

Bases de Datos de interés biológico y Farmacéutico





Ramírez Lab



National
Center for
Biotechnology
Information



¿Porqué las bases de datos (DB)?

- **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 (hipervínculos) -> vínculos con otras DB

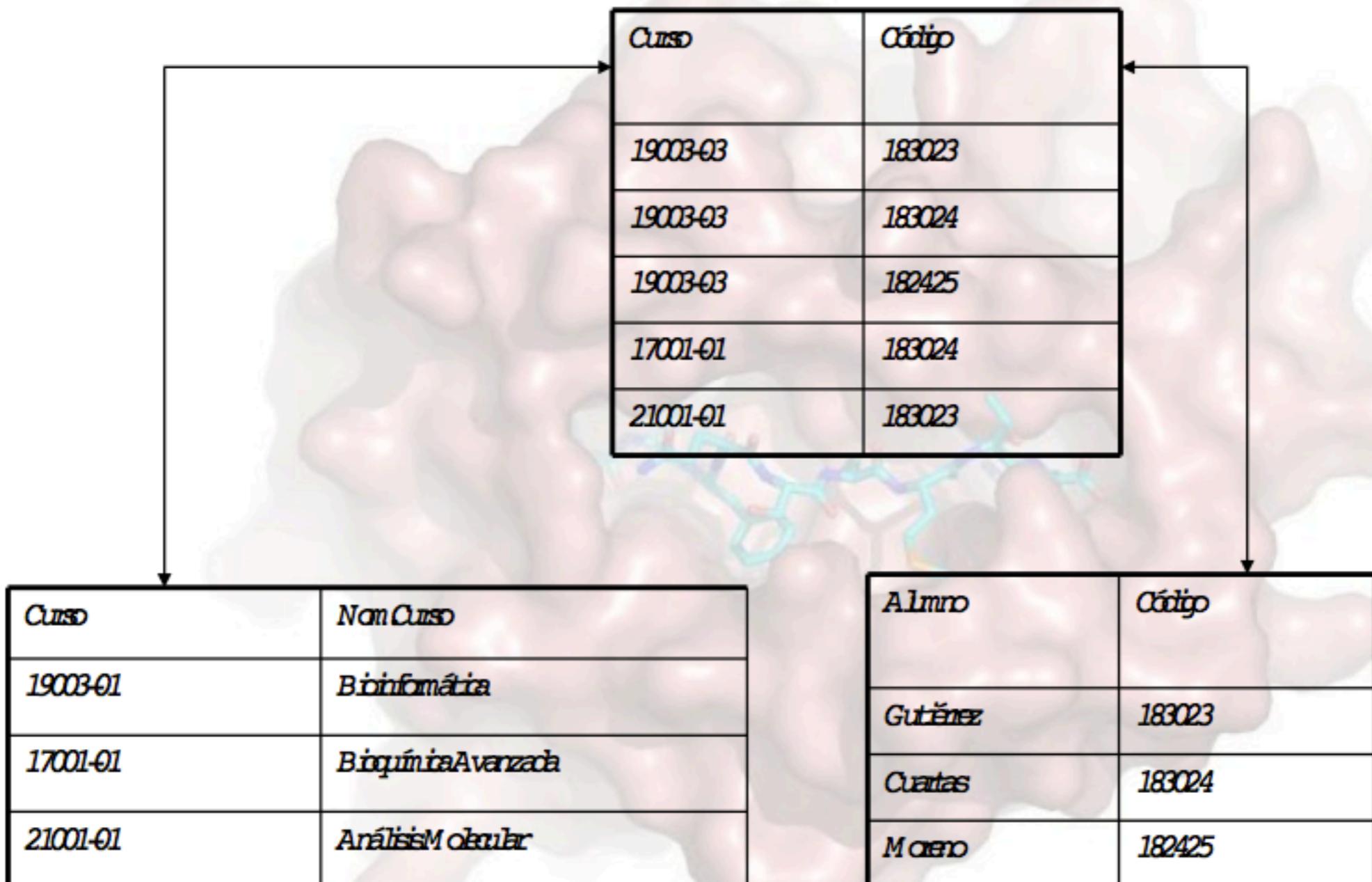
- Incluye la herramientas (software) para acceso, actualización, inserción, borrado.... en la DB
- Almacena datos: Texto plano (flat files) Tablas vinculadas (bases de datos relacionales)

DB: Texto plano “flat file”

Base de datos de estudiantes:
Texto plano, 3 entradas

```
1 Código: 183023
2 Nombre: Julián
3 Apellido : Pulecio
4 Cursos: 19003-01, 21001-01 Email: jpul@ibun.unal.edu.co //
5 //
6 Código: 183024
7 Nombre: Sonia
8 Apellido : Cuartas
9 Cursos : 19003-01, 17001-01 Email: soniacol@hotmail.com
10 //
11 Código: 183025
12 Nombre: Jaime
13 Apellido : Moreno
14 Cursos : 19003-01
15 Email: pm186111@ibun.unal.edu.co //
```

Fácil acceso, fácil de manejar.
Todas las entradas se pueden ver al mismo tiempo!



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
 - Proteínas: 1 Gb
 - Estructuras 3D : 5 Gb
 - Otras: Pequeñas

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 integración de las herramientas de cómputo y conocimiento biológico
 - por ejemplo, genes conocidos y predichos
- Registros añadidos solo después de verificar su precisión y las anotaciones
- Ejemplo :
SWISS-PROT, OMIM, RefSeq, LocusLink



EMBL - European Bioinformatics Institute (EBI)

The home for big data in biology

About this image: An entry from the Tara Oceans expedition in the prototype Image Data Repository, built by scientists at the University of Dundee, EMBL-EBI, the University of Bristol and the University of Cambridge. [Learn more >](#)

Our unique Search service helps you explore dozens of biological data resources.

Find a tool for your data analysis.

Share your scientific data with the world.

All ▾ Find a gene, protein or chemical

Example searches: [blast](#) [keratin](#) [bf1](#)

[Find a tool >](#)

[Deposit data >](#)

Explore EMBL-EBI and our mission

The European Bioinformatics Institute (EMBL-EBI) shares [data from life science experiments](#), performs [basic research](#) in computational biology and offers an extensive [user training programme](#), supporting researchers in academia and industry. We are part of [EMBL](#), Europe's flagship laboratory for the life sciences. [More about EMBL-EBI and our impact >](#)

<http://www.ebi.ac.uk/>



UniProtKB Advanced Search

BLAST Align Retrieve/ID mapping Peptide search Help Contact

The mission of UniProt is to provide the scientific community with a comprehensive, high-quality and freely accessible resource of protein sequence and functional information.

UniProtKB

UniProt Knowledgebase

Swiss-Prot (555,100)
Manually annotated and reviewed.

TrEMBL (88,032,926)
Automatically annotated and not reviewed.

UniRef

Sequence clusters

UniParc

Sequence archive

Proteomes

Supporting data

Literature citations

Cross-ref. databases

Taxonomy

Diseases

Subcellular locations

Keywords

News

BLOG TWITTER f RSS

Forthcoming changes
Planned changes for UniProt

UniProt release 2017_07
A pseudogene turns into an active DNA methyltransferase dedicated to male fertility

UniProt release 2017_06
Eukaryotic sex: good ideas shared with viruses | Change of cross-references to

News archive



UniProt

UniProtKB ▾ Advanced ▾ Search

BLAST Align Retrieve/ID mapping Peptide search Help Contact

UniProtKB results

Basket ▾

UniProt statistics of the current release

[UniProtKB/Swiss-Prot statistics \(Old Style\)](#)

[UniProtKB/TrEMBL statistics \(Old Style\)](#)

[UniParc statistics](#)

[UniRef statistics](#)

Releases before 2016_01 are partially indexed from the archives

Proteome redundancy reduction caused the number of entries in UniProtKB/TrEMBL to drop from 92 million in release 2015_03 to 46 million in release 2015_04.

◀ 1 to 25 of 315 ▶ Show 25 ▲

Release Statistics

UniProtKB/Swiss-Prot 2017_07 - July 5, 2017
(release news)

UniProtKB/TrEMBL 2017_07 - July 5, 2017
(release news)

UniParc 2017_07 - July 5, 2017
(release news)

UniRef 2017_07 - July 5, 2017
(release news)

UniProtKB/Swiss-Prot 2017_07 - July 5, 2017
(release news)



Ej: taxonomy:"Serpentes (snakes) [8570]" (annotation:(type:"tissue specificity" venom) OR locations:(location:nematocyst)) AND reviewed:yes

UniProtKB - taxonomy:"Serpentes (snakes) [8570]" (annotation:(type:"tissue specificity" venom) OR locations:(location:nematocyst)) AND reviewed:yes Advanced Search

BLAST Align Retrieve/ID mapping Peptide search Help Contact

UniProtKB results

About UniProtKB Basket

Filter byⁱ

Reviewed (2,277) Swiss-Prot

Popular organisms

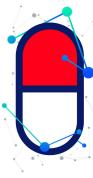
- DENAN (35)
- VIPAA (19)
- BOTJA (58)
- BOTJR (16)
- CRODU (30)

Other organisms

View by

BLAST Align Download Add to basket Columns > 1 to 25 of 2,277 Show 25

<input type="checkbox"/>	Entry	Entry name		Protein names	Gene names	Organism	Length	
<input type="checkbox"/>	Q90249	PA2B1_BOTJR		Basic phospholipase A2 homolog both...		Bothrops jararacussu (Jararacussu)	137	
<input type="checkbox"/>	P00626	PA2BA_VIPAA		Basic phospholipase A2 ammodytoxin ...		Vipera ammodytes ammodytes (Western sand viper)	138	
<input type="checkbox"/>	Q9PW56	BNP2_BOTJA		Bradykinin-potentiating and C-type ...		Bothrops jararaca (Jararaca) (Bothrops jararaca)	265	
<input type="checkbox"/>	P08878	PA1A_CRODU		Phospholipase A2 homolog crot toxin a...		Crotalus durissus terrificus (South American rattlesnake)	138	
<input type="checkbox"/>	Q6LEM5	BNP1_BOTJA		Bradykinin-potentiating and C-type ...		Bothrops jararaca (Jararaca) (Bothrops jararaca)	256	
<input type="checkbox"/>	P00982	VKTHD_DENAN		Kunitz-type serine protease inhibit...		Dendroaspis angusticeps (Eastern green mamba) (Naja)	57	

[NCBI Home](#)[Resource List \(A-Z\)](#)[All Resources](#)[Chemicals & Bioassays](#)[Data & Software](#)[DNA & RNA](#)[Domains & Structures](#)[Genes & Expression](#)[Genetics & Medicine](#)[Genomes & Maps](#)[Homology](#)[Literature](#)[Proteins](#)[Sequence Analysis](#)[Taxonomy](#)[Training & Tutorials](#)[Variation](#)

Welcome to NCBI

The National Center for Biotechnology Information advances science and health by providing access to biomedical and genomic information.

[About the NCBI](#) | [Mission](#) | [Organization](#) | [NCBI News & Blog](#)

Submit

Deposit data or manuscripts into NCBI databases



Download

Transfer NCBI data to your computer



Learn

Find help documents, attend a class or watch a tutorial



Develop

Use NCBI APIs and code libraries to build applications



Analyze

Identify an NCBI tool for your data analysis task



Research

Explore NCBI research and collaborative projects



Popular Resources

[PubMed](#)[Bookshelf](#)[PubMed Central](#)[PubMed Health](#)[BLAST](#)[Nucleotide](#)[Genome](#)[SNP](#)[Gene](#)[Protein](#)[PubChem](#)

NCBI News & Blog

dbSNP architecture redesign supports future human variation data expansion; changes to be introduced over the next year

07 Jul 2017

GenBank release 220.0 is available via FTP

07 Jul 2017

GenBank release 220.0 (6/18/2017) has



All Databases ▾

Search

NCBI Home

Resource List (A-Z)

All Resources

Chemicals & Bioassays

Data & Software

DNA & RNA

Domains & Structures

Genes & Expression

Genetics & Medicine

Genomes & Maps

Homology

Literature

Proteins

Sequence Analysis

Taxonomy

Training & Tutorials

Variation

All Resources

[All](#)[Databases](#)[Downloads](#)[Submissions](#)[Tools](#)[How To](#)

Databases

Assembly

A database providing information on the structure of assembled genomes, assembly names and other meta-data, statistical reports, and links to genomic sequence data.

BioCollections

A curated set of metadata for culture collections, museums, herbaria and other natural history collections. The records display collection codes, information about the collections' home institutions, and links to relevant data at NCBI.

BioProject (formerly Genome Project)

A collection of genomics, functional genomics, and genetics studies and links to their resulting datasets. This resource describes project scope, material, and objectives and provides a mechanism to retrieve datasets that are often difficult to find due to inconsistent annotation, multiple independent submissions, and the varied nature of diverse data types which are often stored in different databases.

BioSample

The BioSample database contains descriptions of biological source materials used in experimental assays.

BioSystems

Database that groups biomedical literature, small molecules, and sequence data in terms of biological relationships.

Bookshelf

A collection of biomedical books that can be searched directly or from linked data in other NCBI databases. The collection includes biomedical textbooks, other scientific titles, genetic resources such as *GeneReviews*, and NCBI help manuals.



All Databases

Search

NCBI Home

Resource List (A-Z)

All Resources

Chemicals & Bioassays

Data & Software

DNA & RNA

Domains & Structures

Genes & Expression

Genetics & Medicine

Genomes & Maps

Homology

Literature

Proteins

Sequence Analysis

Taxonomy

Training & Tutorials

Variation

All Resources

All

Databases

Downloads

Submissions

Tools

How To

Tools

[1000 Genomes Browser](#)

An interactive graphical viewer that allows users to explore variant calls, genotype calls and supporting evidence (such as aligned sequence reads) that have been produced by the [1000 Genomes Project](#).

[Amino Acid Explorer](#)

This tool allows users to explore the characteristics of amino acids by comparing their structural and chemical properties, predicting protein sequence changes caused by mutations, viewing common substitutions, and browsing the functions of given residues in conserved domains.

[Assembly Archive](#)

Links the raw sequence information found in the Trace Archive with assembly information found in publicly available sequence repositories (GenBank/EMBL/DDBJ). The Assembly Viewer allows a user to see the multiple sequence alignments as well as the actual sequence chromatogram.

[BLAST Microbial Genomes](#)

Performs a BLAST search for similar sequences from selected complete eukaryotic and prokaryotic genomes.

[BLAST RefSeqGene](#)

Performs a BLAST search of the genomic sequences in the [RefSeqGene](#)/LRG set. The default display provides ready navigation to review alignments in the Graphics display.

[BLAST Tutorials and Guides](#)

This page links to a number of BLAST-related tutorials and guides, including a selection guide for BLAST algorithms, descriptions of BLAST output formats, explanations of the parameters for stand-alone BLAST, directions for setting up

BLAST on local machines and using the BLAST URL API.



Amino Acid Explorer

Learn Page

PSSM Viewer

Key to Symbols

Description of
Displayed Data

Mutation Analyzer

Compare

A - Ala

to

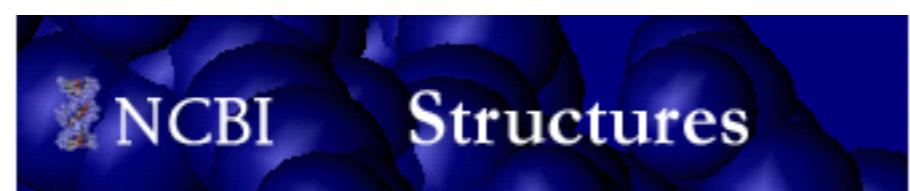
C - Cys

using

text

Compare

Questions or
comments



Amino Acid Explorer

Biochemical Properties

View a table displaying various properties of all 20 amino acids.

[Display Table](#)

Common Substitutions

Using data from the BLOSUM62 matrix, view a list of amino acids ranked by how often they substitute for a given amino acid.

Choose an amino acid:

[View Substitutions](#)

Amino Acids at Work

Using data from NCBI curated CD records, explore functional sites within proteins in which a given amino acid plays a pivotal part.

Choose an amino acid:

Structure and Chemistry

View structural views and detailed properties of a given amino acid.

Choose an amino acid:

[View Properties](#)

Mutation Analyzer

Interactively discover what amino acid substitutions result from selected codon mutations.

[Analyze Mutations](#)

Amino Acids as Ligands

Using Entrez Structure, retrieve 3D protein structures containing a given amino acid as a ligand.

Choose an amino acid:

[Detailed Search](#)



KEGG Kyoto Encyclopedia of Genes and Genomes

KEGG | Search | Help | » Japanese

KEGG Home
Release notes
Current statistics
Plea from KEGG

KEGG Database
KEGG overview
Searching KEGG
KEGG mapping
Color codes

KEGG Objects
Pathway maps
Brite hierarchies
KEGG DB links

KEGG Software
KegTools
KEGG API
KGML

KEGG FTP
Subscription

GenomeNet
DBGET/LinkDB
Feedback
Copyright request

KEGG: Kyoto Encyclopedia of Genes and Genomes

KEGG is a database resource for understanding high-level functions and utilities of the biological system, such as the cell, the organism and the ecosystem, from molecular-level information, especially large-scale molecular datasets generated by genome sequencing and other high-throughput experimental technologies. See [Release notes](#) (July 1, 2017) and our new message.

New article
[KEGG: new perspectives on genomes, pathways, diseases and drugs](#)

Main entry point to the KEGG web service

KEGG2 KEGG Table of Contents [Update notes]

Data-oriented entry points

KEGG PATHWAY	KEGG pathway maps	Subject-oriented entry points
KEGG BRITE	BRITE hierarchies and tables	KEGG Cancer
KEGG MODULE	KEGG modules	KEGG Pathogen
KEGG ORTHOLOGY	KO functional orthologs	KEGG Virus
KEGG GENOME	Genomes [Release history]	KEGG Plant
KEGG GENES	Genes and proteins	KEGG Annotation
KEGG COMPOUND	Small molecules	KEGG RModule
KEGG GLYCAN	Glycans	KEGG SeqData
KEGG REACTION	Biochemical reactions	
KEGG ENZYME	Enzyme nomenclature	
KEGG DISEASE	Human diseases	
KEGG DRUG		

K[GG] Compounds with Biological Roles

[Brite menu | Download htext]

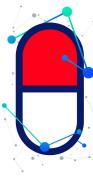
▼ ▼ ▼ ▼ One-click mode

- ▶ **Organic acids**
- ▶ **Lipids**
- ▶ **Carbohydrates**
- ▶ **Nucleic acids**
- ▶ **Peptides**
- ▶ **Vitamins and Cofactors**
- ▶ **Steroids**
- ▶ **Hormones and transmitters**
- ▶ **Antibiotics**

[[BRITE](#) | [KEGG2](#) | [KEGG](#)]

Last updated: May 22, 2015

» [Japanese version](#)

[Browse](#)[Search](#)[Downloads](#)[About](#)[Help](#)[Contact Us](#)

Get DrugBank to go! The DrugBank app for iOS and Android is coming soon.

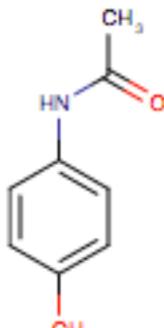
[Sign up to get early access](#)

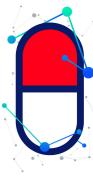


DrugBank Version 5.0

The DrugBank database is a unique bioinformatics and cheminformatics resource that combines detailed drug (i.e. chemical, pharmacological and pharmaceutical) data with comprehensive drug target (i.e. sequence, structure, and pathway) information. The database contains 8261 drug entries including 2021 FDA-approved small molecule drugs, 233 FDA-approved biotech (protein/peptide) drugs, 94 nutraceuticals and over 6000 experimental drugs. Additionally, 4338 non-redundant protein (i.e. drug target/enzyme/transporter/carrier) sequences are linked to these drug entries. Each DrugCard entry contains more than 200 data fields with half of the information being devoted to drug/chemical data and the other half devoted to drug target or protein data. [More about DrugBank](#)

Identification

Name	Acetaminophen
Accession Number	DB00316 (APRD00252)
Type	Small Molecule
Groups	Approved
Description	Acetaminophen, also known as paracetamol, is commonly used for its analgesic and antipyretic effects. Its therapeutic effects are similar to salicylates, but it lacks anti-inflammatory, antiplatelet, and gastric ulcerative effects.
Structure	 🔍 MOL SDF PDB SMILES InChI
Synonyms	4-(Acetylamino)phenol 4-acetamidophenol 4'-hydroxyacetanilide Acenol



Showing BioInteractions for DB00316 (Acetaminophen)

i *BioInteractor* utilizes data on drug-target, -enzyme and -transporter associations to provide insight on drug-drug interactions. It allows you to identify, for instance, which drugs act similarly on the same target. Such drugs may have additive pharmacodynamic effects if given concomitantly. Conversely, two drugs may antagonize the beneficial effects of each other by having opposite actions on a specific drug target. *BioInteractor* uses ranked drug-enzyme association information to predict enzyme-mediated drug interactions that may be clinically relevant.

3 Target Mediated Interactions

19 Enzyme Mediated Interactions

3 Transporter Mediated Interactions

Interacting Group

Interacting Drugs

Acetaminophen is a Prostaglandin G/H synthase 1 inhibitor

1 Prostaglandin G/H synthase 1 **inhibitors**

Aceclofenac, Acetylsalicylic acid, Antipyrine, Antrafenine, Balsalazide, Bromfenac, Carprofen, Choline magnesium trisalicylate, Dexibuprofen, Diclofenac, Diethylcarbamazine, Diflunisal, Dihomo-gamma-linolenic acid, Etodolac, Fenoprofen, Flurbiprofen, Hyperforin, Ibuprofen, Icosapent, Indomethacin, Ketoprofen, Ketorolac, Lornoxicam, Lumiracoxib, Magnesium salicylate, Meclofenamic acid, Mefenamic acid, Meloxicam, Mesalazine, Nabumetone, Naproxen, Nepafenac, Oxaprozin, Phenylbutazone, Piroxicam, Resveratrol, Salicylic acid, Salsalate, Sulfasalazine, Sulindac, Suprofen, Tenoxicam, Tiaprofenic acid, Tolmetin

2 Prostaglandin G/H synthase 1 **inducers**

Desmopressin, Minoxidil



Drug group	Released on	Version	Size	Command	Download (SDF Format)
All	2017-07-06	5.0.7	6.26 MB	Example	Download
Approved	2017-07-06	5.0.7	2.1 MB	Example	Download
Experimental	2017-07-06	5.0.7	2.97 MB	Example	Download
Nutraceutical	2017-07-06	5.0.7	118 KB	Example	Download
Illicit	2017-07-06	5.0.7	117 KB	Example	Download
Withdrawn	2017-07-06	5.0.7	125 KB	Example	Download
Investigational	2017-07-06	5.0.7	1.41 MB	Example	Download


[myBDB logout](#)

Search and Browse

- [Target](#)
- [Sequence](#)
- [Name &](#)
- [Ki IC50 Kd EC50](#)
- [Rate constants](#)
- [ΔG° ΔH° -TΔS°](#)
- [pH \(Enzymatic Assay\)](#)
- [pH \(ITC\)](#)
- [Substrate or Competitor](#)
- [Compound Mol. Wt.](#)
- [Chemical Structure](#)
- [Pathways](#)
- [Source Organism](#)
- [Number of Compounds](#)
- [Monomer List in csv](#)
- [Het List in SDF](#)
-
- [Compound](#)
- [FDA Drugs](#)
- [Important Compounds](#)
- [Chemical Structure](#)
- [Name](#)
- [SMILES](#)
- [Number of Data / Targets](#)

The Binding Database

[Home](#) [Info](#) [Download](#) [About us](#) [Email us](#) [Contribute data](#) [Web Services](#)

BindingDB News

September 2016. BindingDB's Advanced Search results now include a new "Diseases" tab, with information about the probable disease-relatedness of the Targets found in your search. This information is drawn from the source Articles and structured based on Disease Ontology. Please give it a try and let us know what you think of it!

May 2016. We have added a new Webservice, [getLigandsByUniprot](#), which accepts list of UniProt IDs and returns all ligands for the proteins in the list that bind better than a user-specified threshold. A switch allows selection of results for all ligands, only ligands identified as commercially available, or only ligands identified as FDA-approved drugs. Another switch allows the default XML format to be replaced by JSON.

May 2016. The Target Names page has a new column, Commercially

BindingDB is a public, web-accessible database of measured binding affinities, focusing chiefly on the interactions of protein considered to be drug-targets with small, drug-like molecules. BindingDB contains 1,357,744 binding data, for 7,140 protein targets and 605,839 small molecules.

There are 2291 protein-ligand crystal structures with BindingDB affinity measurements for proteins with 100% sequence identity, and 5816 crystal structures allowing proteins to 85% sequence identity.

Simple Search

Article Titles, Authors,
Assays, Compound
Names, Target Names

Use ? for single-letter wild-card or * for general wild-card.

For example, "adeny*" or "adeny?". Query cannot start with wild card.

Advanced Search

Combine multiple search criteria, such as chemical structures, target names, and numerical affinities; restrict searches by data source, such as BindingDB, ChEMBL, PubChem, and Patents.

Messages

We are pleased to report that the NIH has renewed its support for BindingDB. Thanks to all who filled out our survey and provided supporting messages! (June 2017)

Drug Design Data Resource (D3R) datasets have been integrated into BindingDB and are also available here: <https://www.bindingdb.org/bind/ByD3R.jsp> (June 2017)

Patent Curation by BindingDB

BindingDB curates US Patents with protein-small molecule binding data. As of July 2017, BindingDB's patent dataset comprises:

Patents: 1,639
Binding measurements: 173,275
Compounds: 116,165
Target proteins: 1,066
Assays: 2,273



Ramírez Lab

Bioorganic & Medicinal Chemistry Letters 24 (2014) 3968–3973



ELSEVIER

Contents lists available at ScienceDirect

Bioorganic & Medicinal Chemistry Letters

journal homepage: www.elsevier.com/locate/bmcl



Potent and selective inhibitors of the TASK-1 potassium channel through chemical optimization of a bis-amide scaffold



Daniel P. Flaherty ^a, Denise S. Simpson ^a, Melissa Miller ^{b,c}, Brooks E. Maki ^a, Beiyan Zou ^{b,c}, Jie Shi ^{b,c}, Meng Wu ^c, Owen B. McManus ^c, Jeffrey Aubé ^a, Min Li ^{b,c}, Jennifer E. Golden ^{a,*}

^a University of Kansas Specialized Chemistry Center, Lawrence, KS 66047, USA

^b Johns Hopkins University, School of Medicine, The Solomon H. Snyder Department of Neuroscience, Baltimore, MD 21205, USA

^c Johns Hopkins Ion Channel Center, Baltimore, MD 21205, USA



Simple Search

Article Titles, Authors,
Assays, Compound
Names, Target Names

nnel through chemical optimization of a bis-amide scaffold

Use ? for single-letter wild-card or * for general wild-card.
For example, "adeny*" or "adeny?". Query cannot start with wild card.

Go



The Binding Database

[Home](#) [Info](#) [Download](#) [About us](#) [Email us](#) [Contribute data](#) [Web Services](#)

myBDB logout

• Search and Browse

Target

Sequence

Name &

Rate constants

$$\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ$$

pH (Enzymatic Assay)

pH (ITC)

Substrate or Competitor

Compound Mol. Wt

Chemical

Pathways

Source Organism

Number of Compounds

Monomer List in

Compound

FDA Drugs

Important Compounds

Chemical Structure

Name _____

SMILES

[Make Data Set](#) [Compile data set for download or QSAR](#)

 E-MAIL

Found 148 hits of Enzyme Inhibition Constant Data

Sort by KI

Target (Institution)	Ligand	Target Links	Ligand Links	Trg + Lig Links	Ki nM	ΔG° kJ/mole	IC50 nM	Kd nM	EC50/IC50 nM	k_{off} s^{-1}	k_{on} $M^{-1}s^{-1}$	pH	Temp °C
Potassium channel protein TASK-1 (Homo sapiens (Human))	BDBM50050546				n/a	n/a	1	n/a	n/a	n/a	n/a	n/a	n/a
University of Kansas Specialized Chemistry Center		KEGG UniProtKB/SwissProt DrugBank antibodypedia GoogleScholar AffyNet	PC cid PC sid UniChem Patents Similar AffyNet	Article PubMed	Assay Description Inhibition of TASK-1 (unknown origin) expressed in CHO cells by thallium flux assay				Citation and Details				
Curated by ChEMBL	(CHEMBL3182699) Show SMILES Show InChI				More data for this Ligand-Target Pair								
Potassium channel protein TASK-1 (Homo sapiens (Human))	BDBM50050547				n/a	n/a	2	n/a	n/a	n/a	n/a	n/a	n/a
University of Kansas Specialized Chemistry Center		KEGG UniProtKB/SwissProt DrugBank antibodypedia GoogleScholar AffyNet	PC cid PC sid UniChem Patents Similar AffyNet	Article PubMed	Assay Description Inhibition of TASK-1 (unknown origin) expressed in CHO cells by thallium flux assay				Citation and Details				

RCSB PDB Deposit Search Visualize Analyze Download Learn More MyPDB Login

RCSB PDB PROTEIN DATA BANK An Information Portal to 131693 Biological Macromolecular Structures

PDB-101 Worldwide Protein Data Bank EMDDataBank Nucleic Acid Database StructuralBiology Knowledgebase Worldwide Protein Data Bank Foundation

Search by PDB ID, author, macromolecule, sequence, or ligands Go Advanced Search | Browse by Annotations

f t y o

Welcome Deposit Search Visualize Analyze Download Learn

A Structural View of Biology

This resource is powered by the Protein Data Bank archive-information about the 3D shapes of proteins, nucleic acids, and complex assemblies that helps students and researchers understand all aspects of biomedicine and agriculture, from protein synthesis to health and disease.

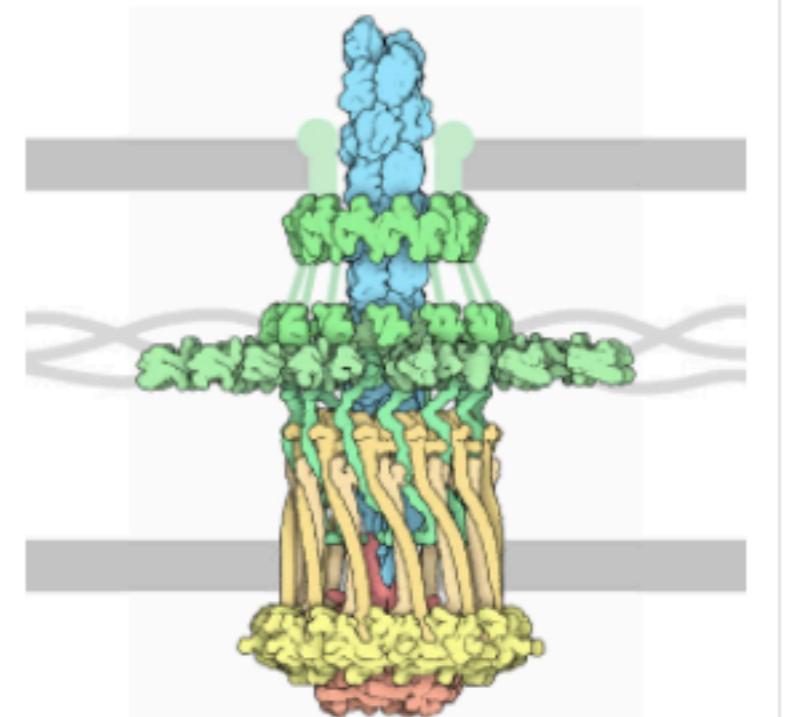
As a member of the wwPDB, the RCSB PDB curates and annotates PDB data. The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.

Zika Illustration Named People's Choice



VIZZIES
VISUALIZATION CHALLENGE
People's Choice Award Winner
Category: Illustration
Zika Virus
David S. Goodsell

July Molecule of the Month



Pilus Machine



RCSB PDB-101

Molecular explorations
through biology and medicine

Educational portal of PROTEIN DATA BANK

Search Molecule of the Month articles and more

Go



Guide to Understanding PDB Data

[Introduction](#) >

[Biological Assemblies](#) >

[Dealing with
Coordinates](#) >

[Methods for
Determining Structure](#) >

[Missing Coordinates
and Biological
Assemblies](#) >

[Molecular Graphics
Programs](#) >

Introduction to PDB Data

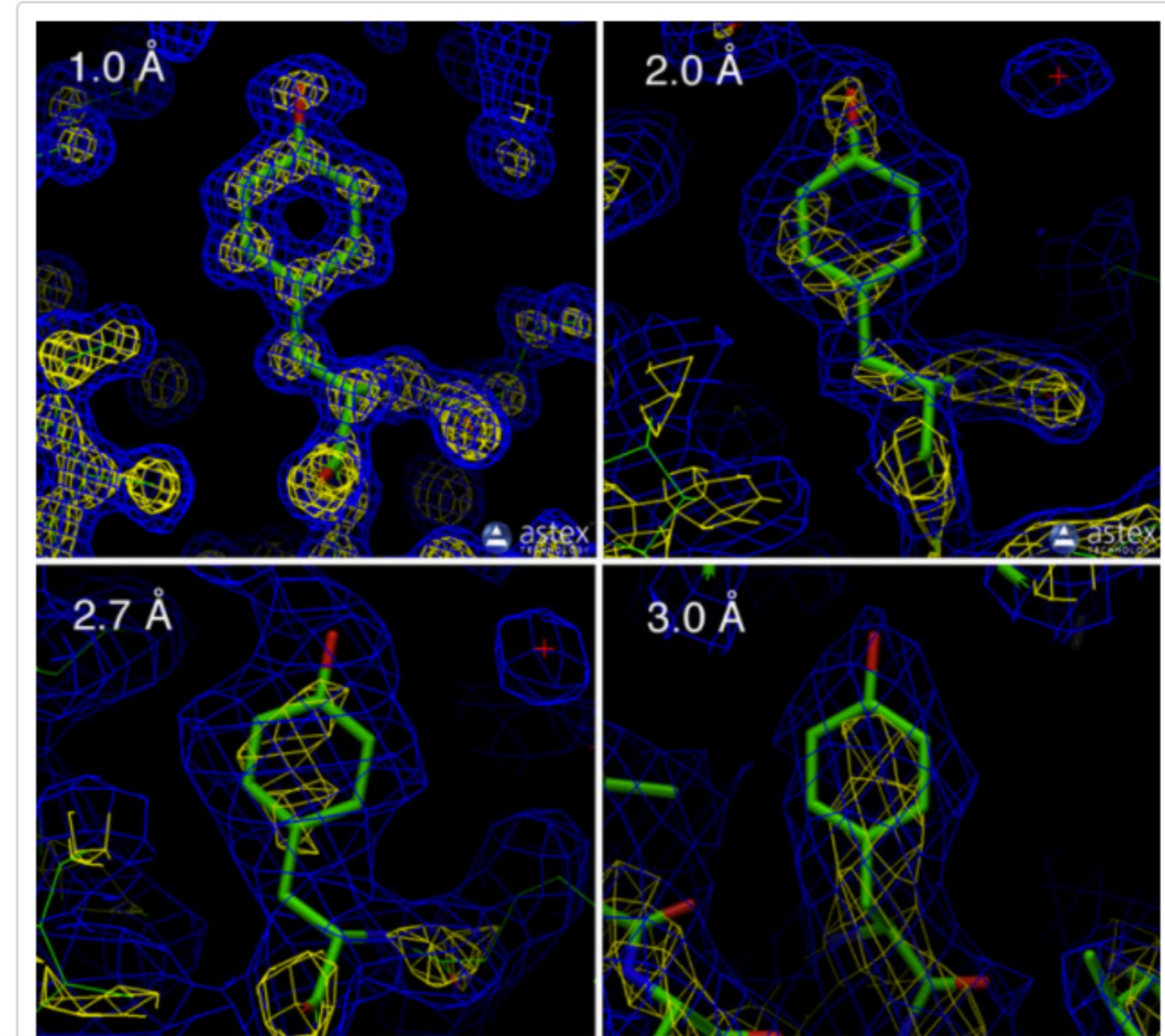
The PDB archive is a repository of atomic coordinates and other information describing proteins and other important biological macromolecules. Structural biologists use methods such as [X-ray crystallography](#), [NMR spectroscopy](#), and [cryo-electron microscopy](#) to determine the location of each atom relative to each other in the molecule. They then deposit this information, which is then annotated and publicly released into the archive by the wwPDB.

The constantly-growing PDB is a reflection of the research that is happening in laboratories across the world. This can make it both exciting and challenging to use the database in research and education. Structures are available for many of the proteins and nucleic acids involved in the central processes of life, so you can go to the PDB archive to find structures for ribosomes, oncogenes, drug targets, and even whole viruses. However, it can be a challenge to find the information that you need, since the PDB archives so many different structures. You will often find multiple structures for a given molecule, or partial structures, or structures that have been modified or inactivated from their native form.

Looking at Structures is designed to help you get started with charting a path through this material, and help you avoid a few common pitfalls. These chapters are intertwined with one another. To begin, select a topic from the right menu, or select a topic from below:

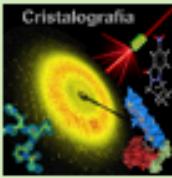
- PDB Data

The primary information stored in the PDB archive consists of [coordinate files](#) for biological molecules. These files list the atoms in each protein, and their 3D location in space. These files are available in several



7. Resolución estructural

Si a la izquierda de la pantalla no se muestra el menú de estos apuntes, [use este enlace](#).



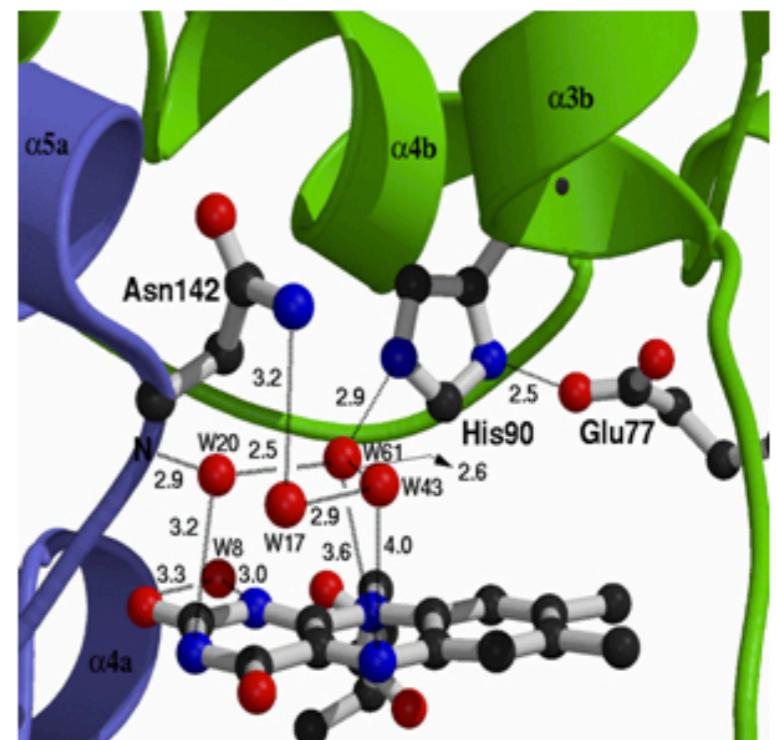
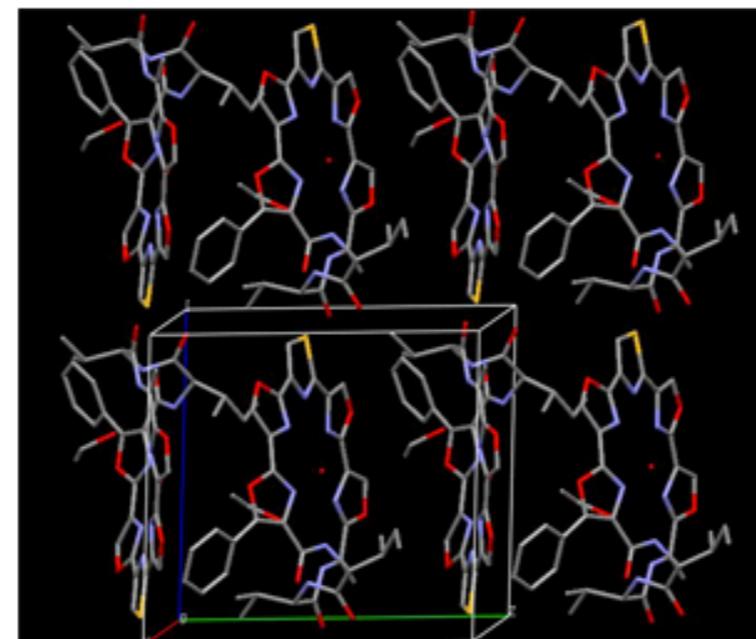
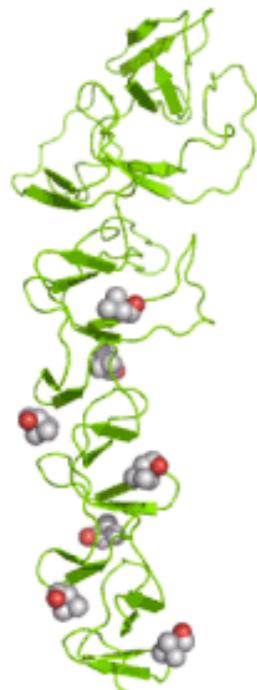
La pregunta que implícitamente nos estamos planteando desde los primeros capítulos de estas páginas es:

¿Podemos "ver" la estructura interna de los cristales?

ó, en definitiva,

¿Podemos "ver" los átomos y las moléculas que están dentro de los cristales?

iii) La respuesta es, definitivamente, **SÍ !!!**



Estructura molecular de un enzima presente en la superficie del neumococo

Empaquetamiento cristalino de una molécula orgánica sencilla, mostrando la celdilla elemental

Detalles geométricos de la interacción entre moléculas en un fragmento de una proteína



Advanced Search Interface

Structure Title ? -

Search by title record (PDB 'TITLE' record or mmCIF_struct.title value)

Contains: Acetylcholinesterase Result Count

AND

X-ray Resolution ? -

Search by X-ray resolution (mmCIF item _refine.ls_d_res_high)

Between 1 and 2 Result Count

AND

Has Ligand(s) ? -

Search based on whether or not the structure contains any free ligands

Has Ligands Yes Result Count

Add Search Criteria +

Retrieve only representatives at 90% sequence identity ?

Match all of the above conditions.

Results Structures Clear All Parameters Submit Query



The screenshot shows the RCSB PDB homepage with the 'Analyze' dropdown menu open. The 'PDB Statistics' option is highlighted. The main search bar is visible, along with social media icons and a map of the world.

- Sequence & Structure Alignment
- Protein Symmetry
- Structure Quality
- Map Genomic Position to Protein
- PDB Statistics
- Third Party Tools

PDB Statistics

With the exception of "Status of Unreleased Entries", all the following statistics are for the current holdings of experimentally-determined structures.

- Content Distribution
 - [Summary Table of Released Entries](#)
 - [Drill-down all Released Entries](#)
 - [Status of Unreleased Entries](#)
 - [Obsoleted PDB Entries](#)
 - [Proteins Solved by Multiple Experimental Methods](#)
 - [Redundancy Based on Sequence Similarity](#)
 - [By Resolution](#)
 - [By Software](#)
 - [By R Free](#)
 - [By Space Group](#)
 - [By Source Organism \(Natural Source\)](#)
 - [By Source Organism \(Gene Source\)](#)
 - [By Expression Organism \(Gene Source\)](#)
 - [By Journal](#)
 - [By Structural Genomics Centers](#)
 - [By Molecular Weight \(Structure\)](#)
 - [By Molecular Weight \(Entity\)](#)
 - [By Residue Count](#)
 - [By Atom Count](#)
 - [By Enzyme Classification](#)

Structure Summary 3D View Annotations Sequence Sequence Similarity Structure Similarity Experiment

Biological Assembly 1 ?

5099

Unconventional SH3 domain from the postsynaptic density scaffold protein Shank3

DOI: 10.22110/pdb5099/pdb

Classification: [PROTEIN BINDING](#)

Deposited: 2017-06-16 Released: 2017-07-05

Deposition author(s): [Ponna, S.K.](#), [Myllykoski, M.](#), [Boeckers, T.M.](#), [Kursula, P.](#)

Organism: [Rattus norvegicus](#)

Expression System: Escherichia coli

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
Resolution: 0.87 Å
R-Value Free: 0.117
R-Value Work: 0.097

View in 3D: [NGL](#) or [JSmol](#) or [PV](#) (in Browser)

Standalone Viewers

Display Files  Download Files 

wwPDB Validation

3D Report Full Report

Metric	Percentile Ranks	Value
Rfree	0	0.116
Clashscore	2	0
Ramachandran outliers	0	0
Sidechain outliers	0	0
RSRZ outliers	1.7%	0

Horse: 
Human: 

Chain B: SH3 and multiple ankyrin repeat domains protein 3

Chain Downloadable Files

[Download FASTA File](#)

[View Sequence & DSSP Image](#)

[Download Sequence Chain Image](#)

Chain Info

Polymer: 1
 Length: 60 residues
 Chain Type: polypeptide(L)
 Reference: UniProtKB (Q9JLU4)

Up-to-date UniProt IDs are provided by the SIFTS project

Display Parameters

Identical Chains

[Show A chain](#) [Show all chains](#)

Mouse over an annotation to see more details. Click on any annotation to enable Jmol.

Annotations	Details
Secondary Structure:DSSP [hide] [reference]	5% helical (1 helices; 3 residues) 48% beta sheet (8 strands; 29 residues)
Structural Feature:Site Record [hide] [reference]	5O99_B_AC1_8 binding site for residue BTB A 601 (Software)

Sequence Chain View

DSSP


DSSP Legend

- binding site for residue BTB A 601 (Software)
- empty; no secondary structure assigned
- ▶ B: beta bridge
- S: bend
- T: turn
- ▶ E: beta strand
- G: 3/10-helix

Structure Summary 3D View Annotations Sequence Sequence Similarity Structure Similarity Experiment

Biological Assembly 1 ?

5VOC

Crystal structure of HCMV Pentamer in complex with neutralizing antibody 8I21 - Low resolution dataset for initial phasing by SAD

DOI: [10.22110/pdb5voc/pdb](https://doi.org/10.22110/pdb5voc/pdb)

Classification: [Viral Protein / Immune System](#)
 Deposited: 2017-05-02 Released: 2017-07-05
 Deposition author(s): [Malito, E., Chandramouli, S.](#)
 Organism: [Human betaherpesvirus 5 | Homo sapiens](#)
 Expression System: Homo sapiens

Experimental Data Snapshot

Method: X-RAY DIFFRACTION
 Resolution: 3.99 Å
 R-Value Free: 0.276
 R-Value Work: 0.259

wwPDB Validation

Metric	Percentile Ranks	Value
Rfree	0.291	10
Clashscore	10	2.1%
Ramachandran outliers	2.1%	14.3%
Sidechain outliers	14.3%	21.6%
RSRZ outliers	21.6%	

View in 3D: [NGL](#) or [JSmol](#) or [PV](#) (in Browser)

Standalone Viewers

[Simple Viewer](#) [Protein Workshop](#)

Display Files **Download Files**

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....)