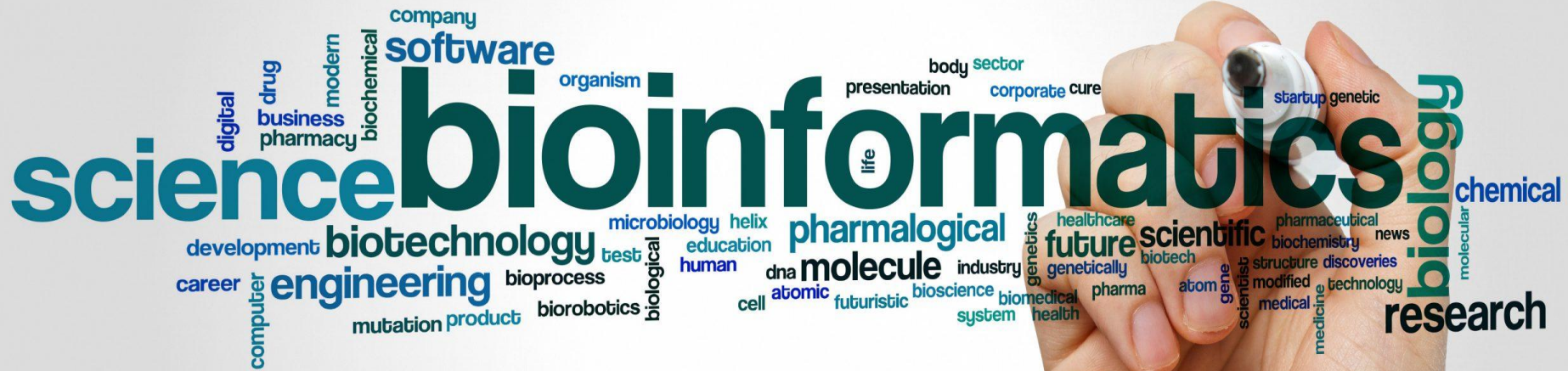




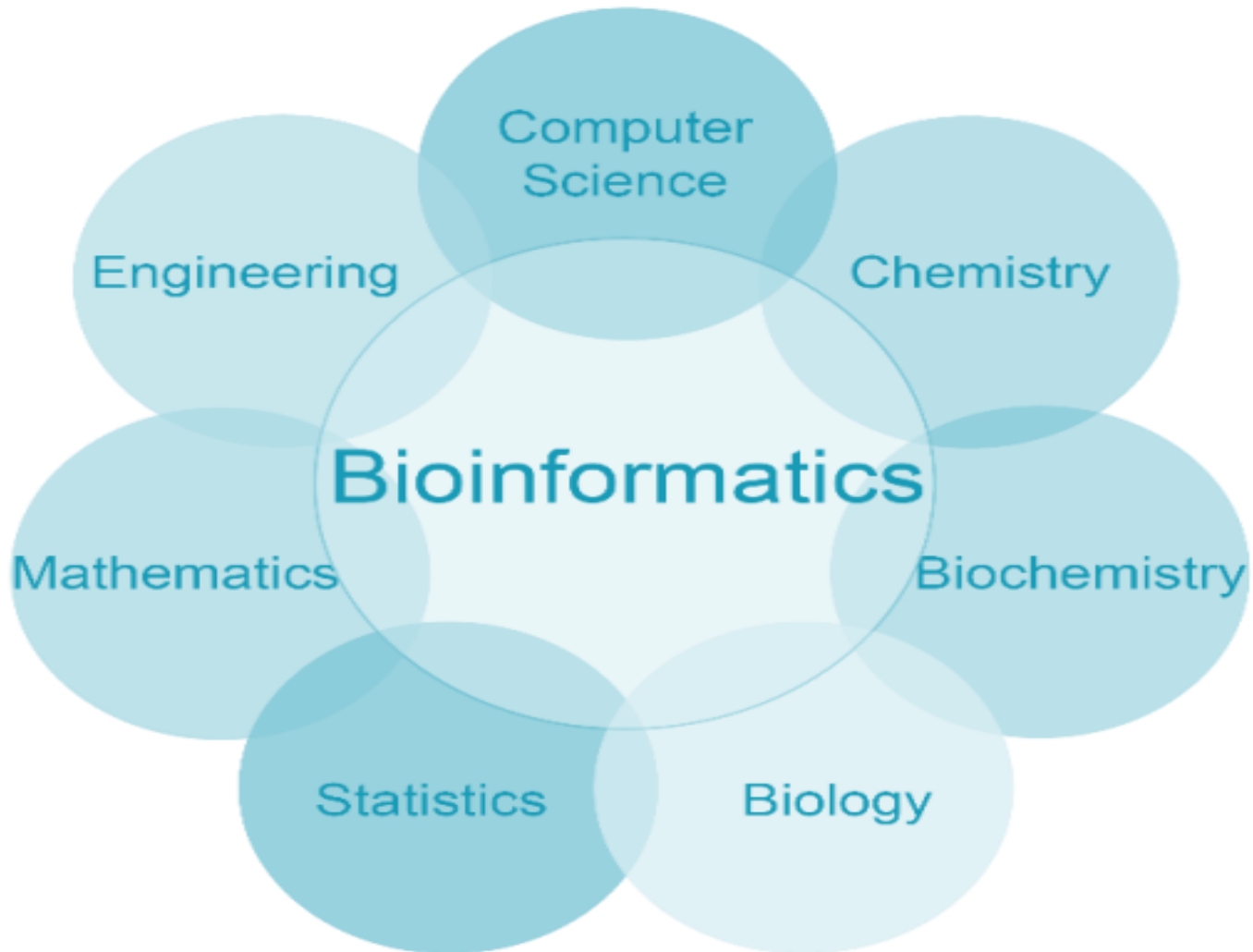
م.م. شيرين نزار قاسم
كلية المعلوماتية الطبية الحيوية
قسم الانظمة الطبية الذكية

DEFINITION OF BIOINFORMATICS

A field of science that uses computers, databases, math, and statistics to collect, store, organize, and analyse large amounts of biological, medical, and health information.

Its deals with DNA microarrays, comparative, functional and structural genomics, proteomics & medical information's

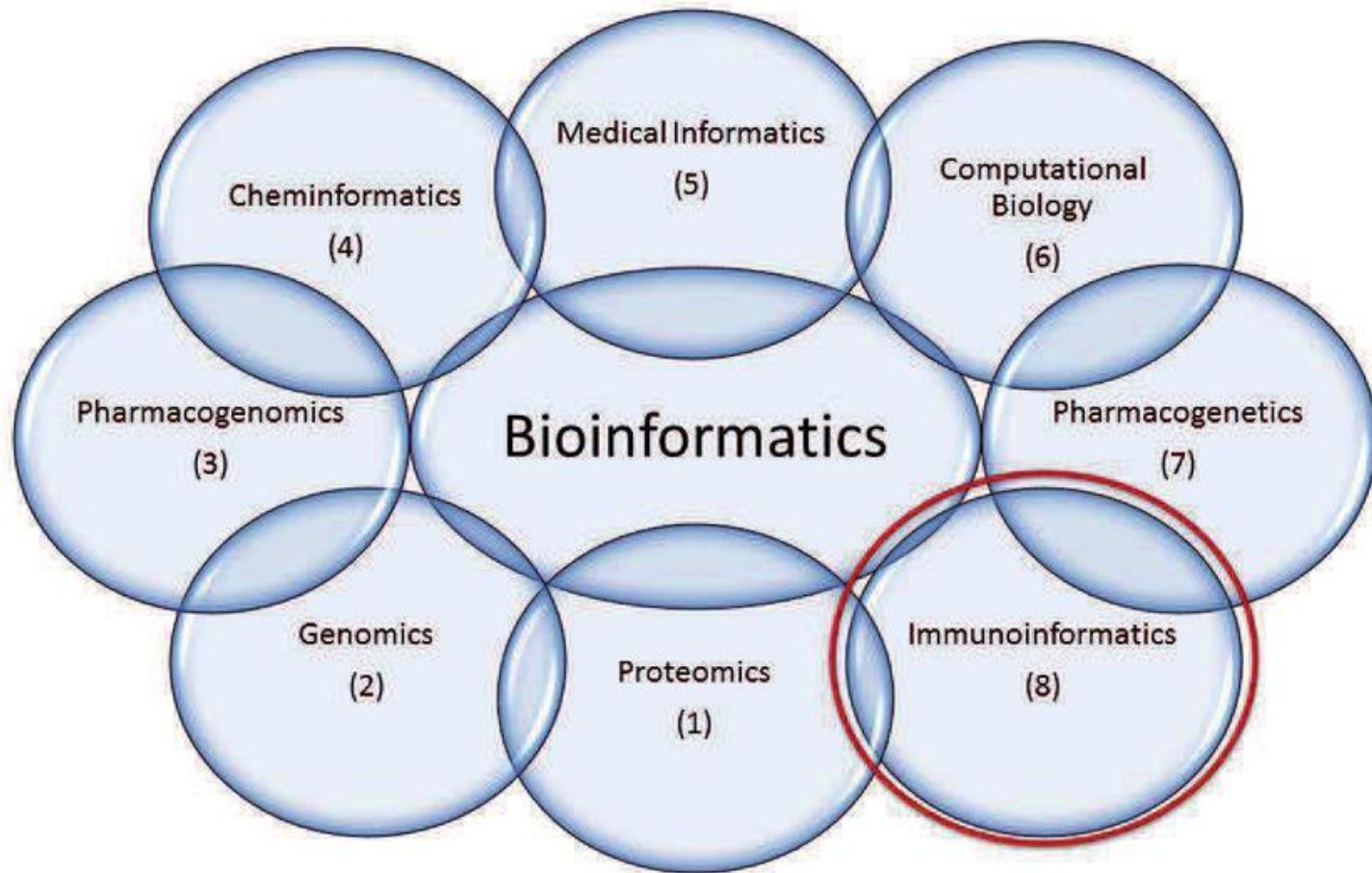
Interaction with other fields



METHODS OF PERFORMING EXPERIMENTS:

- before the era of bioinformatics, only two ways of performing biological experiments were available: within a living organism (**so-called in vivo**) or in an artificial environment (**so-called in vitro**) from the Latin in glass.
- Taking the analogy further, we can say that bioinformatics is in fact **in silico** biology, from the silicon chips on which microprocessors are built.

FIELDS RELATED TO BIOINFORMATICS



FIELDS RELATED TO BIOINFORMATICS

- **What is Biophysics?**

- An interdisciplinary field which applies techniques from the physical sciences to understanding biological structure and function”

- **What is Cheminformatics?**

- "the combination of chemical synthesis, biological screening, and data-mining approaches used to guide drug discovery and development"

- **What is Computational Biology?**

- Computational biology is not a "field", but an "approach" involving the use of computers to study biological processes and hence it is an area as diverse as biology itself.“

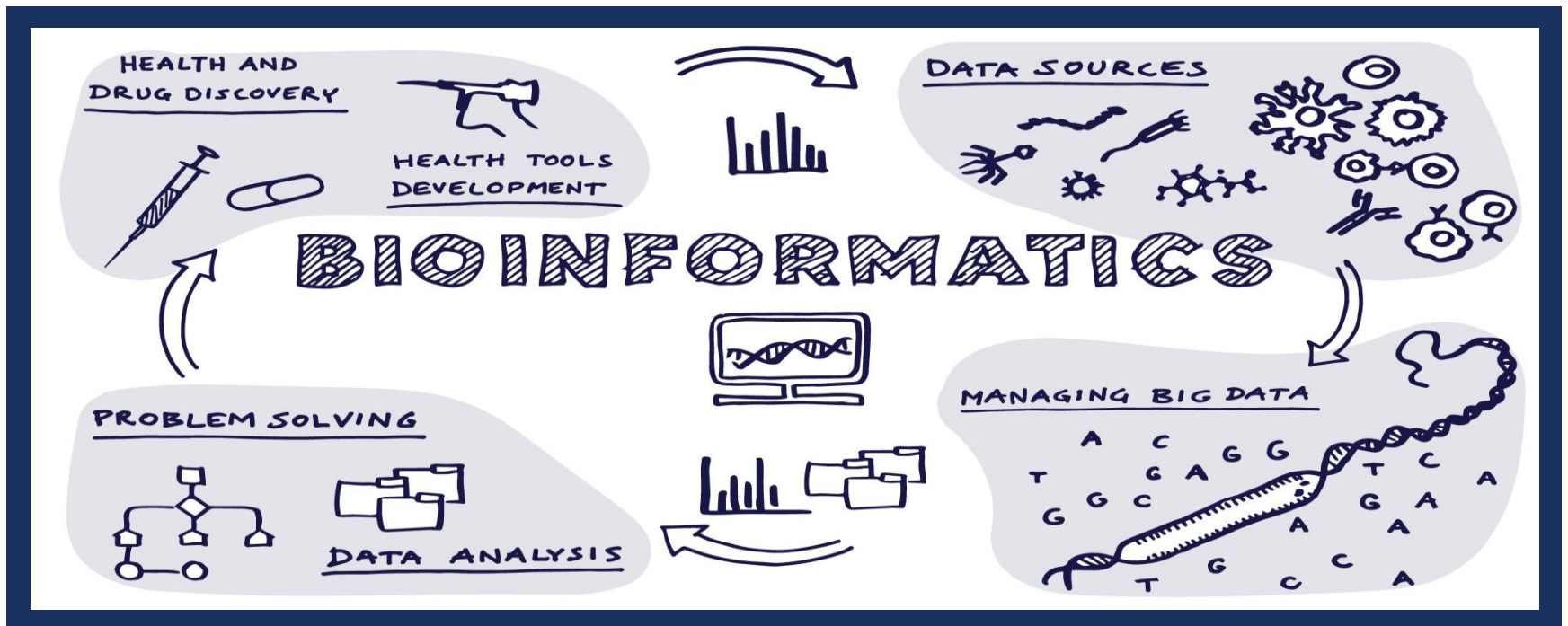
FIELDS RELATED TO BIOINFORMATICS

- **What is Genomics?**
- "Genomics is any attempt to analyze or compare the entire genetic complement of a species or species (plural)".
- **What is Medical informatics/ Med informatics?**
- "Study, invention, and implementation of structures and algorithms to improve communication, understanding and management of medical information."
- **What is Pharmacogenomics?**
- "Pharmacogenomics is the application of genomic approaches and technologies to the identification of drug targets".

BIOINFORMATICS HISTORY

- The father and mother of Bioinformatics, Dr. Margaret Belle Dayhoff (March 11, 1925 – February 5, 1983) was an American biophysicist and a pioneer in the field of bioinformatics. She engineered the application of mathematics and computational methods to the field of biochemistry.
- Her work of collection the protein sequence (**Dayhoff's Atlas of Protein Sequence and Structure, 1954-1965**)
- The EMBL established their data library in 1980 to collect, organize and distribute nucleotide sequence data and related information.
- • NCBI was established in U.S.A. NCBI serves as primary information databank and provider of information.
- • The National Biomedical Research Foundation established the PIR in 1984.

Some Applications for Bioinformatics



Finding genes structures and sequences



National Library of Medicine
National Center for Biotechnology Information

Log in

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

Welcome to NCBI

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

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libraries to build applications



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Identify an NCBI tool for your
data analysis task



Research

Explore NCBI research and
collaborative projects



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[Nucleotide](#)

[Genome](#)

[SNP](#)

[Gene](#)

[Protein](#)

[PubChem](#)

NCBI News & Blog

GenBank Release 264.0 Now Available!

23 Dec 2024

GenBank release 264.0 (12/19/2024) is now available on the NCBI FTP site. This release has 38 97 trillion bases and 5 36

Now Available! NCBI Hidden Markov Models (HMM) Release 17.0

18 Dec 2024

Download release 17.0 of the NCBI protein profile Hidden Markov models

NCBI Taxonomy: Upcoming Changes to Viruses

11 Dec 2024

To reflect changes to the International Code of Virus Classification and

Search NCBI databases

[Help](#)

Results found in 28 databases for "homo sapiens tpo"

Literature

Books	68	books and reports
MeSH	0	ontology used for PubMed indexing
NLM Catalog	1	books, journals and more in the NLM Collections
PubMed	3,478	scientific & medical abstracts/citations
PubMed Central	3,790	full-text journal articles

Health

ClinVar	0	human variations of clinical significance
dbGaP	0	genotype/phenotype interaction studies
GTR	0	genetic testing registry
MedGen	0	medical genetics literature and links
OMIM	0	online mendelian inheritance in man
PubMed Health	7	clinical effectiveness, disease and drug reports

Genomes

Genes

EST	2	expressed sequence tag sequences
Gene	49	collected information about gene loci
GEO DataSets	1,230	functional genomics studies
GEO Profiles	50,081	gene expression and molecular abundance profiles
HomoloGene	3	homologous gene sets for selected organisms
PopSet	1	sequence sets from phylogenetic and population studies
UniGene	4	clusters of expressed transcripts

Proteins

Conserved Domains	0	conserved protein domains
Protein	752	protein sequences
Protein Clusters	14	sequence similarity-based protein clusters
Structure	21	experimentally-determined biomolecular structures

Finding protein structures and sequences

RCSB PDB Deposit ▾ Search ▾ Visualize ▾ Analyze ▾ Download ▾ Learn ▾ About ▾ Careers COVID-19

Help

Contact us

MyPDB ▾

RCSB
PDB
PROTEIN DATA BANK

230,083 Structures from the PDB

1,068,577 Computed Structure Models (CSM)

Enter search term(s), Entry ID(s), Ligand ID or sequence

Include CSM ? ☐



[Advanced Search](#) | [Browse Annotations](#)

[Help](#)

PDB-101

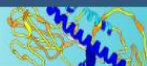
wwPDB

EMDataResource

NAKB

wwPDB
Foundation

PDB-IHM



Access Computed Structure Models (CSMs) of available model organisms

[Learn more](#)

Welcome

Deposit

Search

Visualize

Analyze

Download

Learn

RCSB Protein Data Bank (RCSB PDB) enables breakthroughs in science and education by providing access and tools for exploration, visualization, and analysis of:



Experimentally-determined 3D structures from the **Protein Data Bank (PDB)** archive

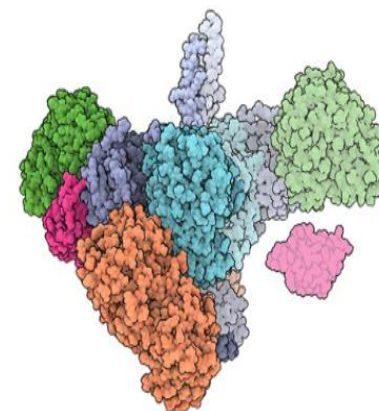


Computed Structure Models (CSM) from AlphaFold DB and ModelArchive

These data can be explored in context of external annotations providing a structural view of biology.



January Molecule of the Month



Assembly Line Polyketide Synthases

UniProt is the world's leading high-quality, comprehensive and freely accessible resource of protein sequence and functional information.

Find your protein

UniProtKB -

Advanced | List

Search

Examples: Insulin, APP, Human, P05067, organism_id:9606

UniProt is the world's leading high-quality, comprehensive and freely accessible resource of protein sequence and functional information. [Cite UniProt](#)™

Proteins UniProt Knowledgebase


Reviewed
(Swiss-Prot)
572,619


Unreviewed
(TrEMBL)
253,882,368

Species Proteomes

Protein sets for species with sequenced
genomes from across the tree of life

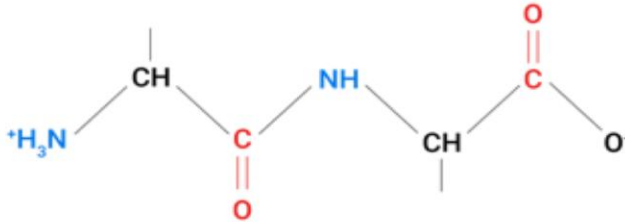
Protein Clusters UniRef

Clusters of protein sequences at 100%,
90% & 50% identity

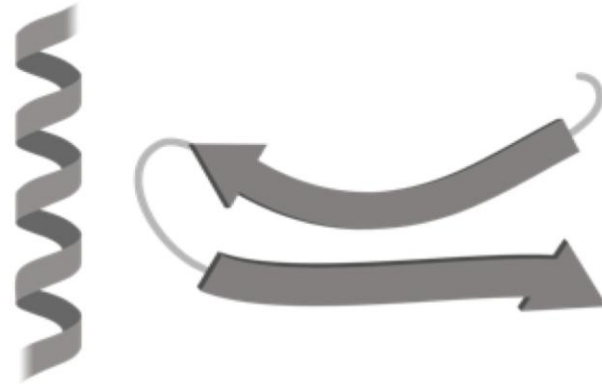
Sequence archive UniParc

Non-redundant archive of publicly
available protein sequences seen across
different databases

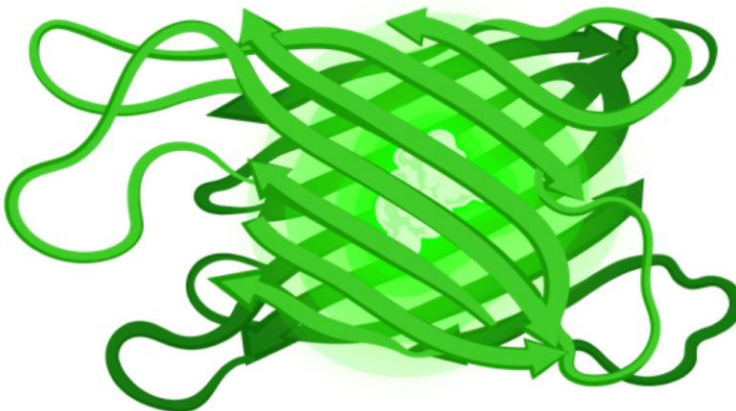
Primary



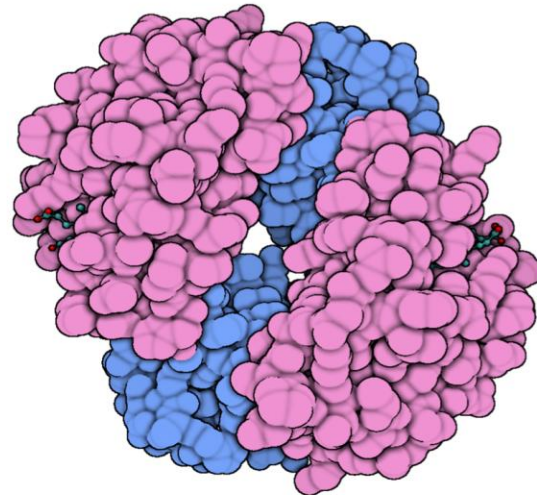
Secondary

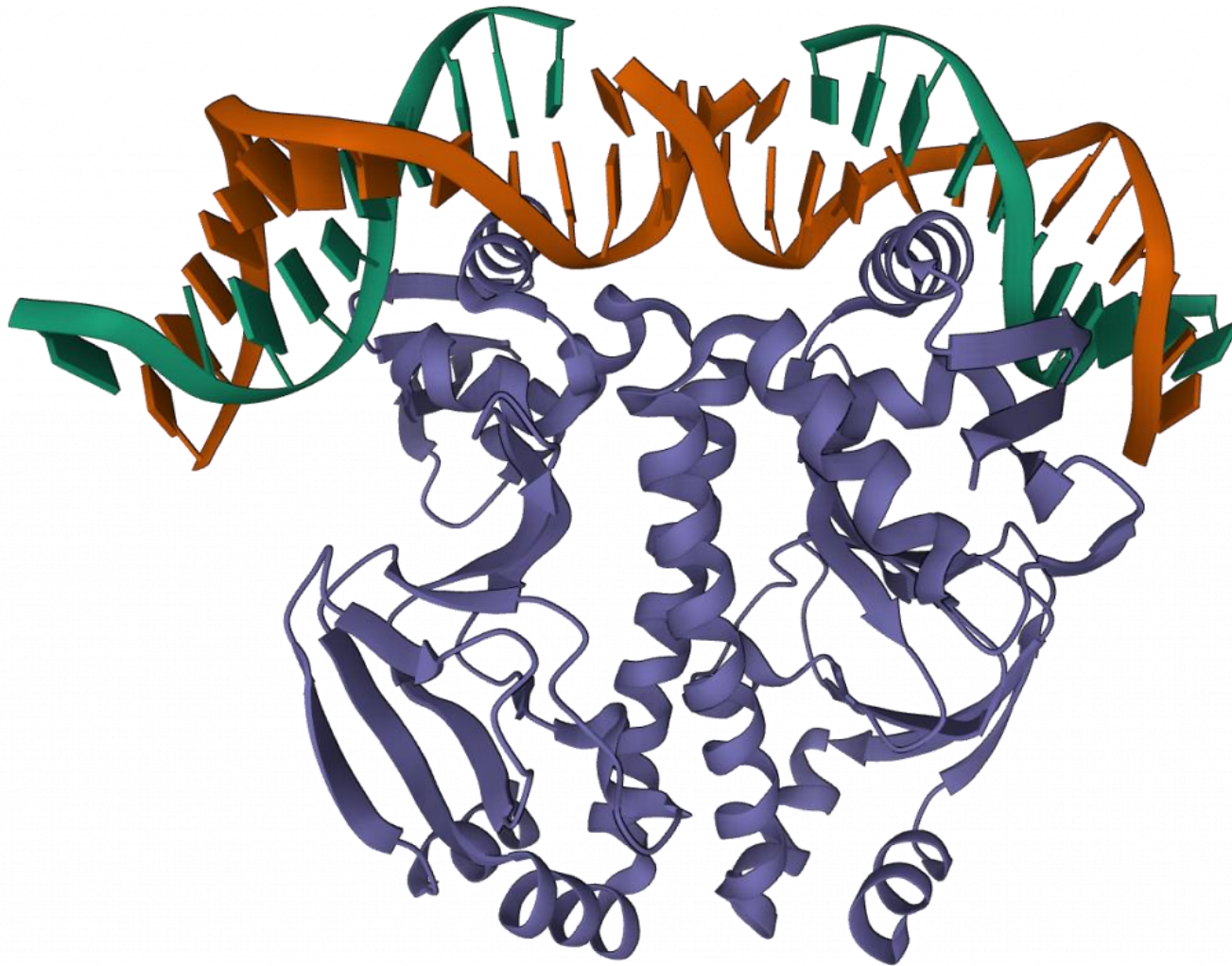


Tertiary



Quaternary





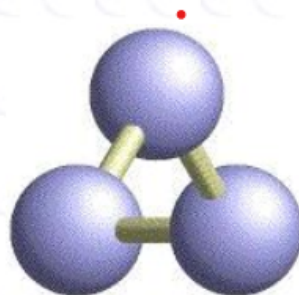
RasMol is an important scientific tool for molecular graphics visualisation

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[RasMol Manual](#)	[RasMol Blog](#)	[Frequently Asked Questions](#)	[RasMol 2.7 Series History](#)	[RasMol and OpenRasMol](#)
[SourceForge OpenRasMol Site](#)	[Click Here to Make a Donation](#)	[RasMol SourceForge Site](#)		

Home Page for RasMol and OpenRasMol

Molecular Graphics Visualisation Tool

- [RasMol Latest Windows Installer](#)
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- [RasMol 2.7.5 Windows Installer](#)
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Swiss-PdbViewer (aka DeepView) is an application that provides a user friendly interface allowing to analyse several proteins at the same time. The proteins can be superimposed in order to deduce structural alignments and compare their active sites or any other relevant parts. Amino acid mutations, H-bonds, angles and distances between atoms are easy to obtain thanks to the intuitive graphic and menu interface.

Swiss-PdbViewer

aka DeepView

v4.1

by Nicolas Gueux , Alexandre Diemand , Manuel C. Peitsch , & Torsten Schwede



Information for MacOS Catalina (10.15.*) [October 9th, 2019]

- Please note that Swiss-PdbViewer is a 32 bits application and will *** NOT *** run on OSX Catalina or more recent OSX. If you absolutely need it, refrain from updating, boot from an older OSX version, or use the PC version within a virtual machine. For example, it is possible to use the PC version with Crossover or with PlayOnMac. I currently have no plan to update it to run on OSX 10.15.
- For information, v4.1.1 works up to OSX Mojave (10.14).

CATH is a classification of protein structures downloaded from the Protein Data Bank.



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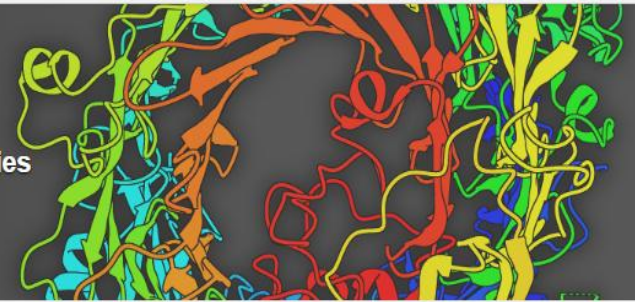
Search CATH by keywords or ID

CATH / Gene3D v4.4

151 million protein domains classified into 6,573 superfamilies

Search by keywords, PDB code, GO term, etc

Search



Putative CATH annotations for predicted structural domains in AlphaFold DB are available in [The Encyclopedia of Domains \(TED\)](#). Annotations for the 21 model organisms predicted by AlphaFold (v2) are [available to download \(doi:10.1038/s42003-023-04488-9\)](#). Core classification files for the latest version of CATH-Plus (v4.4) are [available to download](#). [Daily updates](#) of our very latest classifications [are also available](#).



3D Structure

Find out what 3D structure your protein adopts

Find out more

Go



Protein Evolution

Learn about a particular protein family and how it evolved

Find out more



Protein Function

Investigate the function of your protein

Find out more

Go



Conserved Sites

Look at protein sites that are highly conserved and implicated in function

Find out more

Go



Download Data

Download data files and query CATH via web services

Go



Learn more

Find out how CATH is created and maintained, how to link to CATH and more

Go

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

DALI

PROTEIN STRUCTURE COMPARISON SERVER

[About](#) [PDB search](#) [PDB25](#) [AF-DB search](#) [Pairwise](#) [All against all](#) [Tutorials](#) [References](#) [Statistics](#) [Download](#)

The Dali server is a network service for comparing protein structures in 3D. You submit the coordinates of a query protein structure and Dali compares them against those in the Protein Data Bank (PDB). In favourable cases, comparing 3D structures may reveal biologically interesting similarities that are not detectable by comparing sequences.

Check queue status [here](#). Megausers please consider downloading the standalone program.

You can perform three types of database searches:

- Heuristic **PDB search** - compares one query structure against those in the Protein Data Bank
- Exhaustive **PDB25** search - compares one query structure against a representative subset of the Protein Data Bank
- Hierarchical **AF-DB** search - compares one query structure against a species subset of the AlphaFold Database v2
- beta testing:**AF-DB heuristic** - search AlphaFold Database v2 in minutes

and two types of structure comparisons of user selected structures:

- **Pairwise** structure comparison - compares one query structure against those specified by the user
- **All against all** structure comparison - returns a structural similarity dendrogram for a set of structures specified by the user

SCOPe is a database for (Structural Classification of Proteins — extended)

SCOPe

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Welcome to **SCOPe**!

SCOPe (Structural Classification of Proteins — extended) is a database developed at the Berkeley Lab and UC Berkeley to extend the development and maintenance of SCOP. SCOP was conceived at the MRC Laboratory of Molecular Biology, and developed in collaboration with researchers in Berkeley. Work on SCOP (version 1) concluded in June 2009 with the release of SCOP 1.75.

SCOPe classifies many newer structures through a combination of automation and manual curation, and corrects some errors in SCOP, aiming to have the same accuracy as the hand-curated SCOP releases. **SCOPe** also incorporates and updates the ASTRAL database.

[About **SCOPe**](#)

[Stats & Prior Releases](#)

News

2023-01-06: New **PDB** entries were added in a periodic update; for more info on these updates, see the [online documentation](#).

2022-01-07: We published a [paper describing the new features in **SCOPe 2.08-stable**](#). [\[PDF\]](#).

2021-09-20: **SCOPe 2.08-stable** has been released, with nearly 20,000 new **PDB** entries added since the last stable release. Important features include [genetic variant search tools](#) and [annotations of structural heterogeneity and repeat units](#). Click either the [About](#) or [Stats & History](#) links for more details on what's new!

2018-11-30: We published a [paper describing updates to **SCOPe**](#), focusing on our findings from classifying large structures. [\[PDF\]](#).

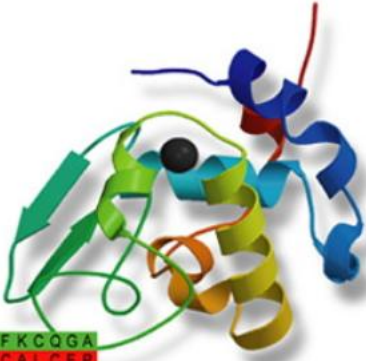
MODELLER is used for homology or comparative modelling of protein three-dimensional structures

The user provides an alignment of a sequence to be modelled with known related structures and MODELLER automatically calculates a model containing all non-hydrogen atoms.

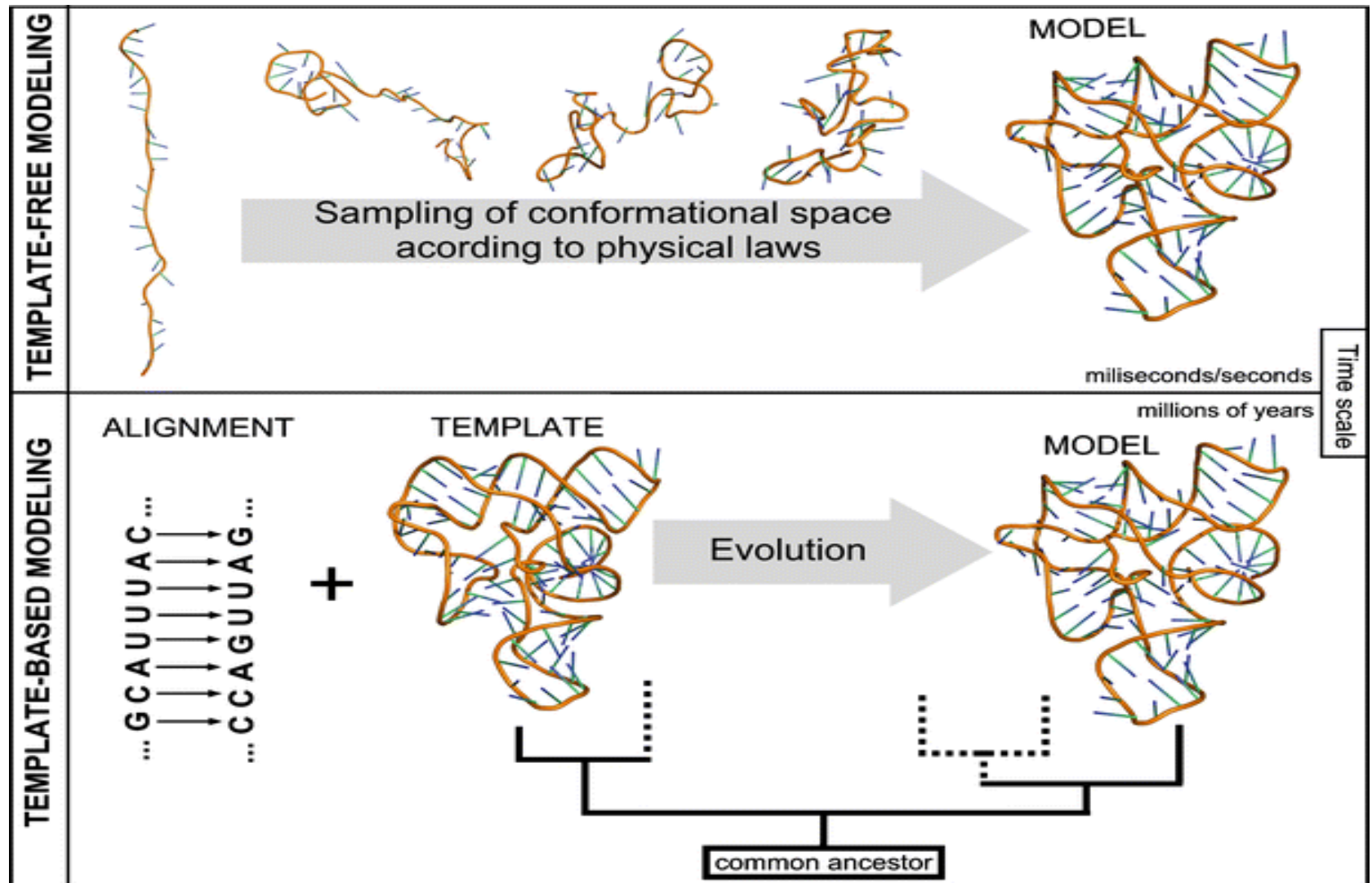
MODELLER implements comparative protein structure modelling by satisfaction of spatial restraints and can perform many additional tasks, including de novo modelling of loops in protein structures, optimization of various models of protein structure with respect to a flexibly defined objective function, multiple alignment of protein sequences and/or structures, clustering, searching of sequence databases, comparison of protein structures, etc

Modeller

Program for Comparative Protein
Structure Modelling by Satisfaction
of Spatial Restraints



A	I	L	V	G	S	M	P	R	R	D	G	M	E	R	K	D	L	L	K	A	N	V	K	I	F	K	C	Q	G	A
V	E	V	C	P	V	D	C	F	Y	E	G	P	N	F	L	V	I	H	P	D	E	C	I	D	C	A	L	C	E	
C	A	C	K	P	E	C	P	V	N	I	Q	G	S	-	-	Y	A	I	D	A	S	C	I	D	C	G	S	-		
C	-	-	I	A	C	G	A	C	K	P	E	C	P	V	N	I	Q	G	S	-	-	I	Y	A	I	D	A	D	S	



Protein Homology/analogy Recognition Engine

Phyre2.2

Protein Homology/analogy Recognition Engine V 2.2

Subscribe to Phyre at Google Groups

Email:

Visit Phyre at Google Groups

 Follow @Phyre2server



gives you access to our *Expert Mode* features. 

We are pleased to announce the release of Phyre2.2, which contains a number of new features (see the help menu for more details).

If you really need to use the old version, checking the "Traditional Phyre2" button will allow this.

One-to-One Threading  (which models your sequence against a user-supplied model) can now use models directly from the [AlphaFold Protein Structure Database](#) .

Please do not use "intensive mode" unless your search using "normal mode" indicates that a single model does *not* cover most of your sequence. 

Current Phyre2 server load = 2% (normal running) 

AlphaFold Is An AI System Developed By Google Deepmind That Predicts A Protein's 3D Structure From Its Amino Acid Sequence. It Regularly Achieves Accuracy Competitive With Experiment.

AlphaFold Protein Structure Database

Developed by Google DeepMind and EMBL-EBI

Search for protein, gene, UniProt accession or organism or sequence search

BETA

Search

Examples: MENFQKEKIGEGTYGV...

Free fatty acid receptor 2

At1g58602

Q5VSL9

E. coli

See search help →

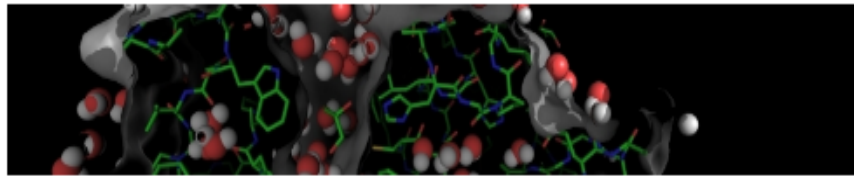
Go to online course →

See our updates – September 2024

ELNÉMO Allows You To View 3-D Animations Of The Protein Movement



IN Nantes
Université



[home](#) | [start a new run](#) | [job status](#) | [references&downloads](#) | [examples](#) | [help](#)

Should you encounter any unexpected behaviour,
please let [us](#) know.

Welcome to *elNémo* !

elNémo is the Web-interface to the *Elastic Network Model* (ENM), a fast and simple way for computing the low frequency normal modes of a macromolecule ([Tirion, 1996](#)). Note that, thanks to the RTB approximation ([Durand et al., 1994](#); [Tama et al., 2000](#)), this server can perform calculations for all-atom systems.

Predicting interactions (molecular docking)

Two different protein molecules (or a protein and a small molecule) might interact with each other. This is technically referred to as molecular docking.

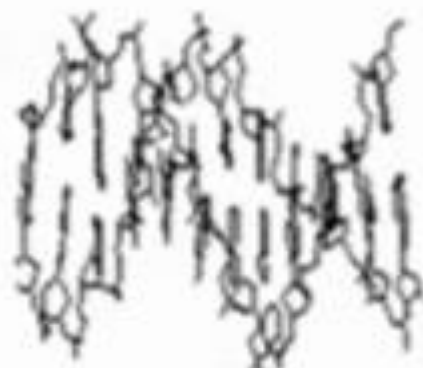


Hex Protein Docking

November 2013 - Hex 8.0.0 now available for Linux-64, Windows, and IntelMac!

About *Hex*

Prediction of Protein 3D structure



0101#01001010#10111010#
01010001#10010#1001#101
10010#100100100101011#0

Residue	ϕ	ψ	ω
THR	0.0	147.7	172.9
THR	107.2	-125.3	187.4
CYS	123.4	63.6	103.7
PSO	60.3	83.9	-116.7

DNA $\longrightarrow$ **Algorithm** $\longrightarrow$ **Protein Model**

Natural Evolution $\longrightarrow$





Biopython

(Redirected from [Main Page](#))

Introduction

Biopython is a set of freely available tools for biological computation written in [Python](#) by an international team of developers.

It is a distributed collaborative effort to develop Python libraries and applications which address the needs of current and future work in bioinformatics. The source code is made available under the [Biopython License](#), which is extremely liberal and compatible with almost every license in the world. We work along with the [Open Bioinformatics Foundation](#), who generously host our website, bug tracker, and mailing lists.

This wiki will help you download and install Biopython, and start using the libraries and tools.

Get Started

- [Download Biopython](#)
- [Installation help](#) (PDF)

Get help

- [Tutorial](#) (PDF)
- [Documentation on this wiki](#)
- [Cookbook](#) (working examples)
- [Discuss and ask questions](#)

Contribute

- [What's being worked on](#)
- [Developing on Github](#)
- [Google Summer of Code](#)

OBIF News

- [Biopython 1.55 beta released](#)
- [Biopython 1.54 released](#)
- [OBIF Google Summer of Code Accepted Students](#)
- [Burnia FASTQ files: Read Segment Quality Control Indicator](#)
- [Partial sequence files with Biopython](#)
- [Making Biopython SeqIO and AlignIO easier](#)
- [Biopython 1.54 beta released](#)
- [OBIF in Google Summer of Code](#)
- [Sanger FASTQ format and the Solexa/Illumina variants](#)
- [Biopython 1.53 released](#)

See also our [news page](#), and [twitter](#).

The latest release is [Biopython 1.55 beta](#), released on 10 August 2010.

Navigation

- [Main Page](#)
- [Downloads](#)
- [Mailing lists](#)
- [Documentation](#)
- [Cookbook](#)
- [News](#)
- [Bugs](#)
- [Source Code](#)
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Search

HOMEWORK

As seen in Slide -3- the interaction of bioinformatics with other fields, write a short essay about one of them