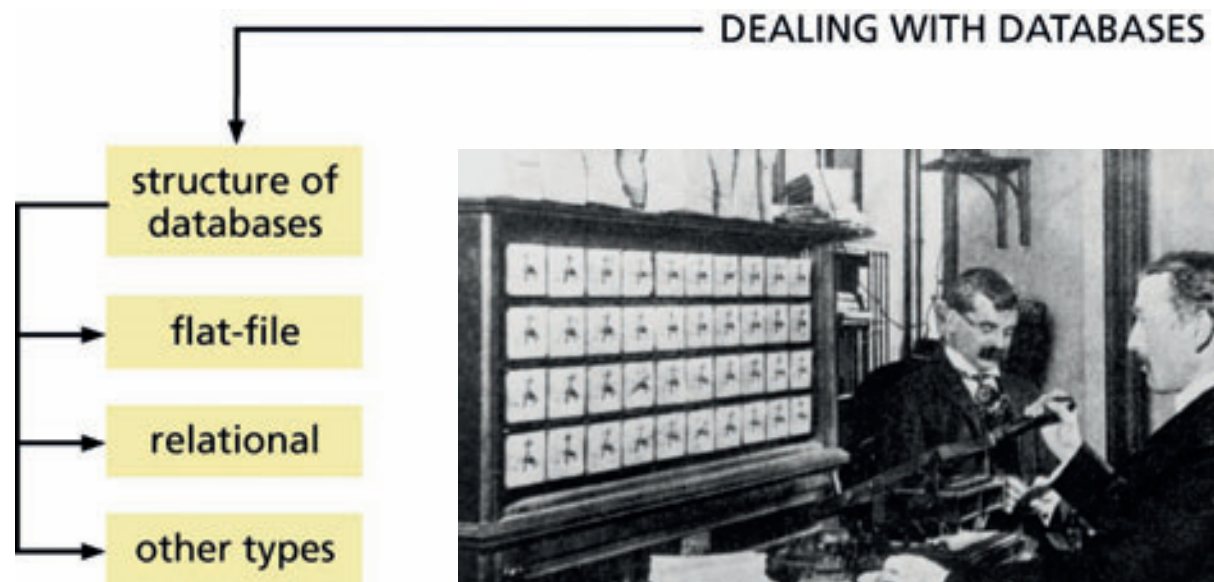


# Biological Databases

1. <http://www.ploscompbiol.org/article/info%3Adoi%2F10.1371%2Fjournal.pcbi.0010034>
2. [http://en.wikipedia.org/wiki/Biological\\_databases](http://en.wikipedia.org/wiki/Biological_databases)
3. <http://www.uniprot.org/help/about>
4. Some basic bioinformatics databases, see course page

# Databases



# What is a database

- **Structured** collection of information.
- Consists of basic units called records or entries.
- Each record consists of fields, which hold **pre-defined** data related to the record.
- For example, a protein database would have protein entries as records and protein properties as fields (e.g., name of protein, length, amino-acid sequence)

# Types of databases

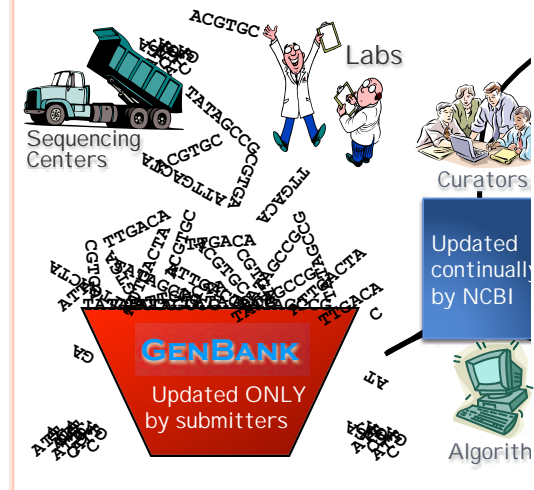
## Primary Databases

Original submissions by experimentalists

Content controlled by the **submitter**

Examples: GenBank, Trace, SRA, SNP, GEO

## PRIMARY VS. DERIVATIVE SEC DATABASES



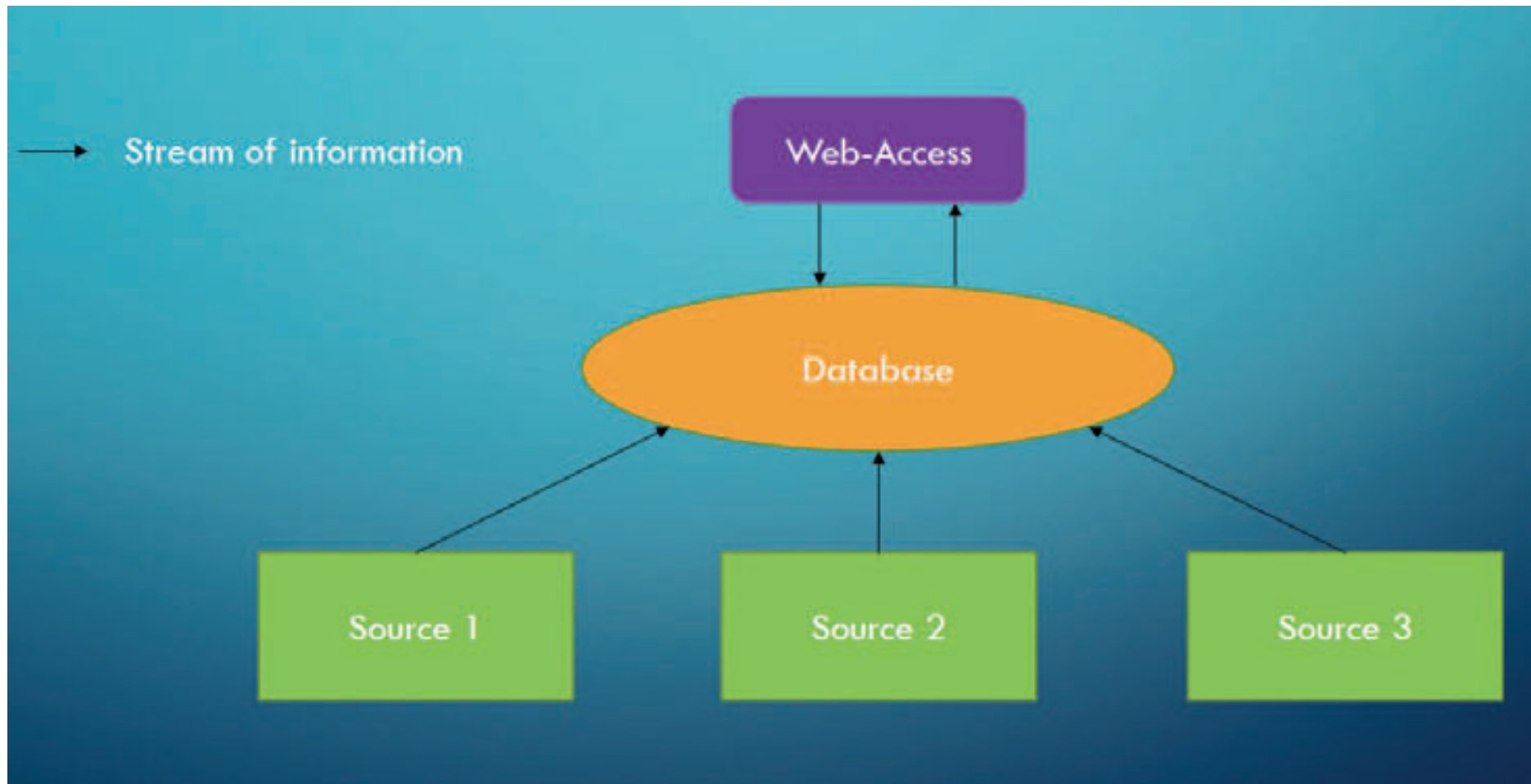
## Derivative Databases

*Derived* from primary data

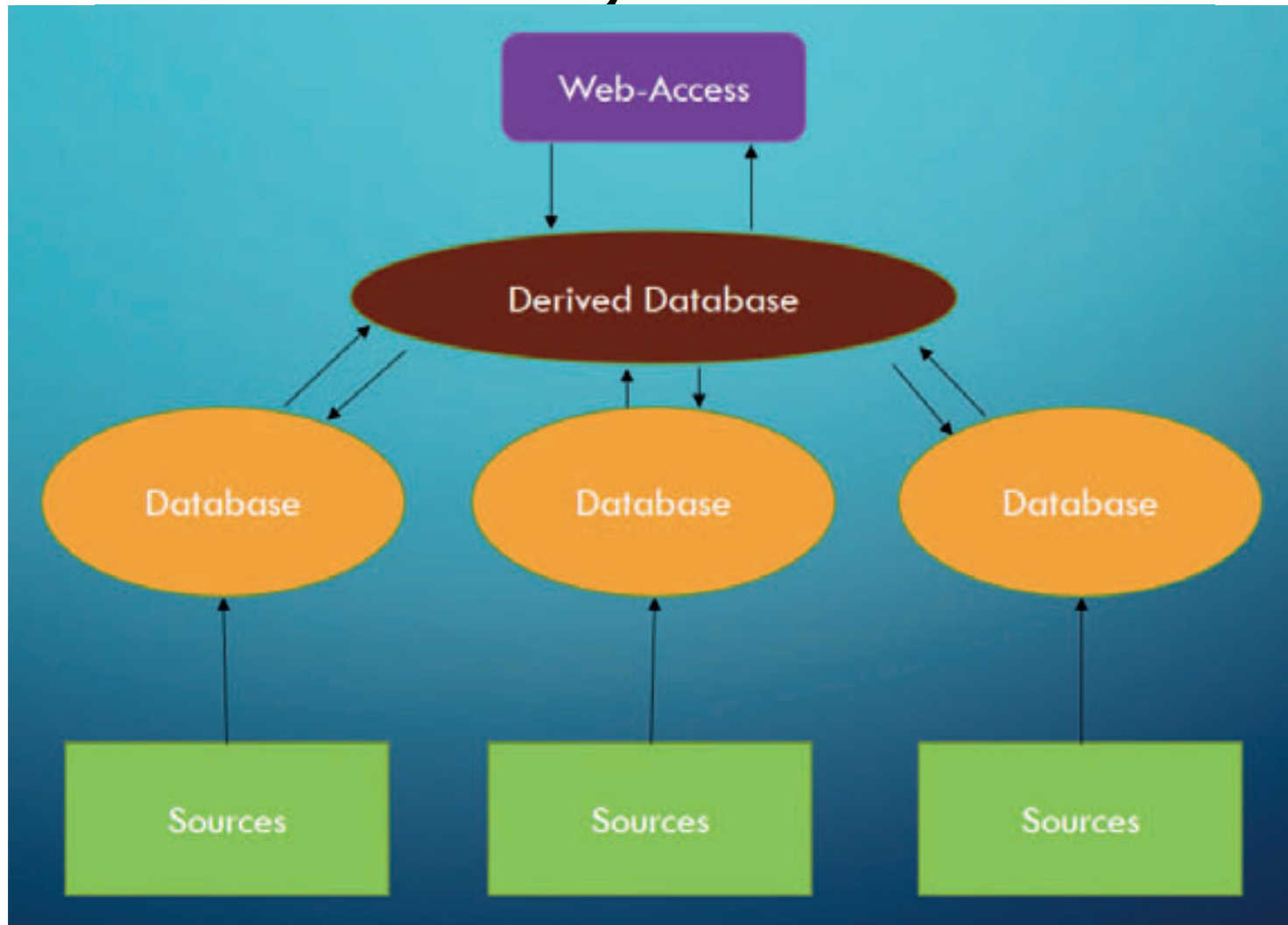
Content controlled by **third party** (NCBI)

Examples: NCBI Protein, Refseq, TPA, RefSNP, GEO datasets, UniGene, Homologene, Structure, Conserved Domain

# Primary databases



# Secondary databases



# A flat-file database

(A)

NAME	TELEPHONE	ADDRESS
S. Claus	0203 450	The North Pole, Lapland
M. Mouse	0202 453	Disneyworld, Florida
A. Moonman	0104 459	Craterland, The Moon

(B) GenBank Flat-File Format

```
LOCUS      SCU49845      5028 bp      DNA
DEFINITION Saccharomyces cerevisiae TCP1-beta gene, partial cds, and
            Ax12p
            (AXL2) and Rev7p (REV7) genes, complete cds.
ACCESSION  U49845
VERSION    U49845.1  GI:1293613
KEYWORDS   .
SOURCE     Saccharomyces cerevisiae (baker's yeast)
  ORGANISM Saccharomyces cerevisiae
            Eukaryota; Fungi; Ascomycota; Saccharomycotina;
            Saccharomycetes;
            Saccharomycetales; Saccharomycetaceae; Saccharomyces.
```

# Relational databases

protab1			
Protein-code	Protein-name	Length	Species-origin
P1001	Hemoglobin	145	Bovine
P1002	Hemoglobin	136	Ovine
P1003	Eye Lens Protein	234	Human
.....			

protab2	
Protein-code	Protein-sequence
P1001	MDRTTHGFDLKLLSPRTVNQWLMLALFFGHS...
P1002	MDKTSHGFEIKLLTPKKLQQWLMIAIYFGHT...
P1003	SRTHEEEGKLMQWPPRPLYIALFTEPPYP...
.....	

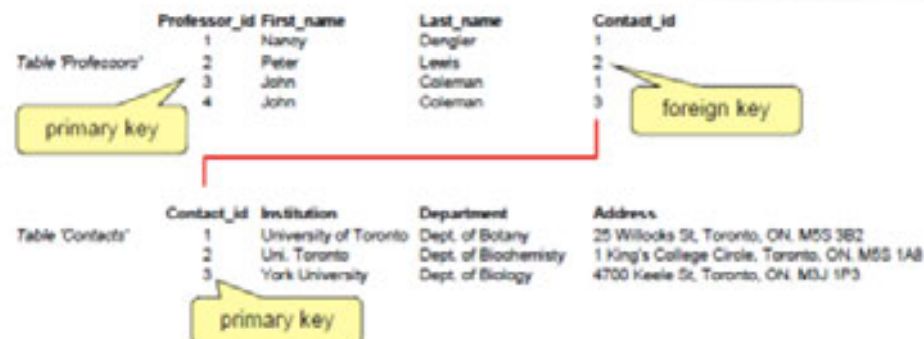
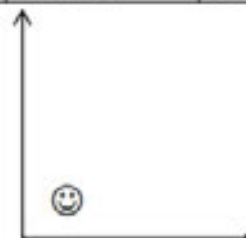


# Relational database

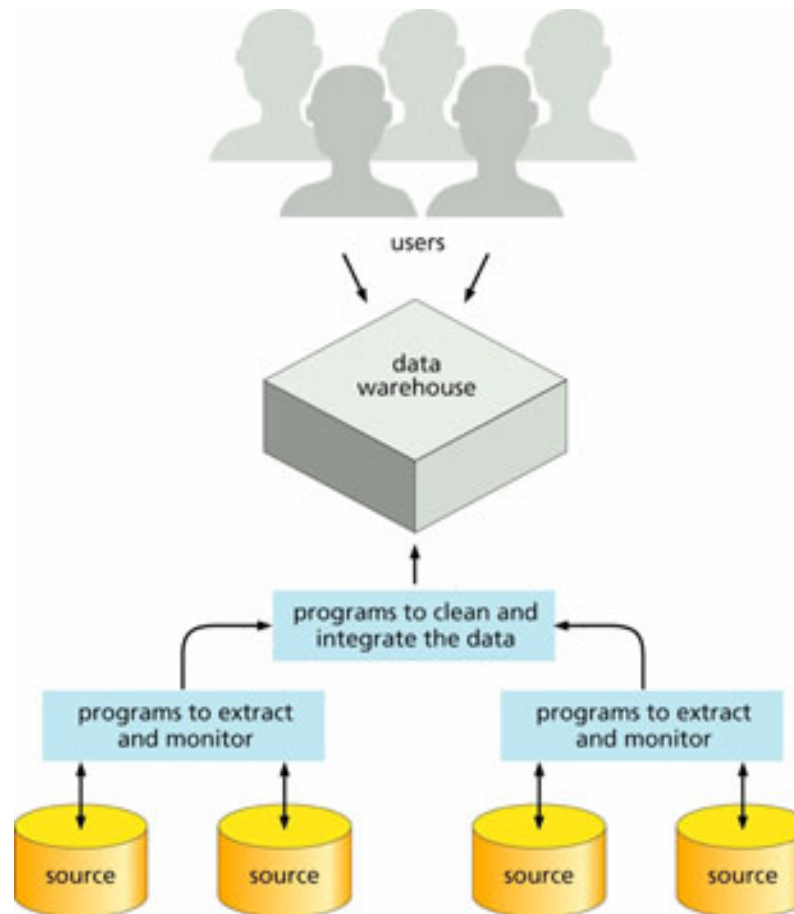
- A relational database consists of a relations (tables) containing attributes (fields or columns). Each row in a table is known as a tuple or a record.
- Information should be 'normalized' so that it is non-redundant this means that every row should be unique, although this ideal is not always observed.

Nancy|Dengler|Botany|University of Toronto|25 Willocks St, Toronto, ON, M5S 3B2  
 Peter|Lewis|Dept. of Biochemistry|Uni. Toronto|1 King's College Circle, Toronto, ON, M5S 1A8  
 John|Coleman|Department of Botany|University of Toronto|25 Willocks St, Toronto, ON, M5S 3B2  
 John|Coleman|Dept. of Biology|York University|4700 Keele St, Toronto, ON, M3J 1P3

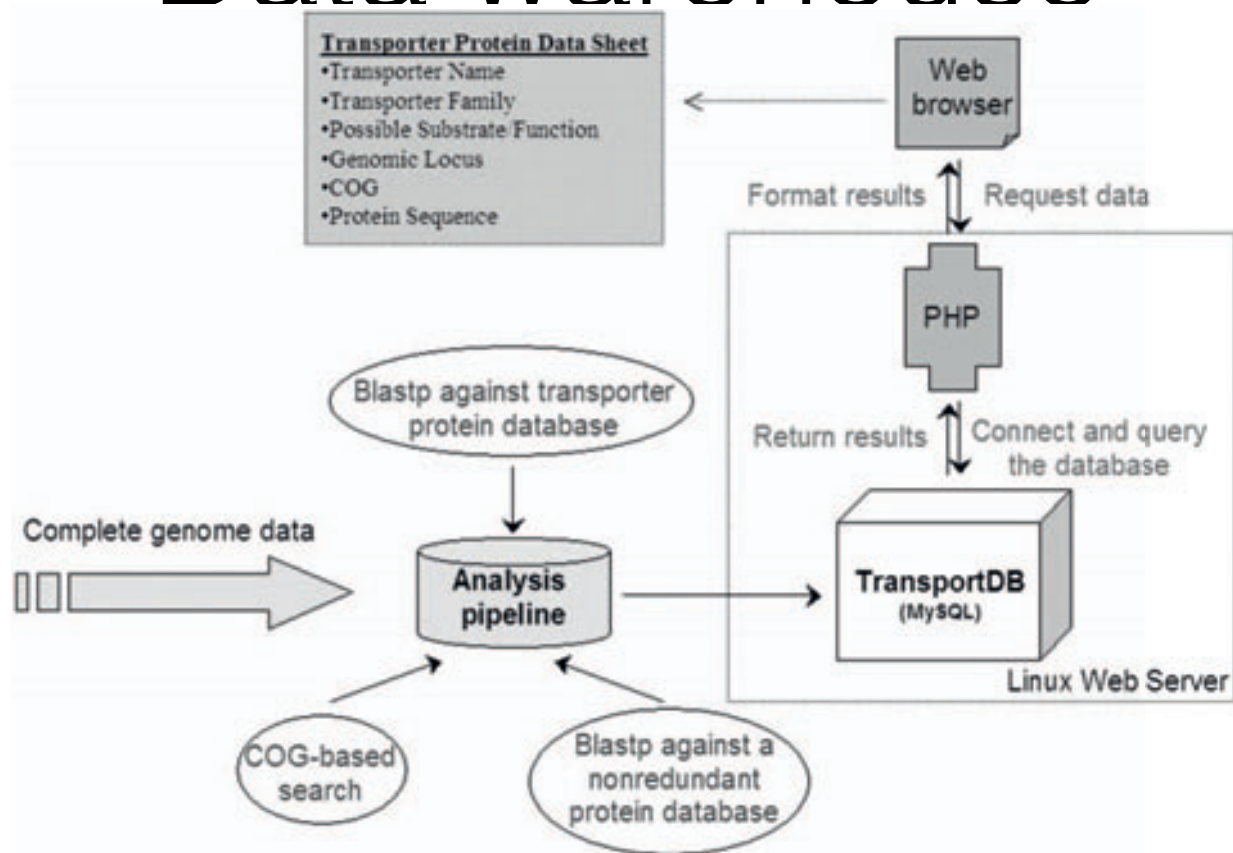
First_name	Last_name	Institution	Department	Address
Nancy	Dengler	University of Toronto	Botany	25 Willocks St, Toronto, ON, M5S 3B2
Peter	Lewis	Uni. Toronto	Dept. of Biochemistry	1 King's College Circle, Toronto, ON, M5S 1A8
John	Coleman	University of Toronto	Department of Botany	25 Willocks St, Toronto, ON, M5S 3B2
John	Coleman	York University	Dept. of Biology	4700 Keele St, Toronto, ON, M3J 1P3



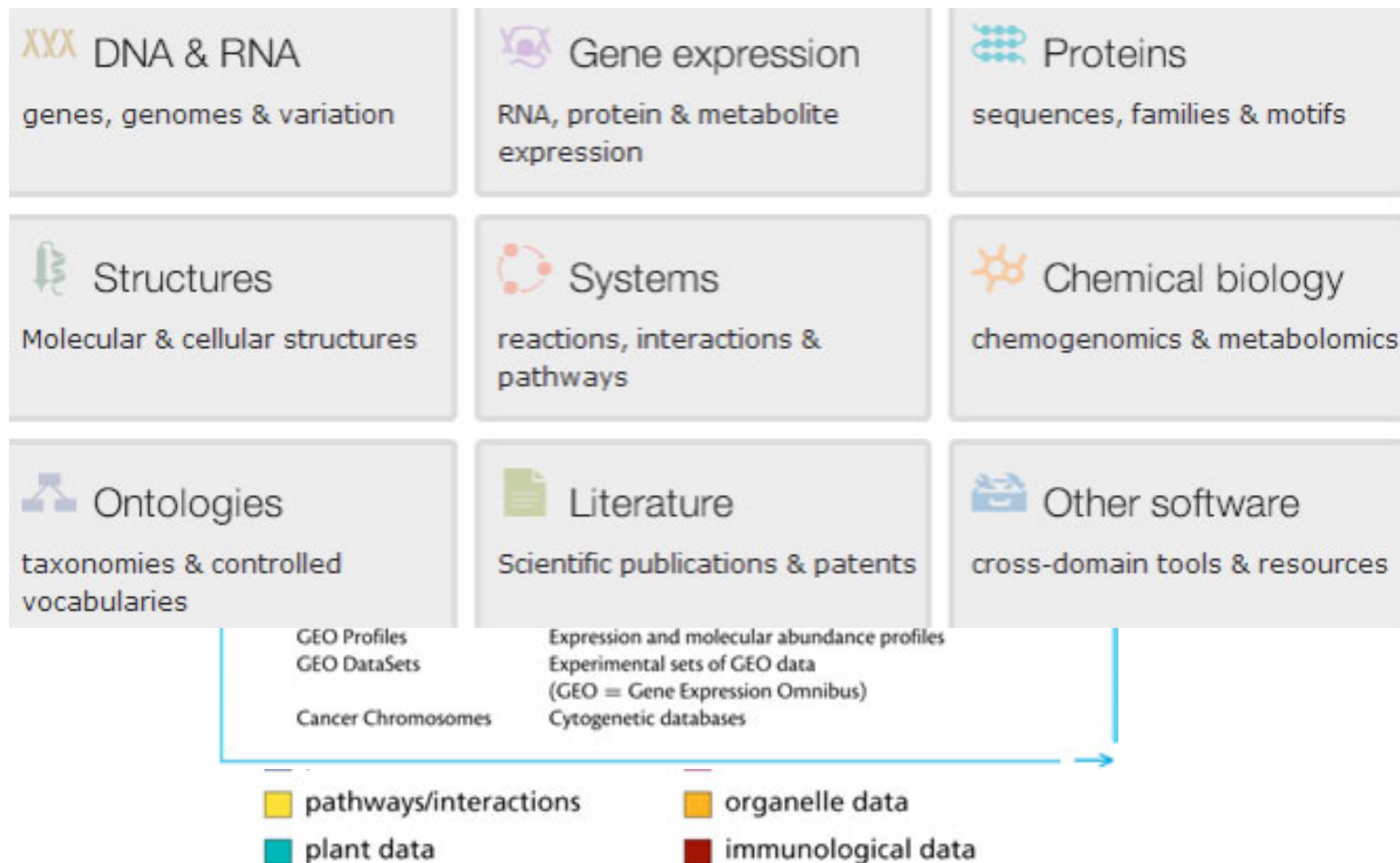
# Data warehouse



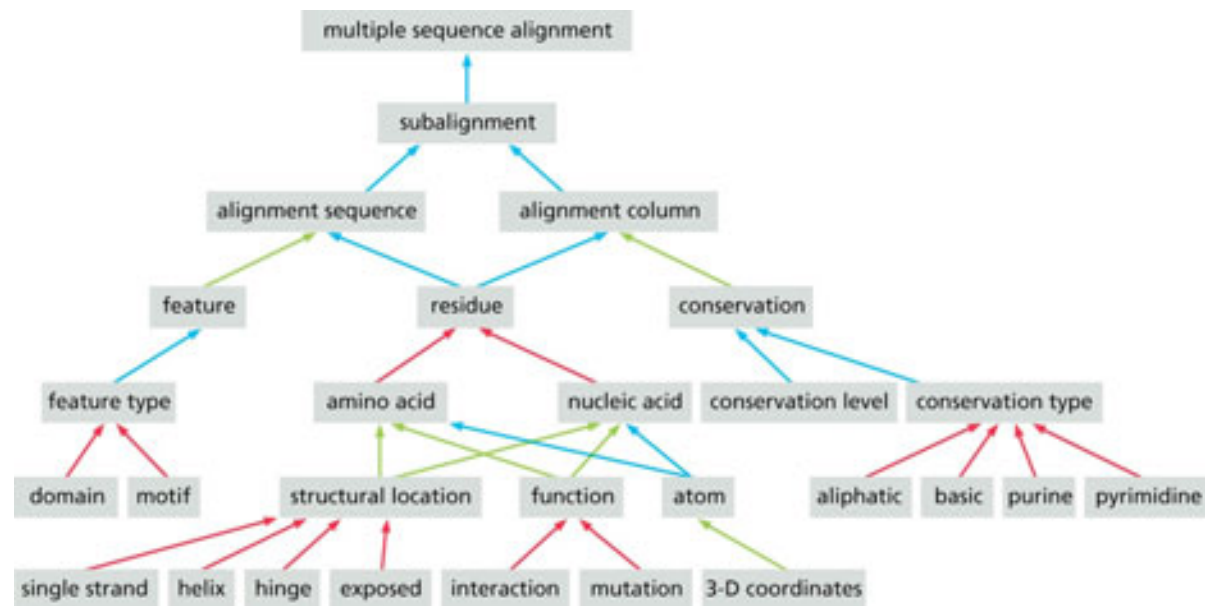
# Data warehouse



# Types of databases



# MAO ontology





# Database providers

- The National Center for Biotechnology Information (NCBI) offers data banks, databases and tools at the USA
- The European Bioinformatics Institute (EBI) does a similar function in Europe
- GenomeNet gathers several databases from Japan



# Data quality

- How are things entered
- What are the evidence ?
- How new is the data.
- Can the data be secret ?
- Redundant or non-redundant ?







# Database providers

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- GenomeNet gathers several databases from Japan



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### NCBI Announcements

Milestone: NCBI annotates 150th eukaryotic genome

Aug 28, 2014

NCBI has now completed the genome annotation for 150 different eukaryotes

The new NCBI Genomes FTP site is here!

Aug 26, 2014

NCBI has released a major revision of the

# The European Bioinformatics Institute

Part of the European Molecular Biology Laboratory

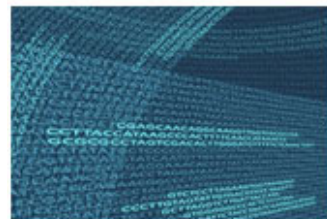
EMBL-EBI provides freely available [data from life science experiments](#), performs [basic research](#) in computational biology and offers an extensive [user training](#) programme, supporting researchers in [academia](#) and [industry](#).

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Examples: [blast](#), [keratin](#), [bfi1](#)...

## News from EMBL-EBI



### The new, improved human genome

Ensembl has incorporated a vast amount of knowledge into a fully annotated reference human genome, GRCh38, providing a solid foundation for future genomics research.



### New Genomics API from the Global Alliance for Genomics and Health

New software allows researchers to share anonymised genetic data seamlessly across platforms.



### Marmoset genome sheds light on chimeral twins

Initial analyses of the marmoset genome provide insight into this tiny primate's reproductive system, which is well adapted to multiple births. The marmoset sequence is freely available in the Ensembl genome explorer.

[Read more press release](#)

European Molecular Biology Laboratory

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Sep 23 2014

Registration deadline: Sep 16 2014

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Sep 29 2014 - Sep 30 2014

Registration deadline: Sep 12 2014

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**GenomeNet**

About GenomeNet  
Release notes  
Acknowledgments

**DBGET**

Overview  
DB release info

**KEGG****varDB****Community DBs**

**Bioinformatics tools**  
Other tools

**FTP****Feedback****GenomeNet Database Resources****DBGET:** Integrated Database Retrieval System

DBGET search

LinkDB search SPARQL endpoint available *New!***KEGG:** Kyoto Encyclopedia of Genes and Genomes

KEGG2 - Table of contents

KEGG PATHWAY - Systems information: pathways

KEGG BRITE - Systems information: ontologies

KEGG Organisms - Organism-specific entry points

KEGG GENES - Genomic information

KEGG LIGAND - Chemical information

KEGG MEDICUS - Health information

**Reaction Ontology:** Reaction classifications**varDB:** Antigenic variation database**Community Databases**

CYORF - Cyanobacteria annotation database

BSORF - Bacillus subtilis genome database

EXPRESSION - Gene expression profile database

**BRITE Functional Hierarchies**

KEGG Pathway Maps

KEGG Organisms

**Genome Catalogs**

Complete (KEGG GENES)

Draft (KEGG DGENES)

Meta (KEGG MGENES)

Viral (KEGG VGENES)

EST (EGENES)

Ortholog Clusters (OC)



Database links

**GenomeNet Bioinformatics Tools****Sequence Analysis**

BLAST / FASTA - Sequence similarity search

Ribosomal databases are available *Updated!*

MOTIF - Sequence motif search

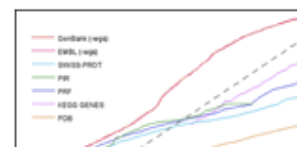
CLUSTALW / MAFFT / PRN - Multiple alignment

**Genome Analysis**OC Viewer - KEGG ortholog clusters *Updated!*

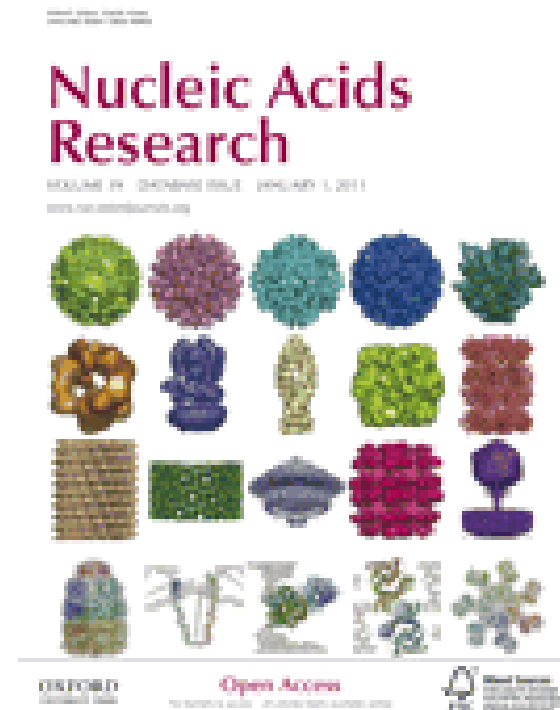
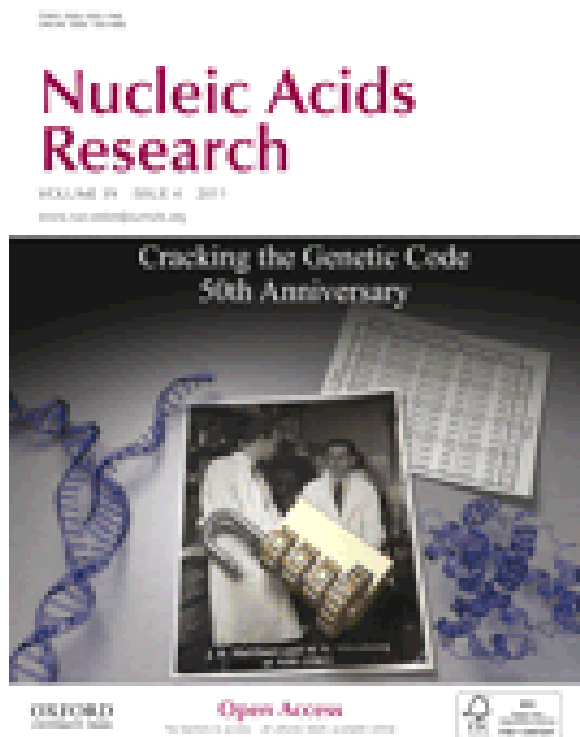
REST service is available

KAAS - KEGG automatic annotation server

MAGE - Functional annotation



# NAR database issue







# Nucleotide databases



- International nucleotide sequence database collaborations

- Genbank
- EMBL
- DDBJ

The nucleotide sequence databases are data repositories, accepting nucleic acid sequence data from the scientific community and making it freely available. The databases strive for completeness, with the aim of recording every publicly known nucleic acid sequence. These data are heterogenous, they vary with respect to the source of the material (e.g. genomic versus cDNA), the intended quality (e.g. finished versus single pass sequences), the extent of sequence annotation and the intended completeness of the sequence relative to its biological target (e.g. complete versus partial coverage of a gene or a genome). The nucleotide databases are distributed free of charge over the internet.

# Genbank entry

```
LOCUS       NM_005358               7235 bp    mRNA      linear   PRI 02-AUG-2006
DEFINITION   Homo sapiens LIM domain 7 (LMO7), mRNA.
ACCESSION    NM_005358
VERSION      NM_005358.4      GI:111119012
KEYWORDS     .
SOURCE       Homo sapiens (human)
  ...
  gene       1..7235
            /gene="LMO7"
            /note="synonyms: LOMP, FBX20, FBXO20, KIAA0858"
            /db_xref="GeneID:4008"
            /db_xref="HGNC:6646"
            /db_xref="HPRD:05078"
            /db_xref="MIM:604362"
CDS          1261..5310
            /gene="LMO7"
ORIGIN
1  ggaataaagt ggaataatta ggaacctagg gtggggtagg gtgacgagac atttcaaa
61  ttaaatgagca tatgagattc caggctctgt taaaaatgca attctgtatt agctgtgtag
121  tgaggtctga gattgtgcat ttctaaacaa cactcagata attctaaagg tgttggccc
181  aggggtcacac tatagtgat ttctagaac ccaagtgggg aagtgaatct tgggcaggag
241  aaatacacac ctctctgcat gagtttgagg atctcatctg atataacttt ttaagaagaa
301  aaaaatttt tccaaatatt caattgataa gctttcccaa taagtggctt tcccactaag
361  tggctcggtt atgaaaattg ctctcaattg aaactctctg tcttggtaat atagaaattc
421  ttgtttctca cagtgtctga ttgagttat gatattgaga ttatggcata aaatatagtg
481  actgtacaaa aaaaaataca ttattaggat ctctaaacat tatgtaaaag tcaattgttc
541  actggttaga ctcaaacctt ggtgtgagac ctggttttat tcttggaact tcatctgagt
601  tgtcttaggc aaattaatac cttaagcaaa aaatatctca tgtacatttt acatgagaat
661  tataaataaa gttacagatt gatgaattc aaatatgtgc tacaagtata gggcaagtgc
721  aagactgcga tcagctatag tgaagtagt ctcaaaagat gtttcatata tcatcagatt
781  cacctaattt tctaaagaat ttaataaagg agatggaatg aatagattgc attttgtttc
841  catgcacagg ggaactgtgc atatttcttc tgtgactcgg aaatggttta ctttttaaaa
901  atctccgaat tctaaagaat tcaataaagg actgctcat atgccaacac ttttatgtga
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2461 gatcagaagt ggcaggatga ccttgcaaaa tggaaaagat gtcgcaaaa gtacaactta
2521 gatctcgaga agaaaaaaga agagagagaa gaaattgaaa agcaggcatg ttacagattc
2581 aagaagaact ctaagacggt taaggaaatg ctgcaggaca ggaatcccaa aaatacaaaa
2641 tctaaccttc ctcaactctc ctgtctgata ctgtctgtgc ggaagtgcg atgtgcagct
2701 gcacccccta caagtactgt ctgacagaa agttaccaga gtgagagagt aagaagagaag
2761 ggagcaactt atccttcaga aattccccaa gaagattcta ccaattttgc aaaaagagag
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2881 gctctcttgt ctcaactctc ctcaactctc atcactcttc caagctttac ttctcagagt
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3181 gagtagcag caacagaaga aggtgcctct ctctcacttc cccctctcca
3241 tctctttccc aagaccaggc tgccactctt aaagccactt tgtcttccac attctgtctt
3301 gatttaagt ctgaatcagt aagaaggaaa atctccccac aaagaagaat ctcaagatcc
3361 cagatcttgt ctcaactctc ctcaactctc atcactcttc ctctcacttc acactctctc
3421 tttggtttta caataaaaat ggaattctct gggattcttc tagctcaggt tgaagcaggt
3481 agcccgacg aattttctca gctacaagta gatgatgaaa ttattgtatt taaacaacac
3541 aagttttcat ataacgattc aaaaagtggt gaggaagcca tggctaaagg tcaagaanaa
3601 ggacacctag tgatggatgt gaggcgctat gaaaaggctg gttcaactga acaaaaatgg
```



# Genbank details

```
LOCUS      NM_005358                7235 bp    mRNA    linear    PRI 02-AUG-2006
DEFINITION Homo sapiens LIM domain 7 (LMO7), mRNA.
ACCESSION  NM_005358
VERSION    NM_005358.4   GI:111119012
KEYWORDS   .
SOURCE     Homo sapiens (human)
```

...


```
gene       1..7235
           /gene="LMO7"
           /note="synonyms: LOMP, FBX20, FBXO20, KIAA0858"
           /db_xref="GeneID:4008"
           /db_xref="HGNC:6646"
           /db_xref="HPRD:05078"
           /db_xref="MIM:604362"

CDS        1261..5310
           /gene="LMO7"
```

ORIGIN


```
1 ggaaagaagt ggaataatta ggaacctagg gtggggtagg gtagcaggac atttcaaaca
```

# Genome specific databases



UNIVERSITY OF CALIFORNIA SANTA CRUZ UCSC Genome Browser

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interactively visualize genomic data
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rapidly align sequences to the genome
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download data from the Genome Browser database
- **Variant Annotation Integrator**  
get functional effect predictions for variant calls
- **Data Integrator**  
combine data sources from the Genome Browser database
- **Gene Sorter**  
find genes that are similar by expression and other metrics
- **Genome Browser in a Box (GBIB)**  
run the Genome Browser on your laptop or server
- **In-Silico PCR**  
rapidly align PCR primer pairs to the genome
- **LiftOver**  
convert genome coordinates between assemblies
- **VisiGene**  
interactively view in situ images of mouse and frog

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Search: All species for Go  
e.g. BRCA2 or rat S:52797383-63627988 or rs696 or coronary heart disease

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 <b>Mouse</b> GRCm38.p6	 <b>Zebrafish</b> GRCz10

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

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 <b>Anole lizard</b> <i>Anolis carolinensis</i> AnoCar2.0	 <b>Gorilla</b> <i>Gorilla gorilla</i> gorGor3.1	 <b>Platypus</b> <i>Ornithorhynchus anatinus</i> OANAS
 <b>Armadillo</b> <i>Dasypus novemcinctus</i> dasNov2	 <b>Guinea Pig</b> <i>Cavia porcellus</i> cavPor3	 <b>Rabbit</b> <i>Oryctolagus cuniculus</i> oryGus2
 <b>Baboon</b> ( <a href="#">preview...assembly only</a> ) <i>Papio hamadryas</i> Pham	 <b>Hedgehog</b> <i>Eriochrome europaeus</i> HEEDGEHOG	 <b>Rat</b> ( <a href="#">preview...new assembly (Rnor_5.0)</a> ) <i>Rattus norvegicus</i> RNO5.0.4
 <b>Budgerigar</b> ( <a href="#">preview...assembly only</a> ) <i>Melopsittacus undulatus</i> MelUnd0.3	 <b>Horse</b> <i>Equus caballus</i> EquCab2	 <b>Saccharomyces cerevisiae</b> <i>Saccharomyces cerevisiae</i> EF4
 <b>Bushbaby</b> <i>Otilomys Garretti</i> OtiGar3	 <b>Human</b> <i>Homo sapiens</i> GRCh37	 <b>Sheep</b> ( <a href="#">preview...assembly only</a> ) <i>Ovis aries</i> oviAri1
 <b>Clonostroma</b> <i>Clonostroma</i> Clon	 <b>Myxine</b> <i>Procris capensis</i> proCap1	 <b>Shrew</b> <i>Sorex araneus</i> COMMON_SHREW1
 <b>Clonostroma</b> <i>Clonostroma</i> Clon	 <b>Kangaroo rat</b> <i>Dipodomys ordii</i> dipOrd1	 <b>Sieth</b> <i>Chiropterus Hoffmanni</i> chiHof1
 <b>Caenorhabditis elegans</b> <i>Caenorhabditis elegans</i> WbIs215	 <b>Lamprey</b> <i>Petromyzon Marinus</i> Pmarinus_7.0	 <b>Spotted Gar</b> ( <a href="#">preview...assembly only</a> ) <i>Lepisosteus oculatus</i> lepOcu1
 <b>Cat</b> ( <a href="#">preview...new assembly (Felis_satus-5.0)</a> ) <i>Felis catus</i> CAT	 <b>Lesser hedgehog tenrec</b> <i>Echinops telfairi</i> TENREC	 <b>Squirrel</b> <i>Sciurus hudsonicus</i> sqhH2
 <b>Chicken</b> ( <a href="#">preview...new assembly (Gallus_gallus)</a> ) <i>Gallus gallus</i> WASHUC2	 <b>Macaque</b> <i>Macaca mulatta</i> MMA_1	 <b>Squirrel monkey</b> ( <a href="#">preview...assembly only</a> ) <i>Saimiri boliviensis</i> SaiBol1.0
 <b>Chimpanzee</b> ( <a href="#">preview...new assembly (Pan_troglodytes_2.1.0)</a> ) <i>Pan troglodytes</i>	 <b>Marmoset</b> <i>Callithrix jacchus</i>	 <b>Stickleback</b> <i>Gasterosteus aculeatus</i>



# Protein Databases

- Sequences are in Uniprot
- Structures are in PDB
- Enzyme classifications EC
- Protein families: Pfam, Interpro etc

	<b>UniProt: The Universal Protein Resource</b> The gold-standard, comprehensive resource for protein sequence and functional annotation data.
	<b>PRIDE: The Proteomics Identifications Database</b> An archive of protein expression data determined by mass spectrometry.
	<b>InterPro</b> A database for the classification of proteins into families, domains and conserved sites.
	<b>Pfam</b> A database of hidden Markov models and alignments to describe conserved protein families and domains.
	<b>Clustal Omega</b> Multiple sequence alignment of DNA or protein sequences. Clustal Omega replaces the older ClustalW alignment tools.
	<b>InterProScan 5</b> InterProScan 5 searches sequences against InterPro's predictive protein signatures. Please note that <u>InterProScan 4.6 has been retired</u> .
	<b>Clustal Phylogeny</b> Commonly used phylogenetic tree generation methods provided by the ClustalW2 program.
	<b>NCBI BLAST (protein)</b> Fast local similarity search tool for protein sequence databases.
	<b>Protein Data Bank in Europe</b> The European resource for the collection, organisation and dissemination of 3D structural data (from PDB and EMDB) on biological macromolecules and their complexes.

# Uniprot

## [UniProtKB](#)

Protein knowledgebase, consists of two sections:

1. Swiss-Prot, which is manually annotated and reviewed.
2. TrEMBL, which is automatically annotated and is **not** reviewed.

Includes [complete and reference proteome sets](#).

## [UniRef](#)

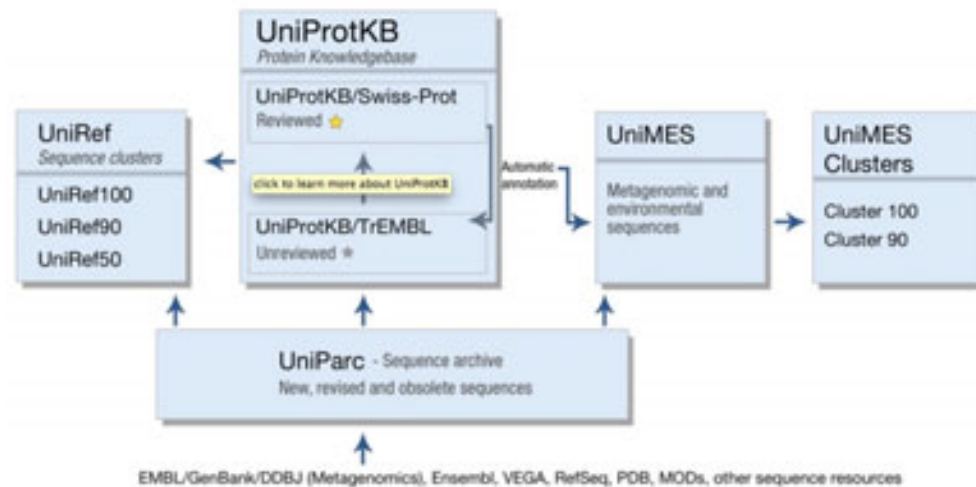
Sequence clusters, used to speed up sequence similarity searches.

## [UniParc](#)

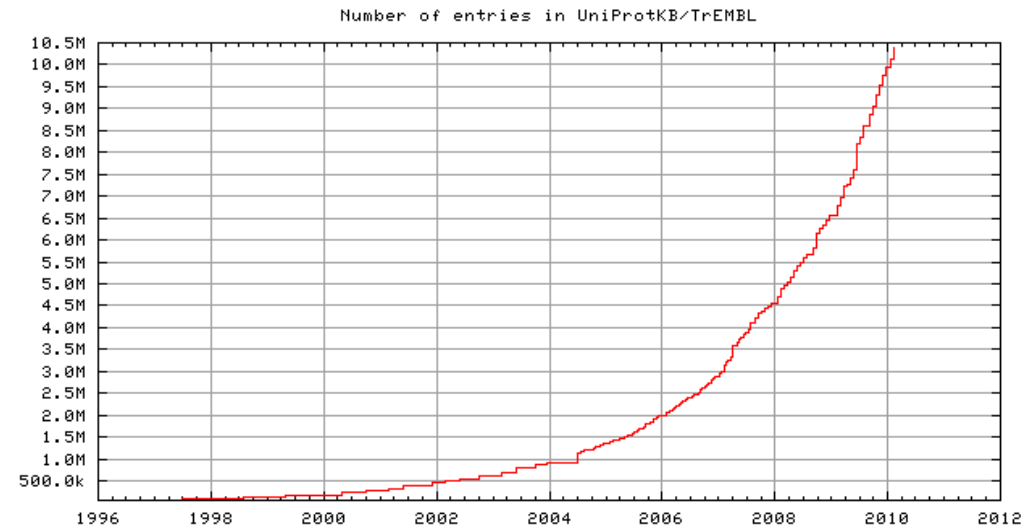
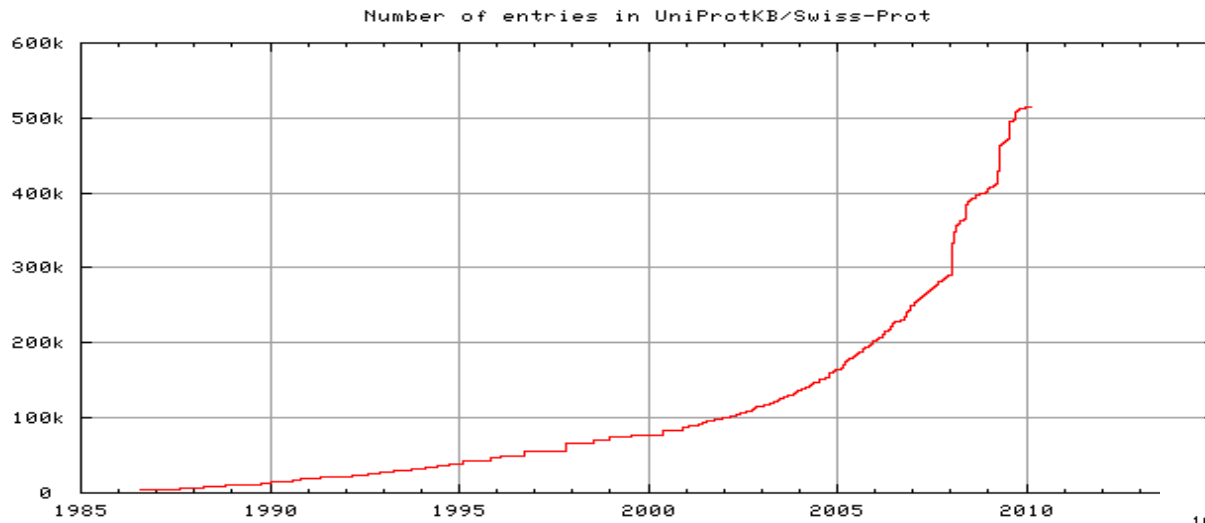
Sequence archive, used to keep track of sequences and their identifiers.

Supporting data

[Literature citations](#), [taxonomy](#), [keywords](#), [subcellular locations](#), [cross-referenced databases](#) and [more](#).



# Growth of Protein sequences



# One uniprot entry

www.uniprot.org/uniprot/Q7ZWK8

Uniprot - UniProtKB

Search in: Protein Knowledgebase (UniProtKB) Query Search Advanced Search Clear

**Q7ZWK8 (OTOP1\_DANRE)** Reviewed, UniProtKB/Swiss-Prot  
Last modified April 18, 2012, Version 44 History

Clusters with 100%, 90%, 50% identity | Documents (2) | Third-party data

Names Attributes General annotation Ontologies Sequence annotation Sequences References Web links Cross-refs Entry info Documents Customize order

### Names and origin

Protein names	Recommended name: <b>Otopetrin-1</b>
Gene names	Name: <i>otop1</i>
Organism	<i>Danio rerio</i> (Zebrafish) ( <i>Brachydanio rerio</i> ) [Reference proteome]
Taxonomic identifier	7955 [NCBI]
Taxonomic lineage	Eukaryota • Metazoa • Chordata • Olfactores • Vertebrata • Euteleostomi • Actinopterygii • Neopterygii • Teleostei • Ostariophysi • Cypriniformes • Cyprinidae • Danio

### Protein attributes

Sequence length	586 AA
Sequence status	Complete
Protein existence	Evidence at protein level

### General annotation (Comments)

Function	Inhibits P2Y purinoceptors. Modulates calcium homeostasis and influx of calcium in response to extracellular ATP [By similarity]. Essential for the formation of otoliths in the inner ear of developing larvae and for the perception of gravity and acceleration. [Ref.1] [Ref.4]
Subcellular location	Membrane; Multi-pass membrane protein. Secreted • extracellular space [By similarity] [Ref.1]
Developmental stage	First detected in the otic placode at 18.5 hours post-fertilization (hpf). Detected in the developing inner ear sensory epithelium at 24 hpf. Detected in hair cells of the sensory epithelium at 4 days post-fertilization (dpf). At 5 dpf, levels are much reduced in the otolith organs, and not detectable at 7 dpf. Detected in neuromasts and in the lateral line system at 5 dpf and 7 dpf. [Ref.1] [Ref.4]
Disruption phenotype	Fishes display the backstroke phenotype. Mutant fish exhibit otolith agenesis without additional effects on the sensory epithelium or other inner ear structures. Otoliths are essential for the perception of gravity and acceleration. Larvae without otoliths are unable to orient dorsal side up and rest mostly on their side in contact with the ground. [Ref.1] [Ref.4]
Miscellaneous	Otoliths are structures composed of proteins and calcium carbonate that are found in the fish inner ear in contact with the otic epithelium. They are essential for the perception of gravity and acceleration.
Sequence similarities	Belongs to the <i>otopetrin</i> family.

### Ontologies

Keywords	
Biological process	Biomineralization
Cellular component	Membrane Secreted
Domain	Transmembrane Transmembrane helix
Technical term	Complete proteome Reference proteome



PDB

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# An Information Portal to Biological Macromolecular Structures

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☒ PDB ID or keyword 
 ☐ Author 
 
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- Deselect All
- Download Selected
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- Narrow Query
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- Results per Page
- Show Query Details
- Results Help

91 Structure Hits
127 Web Page Hits
1 Unreleased Structure


1 2 3 4 5 .. 10 ↻

<input checked="" type="checkbox"/> 1X6Z	 Characteristics Classification Compound Authors	<b>Solution structure of the LIM domain of carboxyl terminal LIM domain protein 1</b>  Release Date: 17-Nov-2005 Exp. Method: NMR 20 Structures <b>Structural Protein</b> Mol. Id: 1 Molecule: C Terminal Lim Domain Protein 1 Fragment: Lim Domain Qin, X.R., Nagashima, T., Hayashi, F., Yokoyama, S.
<input checked="" type="checkbox"/> 1X4K	 Characteristics Classification Compound Authors	<b>Solution structure of LIM domain in LIM-protein 3</b>  Release Date: 14-Nov-2005 Exp. Method: NMR 20 Structures <b>Metal Binding Protein</b> Mol. Id: 1 Molecule: Skeletal Muscle Lim Protein 3 Fragment: Lim Domain He, F., Muto, Y., Inoue, M., Kigawa, T., Shirouzu, M., Terada, T., Yokoyama,
<input checked="" type="checkbox"/> 1X4L	 Characteristics Classification Compound Authors	<b>Solution structure of LIM domain in Four and a half LIM domains protein 2</b>  Release Date: 14-Nov-2005 Exp. Method: NMR 20 Structures <b>Metal Binding Protein</b> Mol. Id: 1 Molecule: Skeletal Muscle Lim Protein 3 Fragment: Lim Domain He, F., Muto, Y., Inoue, M., Kigawa, T., Shirouzu, M., Terada, T., Yokoyama,

# PDB



PROTEIN DATA BANK

A MEMBER OF THE 

An Information Portal to Biological Macromolecular Structures

As of Tuesday Aug 07, 2001 there are 45055 Structures | PDB Statistics

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- 1FAA
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**Quick Tips:**

When exploring a structure, select Structure Analysis and then Geometry from the left menu to view a Ramachandran Plot.

Are you missing data updates? The PDB archive has moved to [ftp://ftp.wwpdb.org](http://ftp.wwpdb.org). For more information click here.

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**1faa**   DOI: 10.2210/pdb/1faa/pdb

Red - Derived information

Title	CRYSTAL STRUCTURE OF THOREDOXIN F FROM SPINACH CHLOROPLAST (LONG FORM)										
Authors	Capitant, G., Markovic-Housley, Z., DeVal, G., Morris, M., Janssens, J.N., Schumann, P.										
Primary Citation	Capitant, G., Markovic-Housley, Z., DeVal, G., Morris, M., Janssens, J.N., Schumann, P. Crystal structures of two functionally different thoredoxins in spinach chloroplasts. <i>J.Mol.Biol.</i> #502 pp. 133-154, 2000 [Abstract]										
History	Deposition	2000-07-13	Release 2000-09-20								
Experimental Method	Type	X-RAY DIFFRACTION Data [ EDS ]									
Parameters	Resolution [Å]	R-value	R-free								
	1.85	0.209 (work)	0.258								
		Space Group	P 2 <sub>1</sub> (P 1 2 <sub>1</sub> 1)								
Unit Cell	Length [Å]	a	30.60								
	Angles [°]	alpha	90.00								
		beta	116.70								
		gamma	90.00								
Molecular Description Asymmetric Unit	Polymer: 1 Molecule: THOREDOXIN F Fragment: LONG FORM Mutation: M1L, Q3L Chain: A										
Classification	Electron Transport										
Source	Polymer: 1 Scientific Name: <b>Spinacia oleracea</b> Common Name: <b>Spinach</b> Expression system: <b>Escherichia coli</b>										
Related PDB Entries	<table border="1"> <tr> <th>ID</th> <th>Details</th> </tr> <tr> <td>1F86</td> <td>thoredoxin m from spinach chloroplast (oxidized form)</td> </tr> <tr> <td>1F80</td> <td>thoredoxin m from spinach chloroplast (reduced form)</td> </tr> <tr> <td>1F9M</td> <td>thoredoxin f from spinach chloroplast (short form)</td> </tr> </table>			ID	Details	1F86	thoredoxin m from spinach chloroplast (oxidized form)	1F80	thoredoxin m from spinach chloroplast (reduced form)	1F9M	thoredoxin f from spinach chloroplast (short form)
ID	Details										
1F86	thoredoxin m from spinach chloroplast (oxidized form)										
1F80	thoredoxin m from spinach chloroplast (reduced form)										
1F9M	thoredoxin f from spinach chloroplast (short form)										
SCOP Classification (version 1.75)	Domain info	Class	Fold								
	1faa_	alpha and beta proteins	Thoredoxin fold								
			Thoredoxin like								
			Thioredoxinase								
			Thoredoxin								
			Spinacia oleracea, thoredoxin f								
CATH Classification (version 3.1.1)	Domain	Class	Architecture								
	1faa400	alpha beta	3-Layer/alpha Sandwich								
Topology	Gutted down										
Homology	Gutted down										
GO Terms	Polymer	Molecular Function	Biological Process								
	THOREDOXIN F (1FAA)	• none	<ul style="list-style-type: none"> <li>cell redox homeostasis</li> <li>cell redox homeostasis</li> </ul>								
			Cellular Component								
			• none								

Images and Visualization

<< Biological Molecule >>



Display Options

☐ RING  
☐ mol  
☐ WorkSet  
☐ RST Superimpose  
☐ RST Protein Workshop  
☐ QuickPDB  
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 \* Capable of displaying biological molecules

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# Pfam



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## Family: 7tm\_1 (PF00001)

326 architectures   28505 sequences   0 interactions   164 species   215 structures

### Summary

[Domain organisation](#)

[Clan](#)

[Alignments](#)

[HMM logo](#)

[Trees](#)

[Curation & model](#)

[Species](#)

[Interactions](#)

[Structures](#)

Jump to... ↓

enter ID/acc

Go

### Summary: 7 transmembrane receptor (rhodopsin family)

Pfam includes annotations and additional family information from a range of different sources. These sources can be accessed via the tabs below.

[Wikipedia: Rhodopsin-like receptors](#)

[Pfam](#)

[InterPro](#)

This is the Wikipedia entry entitled "[Rhodopsin-like receptors](#)". [More...](#)

### Rhodopsin-like receptors [Edit Wikipedia article](#)

**Rhodopsin-like receptors** are a family of proteins that comprise the largest group of G protein-coupled receptors.<sup>[2]</sup>

Contents [\[hide\]](#)

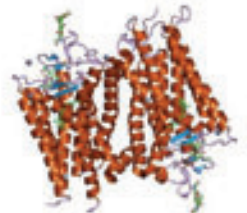
1 Scope

2 Function

3 Classes

- 3.1 Subfamily A1
- 3.2 Subfamily A2
- 3.3 Subfamily A3
- 3.4 Subfamily A4
- 3.5 Subfamily A5
- 3.6 Subfamily A6
- 3.7 Subfamily A7
- 3.8 Subfamily A8
- 3.9 Subfamily A9
- 3.10 Subfamily A10
- 3.11 Subfamily A11
- 3.12 Subfamily A12
- 3.13 Subfamily A13
- 3.14 Subfamily A14
- 3.15 Subfamily A15
- 3.16 Subfamily A16
- 3.17 Subfamily A17
- 3.18 Subfamily A18
- 3.19 Subfamily A19

### Rhodopsin-like receptors



Structure of rhodopsin: A G protein-coupled receptor.<sup>[1]</sup>

#### Identifiers

Symbol	7tm_1
Pfam	PF00001 <a href="#">↗</a>
InterPro	IPR000276 <a href="#">↗</a>
PROSITE	PDOC00211 <a href="#">↗</a>
SCOP	1f88 <a href="#">↗</a>
SUPERFAMILY	1f88 <a href="#">↗</a>
OPM superfamily	6 <a href="#">↗</a>
OPM protein	1gzm <a href="#">↗</a>

# CATH (and related databases such as SCOP, ECOD)

## Browse CATH-Gene3D Hierarchy

BROWSE LINKS

**Browse Hierarchy**

[Highly Diverse Superfamilies](#)


[Superfamily Comparison](#)

Select a CATH node...

**A** Orthogonal Bundle

CATH ID

Topologies	288
Superfamilies	542
Domains	33657
Example Domain	<a href="#">1xmkA00 [PDB]</a>



 Tree

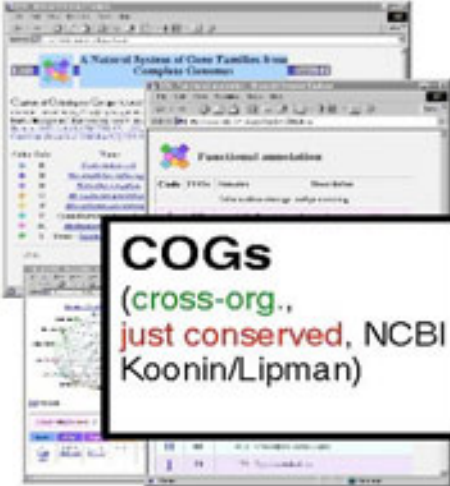
 Sunburst

### Top of CATH Hierarchy (4 Classes)

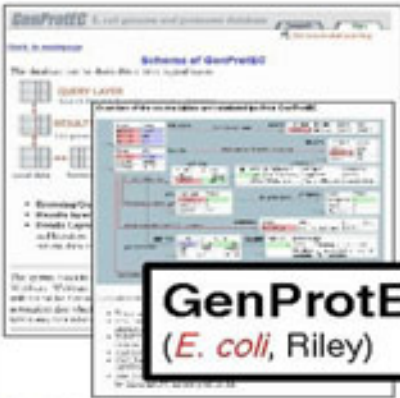
- C 1** Mainly Alpha
  - A 1.10** Orthogonal Bundle
    - 5 Architectures, 397 Folds, 907 Superfamilies, 48121 Domains
  - A 1.20** Up-down Bundle
    - 288 Folds, 542 Superfamilies, 33657 Domains
  - A 1.25** Alpha Horseshoe
    - 101 Folds, 332 Superfamilies, 12774 Domains
  - A 1.40** Alpha solenoid
    - 5 Folds, 27 Superfamilies, 1104 Domains
  - A 1.50** Alpha/alpha barrel
    - 1 Fold, 1 Superfamilies, 11 Domains
- C 2** Mainly Beta
  - 2 Folds, 5 Superfamilies, 575 Domains
- C 3** Alpha Beta
  - 20 Architectures, 241 Folds, 547 Superfamilies, 58944 Domains
- C 4** Few Secondary Structures
  - 14 Architectures, 626 Folds, 1158 Superfamilies, 125772 Domains
- C 4** Few Secondary Structures
  - 1 Architectures, 111 Folds, 126 Superfamilies, 3021 Domains




# Functional Classification



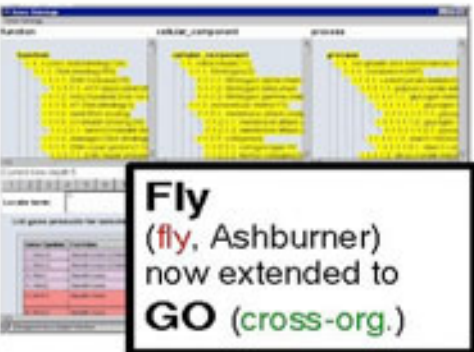
**COGs**  
(**cross-org.**,  
**just conserved**, NCBI  
Koonin/Lipman)



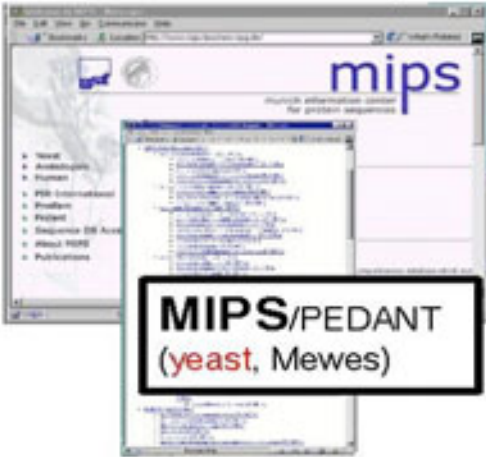
**GenProtEC**  
(*E. coli*, Riley)



**ENZYME**  
(SwissProt  
Bairoch/  
Apweiler,  
**just enzymes**,  
**cross-org.**)



**Fly**  
(**fly**, Ashburner)  
now extended to  
**GO** (**cross-org.**)



**MIPS/PEDANT**  
(**yeast**, Mewes)

Also:  
Other  
SwissProt  
Annotation  
WIT, KEGG  
(**just pathways**)  
TIGR EGAD  
(**human ESTs**)  
SGD (yeast)

# Functional classifications



First figure	Second figure	Third figure
<p><i>A. OXIDOREDUCTASES</i></p> <p>Substrate is oxidised-regarded as the hydrogen or electron donor</p>	Describes substrate acted on by enzyme	Type of acceptor
<p><i>B. TRANSFERASES</i></p> <p>Transfer of a group from one substrate to another</p>	Describes transferred group	Further information on the group transferred
<p><i>C. HYDROLASES</i></p> <p>Hydrolytic cleavage of bond</p>	Describes type of bond	Nature of substrate
<p><i>D. LYASES</i></p> <p>Cleavage of bonds by elimination</p>	Type of bond	Further information on the group eliminated
<p><i>E. ISOMERASES</i></p>	Type of reorganisation	Type of substrate
<p><i>F. LIGASES</i></p> <p>Enzyme catalysing the joining of two molecules in concert with hydrolysis of ATP</p>	Describes type of bond formed	Describes type of compound formed

# EC classifications

# Enzyme Classifications

Class 1. Oxidoreductases

.....

Class 2. Transferases

.....

Class 3. Hydrolases

.....

Class 4. Lyases

.....


Class 5. Isomerases

.....



# Function classifications: GO


← → ↻ amigo.geneontology.org/cgi-bin/amigo/browse.cgi?action=minus\_node&target=GO:0008150&open\_1=GO:0008150,all&session\_id=5155amigo1346402134

 **the Gene Ontology** AmiGO

Search **Browse** BLAST Homolog Annotations Tools & Resources Help

Search GO  ☒ terms ☐ genes or proteins ☐ exact match

### Tree Browser

▼ **Filter tree view** 

Filter by ontology

Ontology


- All
- biological process
- cellular component
- molecular function

Filter Gene Product Counts

Data source	Species
All	All
ASAP	Arabidopsis thaliana
AspGD	Aspergillus fumig...
CGD	Aspergillus niger

View Options

Tree view ☒ Full ☐ Compact

☒ all : all [593966 gene products] 

- ☒ **GO:0008150 : biological\_process [449888 gene products]**
- ☒ GO:0005575 : cellular\_component [418948 gene products]
- ☒ GO:0003674 : molecular\_function [479340 gene products]

Actions...

Last action: Closed

GO:0008150

Graphical View

Permalink

Download...

OBO

RDF/XML

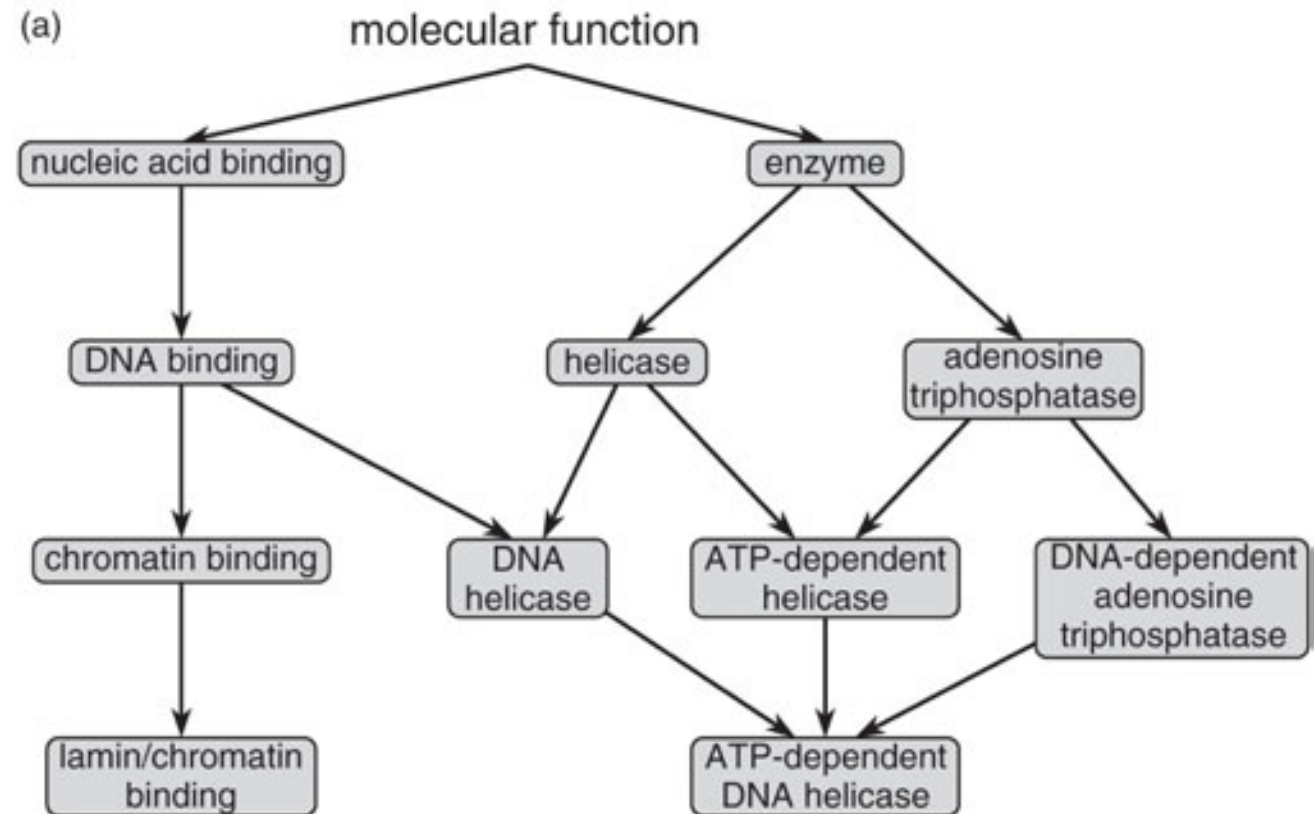
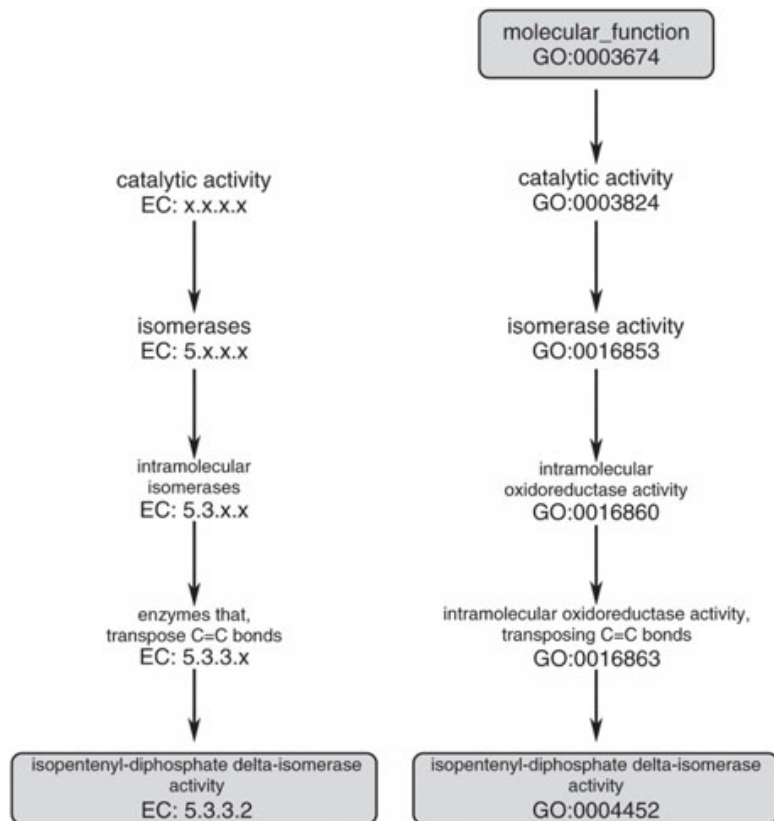
GraphViz dot

AmiGO version: [1.8](#)

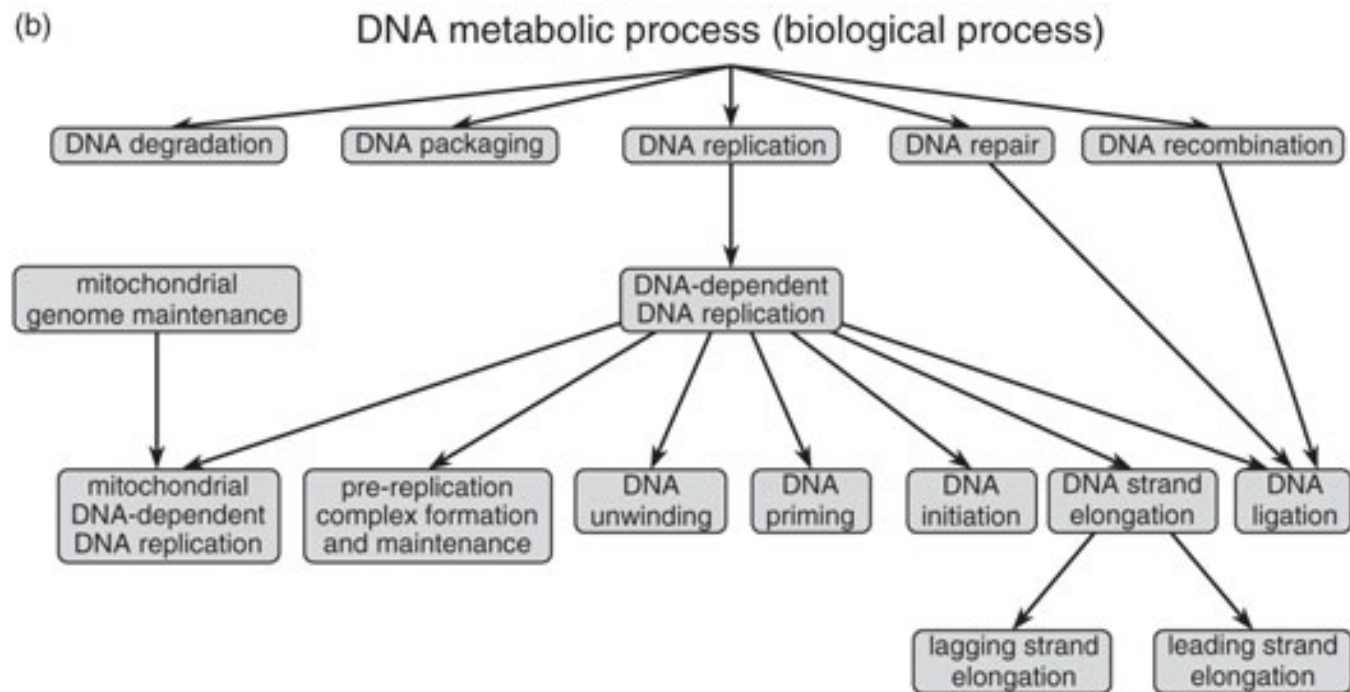
[Try AmiGO Labs](#)

GO database release 2012-08-25  
[Cite this data](#) • [Terms of use](#) • [GO helpdesk](#)  
Copyright © 1999-2010 the Gene Ontology

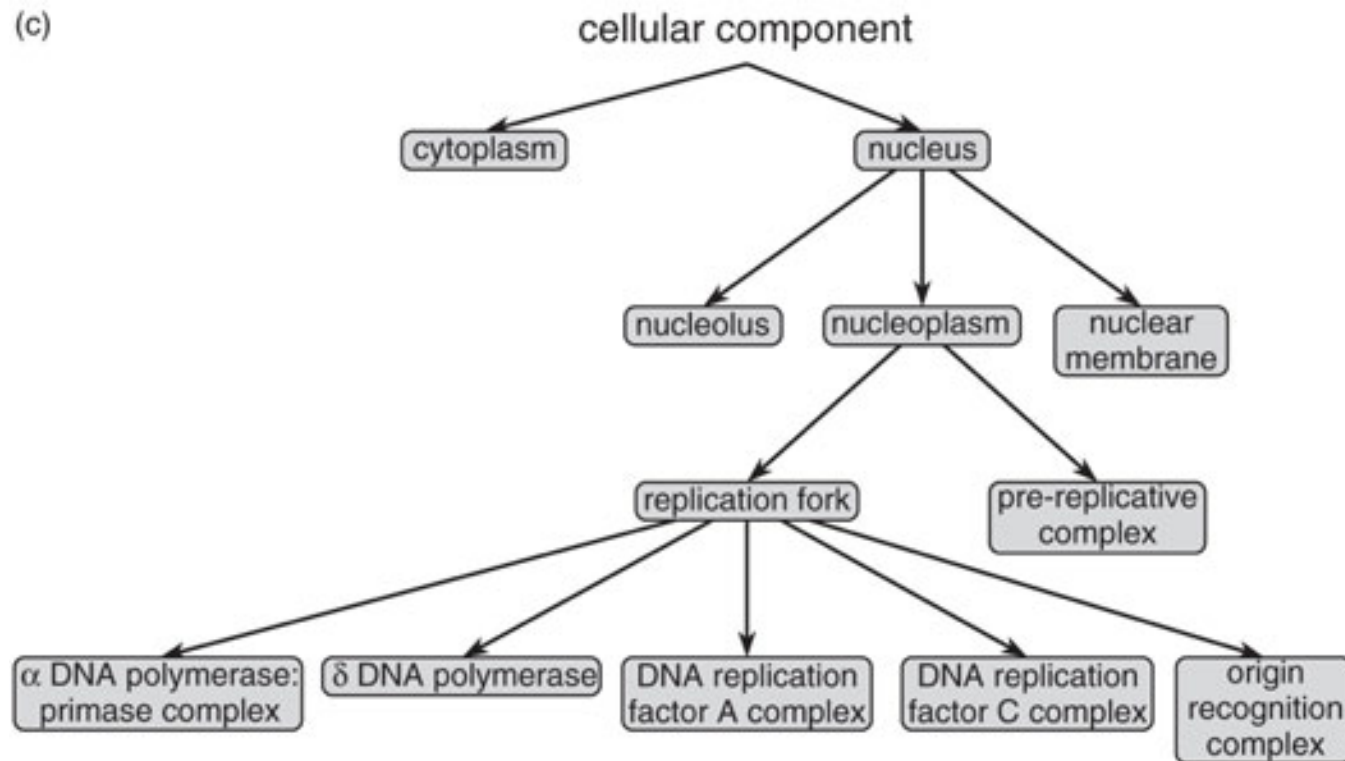
# GO - molecular function



# GO metabolic process



# GO cellular component



# Expression databases

- Gene Expression, GeneExpressAtlas
  - total experiments 3476
  - total genes 692307
- Protein Expression: Pride
  - 25,816 Experiments
  - 11,042,722 Identified Proteins



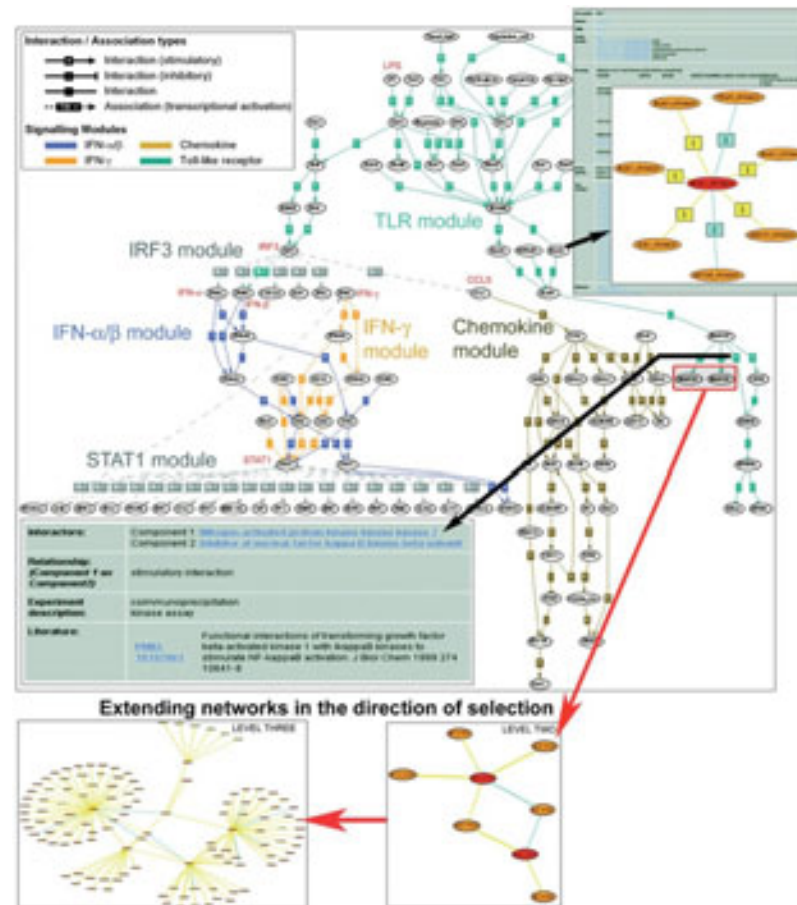
# Molecular Interactions




- Intact:



# Interacting maps



# String Database

[Home](#) • [Download](#) • [Help](#) • [My Data](#) **STRING 9.1**

**STRING - Known and Predicted Protein-Protein Interactions**

search by name

search by protein sequence

multiple names

multiple sequences

protein name: (examples: [#1](#) [#2](#) [#3](#))

(STRING understands a variety of protein names and accessions; you can also try a [random entry](#))


organism:  
auto-detect ▼


interactors wanted:  
☐ COGs ☒ Proteins


please enter your protein of interest...


**What it does ...**

STRING is a database of known and predicted protein interactions. The interactions include direct (physical) and indirect (functional) associations; they are derived from four sources:

Genomic Context  


High-throughput Experiments  


(Conserved) Coexpression  


Previous Knowledge  


STRING quantitatively integrates interaction data from these sources for a large number of organisms, and transfers information between these organisms where applicable. The database currently covers 5'214'234 proteins from 1133 organisms.

**More Info**

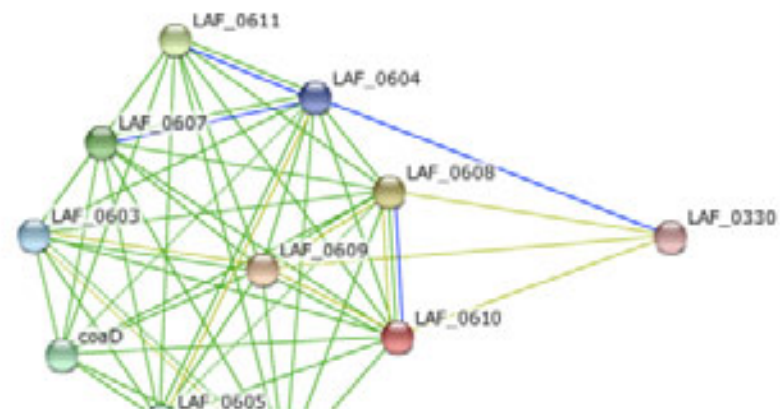
[Funding / Support](#)

[Acknowledgements](#)

[Use Scenarios](#)

STRING (*Search Tool for the Retrieval of Interacting Genes/Proteins*) is being developed at [CPB](#), [EMBL](#), [SIB](#), [KU](#), [TUD](#) and [UZH](#).  
STRING references: [Franceschini et al. 2013](#) / [2011](#) / [2009](#) / [2007](#) / [2005](#) / [2003](#) / [Snel et al. 2000](#).  
Miscellaneous: [Access Statistics](#), [Robot Access Guide](#), [STRING/STITCH Blog](#), [Supported Browsers](#).

**What's New?** This is version 9.1 of STRING - more efficient interolog prediction, and now parsing the *full text* of publications!  
**Sister Projects:** check out [STITCH](#) and [eggNOG](#) - two sister projects built on STRING data!  
**Previous Releases:** Trying to reproduce an earlier finding? Confused? Refer to our [old releases](#).



This is the **evidence view**. Different line colors represent the types of evidence for the association.



(requires flash player 10 or better)

#### Your Input:

- LAF\_0610 competence protein (745 aa)  
(Lactobacillus fermentum)

#### Predicted Functional Partners:

		Neighborhood	Gene Fusion	Cooccurrence	Coexpression	Experiments	Databases	Textmining	[Homology]	Score
LAF_0609	competence protein (159 aa)	•								0.971
LAF_0608	competence protein (324 aa)	•								0.948
LAF_0611	DNA-directed DNA polymerase III delta subunit (342 aa)	•								0.917
LAF_0607	hypothetical protein (349 aa)	•								0.777
coaD	phosphoantennal adenylyltransferase; Reversibly transfers an adenylyl group from ATP to 4'-[...]	•								0.777
LAF_0605	putative N6-adenine-specific methylase (186 aa)	•								0.776
LAF_0603	cell division protein (399 aa)	•								0.776
LAF_0604	hypothetical protein (98 aa)	•								0.677
LAF_0602	GTP-binding protein (615 aa)	•								0.632
LAF_0330	DNA helicase (438 aa)	•								0.632

#### Views:



# Reactions and Pathways

EBI > Databases > Pathways & Networks

## Pathway & Network Databases

The EBI has developed and maintained a number of pathways & networks databases.

Database	Description
<a href="#">BioModels</a>	A database of annotated biological models that allows biologists to store, search and retrieve published mathematical models of biological interests.
<a href="#">IntAct</a>	IntAct is a protein interaction database and analysis system. It provides a query interface and modules to analyse interaction data.
<a href="#">Reactome</a>	A curated database of biological processes in humans. Reactome will not only be useful to general biologists as an online textbook of biology, but also to bioinformaticians for making new discoveries about biological pathways.
<a href="#">Rhea</a> <i>New</i>	Rhea is a freely available, manually annotated database of chemical reactions created in collaboration with the Swiss Institute of Bioinformatics (SIB).



# Gateways

- NCBI - Entrez -Pubmed
- EBI
- SRS
- BioMart
- ExPASy

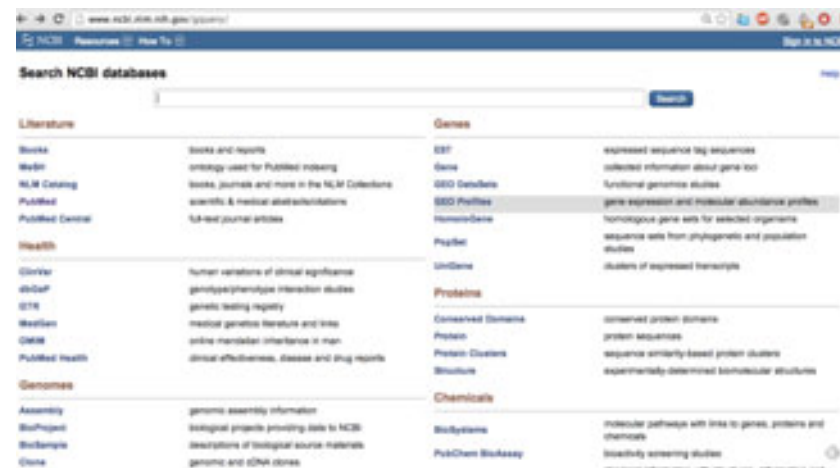


# Entrez

- Entrez searches the following databases:
- PubMed: biomedical literature citations and abstracts, including Medline - articles from full-text resources are provided for articles from the 1990s.
- PubMed Central: free, full-text journal articles
- Site Search: NCBI web and FTP web sites
- Books: online books
- Online Mendelian Inheritance in Man (OMIM)
- Online Mendelian Inheritance in Animals (OMIA)
- Nucleotide: sequence database (GenBank)
- Protein: sequence database
- Genome: whole genome sequences and mapping
- Structure: three-dimensional macromolecular structures
- Taxonomy: organisms in GenBank Taxonomy
- SNP: single nucleotide polymorphism
- Gene: gene-centered information



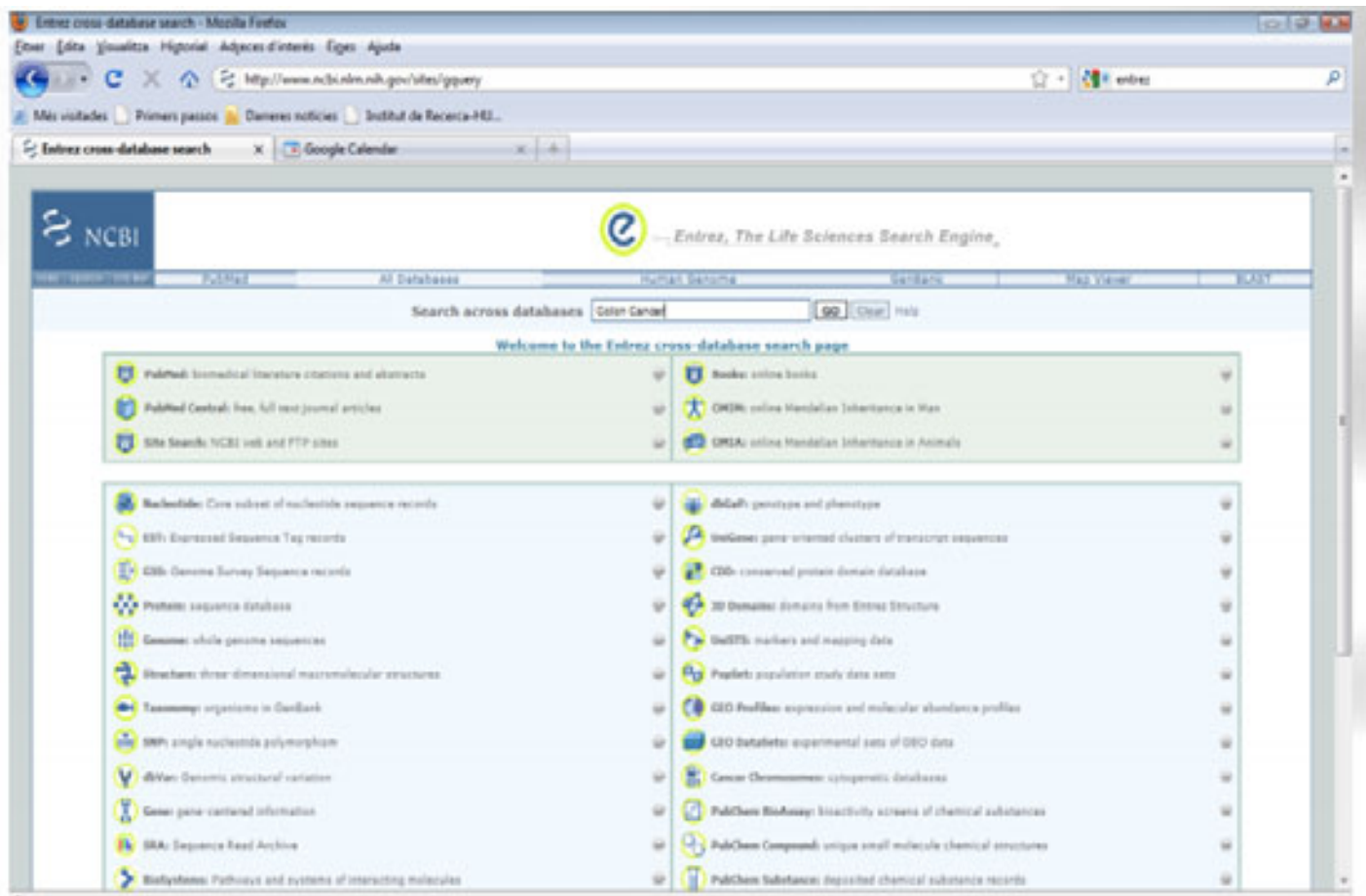
entral and other



From: Alex Sánchez



# Cross search in entrez



# Searching entrez

- Boolean operators: **AND**, **OR**, **NOT**, “”, \*
- **AND** applied by default
- Query by **Accession Numbers (AC)** in
  - Genbank / EMBL / DDBJ:
    - 1 char. + 5 nums. (U12345)
    - 2 char. + 6 nums. (AF123456)
  - SwissProt / PIR:
    - 1 char. + 5 nums. (P12345)
- Refine queries with the reserved word **LIMITS**
- Combine queries with **HISTORY**

# Search fields

Field	Short term	Nucleotide	Available for Database ...			PopSet
			Protein	Genome	Structure	
Accession	ACCN	Yes	Yes	Yes	Yes	Yes
All Fields	ALL	Yes	Yes	Yes	Yes	Yes
Author Name	AUTH	Yes	Yes	Yes	Yes	Yes
EC/RN Number	ECNO	Yes	Yes	Yes	Yes	Yes
Feature Key	FKEY	Yes	No	Yes	No	Yes
Filter	FILT	Yes	Yes	Yes	Yes	Yes
Gene Name	GENE	Yes	Yes	Yes	No	Yes
Issue	ISS	Yes	Yes	Yes	Yes	Yes
Journal Name	JOUR	Yes	Yes	Yes	Yes	Yes
Keyword	KYWD	Yes	Yes	Yes	No	Yes
Modification Date	MDAT	Yes	Yes	Yes	Yes	Yes
Molecular Weight	MOLWT	No	Yes	No	No	No
Organism	ORGN	Yes	Yes	Yes	Yes	Yes
Page Number	PAGE	Yes	Yes	Yes	Yes	Yes
Primary Accession	PACC	Yes	Yes	Yes	No	Yes
Properties	PROP	Yes	Yes	Yes	No	Yes
Protein Name	PROT	Yes	Yes	Yes	No	Yes
Publication Date	PDAT	Yes	Yes	Yes	Yes	Yes
SeqID String	SQID	Yes	Yes	Yes	No	Yes
Sequence Length	SLEN	Yes	Yes	Yes	No	No
Substance Name	SUBS	Yes	Yes	No	Yes	No
Text Word	WORD	Yes	Yes	Yes	Yes	Yes
Title Word	TITL	Yes	Yes	Yes	No	No
UId	UID	No	No	No	No	No
Volume	VOL	Yes	Yes	Yes	Yes	Yes



# PubMed

← → ↻ [www.ncbi.nlm.nih.gov/pubmed](http://www.ncbi.nlm.nih.gov/pubmed) 🔍 ☆ 🌐 📄 📱 📺 📖 📄 📄

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## PubMed

PubMed comprises more than 24 million citations for biomedical literature from MEDLINE, life science journals, and online books. Citations may include links to full-text content from PubMed Central and publisher web sites.

## PubMed COMMONS



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