Bases de datos Biológicas

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¿Por qué las bases de datos?

- Crecimiento exponencial de los datos biológicos
- Datos (secuencias, 3D estructuras, análisis gel 2D, MS análisis....) no son publicados en revistas, pero si en bases de datos
- Son usadas en investigación biológica, como lo eran la revistas científicas!
- Biólogos dependen de los computadores para almacenar, organizar, buscar, manipular, y recuperar los datos
- Libre Acceso es clave
- Base de todas las herramientas bioinformáticas



¿Qué es una base de datos?

- Una colección
 - estructurada
 - De fácil búsqueda (indexada) -> tabla de contenido
 - Actualizada periódicamente (release) -> Nuevas ediciones
 - Referencias cruzadas (<u>hipervínculos</u>)
 -> vínculos con otras DB
- Incluye la herramientas (software) para acceso, actualización, inserción, borrado.... en la DB
- Almacena datos: Texto plano (flat files) Tablas vinculadas (bases de datos relacionales)



DB: Texto plano « flat file »

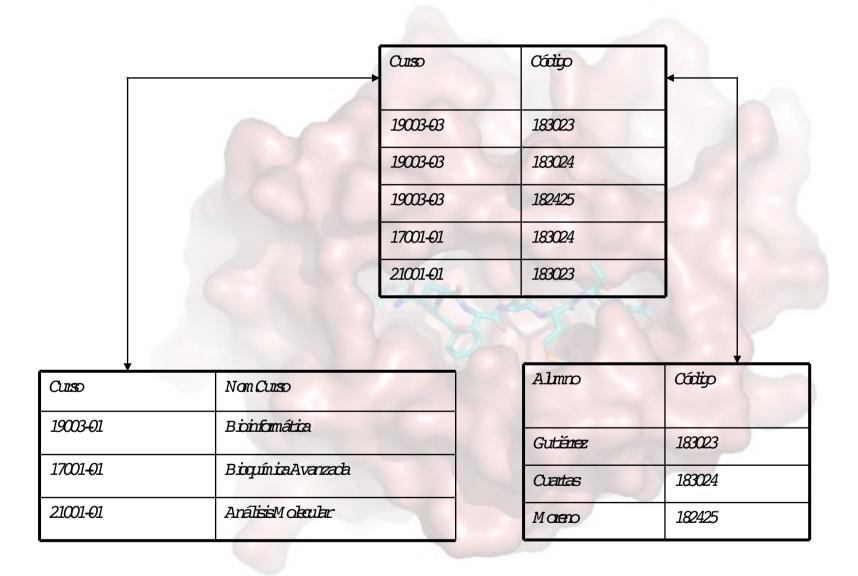
Base de datos de estudiantes: (texto plano, 3 entradas)

```
Código: 183023
Nombre: Julián
Apellido: Pulecio
Cursos: 19003-01, 21001-01
Email: jpul@ibun.unal.edu.co
Código: 183024
Nombre: Sonia
Apellido : Cuartas
Cursos: 19003-01, 17001-01
Email: soniacol@hotmail.com
Código: 183025
Nombre: Jaime
Apellido : Moreno
Cursos: 19003-01
Email: pm186111@ibun.unal.edu.co
//
```

 Facil de manejar: todas las entradas de pueden ver al tiempo!



Bases de datos « relacionales »



Fácil: manejo y selección de la salida



Algunas estadísticas

- Más de 1000 bases de datos
- Generalmente accesibles a través de WEB
 - Biohunt: http://www.expasy.org/BioHunt/
 - Amos' links: www.expasy.ch/alinks.html
- Tamaño variable: 100Kb a 10Gb
 - DNA: > 10 Gb
 - Proteinas: 1 Gb
 - Estructuras 3D: 5 Gb
 - Otras: Pequeñas



Históricamente las bases de datos de proteínas preceden a las de DNA.

- Atlas de secuencias y estructuras protéicas (1965).
- PIR (1997).

Atlas of Protein Sequence and Structure

From the Beginning

A View from 1965

<u>Laying the Foundation for</u> Bioinformatics **DEDICATED**

To those who would know

the biochemical structure, function and origin

of man and would strive to improve his lot.



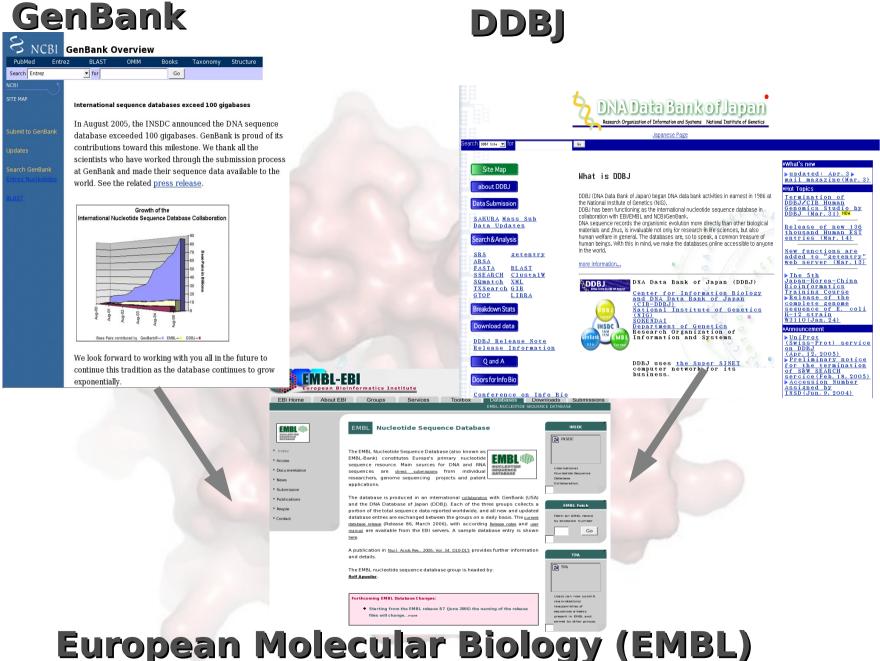
Home Page

http://www.dayhoff.cc/MODAtlasSummary.html



Dr. Margaret Oakley Dayhoff (1925-1983)





1982

International Collaboration of DNA sequence Databases ONE PRINTICAL

Bases de datos primarias y secundarias

Primarias: resultados experimentales sin curaduria. Secundarias: derivadas de las primarias, curadas.

- contienen la secuencia, comentarios, referencias de la literatura, notas sobre experimentos
- Derivadas de la integracion de las herramientas de cómputo y conocimiento biológico
 - por ejemplo, genes conocidos y predichos
- Registros añadidos solo despues de verificar su precision y las anotaciones
- Ejemplo: SWISS-PROT, OMIM, RefSeq, LocusLink



EMBL-BANK



- Release 86 on 28-FEB-2006.
- 69,783,593 entries.
- 126,401,347,060 nucleotides, of which 13,313,896 entries (65,362,911,476 nucleotides) are WGS (whole genome shotgun) data.
- The release 86 files total
 61 GB compressed.



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- Submission
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- Contact

EMBL Nucleotide Sequence Database

The EMBL Nucleotide Sequence Database (also known as EMBL-Bank) constitutes Europe's primary nucleotide sequence resource. Main sources for DNA and RNA sequences are <u>direct submissions</u> from individual researchers, genome sequencing projects and patent applications.



The database is produced in an international <u>collaboration</u> with GenBank (USA) and the DNA Database of Japan (DDBJ). Each of the three groups collects a portion of the total sequence data reported worldwide, and all new and updated database entries are exchanged between the groups on a daily basis. The <u>current database release</u> (Release 86, March 2006), with according <u>Release notes</u> and <u>user manual</u> are available from the EBI servers. A sample database entry is shown here.

A publication in <u>Nucl. Acids Res., 2006, Vol. 34: D10-D15</u> provides further information and details.

The EMBL nucleotide sequence database group is headed by: Rolf Apweiler.

Forthcoming EMBL Database Changes:

 Starting from the EMBL release 87 (June 2006) the naming of the release files will change...more

INSDC



International
Nucleotide Sequence
Database
Collaboration.

EMBL Fetch

Fetch an EMBL record by accession number



Go

TPA



Users can now submit re-annotations/ re-assemblies of sequences already present in EMBL and owned by other groups.







- Similarity & Homology
- Protein Functiona Analysis
- Proteomic Services
- Sequence Analysis
- Structural Analysis
- Tools Miscellaneous
- View all Tools

Toolbox at the EBI

The European Bioinformatics Institute (EBI) toolbox area provides a comprehensive range of tools for the field of bioinformatics. These are subdivided into categories in the left menu for convenience.





New Clustr Search Released

We have developed a large numb

A few examples include:

- Similarity & Homology the sequence similarity and i
- Protein Functional Analysis in your protein sequence.
- Proteomic Services NEW U their research results in th
- ◆ Sequence Analysis Clustal\ · Structural Analysis - MSDfc
- structure and compare it ◆ Tools Miscellaneous - Expre and visualisation of gene

Please Note: Wednesday April 5th the EBI will be running at a redu inconvenience



May 25th 2004 - Search against the new version of the Clustr database, searches include:

- 109 proteomes, including 10 Eukaryotes
- 180 mln similarities
- 1.6 mln clusters, which includes clustering groups for all of the 109 proteomes separately, as well as for 'Human and Mouse' and 'All against All'
- 462 thousand proteins, including nearly 50 thousand of IPI-only (Human, Mouse and Rat) proteins (i.e. those which don't occur in UniProt).

SRS3D available



July 31 st 2003 - SRS3D is an integrated environment that allows the end-user to quickly and easily retrieve/visualise sequence structure and also feature data from primary, secondary and tertiary protein databases, is now publicly available from the EBI...more

WSDbfetch available



August 12th 2003- WSDbfetch is a webservice implementation of Dbfetch, a generic DB retrieval system. It aims to provide programmatic access for sequence retrieval. more

'2can Bioinformatics' website available



April 17th 2003- '2can Bioinformatics' website contains simple tutorials on how to use the most common nucleotide/protein bioinformatics search and analysis tools... more

EMBL-BANK (Tools)



SRS is a powerful data integration platform, providing rapid, easy and user friendly access to the large volumes of diverse and heterogeneous Life Science data stored in more than 400 internal and public domain databases.

March 5th 2003 - SRS7 Launched. The new datawarehouse has many new features including sorting of query results and more than 100 applications.

MSDfold - Secondary Structure Matching



MSDfold is a powerful interactive tool for protein structure recognition. In tens of seconds compare structures submitted as PDB or mmCIF files, or identified by PDB code. Structures may be easily visualised using Rasmol or downloaded as PDB files.





The Dali server is a network service for comparing protein structures in 3D.

Expression Profiler



Providing Web-based tools for microarray data analysis, Expression Profiler is a set of tools for clustering, analysis and visualization of gene expression and other genomic data.

Search the UniProt Protein Resource

Text Search

Wu-Blast2

NCBI-Blas±2

UniRef



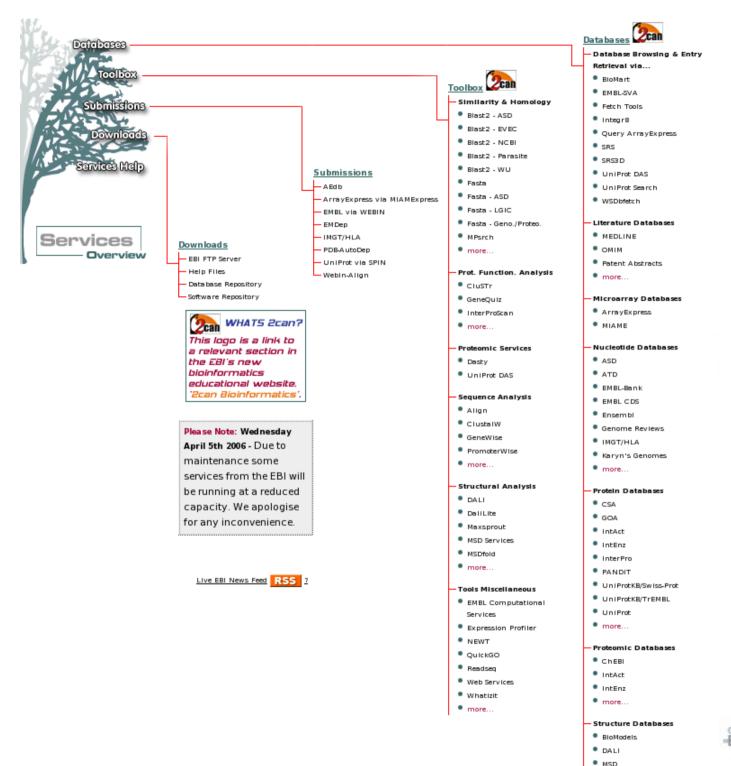
UniProt

- Text Search
- Wu-Blast2
- NCBI-Blast2
- fasta
- MPsrch
- ▶ Scan PS
- Dbfetch

UniParc

- Text Search
- Wu-Blast2
- NCBI-Blast2 ▶ fasta
- MPsrch Dbfetch
- Scan PS
- ▶ fasta MPsrch
 - ▶ ScanPS Dbfetch





BIOINFORMÁTICA

MSDchemMSDIIbe

UNIPROT

Uniprot Knowledge Base
UniprotKB/Swissprot
UniprotKB/TrEMBL

Uniprot reference Clusters

Clusters a partir de UniprotKB y Uniparc (Uniref100, Uniref90, Uniref50).

Uniprot Archive

Todas las secuencias protéicas conocidas, no redundante.



About UniProt

Text Search UniProt Knowledgebase

Text Search

BLAST

Home

FAQ

Help Desk

Download

Welcome to UniProt

Getting Started

UniProt (Universal Protein Resource) is the world's most comprehensive catalog of information on proteins. It is a central repository of protein sequence and function created by joining the information contained in Swiss-Prot, TrEMBL, and PIR.

UniProt is comprised of three components, each optimized for different uses. The **UniProt Knowledgebase (UniProtKB)** is the central access point for extensive curated protein information, including function, classification, and cross-reference. The **UniProt Reference Clusters (UniRef)** databases combine closely related sequences into a single record to speed searches. The **UniProt Archive (UniParc)** is a comprehensive repository, reflecting the history of all protein sequences.

The sequences and information in UniProt are accessible via <u>text search</u>, <u>BLAST similarity search</u>, and <u>FTP</u>.



European Bioinformatics Institute



Swiss Institute of Bioinformatics



Georgetown
University



Celebrating the 20th Anniversary of Swiss-Prot



UNIPROT-SWISSPROT

Anotación:

* Swissprot

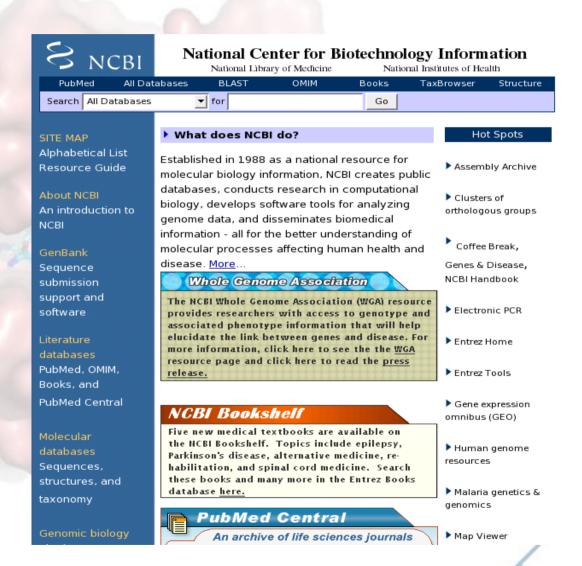
- Function(s) of the protein
- Post-translational modification(s). For example carbohydrates,
- phosphorylation, acetylation, GPI-anchor, etc.
- Domains and sites. For example calcium binding regions, ATPbinding sites,
- zinc fingers, homeobox, kringle, etc.
- Secondary structure
- Quaternary structure. For example homodimer, heterotrimer, etc.
- Similarities to other proteins
- Disease(s) associated with deficiencie(s) in the protein
- Sequence conflicts, variants, etc.



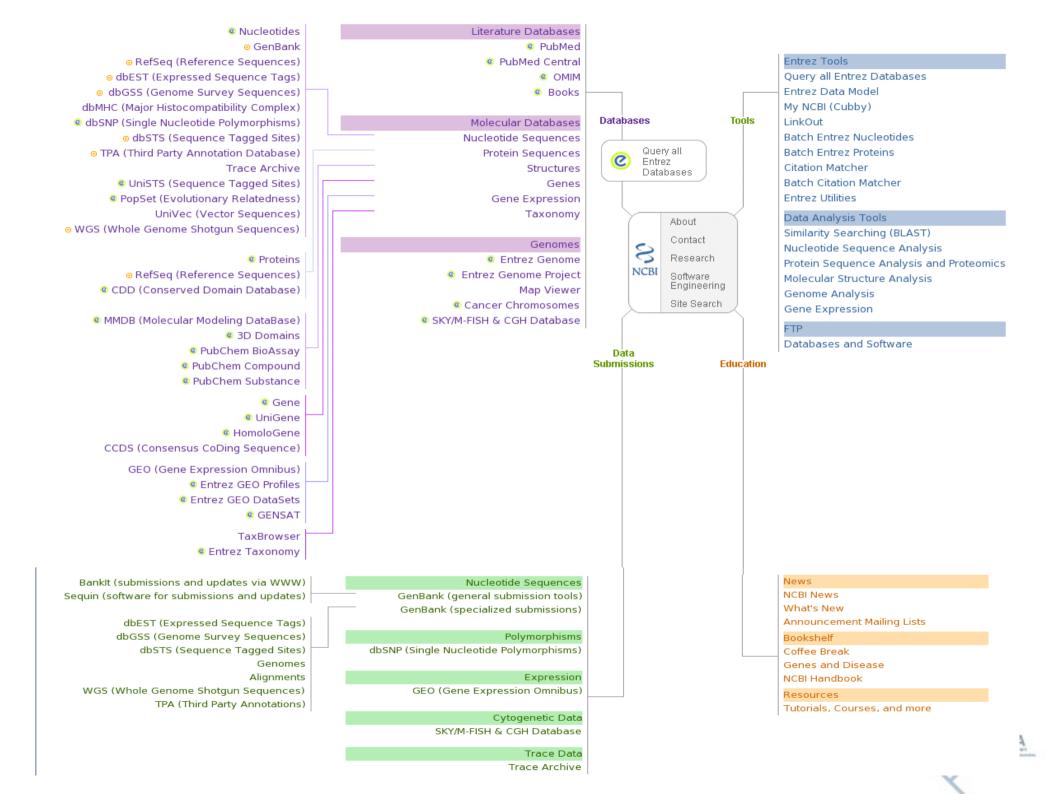
NCBI

National Center for Biotechnology Information

Establecido en 1988. Es recurso nacional (USA) información biológica molecular, el NCBI crea bases de datos públicas, lleva a cabo investigaciones biología computacional, desarrolla herramientas de software para el análisis de información genómica, y da a conocer la información biomédica - todo esto con el propósito de *mejorar nuestro* entendimiento acerca los procesos moleculares que afectan la salud y la enfermedad en los seres humanos.



-BIOINF RMATICA



NCBI- ENTREZ



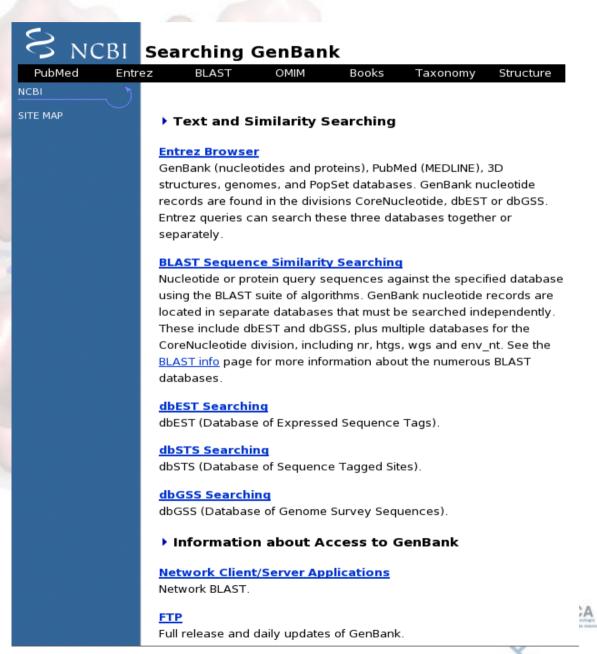


CH SITE	MAP PubMed	All Databases	Human	Genome	GenBank	Map Viewer		
		Search across database	s		GO GLEAR Help			
		Welcome to th	e Entrez cross	-database searc	h page			
W	PubMed: biomedical lite	rature citations and abstracts	2 (B	Books: online books				
	PubMed Central: free, fo	ull text journal articles	2 (**)	OMIM: online Mendelian Inheritance in Man				
	Site Search: NCBI web a	and FTP sites	2	OMIA: online Mendelian Inheritance in Animals				
8	Nucleotide: sequence dat	abase (GenBank)	2 6	UniGene: gene-orie	nted clusters of transcript s	equences	?	
	Protein: sequence databa	se	? 💽	CDD: conserved pro	tein domain database		?	
	Genome: whole genome s	sequences	2	3D Domains: doma	ins from Entrez Structure		?	
3	Structure: three-dimensio	nal macromolecular structures	?	UniSTS: markers and mapping data				
	Taxonomy: organisms in (GenBank	2 👵	PopSet: population study data sets				
(M)	SNP: single nucleotide pol	ymorphism	?	GEO Profiles: expre	ession and molecular abund	dance profiles	?	
(X	Gene: gene-centered infor	mation	?	GEO DataSets: exp	erimental sets of GEO data		?	
###	HomoloGene: eukaryotic	homology groups	2	Cancer Chromoson	nes: cytogenetic database	S	?	
6	PubChem Compound: ur	nique small molecule chemical structures	2 📝	PubChem BioAssay	y: bioactivity screens of ch	emical substances	?	
	PubChem Substance: de	eposited chemical substance records	?	GENSAT: gene expre	ession atlas of mouse centr	al nervous system	?	
E	Genome Project: genome	e project information	2	Probe: sequence-spe	ecific reagents		?	
			<u>'</u>					
	Journals: detailed informati Entrez databases	on <i>about</i> the journals indexed in PubMed ar	nd other	MeSH: detailed info	rmation about NLM's contro	olled vocabulary	?	
(2)	NLM Catalog: catalog of bo	ooks, journals, and audiovisuals in the NLM	collections ?					

NCBI- GENBANK

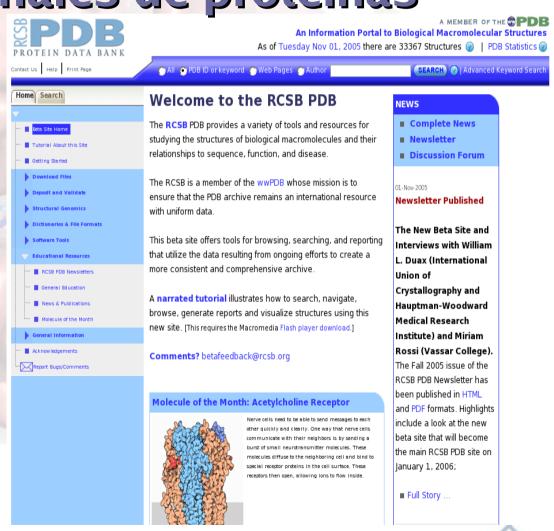
Base de datos pública de todas las secuencias DNA disponibles

59,750,386,305 bases en 54,584,635 entradas de secuencias en la división tradicional de GenBank y 63,183,065,091 bases en 12,465,546 entradas en la división WGS (Febrero de 2006).



Protein Data Bank (PDB) Base de datos de estructuras tridimensionales de proteínas

- Cristalografia de Rayos X.
- 41136 estructuras (Enero 16 de 2007)
- Archivo de coordenadas.



http://www.rcsb.org/pdb/



Sequence Retrieval System

LION SRS					Custom View	QueryHistory	Projects	DatabankInfo	Help?
	Quick Searches	Predefined Queries	Query Builder	Analysis Took					
ick Searches						Start a perma	nent project		
Quick Text Sea	rch								?
Find:					in: Nu	cleic Acid Sequen	ce [EMBL]	IIII	▼ Search
ID Search									?
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or specify a file cor Searching: EMBL	taining identifie	ers:			Ex	xaminar		lui.	▶ Search
Sequence Simi	larity/Homol	ogy Search							?
Search for seque	nces of type:	Nucleotide Se	equences _	<u>-</u>					
(Paste in yo	ur sequence	e here)							
Searching: EMBL (Release)							Ш	⇒ Search
I	nttp:/	/srs.ik	un.ı	ınal.	edu.co	:8080/s	rs81,	"	BIOINFOR

Más bases de datos I



feedback, etc.

Find a Specific Locus:

Más bases de datos II



KEGG: Kyoto Encyclopedia of Genes and Genomes

A grand challenge in the post-genomic era is a complete computer represencell, the organism, and the biosphere, which will enable computational phigher-level complexity of cellular processes and organism behaviors from molecular information. Towards this end we have been developing a biresource named KEGG as part of the research projects of the Kanehisa Lalthe Bioinformatics Center of Kyoto University and the Human Genome C University of Tokyo.





HOMOPHILA

Human Disease to Drosophila Gene Database

Version 2.1 Last update: Fri, 31 Mar 2006 Credits

omophila utilizes the sequence information of human disease genes from the <u>NCBI OMIM (Online Mendelian Inheritance in Man)</u> database in order to determine if sequence homologs of these enes exist in the current *Drosophila* sequence database (<u>FlyBase</u>). Sequences are compared using NCBI's <u>BLAST</u> program. The database is updated weekly and can be searched by human sease, gene name, OMIM number, title, subtitle and/or allelic variant descriptions.

is analysis is discussed in detail in the following publications:

eiter LT, Potocki L, Chien S, Gribskov M, Bier E., "A Systematic Analysis of Human Disease-Associated Gene Sequences In Drosophila melanogaster," Genome Research 11:1114–1125, Cold pring Harbor Labratory Press.

hien S, Reiter LT, Bier E, Gribskov M., "Homophila: human disease gene cognates in Drosophila", Nucleic Acids Research, 2002, Vol. 30, No. 1 149-151

Tab delimited flatfiles are now available for download. See table below for links.

best 5 matches



Más bases de datos III

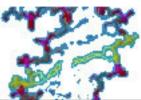
Bases de datos que no pueden ser clasificadas.

ReBase (enzimas restricción),
RepBase (repeticiones)
TRANSFAC (factores de transcripción),
CarbBank, GlycoSuiteDB (Azucares ligados),
Proteína-proteína interacción db (DIR, ProNet, Interact),
Proteasa db (MEROPS), patentes en biotecnología db, etc.;





Single Nucleotide Polymorphism



- NCBI						5.4					
PubMed Nucleotid	e Protein G	enome Str	ucture PopS	et Taxono	my OMIM	Books SNP					
Search for SNP on NCBI Reference Assembly											
Search Entrez SNP	for for				Go						
BUILD 126	dbSNP Search Options										
Have a question about dbSNP?	Entrez SNP	ID Numbers	Submission Info	Batch	Locus Info	Between Markers					
Try searching the SNP FAQ	ANNOUNCEMENT										
Archive!	■ 08/29/2006: dbSNP Genotype Server										
GENERAL SNP SUBMISSION DOCUMENTATION SEARCH	Desumentation.										
Entrez SNP	Search by IDs on All Assemblies										
EUtils API Blast SNP	Note: <u>rs</u> #	# and ss#	must be p								
Batch Query Genotype №	respective	ely (1.e. rs	cluster ID(r	s#) <u>▼</u>							
By Submitter New Batches	Searc	h Reset									



Submission Information

dbSNP

Base de datos de polimorfismos genéticos

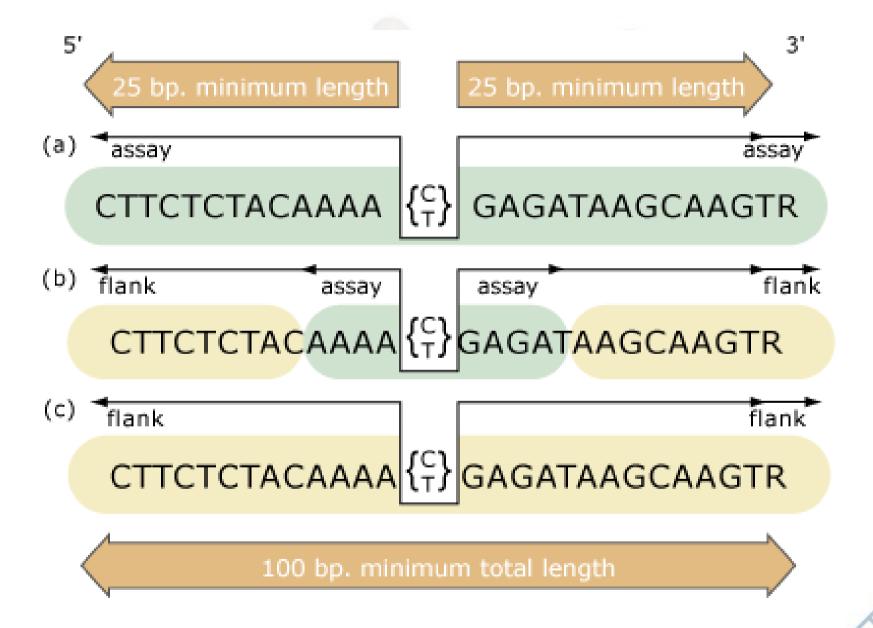
Consta de:

- SNPs: single nucleotide polymorphism
- **DIPs:** deletion insertion polymorphisms.
- SSRs: short tandem repeats.

Cada entrada incluye:

- Contexto.
- Frecuencia del polimorfismo.
- Métodos experimentales para su obtención.





-BIOINF RMÁTICA

Sidebar links to data, Nucleotide Polymorphism documentation, and queries: database information, submission, instructions, link to FTP area, site Go Clear documentation, preconfigured searches, prototype haplotype data History Clipboard Details GENERAL dbSNP Search Options dbSNP Home Page Entrez SNP ID Numbe Batch Locus Info Free Form Easy Form SNP Science Primer NEW Announcements NCBI has moved all FTP services to a Query quick links: dbSNP Summary ftp.ncbi.nih.gov. The full contents of a announcement area FTP SERVER Build History the new address ftp://ftp.ncbi.nih.gov/snj Handle Request Please contact snp-admin@ncbi.nlm.nih.gov to report problems with access to the new ftp area. DOCUMENTATION Single record query: Overview Search by IDs Accession, ID, or cluster How To Submit RefSNP Summary Info Note: rs# and ss# must be prefixed with "rs" or "ss", respectively (ie. rs25, Database Schema bitmal Data formats Search Reset Heterozygosity Advanced ID Search SEARCH Submission Information Entrez SNP Blast SNP By Submitter Submission property Batch query New Batches query: method, paper, By Submitter Method submitter, latest data New Batches Population Method Detail (Description, Handle, and ID) Population Class (Classification based on geographic location) Class Publication Publication Chromosome Report Chromosome Report Locus Information Batch STS Markers Free Form Search Enter List Batch query: retrieve - NCBI Assay ID(ss) Advanced up to 20,000 records Reference SNP ID(rs) of interest at a time Local SNP ID HAPLOTYPE Upload List Specifications NCBI Assay ID(ss) Sample HapSet Reference SNP ID(rs) Sample Individual - Local SNP ID Batch Query Help Locus Information Locus ID Locus query: retrieve Gene Name or Symbol lists of variations in known Gene Product gene regions or mRNA Accession Number transcripts Gene Ontology Biological Process Cellular Location - Molecular Function Locus Query Help Free Form Use the pull-down menu to specify a search field. Enter a term in the text box or select from the option pull-down menu; Select an operator. Click 'Add' to add search field to the query box and 'Go' to view the Free-form (Entrez-like)



and Easy form queries: query the database using descriptor tags with boolean logic, or pick your choices from a set of pull down menus

Para tener en cuenta...

- Cual es la mejor DB para análisis de secuencia?
- Cual tiene la mejor calidad de datos ?
- Cual es la más completa?
- Cual es la más actualizada?
- Cual es la menos redundante?
- Cual es la más indexada (permite búsquedas complejas) ?
- Cual es la que responde más rápido ?

- DB: Muchos errores (Anotaciones automáticas)!
- No todas las DB estan disponibles en todos los servidores
- La frecuencia de actualización es diferente en los distintos servidores; creación de db_new entre releases (ejemplo: EMBLnew; TrEMBLnew....)

