important role. As the bioinformatics field matures there will be a huge demand for outreach to the biological community, as well as the need for individuals with the in-depth biological background necessary to sift through gigabases of genomic sequence in search of novel targets. It will be in these areas that biologists with the necessary computational skills will find their niche.

- A. Molecular biology packages (GCG, BLAST etc),
Web and programming skills including HTML, Perl, JAVA and C++,
Familiar with a variety of operating systems (especially UNIX),
Relational database skills such as SQL, Sybase or Oracle,
Statistics,
Structural biology and modeling,
Mathematical optimization,
Computer graphics theory and linear algebra.
You will need to be able to readily pick up, use and understand the tools and databases designed by computer programmers, and
To communicate biological science requirements to core computer scientists.