BGGN 213

Foundations of Bioinformatics

Barry Grant
UC San Diego

http://thegrantlab.org/bggn213

HELLO
my name is

BARRY

bjgrant@ucsd.edu

HELLO
HER ~~my~~ name is

ILEENA

ileenamitra@eng.ucsd.edu

Introduce Yourself!

Your preferred name,
Place you identify with,
Major area of study/research,
Favorite joke (optional)!

Today's Menu

Course Logistics	Website, screencasts, survey, ethics, assessment and grading.
Learning Objectives	What you need to learn to succeed in this course.
Course Structure	Major lecture topics and specific leaning goals.
Introduction to Bioinformatis	**Introducing the *what*, *why* and *how* of bioinformatics?**
Computer Setup	Ensuring your laptop is all set for future sections of this course.

http://thegrantlab.org/bggn213/

bioboot.github.io/bggn213_f17/

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UC San Diego

BGGN 213

A hands-on introduction to the computer-based analysis of genomic and biomolecular data from the Division of Biological Sciences, UCSD.

- Overview
- Lectures
- Computer Setup
- Learning Goals
- Assignments & Grading
- Ethics Code
- Screen Cast Videos

Foundations of Bioinformatics (BGGN 213, Fall 2017)

Course Director

Prof. Barry J. Grant (Email: bjgrant@ucsd.edu)

Instructional Assistant

Ileena Mitra (Email: ileenamitra@eng.ucsd.edu)

Course Syllabus

Fall 2017 (PDF)

Overview

Bioinformatics is driving the collection and analysis of big data in the biosciences. This course is designed for bioscience graduate students and provides a hands-on introduction to the computer-based analysis of genomic and biomolecular data.

Major topics include:

- Genomic and biomolecular bioinformatic resources,

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What essential concepts and skills should YOU attain from this course?

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Learning Goals

At the end of this course students will:

- Understand the increasing necessity for computation in modern life sciences research.
- Be able to use and evaluate online bioinformatics resources including major biomolecular and genomic databases, search and analysis tools, genome browsers, structure viewers, and select quality control and analysis tools to solve problems in the biological sciences.
- Be able to use the UNIX command line and the R environment to analyze bioinformatics data at scale.
- Understand the process by which genomes are currently sequenced and the bioinformatics processing and analysis required for their interpretation.
- Be familiar with the research objectives of the bioinformatics related sub-disciplines of Genomics, Transcriptomics and Structural bioinformatics.

In short, students will develop a solid foundational knowledge of bioinformatics and be able to evaluate new biomolecular and genomic information using existing bioinformatic tools and resources.

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In short, you will develop a solid foundational knowledge of **bioinformatics** and be able to evaluate new biomolecular and genomic information using **existing bioinformatic tools and resources**.

Specific Learning Goals….

What I want you to know by course end!

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Specific Learning Goals

Teaching toward the specific learning goals below is expected to occupy 60%-70% of class time. The remaining course content is at the discretion of the instructor with student body input. This includes student selected topics for peer presentation as well one student selected guest lecture from an industry based genomic scientist.

All students who receive a passing grade should be able to:

		Lecture(s):
1	Appreciate and describe in general terms the role of computation in hypothesis-driven discovery processes within the life sciences.	1, 2, 20
2	Be able to query, search, compare and contrast the data contained in major bioinformatics databases and describe how these databases intersect (GenBank, GENE, UniProt, PFAM, OMIM, PDB, UCSC, ENSEMBLE).	2, 12, 13
3	Describe how nucleotide and protein sequence and structure data are represented (FASTA, FASTQ, GenBank, UniProt, PDB).	3, 10
4	Be able to describe how dynamic programming works for pairwise sequence alignment and appreciate the differences	4, 5

Course Structure

Derived from specific learning goals

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Lectures

All Lectures are Tu/Th 9:00-12:00 pm in Warren Lecture Hall 2015 (WLH 2015) (Map). Clicking on the class topics below will take you to corresponding lecture notes, homework assignments, pre-class video screen-casts and required reading material.

#	Date	Topics for Fall 2017
1	Th, 09/28	**Welcome to Foundations of Bioinformatics** Course introduction, Leaning goals & expectations, Biology is an information science, History of Bioinformatics, Types of data, Application areas and introduction to upcoming course segments, Student computer setup
2	Tu, 10/03	**Bioinformatics databases and key online resources** NCBI & EBI resources for the molecular domain of bioinformatics, Focus on GenBank, UniProt, Entrez and Gene Ontology. Hands on with BLAST, GenBank, OMIM, GENE, UniProt, Muscle, PFAM and PDB bioinformatics tools and databases

Course Structure

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Class Details

Goals, Class material, Screencasts & **Homework**

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1: Welcome to Foundations of Bioinformatics

Topics:

Course introduction, Leaning goals & expectations, Biology is an information science, History of Bioinformatics, Types of data, Application areas and introduction to upcoming course segments, Student 30-second introductions, Student computer setup.

Goals:

- Understand course scope, expectations, logistics and ethics code.
- Understand the increasing necessity for computation in modern life sciences research.
- Get introduced to how bioinformatics is practiced.
- Complete the pre-course questionnaire.
- Setup your laptop computer for this course.

Material:

- Pre class screen cast,
- Lecture Slides: Large PDF, Small PDF, (To be updated!)
- Handout: Class Syllabus
- Computer Setup Instructions.

Homework

Goals, Class material, Screencasts & **Homework**

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Homework:

- Questions,
- Readings:
  - PDF1: What is bioinformatics? An introduction and overview,
  - PDF2: Advancements and Challenges in Computational Biology,
  - Other: For Big-Data Scientists, 'Janitor Work' Is Key Hurdle to Insights New York Times, 2014.

Screen Casts:

1 Welcome to BGGN-213: Course introduction and logistics.

Homework

Goals, Class material, Screencasts & **Homework**

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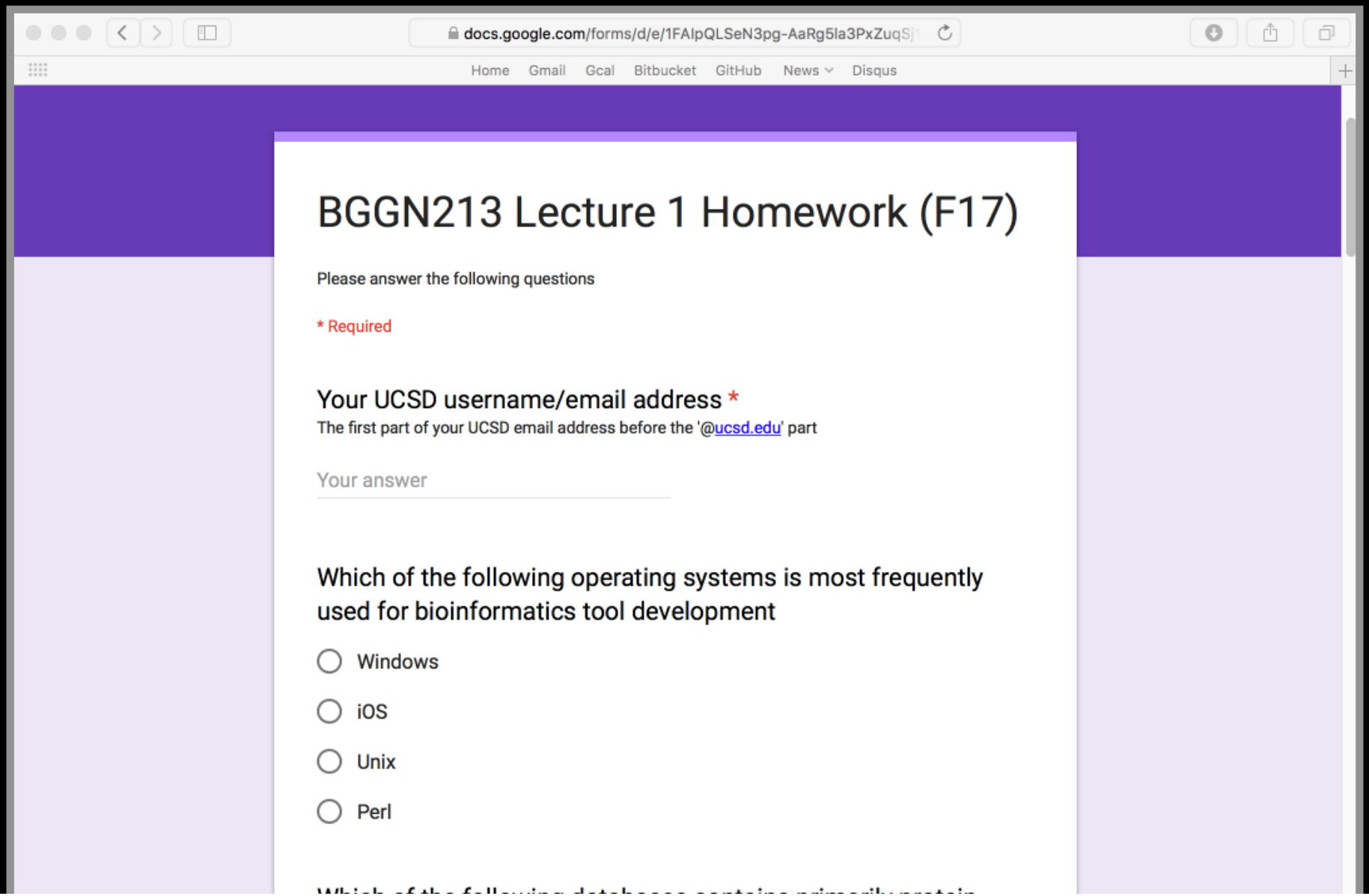

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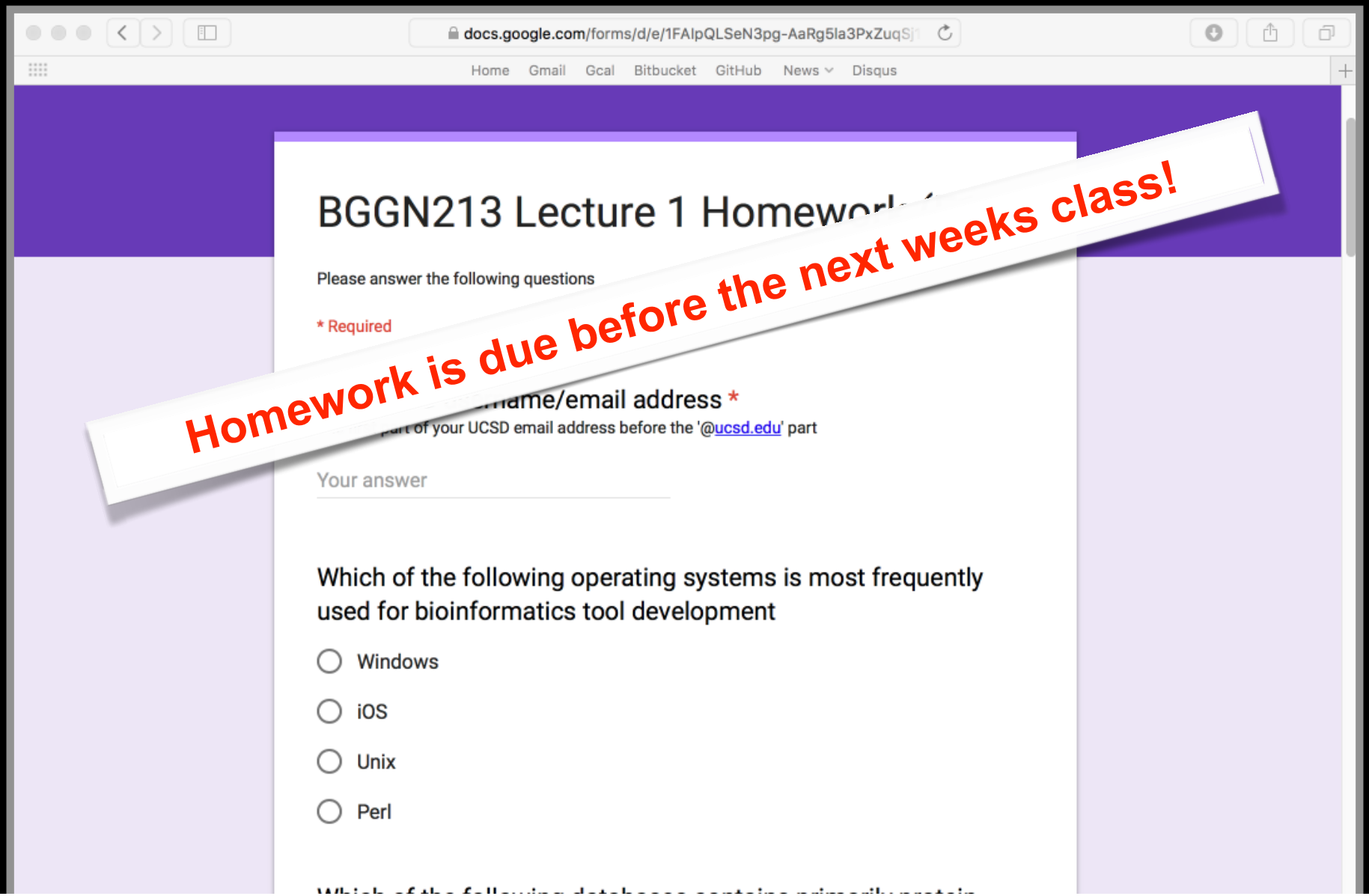

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OUTLINE

Overview of bioinformatics

- The *what*, *why* and *how* of bioinformatics?
- Major bioinformatics research areas.
- Skepticism and common problems with bioinformatics.

Online databases and associated tools

- Primary, secondary and composite databases.
  - Nucleotide sequence databases (GenBank & RefSeq).
  - Protein sequence database (UniProt).
  - Composite databases (PFAM & OMIM).

Database usage vignette

- How-to productively navigate major databases.

Q. What is Bioinformatics?

"*Bioinformatics is the application of computers to the collection, archiving, organization, and analysis of biological data.*"

… Bioinformatics is a hybrid of biology and computer science

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… **Bioinformatics is computer aided biology!**

Q. What is Bioinformatics?

"Bioinformatics is the application of computers to the collection, archiving, organization, and analysis of biological data."

… Bioinformatics is a hybrid of biology and computer science

… **Bioinformatics is computer aided biology!**

Computer based management and analysis of biological and biomedical data with useful applications in many disciplines, particularly genomics, proteomics, metabolomics, etc...

MORE DEFINITIONS

- "Bioinformatics is conceptualizing biology in terms of **macromolecules** and then applying **"informatics" techniques** (derived from disciplines such as applied maths, computer science, and statistics) to **understand** and **organize** the information associated with these molecules, on a **large-scale**.
  Luscombe NM, *et al.* Methods Inf Med. 2001;40:346.

- "Bioinformatics is research, development, or application of **computational approaches** for expanding the use of **biological**, **medical**, **behavioral** or **health data**, including those to **acquire**, **store**, **organize** and **analyze** such data."
  National Institutes of Health (NIH) (http://tinyurl.com/l3gxr6b)

MORE DEFINITIONS

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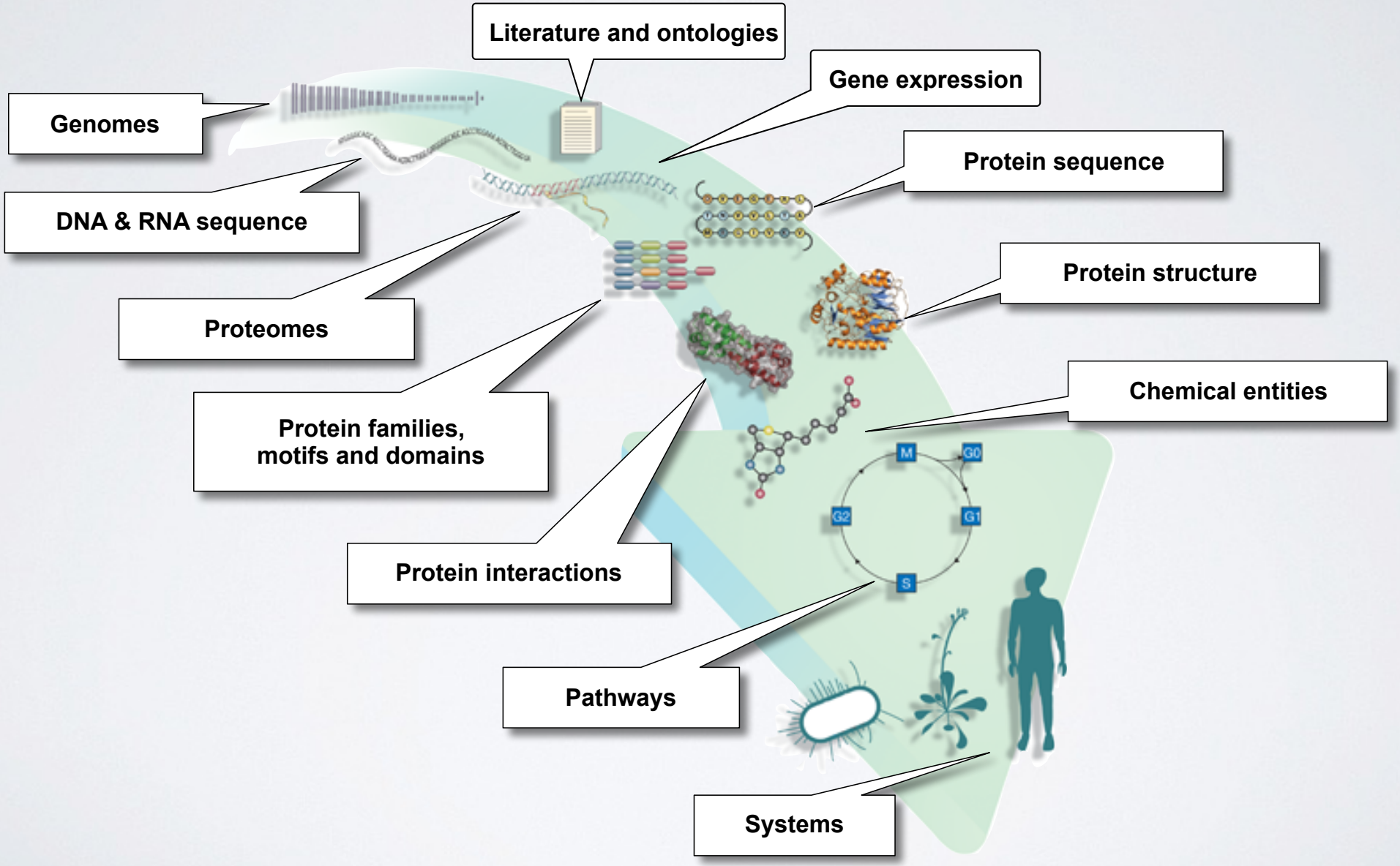
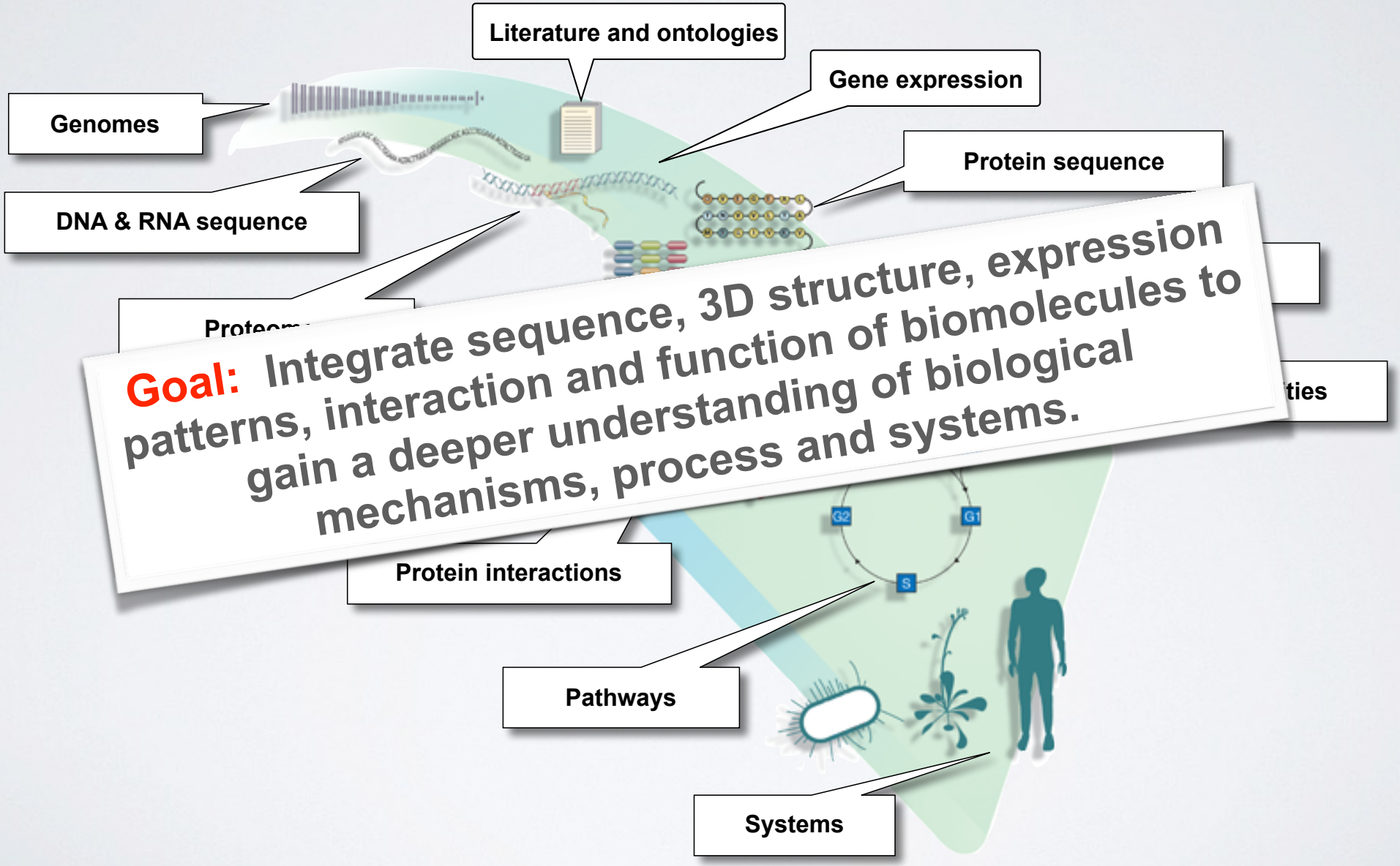
- "Bioinformati[illegible]arch, development, or application of **compu**[illegible] **approaches** for expanding the use of **bi**[illegible], **medical**, **behavioral** or **health data**, including those to a[illegible]**quire**, **store**, **organize** and **analyze** such data." National Institutes of Health (NIH) (http://tinyurl.com/l3gxr6b)

Key Point: Bioinformatics is Computer Aided Biology

Major types of Bioinformatics Data

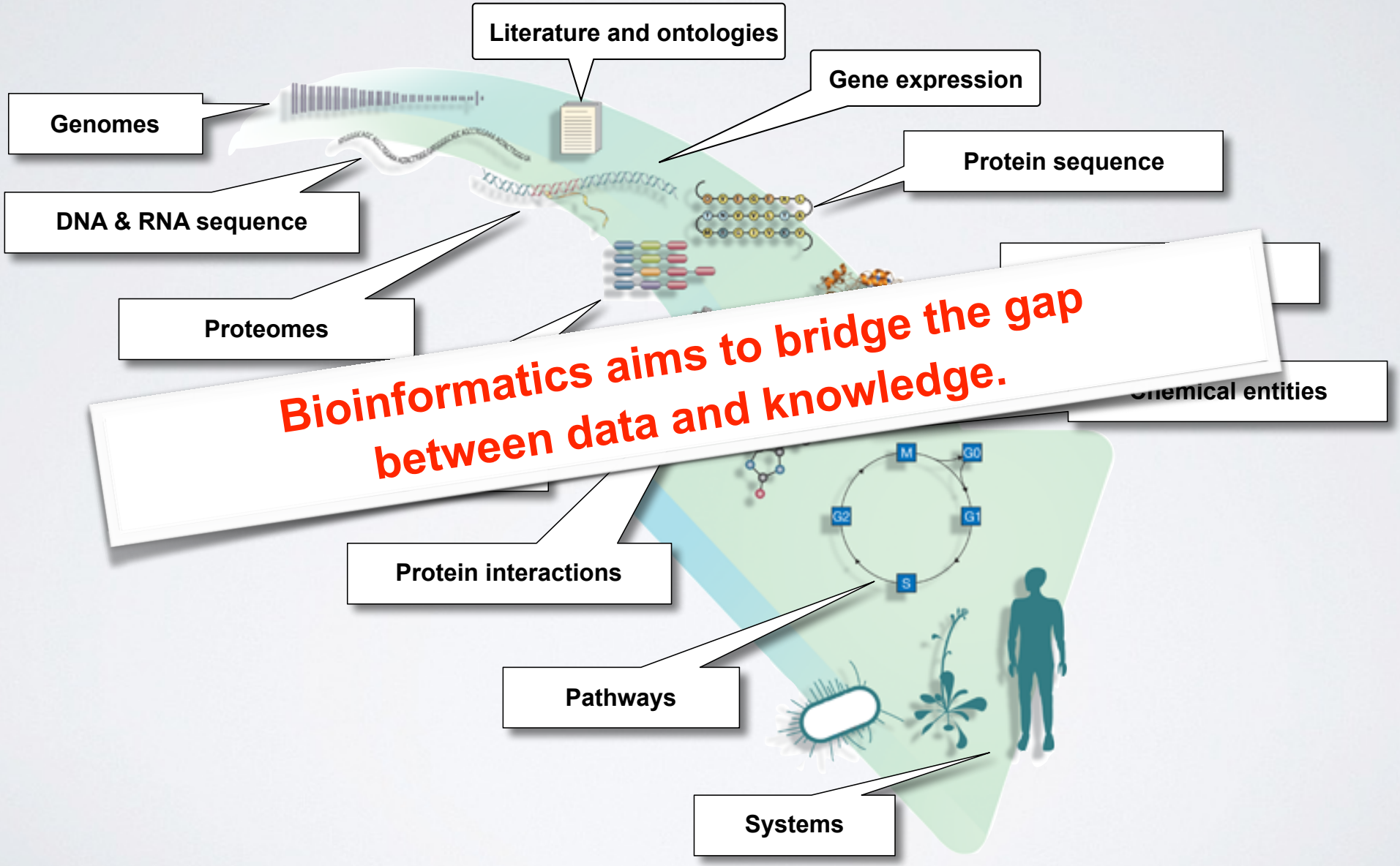


Major types of Bioinformatics Data



Goal: Integrate sequence, 3D structure, expression patterns, interaction and function of biomolecules to gain a deeper understanding of biological mechanisms, process and systems.

Major types of Bioinformatics Data



Bioinformatics aims to bridge the gap between data and knowledge.

BIOINFORMATICS RESEARCH AREAS

Include but are not limited to:

- Organization, classification, dissemination and analysis of biological and biomedical data (particularly '-omics' data).
- Biological sequence analysis and phylogenetics.
- Genome organization and evolution.
- Regulation of gene expression and epigenetics.
- Biological pathways and networks in healthy & disease states.
- Protein structure prediction from sequence.
- Modeling and prediction of the biophysical properties of biomolecules for binding prediction and drug design.
- Design of biomolecular structure and function.

With applications to Biology, Medicine, Agriculture and Industry

Where did bioinformatics come from?

Bioinformatics arose as molecular biology began to be transformed by the emergence of molecular sequence and structural data

Recap: <u>The key dogmas of molecular biology</u>

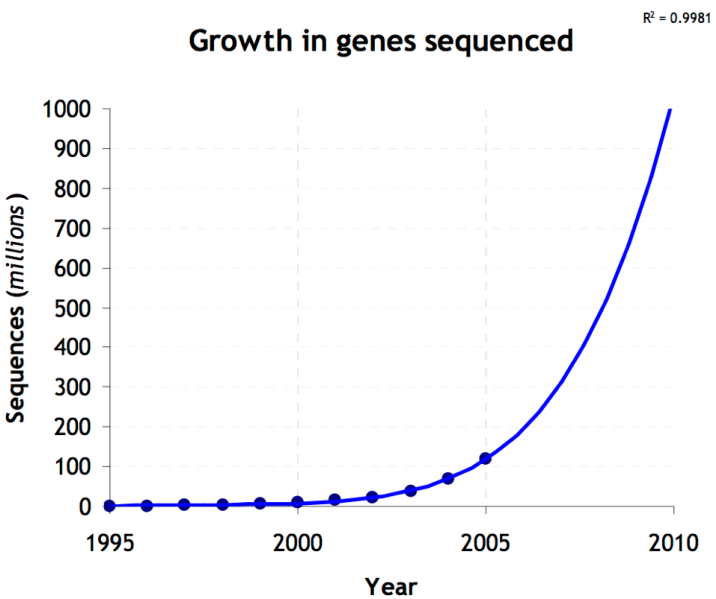
- *DNA sequence* determines *protein sequence.*
- *Protein sequence* determines *protein structure.*
- *Protein structure* determines *protein function.*
- *Regulatory mechanisms* (e.g. gene expression) determine the amount of a particular *function in space and time.*

Bioinformatics is <u>*now*</u> essential for the archiving, organization and analysis of data related to all these processes.

Why do we need Bioinformatics?

Bioinformatics is necessitated by the rapidly expanding quantities and complexity of biomolecular data

- Bioinformatics provides methods for the efficient:
  - **storage**
  - **annotation**
  - **search** and **retrieval**
  - data **integration**
  - data **mining** and **analysis**



E.G. data from sequencing, structural genomics, proteomics, new high throughput assays, *etc…*

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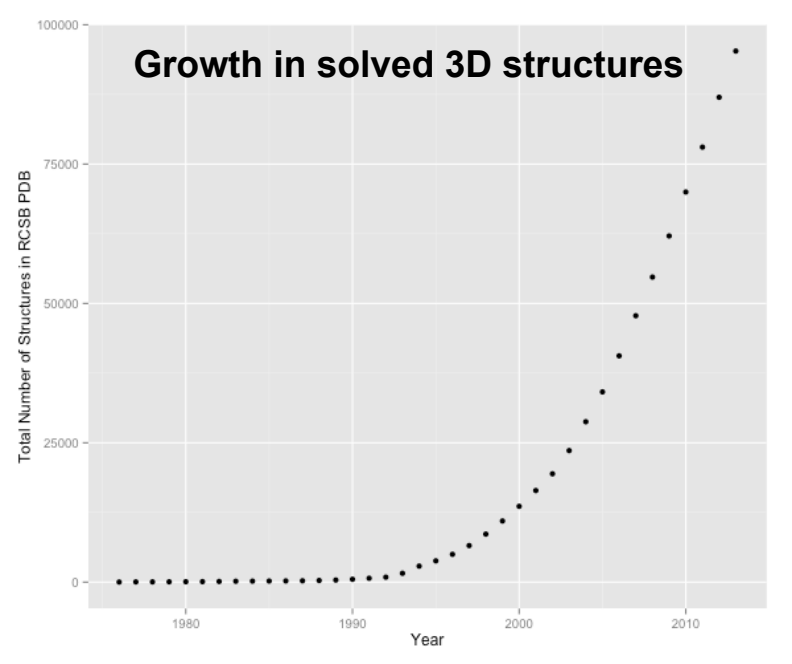


E.G. data from sequencing, structural genomics, proteomics, new high throughput assays, *etc…*

How do we do Bioinformatics?

- A "*bioinformatics approach*" involves the application of **computer algorithms**, **computer models** and **computer databases** with the broad goal of understanding the action of both individual genes, transcripts, proteins and large collections of these entities.

DNA	→	RNA	→	Protein
Genome	→	**Transcriptome**	→	**Proteome**

x 1,000

x 100,000

How do we actually do Bioinformatics?

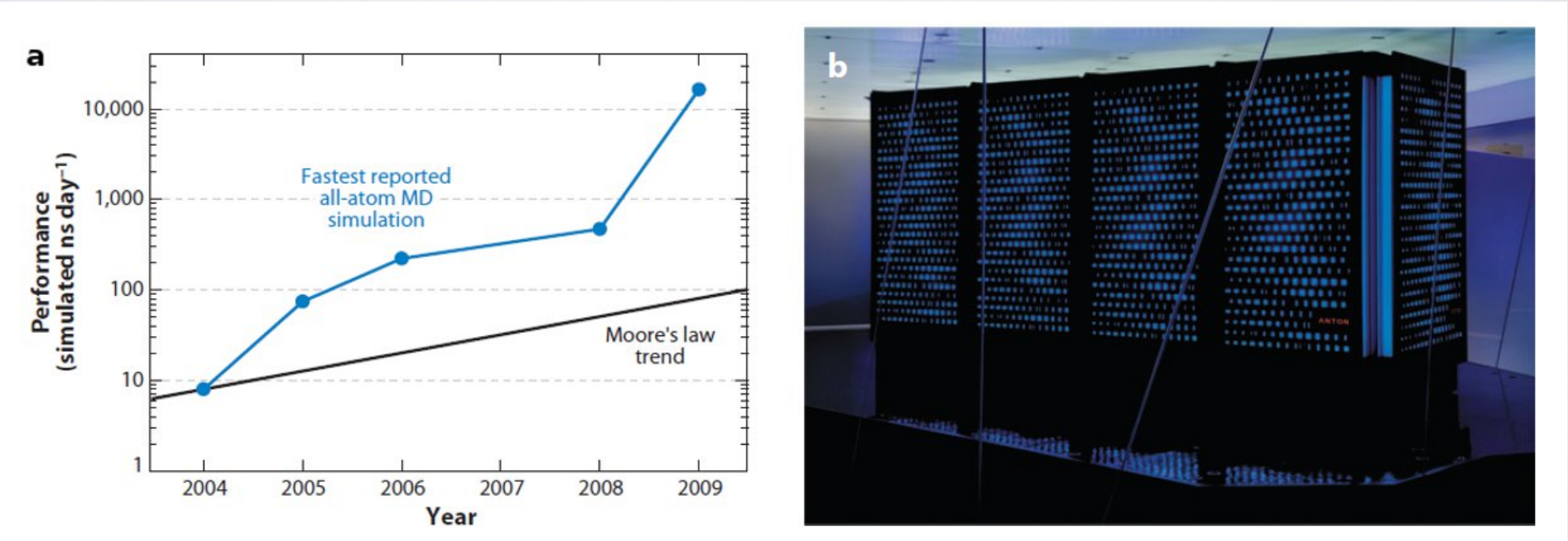
Pre-packaged tools and databases

- Many online
- New tools and time consuming methods frequently require downloading
- Most are free to use

Tool development

- Mostly on a UNIX environment
- Knowledge of programing languages frequently required (Python, **R**, Perl, C Java, Fortran)
- May require specialized or high performance computing resources…

SIDE-NOTE: SUPERCOMPUTERS AND GPUS



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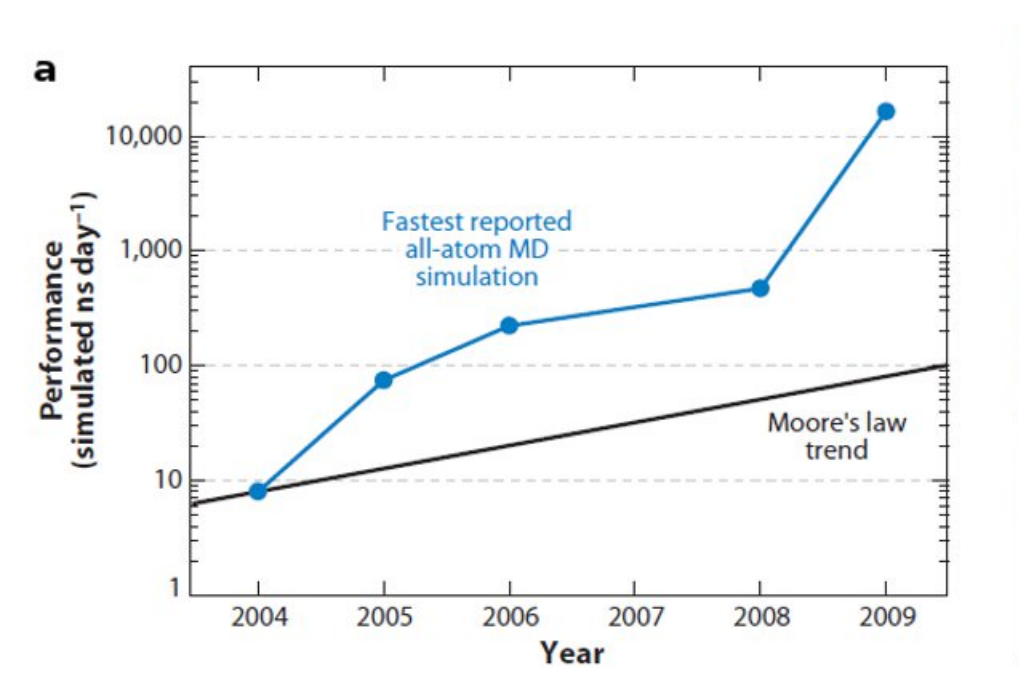


HOW COMPUTERS HAVE CHANGED

DATE	COST	SPEED	MEMORY	SIZE
1967	$40M	0.1 MHz	1 MB	HALL
2013	$4,000	1 GHz	10 GB	LAPTOP
CHANGE	10,000	10,000	10,000	10,000

If cars were like computers then a new Volvo would cost $3, would have a top speed of 1,000,000 Km/hr, would carry 50,000 adults and would park in a shoebox

Skepticism & Bioinformatics

We have to approach computational results the same way we do wet-lab results:

- Do they make sense?
- Is it what we expected?
- Do we have adequate controls, and how did they come out?
- Modeling is modeling, but biology is different...
  What does this model actually contribute?
- Avoid the miss-use of ‘black boxes’

Common problems with Bioinformatics

Confusing multitude of tools available

- Each with many options and settable parameters

Most tools and databases are written by and for nerds

- Same is true of documentation - if any exists!

Most are developed independently

Notable exceptions are found at the:

- **EBI** (European Bioinformatics Institute) and
- **NCBI** (National Center for Biotechnology Information)

Protein BLAST: search protein databases using a protein query

blast.ncbi.nlm.nih.gov/Blast.cgi?PROGRAM=blastp&BLAST_PROGRAMS=blastp&PAGE_TYPE=BlastSearch&SHOW_DEFAULTS=on&LINK_LOC=blasthome

General Parameters

Max target sequences	500 — Select the maximum number of aligned sequences to display
Short queries	☑ Automatically adjust parameters for short input sequences
Expect threshold	10
Word size	3
Max matches in a query range	0

Scoring Parameters

Matrix	BLOSUM62
Gap Costs	Existence: 11 Extension: 1
Compositional adjustments	Conditional compositional sco

Filters and Masking

Filter	☐ Low complexity regions
Mask	☐ Mask for lookup table only ☐ Mask lower case letters

PSI/PHI/DELTA BLAST

Upload PSSM Optional	Choose File — no file selected
PSI-BLAST Threshold	0.005
Pseudocount	0

Even Blast has many settable parameters

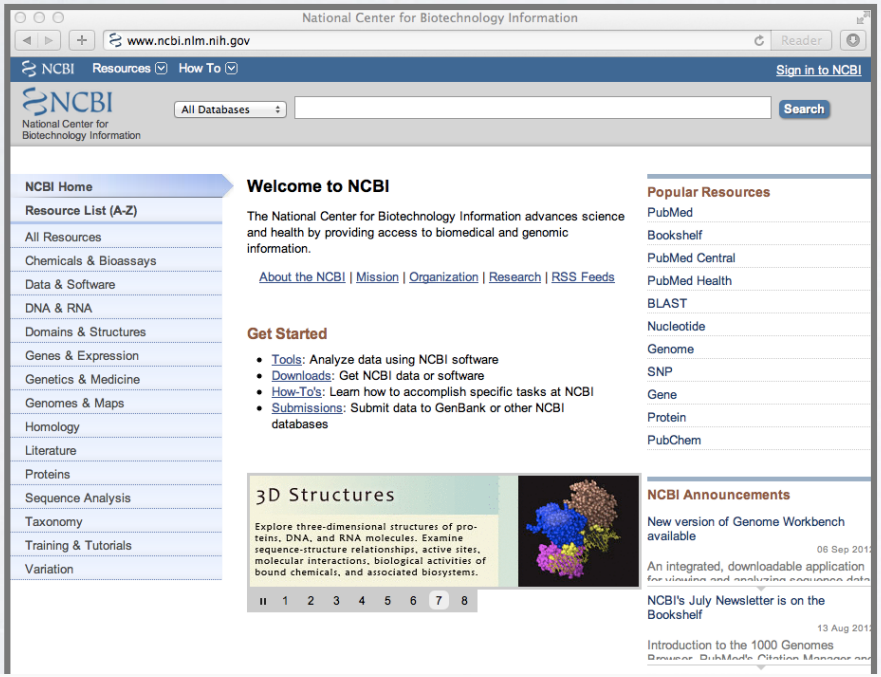
STEP 3 - Set you

Related tools with different terminology

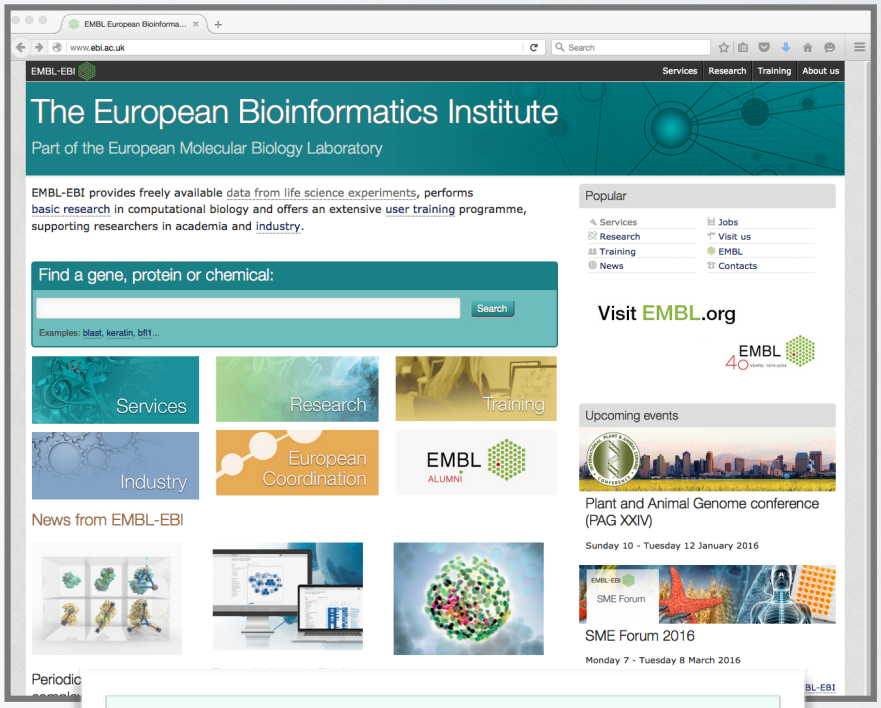
PROGRAM					
FASTA					
MATRIX	**GAP OPEN**	**GAP EXTEND**	**KTUP**	**EXPECTATION UPPER VALUE**	**EXPECTATION LOWER VALUE**
BLOSUM50	-10	-2	2	10	0 (default)
DNA STRAND	**HISTOGRAM**	**FILTER**		**STATISTICAL ESTIMATES**	
N/A	no	none		Regress	
SCORES	**ALIGNMENTS**	**SEQUENCE RANGE**	**DATABASE RANGE**	**MULTI HSPs**	
50	50	START-END	START-END	no	
SCORE FORMAT					
Default					

Key Online Bioinformatics Resources: NCBI & EBI

The NCBI and EBI are invaluable, publicly available resources for biomedical research



http://www.ncbi.nlm.nih.gov



https://www.ebi.ac.uk

National Center for Biotechnology Information (NCBI)

- Created in 1988 as a part of the National Library of Medicine (NLM) at the National Institutes of Health
- NCBI's mission includes:
  - Establish **public databases**
  - Develop **software tools**
  - **Education** on and dissemination of biomedical information

- We will cover a number of core NCBI databases and software tools in the lecture

http://www.ncbi.nlm.nih.gov

National Center for Biotechnology Information

www.ncbi.nlm.nih.gov

NCBI Resources How To Sign in to NCBI

NCBI National Center for Biotechnology Information

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.

About the NCBI | Mission | Organization | Research | RSS Feeds

Get Started

- Tools: Analyze data using NCBI software
- Downloads: Get NCBI data or software
- How-To's: Learn how to accomplish specific tasks at NCBI
- Submissions: Submit data to GenBank or other NCBI databases

Popular Resources

PubMed
Bookshelf
PubMed Central
PubMed Health
BLAST
Nucleotide
Genome
SNP
Gene
Protein
PubChem

3D Structures

Explore three-dimensional structures of proteins, DNA, and RNA molecules. Examine sequence-structure relationships, active sites, molecular interactions, biological activities of bound chemicals, and associated biosystems

NCBI Announcements

New version of Genome Workbench available

06 Sep

An integrated, downloadable applicati

http://www.ncbi.nlm.nih.gov

National Center for Biotechnology Information

www.ncbi.nlm.nih.gov

NCBI Resources How To Sign in to NCBI

NCBI National Center for Biotechnology Information

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 Biotech
and health by providing access
information.

About the NCBI | Mission | Or

Get Started

- Tools: Analyze data using
- Downloads: Get NCBI data
- How-To's: Learn how to acc
- Submissions: Submit data
databases

3D Structures

Explore three-dimensional structures of pro-teins, DNA, and RNA molecules. Examine sequence-structure relationships, active sites, molecular interactions, biological activities of bound chemicals, and associated biosystems

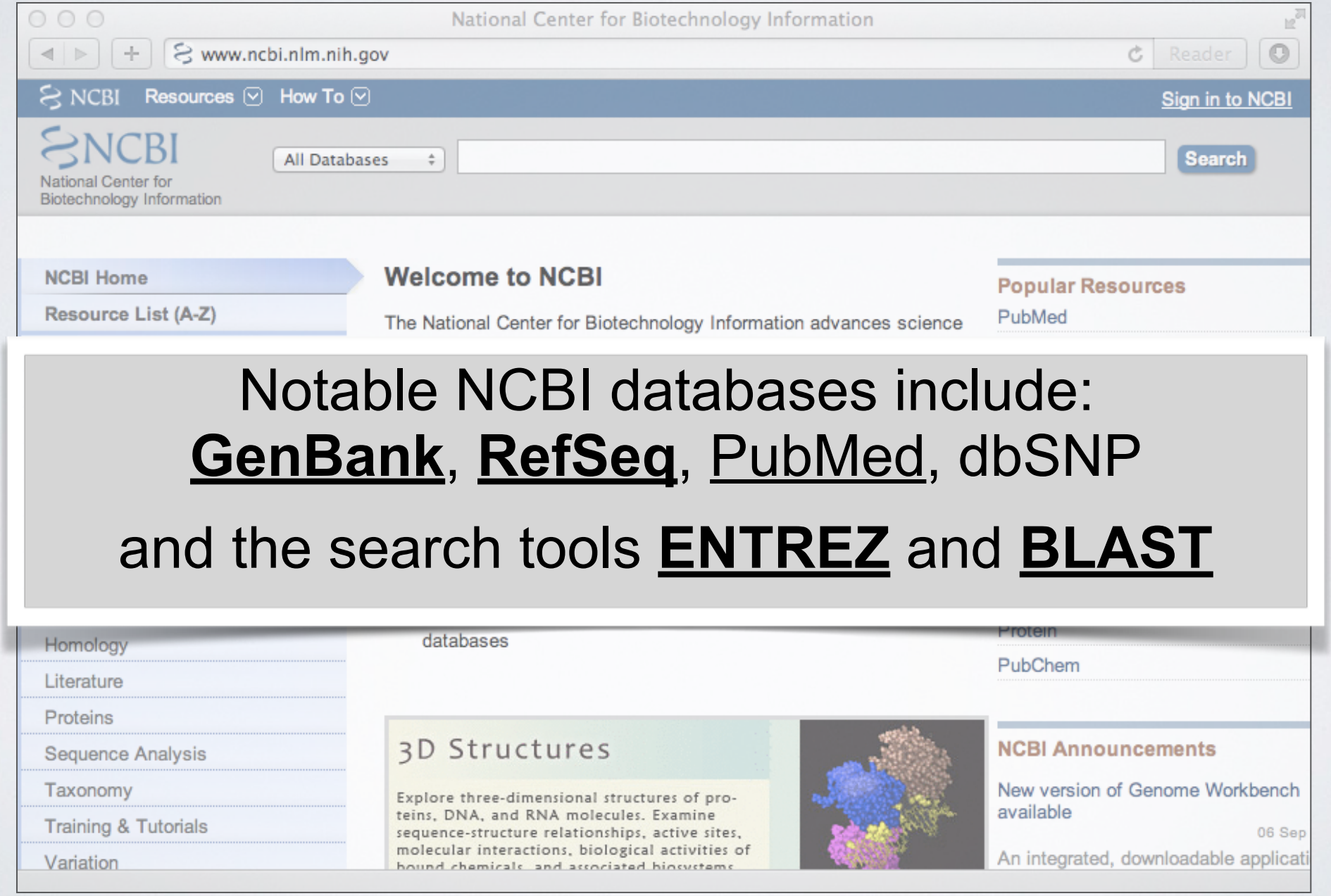
Popular Resources

PubMed
Bookshelf
PubMed Central
PubMed Health
BLAST
Nucleotide
Genome
SNP
Gene
Protein
PubChem

Resources
f
Central
Health
e

nouncements
New version of Genome Workbench available
06 Sep
An integrated, downloadable applicati

http://www.ncbi.nlm.nih.gov

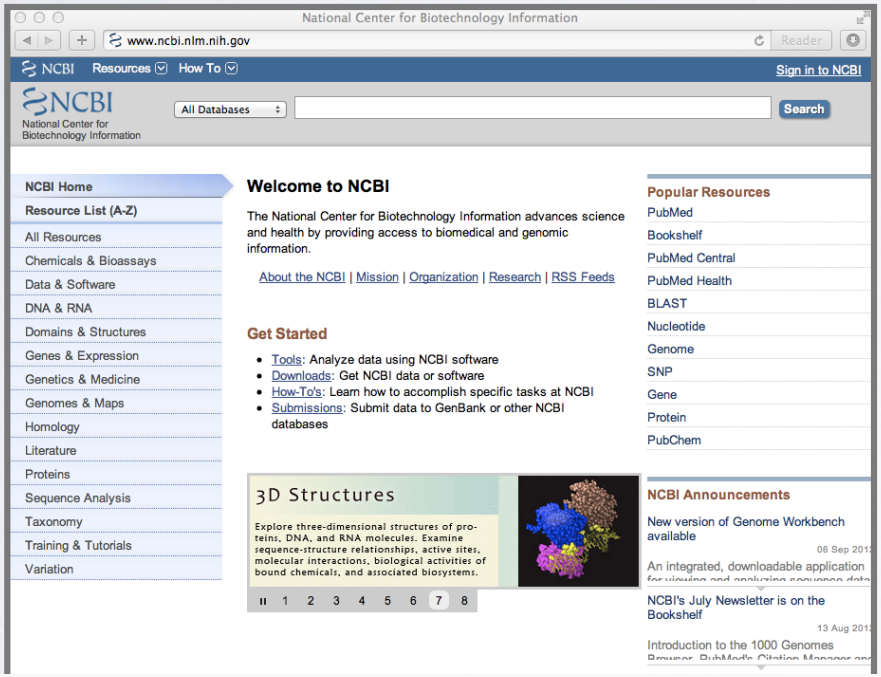


Notable NCBI databases include:
GenBank, **RefSeq**, PubMed, dbSNP

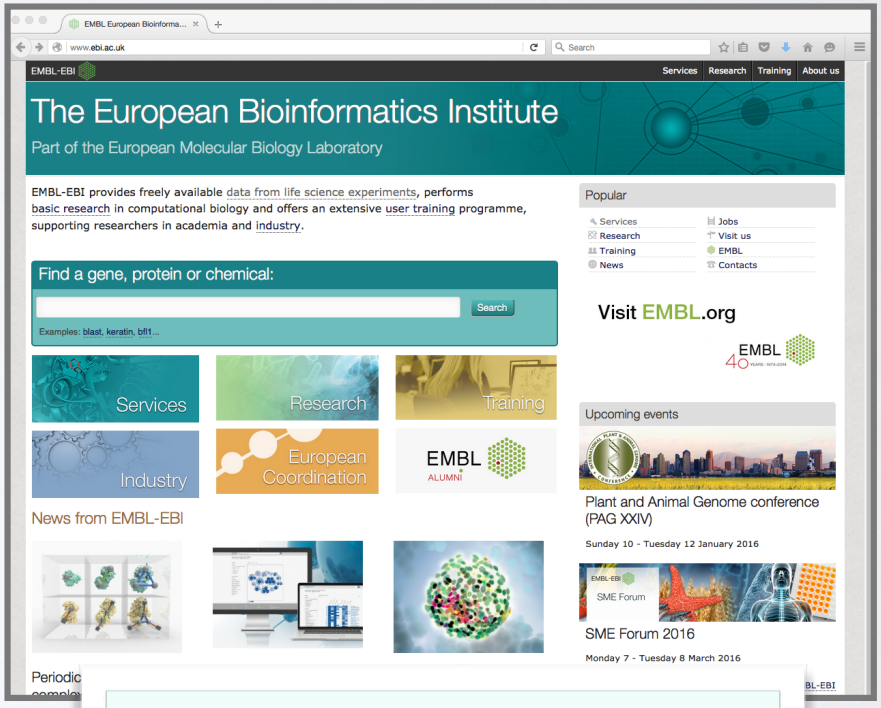
and the search tools **ENTREZ** and **BLAST**

Key Online Bioinformatics Resources: NCBI & EBI

The NCBI and EBI are invaluable, publicly available resources for biomedical research



http://www.ncbi.nlm.nih.gov



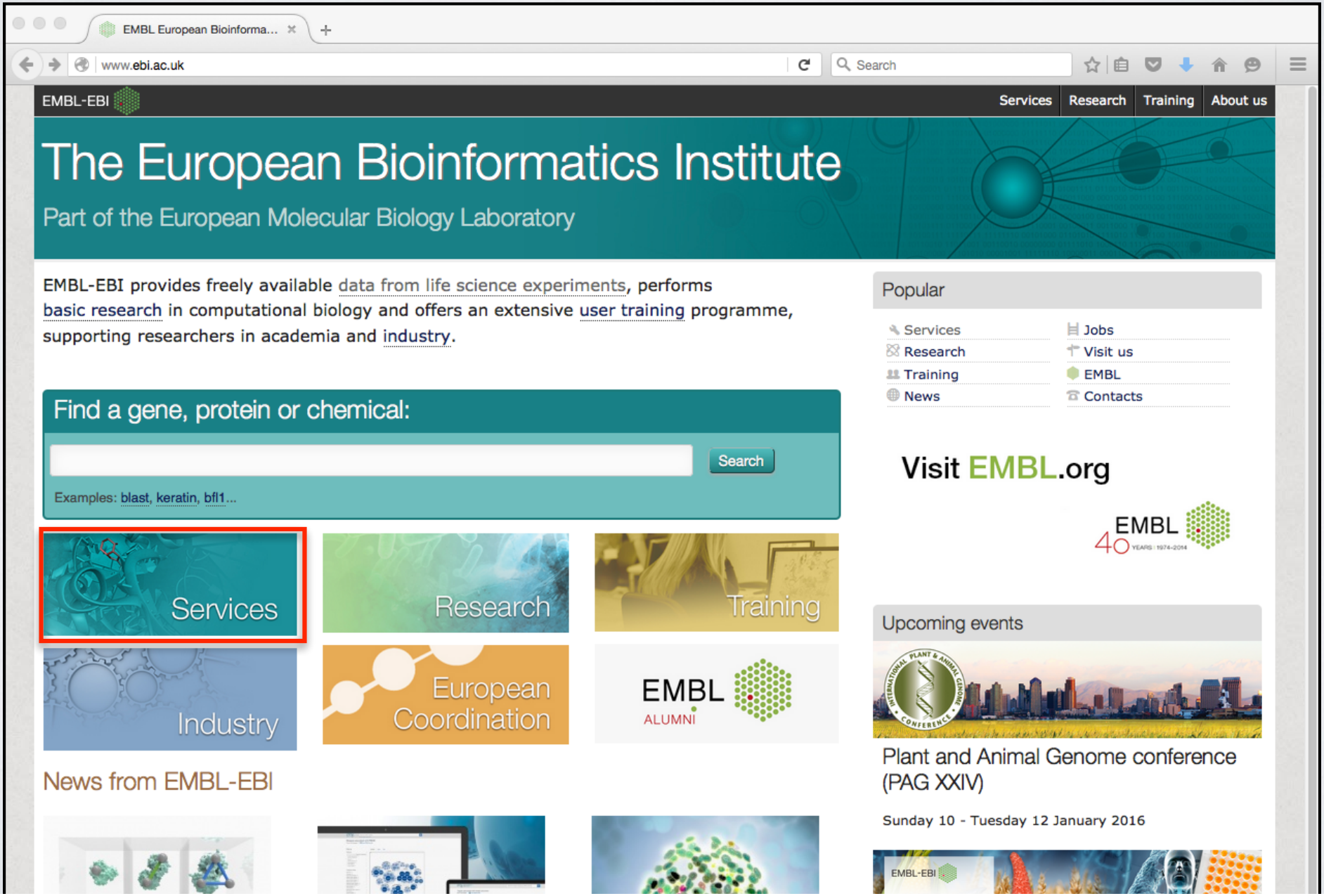
https://www.ebi.ac.uk

European Bioinformatics Institute (EBI)

- Created in 1997 as a part of the European Molecular Biology Laboratory (EMBL)
- EBI's mission includes:
  - providing freely available **data** and **bioinformatics services**
  - and providing advanced **bioinformatics training**

- We will briefly cover several EBI databases and tools that have advantages over those offered at NCBI

The EBI maintains a number of high quality curated **secondary databases** and associated tools



The EBI maintains a number of high quality curated **secondary databases** and associated tools

Services < EMBL-EBI

www.ebi.ac.uk/services

EMBL-EBI | Services | Research | Training | About us

Services

Overview | A to Z | Data submission | Support

Bioinformatics services

We maintain the world's most comprehensive range of **freely available** and up-to-date molecular databases. Developed in collaboration with our colleagues worldwide, our services let you share data, perform complex queries and analyse the results in different ways. You can work locally by downloading our data and software, or use our web services to access our resources programmatically. You can read more about our services in the journal *Nucleic Acids Research*.

DNA & RNA
genes, genomes & variation

Gene expression
RNA, protein & metabolite expression

Proteins
sequences, families & motifs

Structures
Molecular & cellular structures

Systems
reactions, interactions & pathways

Chemical biology
chemogenomics & metabolomics

Ontologies
taxonomies & controlled vocabularies

Literature
Scientific publications & patents

Cross domain
cross-domain tools & resources

Popular

- Ensembl
- UniProt
- PDBe
- ArrayExpress
- ChEMBL
- BLAST
- Europe PMC
- Reactome
- Train online
- Support

Service news

The EBI maintains a number of high quality curated **secondary databases** and associated tools

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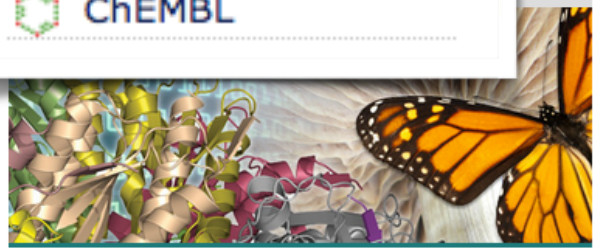
- **DNA & RNA** — genes, genomes & variation
- **Gene expression** — RNA, protein & metabolite expression
- **Proteins** — sequences, families & motifs
- **Structures** — Molecular & cellular structures
- **Systems** — reactions, interactions & pathways
- **Chemical biology** — chemogenomics & metabolomics
- **Ontologies** — taxonomies & controlled vocabularies
- **Literature** — Scientific publications & patents
- **Cross domain** — cross-domain tools & resources

Popular

- Ensembl
- UniProt
- PDBe
- ArrayExpress
- ChEMBL



https://www.ebi.ac.uk

The EBI makes available a wider variety of **online tools** than NCBI

Proteins

Popular services

UniProt: The Universal Protein Resource

The gold-standard, comprehensive resource for protein sequence and functional annotation data.

InterPro

A database for the classification of proteins into families, domains and conserved sites.

PRIDE: The Proteomics Identifications Database

An archive of protein expression data determined by mass spectrometry.

Pfam

A database of hidden Markov models and alignments to describe conserved protein families and domains.

Clustal Omega

Multiple sequence alignment of DNA or protein sequences. Clustal Omega replaces the older ClustalW alignment tools.

HMMER - protein homology search

Fast sensitive protein homology searches using profile hidden Markov models (HMMs). Variety of different search methods for querying against both sequence and HMM target databases.

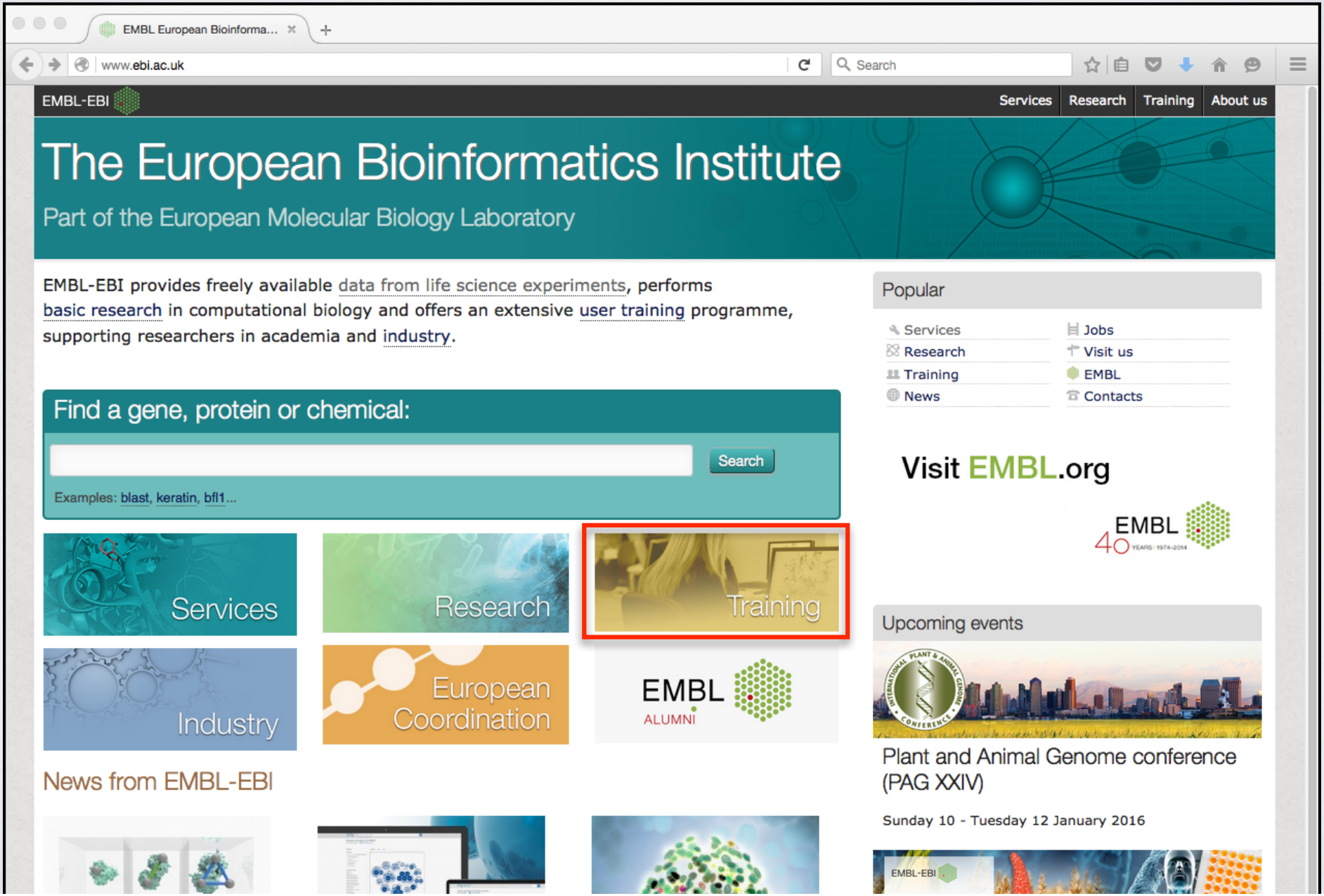
InterProScan 5

InterProScan 5 searches sequences against InterPro's predictive protein signatures. Please note that InterProScan 4.8 has been retired.

Quick links

- Popular services in this category
- All services in this category
- Project websites in this category

The EBI also provides a growing selection of **online tutorials** on EBI databases and tools



The EBI also provides a growing selection of **online tutorials** on EBI databases and tools

Using sequence similarity s...

www.ebi.ac.uk/training/online/course/using-sequence-similarity-searching-tools-embl-ebi

EMBL-EBI | Services | Research | Training | About us

Train online

Training | Train online Home | Course list | Glossary | Support & Feedback | Log in / Register

training » online » course-list » using-sequence-similarity-searching-tools-embl-ebi

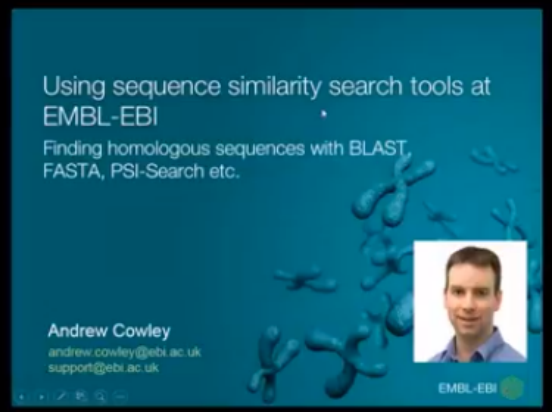
Course content

- Using sequence similarity searching tools at EMBL-EBI: webinar
- Contributors

Print Course

Using sequence similarity searching tools at EMBL-EBI: webinar

Using sequence similarity searching tools at EMBL-EBI: webinar



0:00 / 37:42

This webinar focuses on how to use tools like BLAST and PSI-Search to find homologous sequences in EMBL-EBI databases, including tips on which tool and database to use, input formats, how to change parameters and how to interpret the results pages.

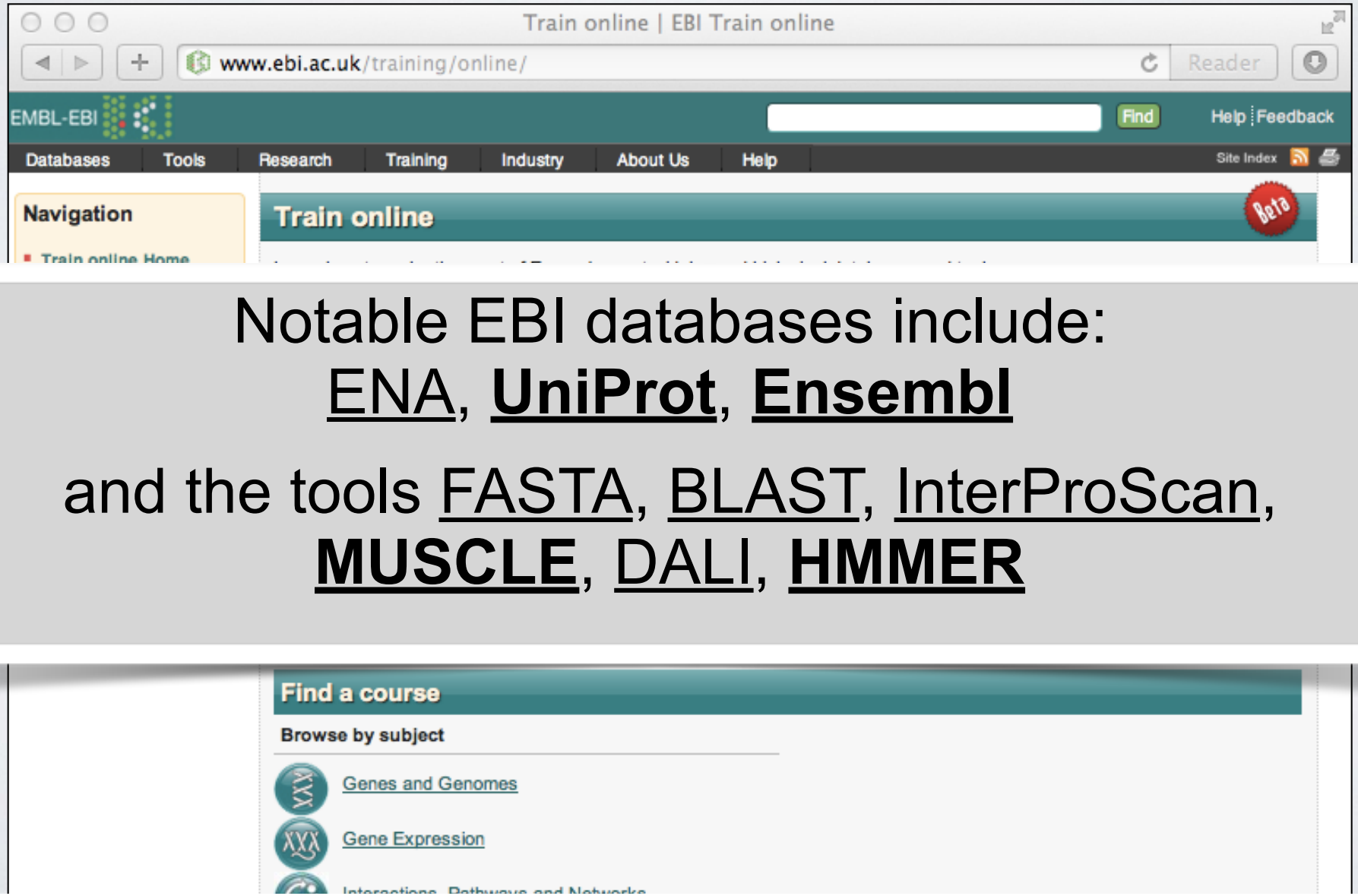
Popular

- Train online
- Find us
- Funding

Find us at...

- Open days and career days
- Conference exhibitions
- EMBL courses and events
- Genome campus events
- Science for schools

The EBI also provides a growing selection of **online tutorials** on EBI databases and tools



Notable EBI databases include:
ENA, **UniProt**, **Ensembl**

and the tools FASTA, BLAST, InterProScan, **MUSCLE**, DALI, **HMMER**

Next Class…

MAJOR BIOINFORMATICS DATABASES AND ASSOCIATED ONLINE TOOLS

Bioinformatics Databases

AATDB, AceDb, ACUTS, ADB, AFDB, AGIS, AMSdb, ARR, AsDb,BBDB, BCGD, Beanref, BioImage, BioMagResBank, BIOMDB, BLOCKS, BovGBASE, BOVMAP, BSORF, BTKbase, CANSITE, CarbBank, CARBHYD, CATH, CAZY, CCDC, CD4OLbase, CGAP, ChickGBASE, Colibri, COPE, CottonDB, CSNDB, CUTG, CyanoBase, dbCFC, dbEST, dbSTS, DDBJ, DGP, DictyDb, Picty_cDB, DIP, DOGS, DOMO, DPD, DPInteract, ECDC, ECGC, EC02DBASE, EcoCyc, EcoGene, EMBL, EMD db, ENZYME, EPD, EpoDB, ESTHER, FlyBase, FlyView, GCRDB, GDB, GENATLAS, Genbank, GeneCards, GenIilesne, GenLink, GENOTK, GenProtEC, GIFTS, GPCRDB, GRAP, GRBase, gRNAsdb, GRR, GSDB, HAEMB, HAMSTERS, HEART-2DPAGE, HEXAdb, HGMD, HIDB, HIDC, HIVdb, HotMolecBase, HOVERGEN, HPDB, HSC-2DPAGE, ICN, ICTVDB, IL2RGbase, IMGT, Kabat, KDNA, KEGG, Klotho, LGIC, MAD, MaizeDb, MDB, Medline, Mendel, MEROPS, MGDB, MGI, MHCPEP5 Micado, MitoDat, MITOMAP, MJDB, MmtDB, MoI-R-Us, MPDB, MRR, MutBase, MycDB, NDB, NRSub, 0-lycBase, OMIA, OMIM, OPD, ORDB, OWL, PAHdb, PatBase, PDB, PDD, Pfam, PhosphoBase, PigBASE, PIR, PKR, PMD, PPDB, PRESAGE, PRINTS, ProDom, Prolysis, PROSITE, PROTOMAP, RatMAP, RDP, REBASE, RGP, SBASE, SCOP, SeqAnaiRef, SGD, SGP, SheepMap, Soybase, SPAD, SRNA db, SRPDB, STACK, StyGene,Sub2D, SubtiList, SWISS-2DPAGE, SWISS-3DIMAGE, SWISS- MODEL Repository, SWISS-PROT, TeIDB, TGN, tmRDB, TOPS, TRANSFAC, TRR, UniGene, URNADB, V BASE, VDRR, VectorDB, WDCM, WIT, WormPep, etc ..... !!!!

Bioinformatics Databases

AATDB, AceDb, ACUTS, ADB, AFDB, AGIS, AMSdb, ARR, AsDb,BBDB, BC Beanref, BioImage, BioMagResBank, BIOMDB, BLOCKS, BovGBASE, BO TKbase, CANSITE, CarbBank, CARBHYD, CATH, CAZY AP, ChickGBASE, Colibri, COPE, CottonDB bEST, dbSTS, DDBJ, DGP, DictyDb, Bi CDC, ECGC, EC02DBASE THER, FlyBase, Fl Link, G DB, HAEMB, H Hivdb, HotMolecBase, H LZRGbase, IMGT, Kabat, KDNA, K DB, Medline, Mendel, MEROPS, MGDB, MGI, MHC TOMAP, MJDB, MmtDB, Mol-R-Us, MPDB, MRR, MutBase, Myc db, 0-lycBase, OMIA, OMIM, OPD, ORDB, OWL, PAHdb, PatBase, PD DB, Pfam, PhosphoBase, PigBASE, PIR, PKR, PMD, PPDB, PRESAGE, PRINTS, ProDom, Prolysis, PROSITE, PROTOMAP, RatMAP, RDP, REBASE, RGP, SBASE, SCOP, SeqAnaiRef, SGD, SGP, SheepMap, Soybase, SPAD, SRNA db, SRPDB, STACK, StyGene,Sub2D, SubtiList, SWISS-2DPAGE, SWISS-3DIMAGE, SWISS- MODEL Repository, SWISS-PROT, TelDB, TGN, tmRDB, TOPS, TRANSFAC, TRR, UniGene, URNADB, V BASE, VDRR, VectorDB, WDCM, WIT, WormPep, etc ..... !!!!

There are lots of Bioinformatics Databases

For a annotated listing of major bioinformatics databases please see the online handout

< Handout_Major_Databases.pdf >

Side-note: Databases come in all shapes and sizes





Databases can be of variable quality and often there are multiple databases with overlapping content.

Primary, secondary & composite databases

Bioinformatics databases can be usefully classified into *primary*, *secondary* and *composite* according to their data source.

- **Primary databases** (or *archival databases*) consist of data derived experimentally.
  - **GenBank**: NCBI's primary nucleotide sequence database.
  - **PDB:** Protein X-ray crystal and NMR structures.
- **Secondary databases** (or *derived databases*) contain information derived from a primary database.
  - **RefSeq**: non redundant set of curated reference sequences primarily from GenBank
  - **PFAM**: protein sequence families primarily from UniProt and PDB
- **Composite databases** (or *metadatabases*) join a variety of different primary and secondary database sources.
  - **OMIM**: catalog of human genes, genetic disorders and related literature
  - **GENE**: molecular data and literature related to genes with extensive links to other databases.

DATABASE VIGNETTE

You have just come out a seminar about gastric cancer and one of your co-workers asks:

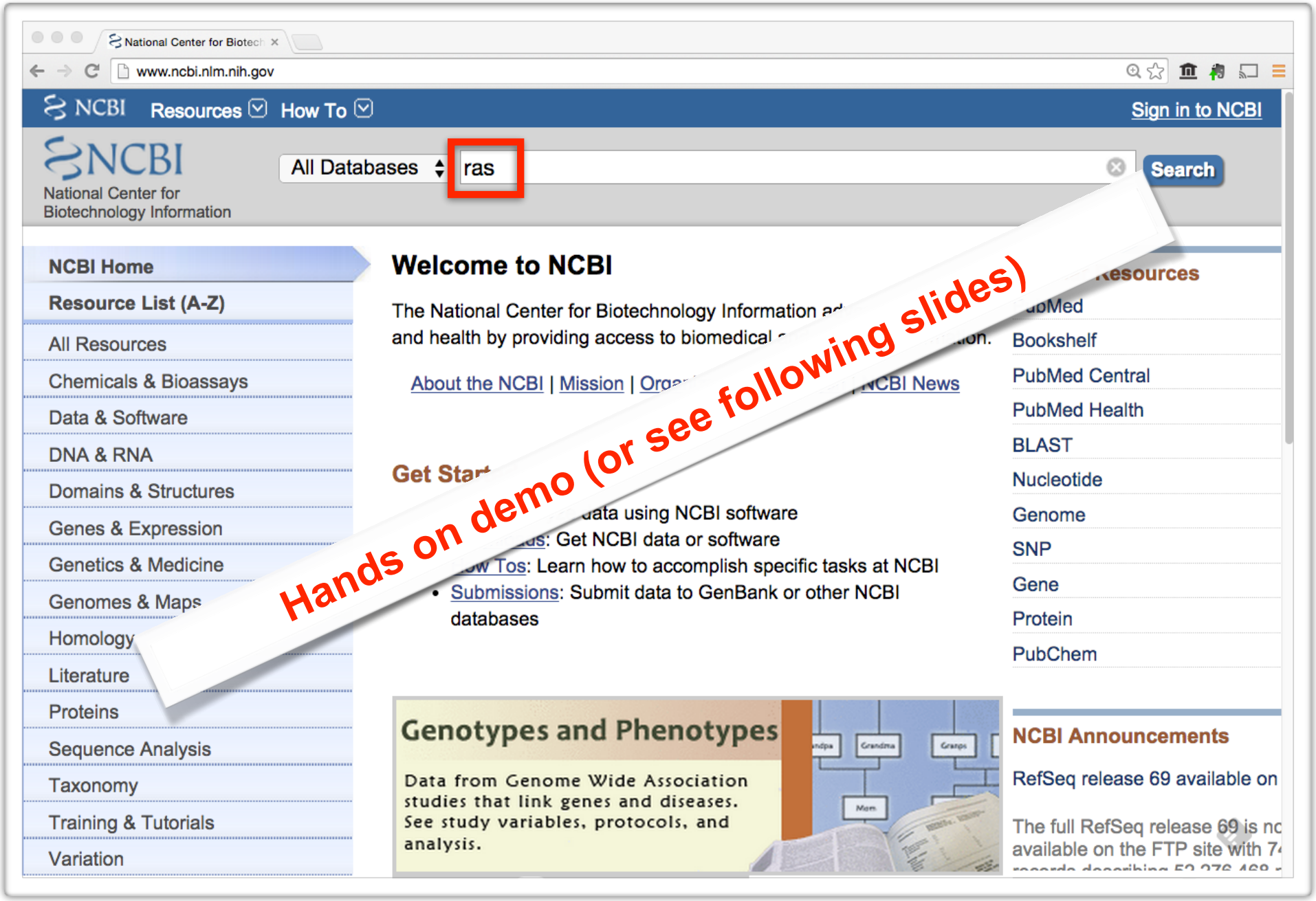
> *"What do you know about that 'Kras' gene the speaker kept taking about?"*

You have some recollection about hearing of 'Ras' before. How would you find out more?

- Google?
- Library?
- **Bioinformatics databases at NCBI and EBI!**

http://www.ncbi.nlm.nih.gov/

http://www.ncbi.nlm.nih.gov/



ras - GQuery: Global Cross

www.ncbi.nlm.nih.gov/gquery/?term=ras

NCBI Resources How To Sign in to NCBI

Search NCBI databases

Help

ras Search

About 2,978,774 search results for "ras"

Literature

Books	1,677	books and reports
MeSH	402	ontology used for PubMed indexing
NLM Catalog	223	books, journals and more in the NLM Collections
PubMed	54,672	scientific & medical abstracts/citations
PubMed Central	96,114	full-text journal articles

Health

ClinVar	759	human variations of clinical significance
dbGaP	120	genotype/phenotype interaction studies
GTR	1,879	genetic testing registry

Genes

EST	3,985	expressed sequence tag sequences
Gene	87,165	collected information about gene loci
GEO DataSets	3,732	functional genomics studies
GEO Profiles	1,622,789	gene expression and molecular abundance profiles
HomoloGene	696	homologous gene sets for selected organisms
PopSet	2,254	sequence sets from phylogenetic and population studies
UniGene	4,770	clusters of expressed transcripts

Proteins

ras - Gene - NCBI

www.ncbi.nlm.nih.gov/gene/?term=ras

NCBI Resources How To Sign in to NCBI

Gene

Gene ras Search

Save search Advanced Help

Show additional filters

Clear all

Gene sources

Genomic
Mitochondria
Organelles
Plasmids
Plastids

Categories

Alternatively spliced
Annotated genes
Non-coding
Protein-coding
Pseudogene

Sequence content

CCDS
Ensembl
RefSeq

Display Settings: Tabular, 20 per page, Sorted by Relevance Send to:

Hide sidebar >>

Did you mean ras as a gene symbol?
Search Gene for ras as a symbol.

<< First < Prev Page 1 of 4282 Next > Last >>

Results: 1 to 20 of 85633

Filters activated: Current only. Clear all to show 87165 items.

Name/Gene ID	Description	Location	Aliases
ras ID: 19412	resistance to audiogenic seizures [*Mus musculus* (house mouse)]		asr
ras ID: 43873	raspberry [*Drosophila melanogaster* (fruit fly)]	Chromosome X, NC_004354.4 (10744502..10749097)	Dmel_CG1799, CG11485, CG1799, Dmel\CG1799, EP(X)1093,

Filters: Manage Filters

Top Organisms [Tree]

Homo sapiens *(1126)*
Mus musculus *(823)*
Rattus norvegicus *(625)*
Oreochromis niloticus *(533)*
Neolamprologus brichardi *(507)*
All other taxa *(82019)*
More...

Find related data

Database:
Select

Find items

Search details

```
ras[All Fields] AND
alive[property]
```

(ras) AND "Homo sapiens"

www.ncbi.nlm.nih.gov/gene

NCBI Resources How To Sign in to NCBI

Gene

Gene

(ras) AND "Homo sapiens"[porgn:__txid9606]

Search

Save search Advanced Help

Show additional filters

Clear all

Gene sources

Genomic

Categories

Alternatively spliced

Annotated genes

Non-coding

Protein-coding

Pseudogene

Sequence content

CCDS

Ensembl

RefSeq

Status clear

✓ **Current only**

Chromosome locations

Select

Display Settings: Tabular, 20 per page, Sorted by Relevance **Send to:**

Hide sidebar >>

Results: 1 to 20 of 1126 << First < Prev Page 1 of 57 Next > Last >>

Filters activated: Current only. Clear all to show 1499 items.

Name/Gene ID	Description	Location	Aliases
NRAS ID: 4893	neuroblastoma RAS viral (v-ras) oncogene homolog [*Homo sapiens* (human)]	Chromosome 1, NC_000001.11 (114704464..114716894, complement)	RP5-1000E10.2, ALPS4, CMNS, N-ras, NCMS1, NS6, NRAS
KRAS ID: 3845	Kirsten rat sarcoma viral oncogene homolog [*Homo sapiens* (human)]	Chromosome 12, NC_000012.12 (25205246..25250923, complement)	C-K-RAS, CFC2, K-RAS2A, K-RAS2B, K-RAS4A, K-RAS4B, KI-RAS1, KRAS2, NS, NS3, RASK2

Filters: Manage Filters

Find related data

Database:

Select

Find items

Search details

```
ras[All Fields] AND "Homo
sapiens"[porgn] AND
alive[property]
```

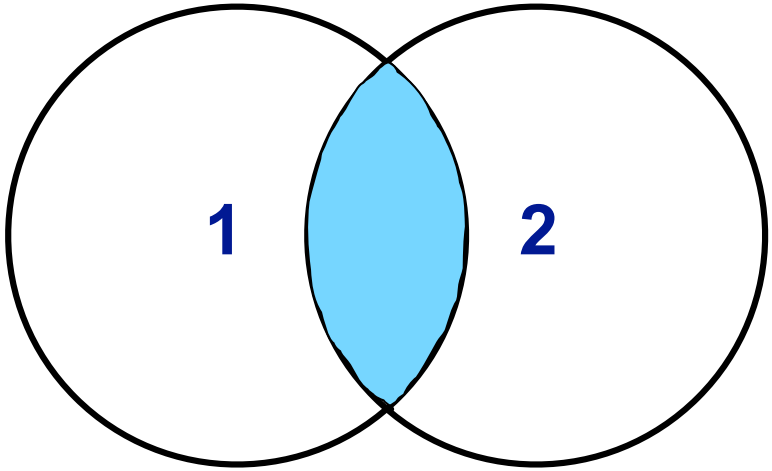
Search

See more...

Recent activity

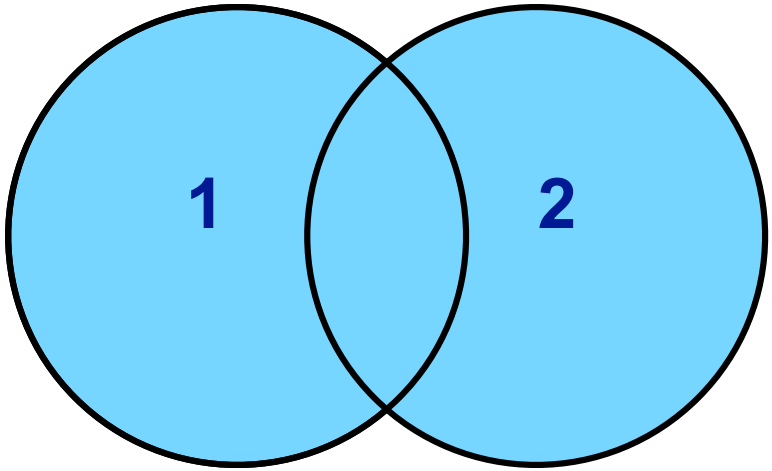
Turn Off Clear

1 AND 2



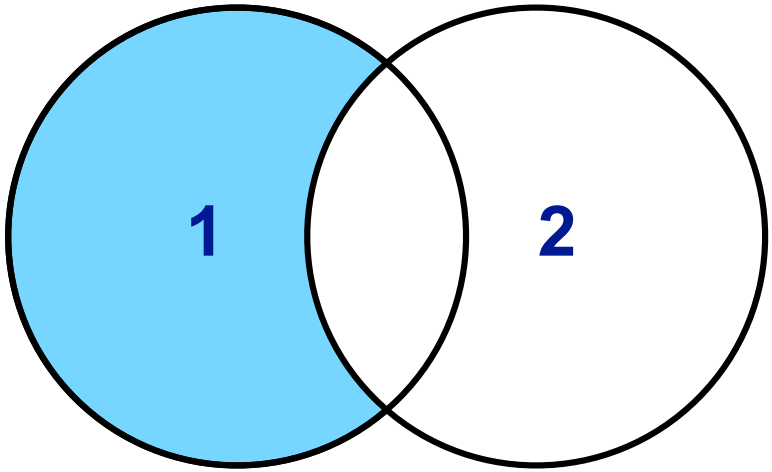
ras AND disease
(1185 results)

1 OR 2



ras OR disease
(134,872 results)

1 NOT 2



ras NOT disease
(84,448 results)

(ras) AND "Homo sapiens"

www.ncbi.nlm.nih.gov/gene

NCBI Resources How To Sign in to NCBI

Gene

Gene (ras) AND "Homo sapiens"[porgn:__txid9606] Search

Save search Advanced Help

Show additional filters

Clear all

Gene sources
Genomic

Categories
Alternatively spliced
Annotated genes
Non-coding
Protein-coding
Pseudogene

Sequence content
CCDS
Ensembl
RefSeq

Status clear
✓ **Current only**

Chromosome locations
Select

Display Settings: Tabular, 20 per page, Sorted by Relevance **Send to:**

Results: 1 to 20 of 1126 << First < Prev Page 1 of 57 Next > Last >>

Filters activated: Current only. Clear all to show 1499 items.

Name/Gene ID	Description	Location	Aliases
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Hide sidebar >>

Filters: Manage Filters

Find related data

Database:
Select

Find items

Search details

```
ras[All Fields] AND "Homo sapiens"[porgn] AND alive[property]
```

Search See more...

Recent activity

Turn Off Clear

KRAS Kirsten rat sarcoma

www.ncbi.nlm.nih.gov/gene/3845

NCBI Resources How To Sign in to NCBI

Gene Gene Search

Advanced Help

Display Settings: Full Report Send to: Hide sidebar >>

KRAS Kirsten rat sarcoma viral oncogene homolog [*Homo sapiens* (human)]

Gene ID: 3845, updated on 4-Jan-2015

Summary

Official Symbol	KRAS provided by HGNC
Official Full Name	Kirsten rat sarcoma viral oncogene homolog provided by HGNC
Primary source	HGNC:HGNC:6407
See related	Ensembl:ENSG00000133703; HPRD:01817; MIM:190070; Vega:OTTHUMG00000171193
Gene type	protein coding
RefSeq status	REVIEWED
Organism	Homo sapiens
Lineage	Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia; Eutheria; Euarchontoglires; Primates; Haplorrhini; Catarrhini; Hominidae; Homo
Also known as	NS; NS3; CFC2; KRAS1; KRAS2; RASK2; KI-RAS; C-K-RAS; K-RAS2A; K-

Table of contents

KRAS Kirsten rat sarcoma

www.ncbi.nlm.nih.gov/gene/3845

NCBI Resources How To Sign in to NCBI

Gene Search Help

Display S

Hide sidebar >>

Example Questions:

What chromosome location and what genes are in the vicinity?

KRAS

(human)

Gene ID: 3845, updated on 4-Jan-2015

Summary

Official Symbol	KRAS provided by HGNC
Official Full Name	Kirsten rat sarcoma viral oncogene homolog provided by HGNC
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Table of contents

KRAS Kirsten rat sarcoma

www.ncbi.nlm.nih.gov/gene/3845#genomic-context

Genomic context

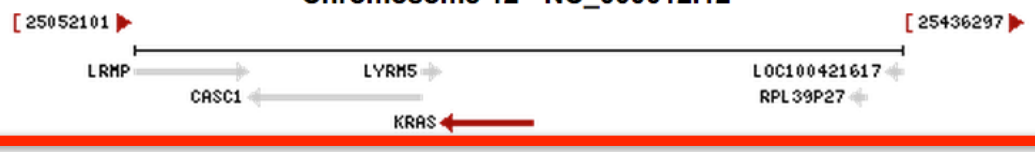
Location: 12p12.1

Exon count: 6

See KRAS in Epigenomics, MapViewer

Annotation release	Status	Assembly	Chr	Location
106	current	GRCh38 (GCF_000001405.26)	12	NC_000012.12 (25205246..25250923, complement)
105	previous assembly	GRCh37.p13 (GCF_000001405.25)	12	NC_000012.11 (25358180..25403870, complement)

Chromosome 12 - NC_000012.12



Genomic regions, transcripts, and products

Go to reference sequence details

Genomic Sequence: NC_000012.12 chromosome 12 reference GRCh38 Primary Assembly

Go to nucleotide: Graphics FASTA GenBank

BioAssay by Target (Summary)
BioAssay, by Gene target
BioAssays, RNAi Target, Active
BioAssays, RNAi Target, Tested
BioProjects
BioSystems
Books
CCDS
ClinVar
Conserved Domains
dbVar
EST
Full text in PMC
Full text in PMC_nucleotide
Gene neighbors
Genome
GEO Profiles
GTR
HomoloGene
Map Viewer
MedGen
Nucleotide

KRAS Kirsten rat sarcoma

www.ncbi.nlm.nih.gov/gene/3845

NCBI Resources How To Sign in to NCBI

Gene Search Help

Display Settin

Hide sidebar >>

KRAS Ki
(human)]

Gene ID: 3845

Summa

Example Questions:

What 'molecular functions', 'biological processes', and 'cellular component' information is available?

Official Symbol	KRAS provided by HGNC
Official Full Name	Kirsten rat sarcoma viral oncogene homolog provided by HGNC
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See related	Ensembl:ENSG00000133703; HPRD:01817; MIM:190070; Vega:OTTHUMG00000171193
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Also known as	NS; NS3; CFC2; KRAS1; KRAS2; RASK2; KI-RAS; C-K-RAS; K-RAS2A; K-

Table of contents

- Summary
- Genomic context
- Genomic regions, transcripts, and products
- Bibliography
- Phenotypes
- Variation
- HIV-1 interactions
- Pathways from BioSystems
- Interactions
- General gene information
  - Markers, Related pseudogene(s), Homology, Gene Ontology
- General protein information
- NCBI Reference Sequences (RefSeq)

KRAS Kirsten rat sarcoma

www.ncbi.nlm.nih.gov/gene/3845#gene-ontology

Gene Ontology Provided by GOA

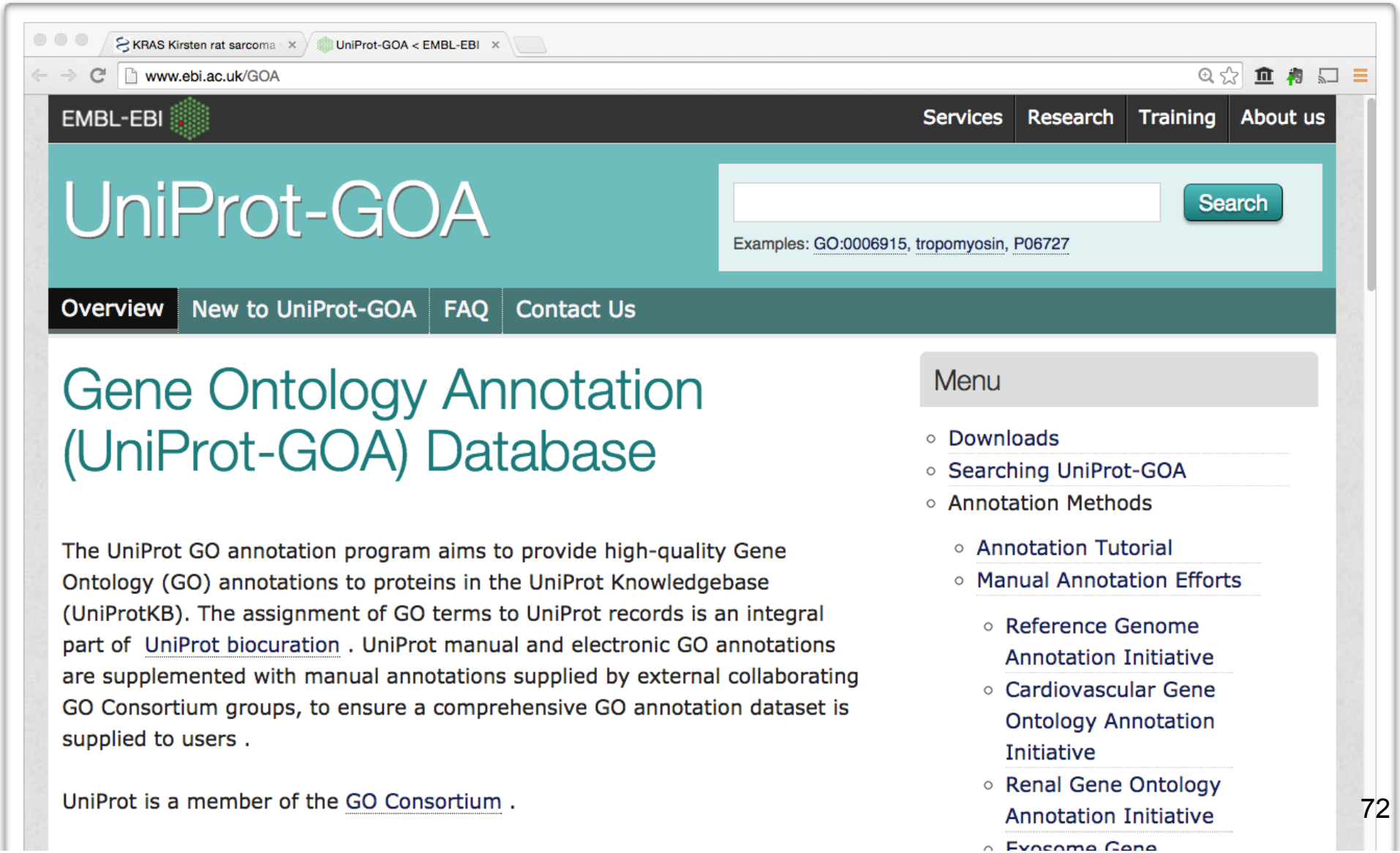
Function	Evidence Code	Pubs
GDP binding	IEA	
GMP binding	IEA	
GTP binding	IEA	
LRR domain binding	IEA	
protein binding	IPI	PubMed
protein complex binding	IDA	PubMed

Items 1 - 25 of 33 < Prev Page 1 of 2 Next >

Process	Evidence Code	Pubs
Fc-epsilon receptor signaling pathway	TAS	
GTP catabolic process	IEA	
MAPK cascade	TAS	
Ras protein signal transduction	TAS	
actin cytoskeleton organization	IEA	
activation of MAPKK activity	TAS	
axon guidance	TAS	
blood coagulation	TAS	

GO: Gene Ontology

GO provides a controlled vocabulary of terms for describing gene product characteristics and gene product annotation data

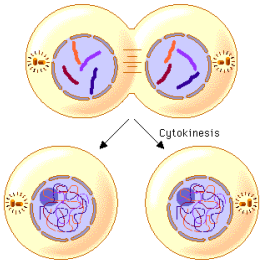


Why do we need Ontologies?

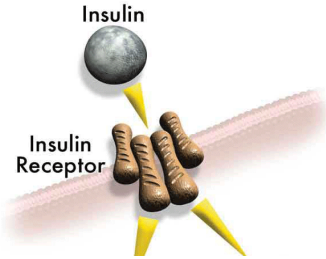
- Annotation is essential for capturing the understanding and knowledge associated with a sequence or other molecular entity
- Annotation is traditionally recorded as “free text”, which is easy to read by humans, but has a number of disadvantages, including:
  - Difficult for computers to parse
  - Quality varies from database to database
  - Terminology used varies from annotator to annotator
- Ontologies are annotations using standard vocabularies that try to address these issues
- GO is integrated with UniProt and many other databases including a number at NCBI

GO Ontologies

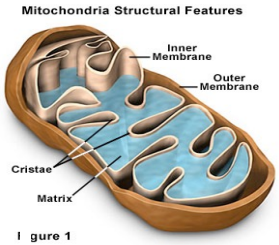
- There are three ontologies in GO:
  - **Biological <u>Process</u>**
    A commonly recognized series of events
    e.g. cell division, mitosis,



  - **Molecular <u>Function</u>**
    An elemental activity, task or job
    e.g. kinase activity, insulin binding



  - **Cellular <u>Component</u>**
    Where a gene product is located
    e.g. mitochondrion, mitochondrial membrane



KRAS Kirsten rat sarcoma

www.ncbi.nlm.nih.gov/gene/3845#gene-ontology

Gene Ontology Provided by GOA

Function	Evidence Code	Pubs
GDP binding		
GMP binding		
GTP binding		
LRR domain binding		
protein binding		
protein complex binding		

The 'Gene Ontology' or GO is actually maintained by the EBI so lets switch or link over to UniProt also from the EBI.

Process	Code	Pubs
Fc-epsilon receptor signaling pathway	TAS	
GTP catabolic process	IEA	
MAPK cascade	TAS	
Ras protein signal transduction	TAS	
actin cytoskeleton organization	IEA	
activation of MAPKK activity	TAS	
axon guidance	TAS	
blood coagulation	TAS	

Scroll down to **UniProt** link

UniProt will detail much more information for protein coding genes such as this one

KRAS Kirsten rat sarcoma

www.ncbi.nlm.nih.gov/gene/3845#gene-ontology

genomic	X01669.1	CAA25828.1

Items 1 - 25 of 43 < Prev Page 1 of 2 Next >

Protein Accession	Links	
	GenPept Link	UniProtKB Link
P01116.1	GenPept	UniProtKB/Swiss-Prot:P01116

Additional links

Scroll down to Very bottom for **UniProt** link

You are here: NCBI > Genes & Expression > Gene

Write to the Help Desk

GETTING STARTED	RESOURCES	POPULAR	FEATURED	NCBI INFORMATION
NCBI Education	Chemicals & Bioassays	PubMed	Genetic Testing Registry	About NCBI
NCBI Help Manual	Data & Software	Bookshelf	PubMed Health	Research at NCBI
NCBI Handbook	DNA & RNA	PubMed Central	GenBank	NCBI News
Training & Tutorials	Domains & Structures	PubMed Health	Reference Sequences	NCBI FTP Site
	Genes & Expression	BLAST	Gene Expression Omnibus	NCBI on Facebook
	Genetics & Medicine	Nucleotide	Map Viewer	NCBI on Twitter
	Genomes & Maps	Genome	Human Genome	NCBI on YouTube
	Homology	SNP	Mouse Genome	
	Literature	Gene	Influenza Virus	
	Proteins	Protein	Primer-BLAST	
	Sequence Analysis	PubChem	Sequence Read Archive	
	Taxonomy			

UniProt will detail much more information for protein coding genes

KRAS - GTPase KRas prec

www.uniprot.org/uniprot/P01116

UniProt

UniProtKB | Advanced

BLAST | Align | Retrieve/ID Mapping | Help | Contact

Basket

P01116 - RASK_HUMAN

Protein	**GTPase KRas**
Gene	**KRAS**
Organism	*Homo sapiens (Human)*
Status	Reviewed - ⦿⦿⦿⦿⦿ - Experimental evidence at protein level[i]

BLAST | Align | Format | Add to basket | History | Feedback | Help video

Display None

- FUNCTION
- NAMES & TAXONOMY
- SUBCELL. LOCATION
- PATHOL./BIOTECH
- PTM / PROCESSING
- EXPRESSION
- INTERACTION
- STRUCTURE
- FAMILY & DOMAINS
- SEQUENCES (2)
- CROSS-REFERENCES

Function[i]

Ras proteins bind GDP/GTP and possess intrinsic GTPase activity. Plays an important role in the regulation of cell proliferation (PubMed:23698361, PubMed:22711838). 2 Publications Curated

Enzyme regulation[i]

Alternates between an inactive form bound to GDP and an active form bound to GTP. Activated by a guanine nucleotide-exchange factor (GEF) and inactivated by a GTPase-activating protein (GAP). Interaction with SOS1 promotes exchange of bound GDP by GTP. 3 Publications

Regions

Feature key	Position(s)	Length	Description	Graphical view	Feature identifier	Actions
Nucleotide binding[i]	10 – 18	9	GTP 2 Publications			
Nucleotide binding[i]	29 – 35	7	GTP 2 Publications			
Nucleotide binding[i]	59 – 60	2	GTP 2 Publications			

KRAS - GTPase KRas prec

www.uniprot.org/uniprot/P01116

UniProt

UniProtKB | Advanced

BLAST Align Retrieve/ID Mapping Help Contact

Basket

P01116 - RASK_HUMAN

Protein	**GTPase KRas**
Gene	**KRAS**
Organism	*Homo sapiens (Human)*
Status	Reviewed -

BLAST Align Fo

Example Questions:

What positions in the protein are responsible for GTP binding?

Display None

- FUNCTION
- NAMES & TAXONOMY
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Nucleotide binding	59 – 60	2	GTP 2 Publications			

Example Questions:

What variants of this enzyme are involved in gastric cancer and other human diseases?

KRAS - GTPase KRas prec

www.uniprot.org/uniprot/P01116

Display None

- FUNCTION
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- CROSS-REFERENCES
- PUBLICATIONS
- ENTRY INFORMATION
- MISCELLANEOUS
- SIMILAR PROTEINS

Top

Pathology & Biotech

Involvement in disease

LEUKEMIA, ACUTE MYELOGENOUS (AML)

[MIM:601626]: A subtype of acute leukemia, a cancer of the white blood cells. AML is a malignant disease of bone marrow characterized by maturational arrest of hematopoietic precursors at an early stage of development. Clonal expansion of myeloid blasts occurs in bone marrow, blood, and other tissue. Myelogenous leukemias develop from changes in cells that normally produce neutrophils, basophils, eosinophils and monocytes. 1 Publication

Note: The disease is caused by mutations affecting the gene represented in this entry.

Feature key	Position(s)	Length	Description	Graphical view	Feature identifier	Actions
Natural variant	10 – 10	1	G → GG in one individual with AML; expression in 3T3 cell causes cellular transformation; expression in COS cells activates the Ras-MAPK signaling pathway; lower GTPase activity; faster GDP dissociation rate. 1 Publication		VAR_034601	

LEUKEMIA, JUVENILE MYELOMONOCYTIC (JMML)

[MIM:607785]: An aggressive pediatric myelodysplastic syndrome/myeloproliferative disorder characterized by malignant transformation in the hematopoietic stem cell compartment with proliferation of differentiated progeny. Patients have splenomegaly, enlarged lymph nodes, rashes, and hemorrhages.

Note: The disease is caused by mutations affecting the gene represented in this entry.

NOONAN SYNDROME 3 (NS3)

[MIM:609942]: A form of Noonan syndrome, a disease characterized by short stature, facial dysmorphic features such as hypertelorism, a downward eyeslant and low-set posteriorly rotated ears, and a high incidence of congenital heart

Example Questions:

Are high resolution protein structures available to examine the details of these mutations?

KRAS - GTPase KRas prec

www.uniprot.org/uniprot/P01116

Display None

- FUNCTION
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- SEQUENCES (2)
- CROSS-REFERENCES
- PUBLICATIONS
- ENTRY INFORMATION
- MISCELLANEOUS
- SIMILAR PROTEINS

Top

Structure

Secondary structure

1 189

Legend: Helix Turn Beta strand

Show more details

3D structure databases

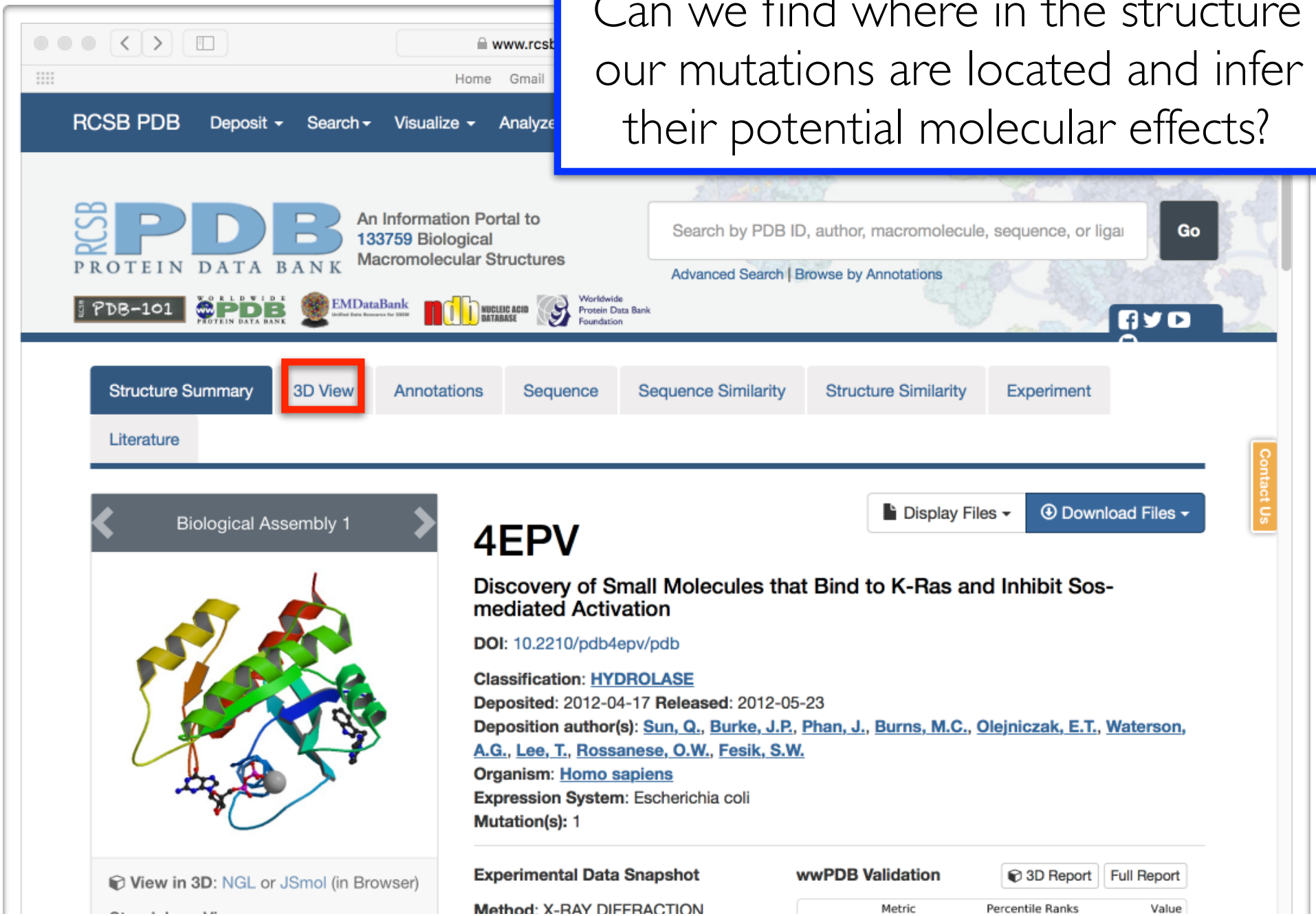
Select the link destinations:

- PDBe
- RCSB PDB
- PDBj

Entry	Method	Resolution (Å)	Chain	Positions	PDBsum
1D8D	X-ray	2.00	P	178-188	[»]
1D8E	X-ray	3.00	P	178-188	[»]
1KZO	X-ray	2.20	C	169-173	[»]
1KZP	X-ray	2.10	C	169-173	[»]
3GFT	X-ray	2.27	A/B/C/D/E/F	1-164	[»]
4DSN	X-ray	2.03	A	2-164	[»]
4DSO	X-ray	1.85	A	2-164	[»]
4EPR	X-ray	2.00	A	1-164	[»]
4EPT	X-ray	2.00	A	1-164	[»]
4EPV	X-ray	1.35	A	1-164	[»]
4EPW	X-ray	1.70	A	1-1	
4EPX	X-ray	1.76	A	1-1	
4EPY	X-ray	1.80	A	1-1	
4L8G	X-ray	1.52	A	1-1	
4LDJ	X-ray	1.15	A	1-164	[»]
4LPK	X-ray	1.50	A/B	1-169	[»]

Open link in a new tab!

Lets view the 3D structure:
Can we find where in the structure our mutations are located and infer their potential molecular effects?



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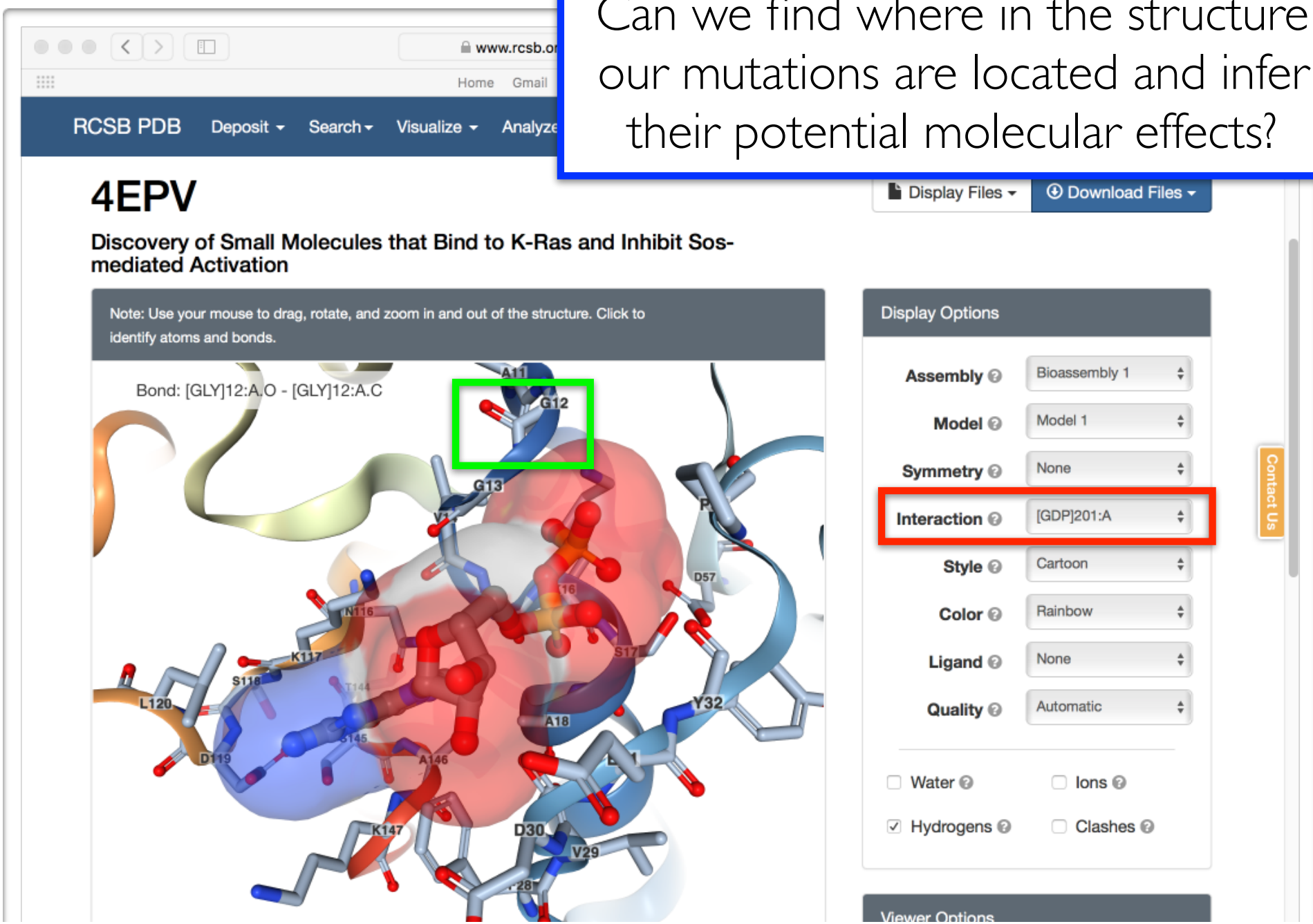

Back to UniProt:

What is known about the protein family, its species distribution, number in humans and residue-wise conservation, etc… ?

KRAS - GTPase KRas prec ×

www.uniprot.org/uniprot/P01116

Display None

- FUNCTION
- NAMES & TAXONOMY
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▲Top

PhylomeDB[i]	P01
TreeFam[i]	TF3

Family and domain databases

Gene3D[i]	3.40.50.300. 1 hit.
InterPro[i]	IPR027417. P-loop_NTPase. IPR005225. Small_GTP-bd_dom. IPR001806. Small_GTPase. IPR020849. Small_GTPase_Ras. [Graphical view]
PANTHER[i]	PTHR24070. PTHR24070. 1 hit.
Pfam[i]	PF00071. Ras. 1 hit. [Graphical view]
PRINTS[i]	PR00449. RASTRNSFRMNG.
SMART[i]	SM00173. RAS. 1 hit. [Graphical view]
SUPFAM[i]	SSF52540. SSF52540. 1 hit.
TIGRFAMs[i]	TIGR00231. small_GTP. 1 hit.
PROSITE[i]	PS51421. RAS. 1 hit. [Graphical view]

PFAM is one of the best protein family databases

Sequences (2)[i]

Sequence status[i]: Complete.

Sequence processing[i]: The displayed sequence is further processed into a mature form.

This entry describes **2** isoforms[i] produced by **alternative splicing**. Align

Example Questions:

What is known about the protein family, its **species distribution**, number in humans and residue-wise conservation, etc… ?

KRAS - GTPase KRas prec × | Pfam: Family: Ras (PF0007 ×

pfam.xfam.org/family/PF00071

EMBL-EBI HOME

Family: *Ras* (PF00071)

332 architectures | 21243 sequences | 30 interactions | 1006 species | 663 structures

- Summary
- Domain organisation
- Clan
- Alignments
- HMM logo
- Trees
- Curation & model
- Species
- Interactions
- Structures

Jump to… enter ID/acc Go

Summary: Ras family

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

Wikipedia: Ras subfamily | Wikipedia: Ras superfamily | Pfam | InterPro

This is the Wikipedia entry entitled "Ras subfamily". More...

Ras subfamily

Edit Wikipedia article

This article is about p21/Ras protein. For the p21/waf1 protein, see p21.

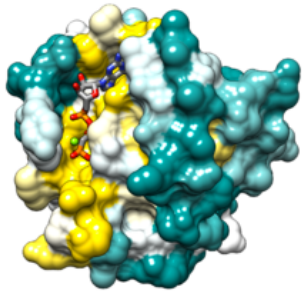
Ras is the name given to a family of related proteins which is ubiquitously expressed in all cell lineages and organs. All Ras protein family members belong to a class of protein called small GTPase, and are involved in transmitting signals within cells (cellular signal transduction). Ras is the prototypical member of the Ras superfamily of proteins, which are all related in 3D structure and regulate diverse cell behaviours.

The name 'Ras' is an abbreviation of 'Rat sarcoma', reflecting the way the first members of the protein family were discovered. The name ras is also used to refer to the family of genes encoding those proteins.

When Ras is 'switched on' by incoming signals, it subsequently switches on other proteins, which ultimately turn on genes involved in cell growth, differentiation and survival. As a result, mutations in ras genes can lead to the production of permanently activated Ras proteins. This can cause unintended and overactive signalling inside the cell, even in the absence of incoming signals.

Because these signals result in cell growth and division, overactive Ras signaling can ultimately lead to cancer.[1] The 3 Ras genes in humans (HRAS, KRAS, and NRAS) are the most common oncogenes in human cancer; mutations that permanently activate Ras are found in 20% to 25% of all human tumors and up to 90% in certain types of cancer (e.g., pancreatic cancer).[2] For this reason, Ras inhibitors are being studied as a treatment for cancer, and other diseases with Ras overexpression.

Contents [hide]

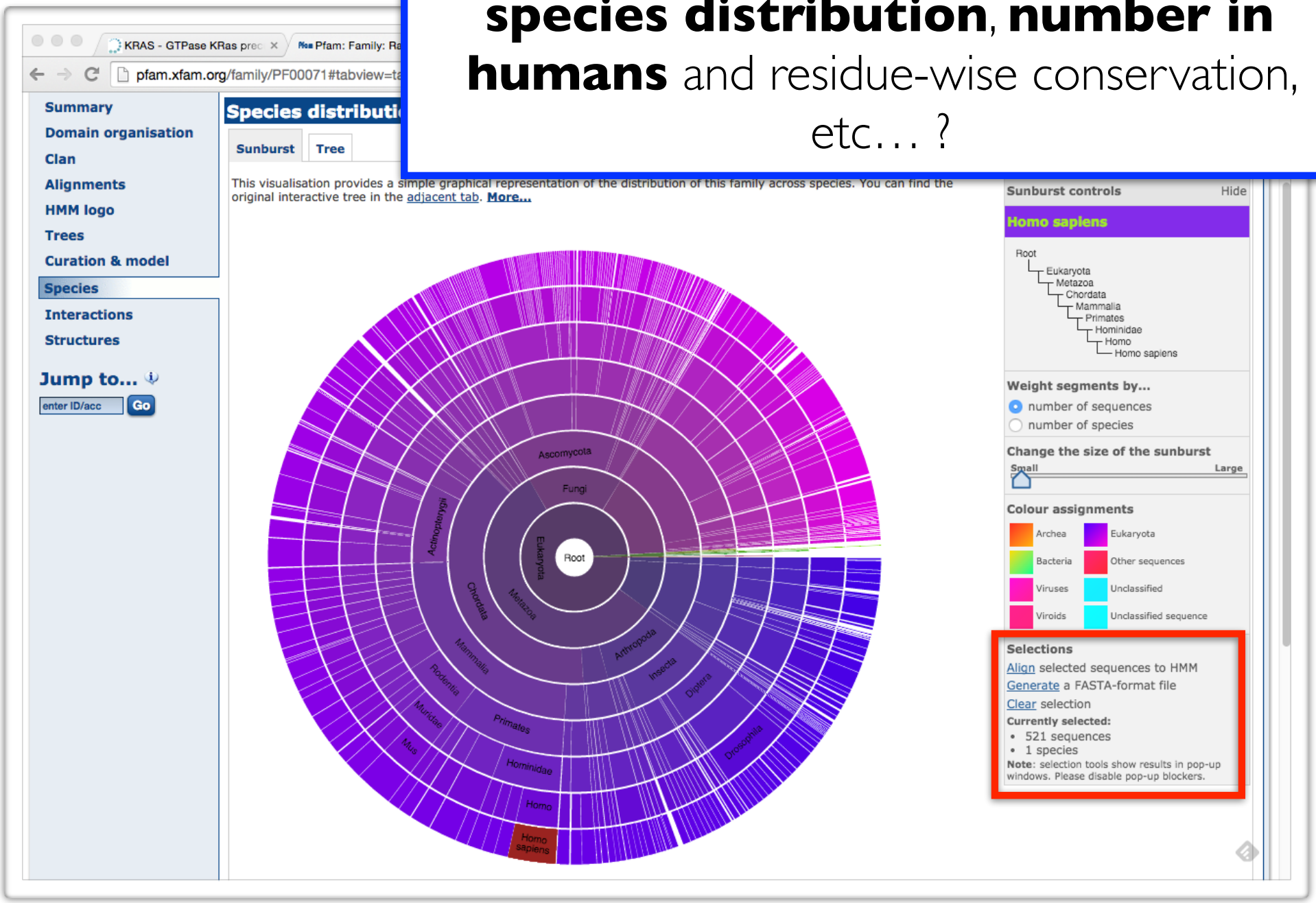


H-Ras structure PDB 121p, surface colored by conservation in Pfam seed alignment: gold, most conserved; dark cyan, least conserved.

Identifiers	
Symbol	Ras
Pfam	PF00071
InterPro	IPR013753
PROSITE	PDOC00017
SCOP	5p21
SUPERFAMILY	5p21

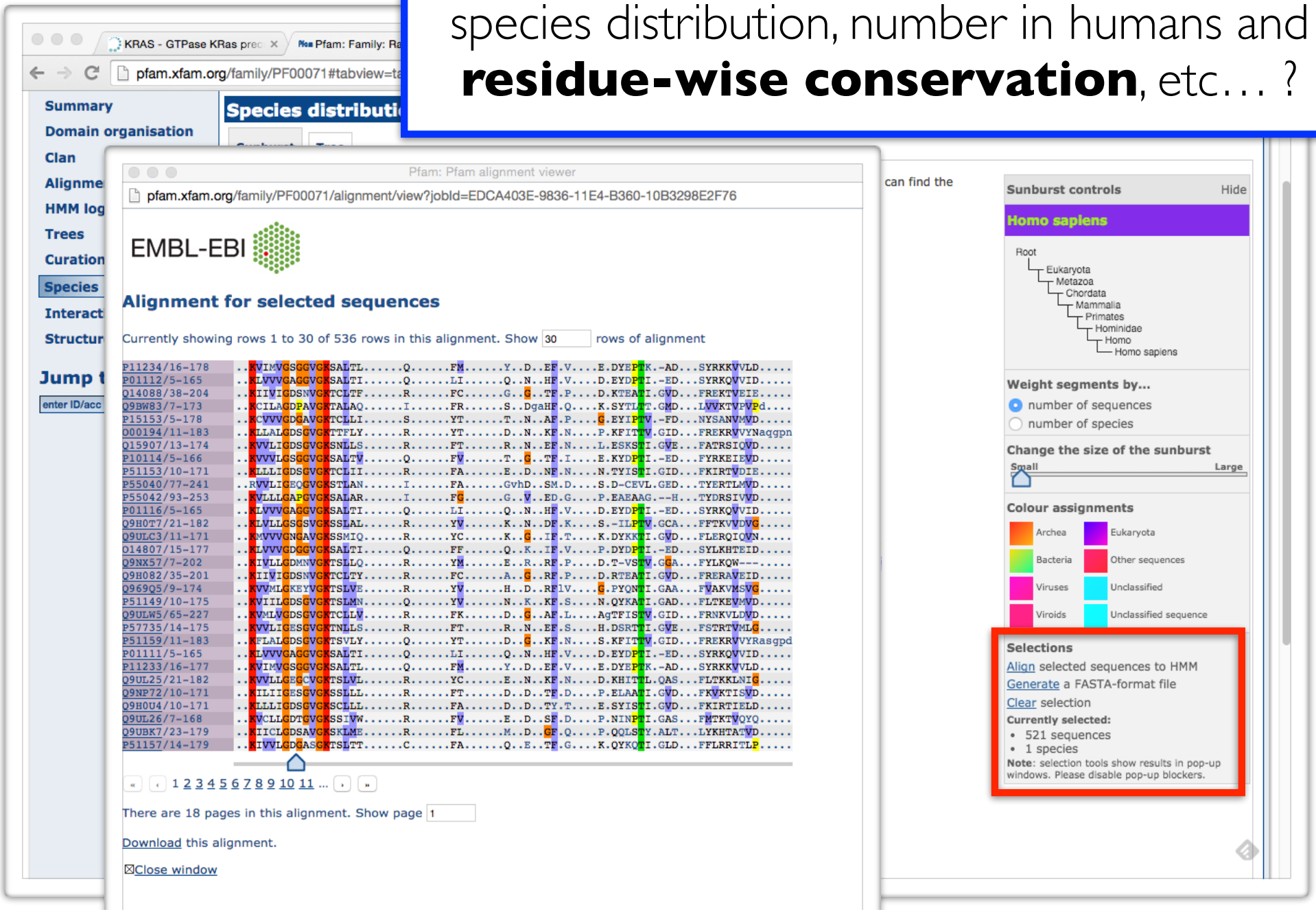
Example Questions:

What is known about the protein family, its **species distribution**, **number in humans** and residue-wise conservation, etc… ?



Example Questions:

What is known about the protein family, its species distribution, number in humans and **residue-wise conservation**, etc… ?



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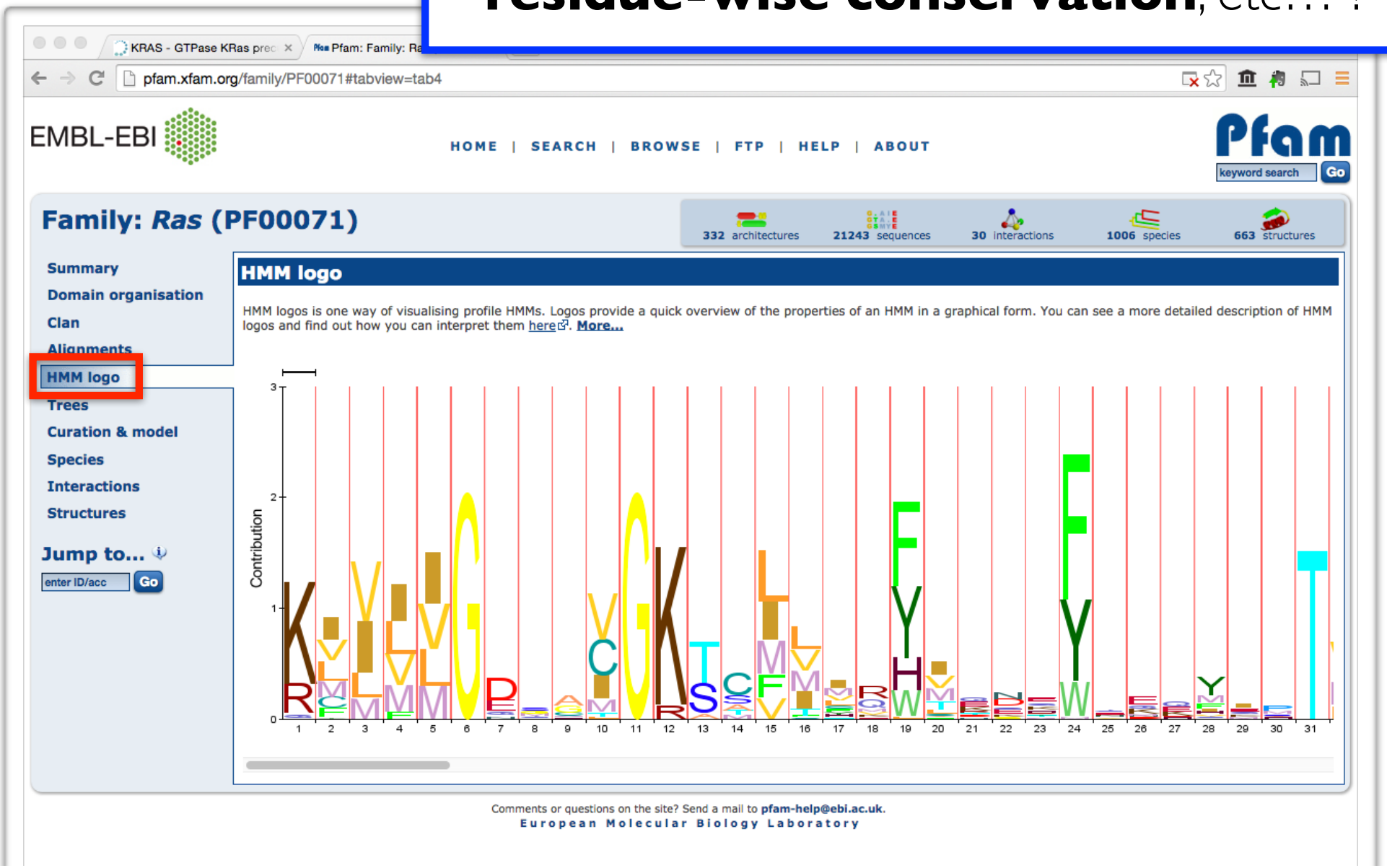
What is known about the protein family, its species distribution, number in humans and **residue-wise conservation**, etc… ?



Family: *Kinesin* (PF00225)

Loading page components (1 remaining)...

126 architectures 4150 sequences 6 interactions 248 species 114 structures

Summary
Domain organisation
Clans
Alignments
HMM logo
Trees
Curation & models
Species
Interactions
Structures

Jump to...
enter ID/acc Go

Interactions

There are **6** interactions for this family. More...

Tubulin Tubulin_C	Tubulin_C	Kinesin	Tubulin	Kinesin

Family: *Kinesin* (PF00225)

Structures

For those sequences which have a structure in the Protein DataBank, we use the mapping between UniProt, PDB and Pfam coordinate systems from the PDBe group, to allow us to map Pfam domains onto UniProt sequences and three-dimensional protein structures. The table below shows the structures on which the **Kinesin** domain has been found.

UniProt entry	UniProt residues	PDB ID	PDB chain ID	PDB residues	View
A8BKD1_GIALA	11 - 335	2vvq	A	11 - 335	Jmol AstexViewer SPICE
			B	11 - 335	Jmol AstexViewer SPICE
CENPE_HUMAN	12 - 329	1t5c	A	12 - 329	Jmol AstexViewer SPICE
			B	12 - 329	Jmol AstexViewer SPICE
KAR3_YEAST	392 - 723	1f9t	A	392 - 723	Jmol AstexViewer SPICE
		1f9u	A	392 - 723	Jmol AstexViewer SPICE
		1f9v	A	392 - 723	Jmol AstexViewer SPICE
		1f9w	A	392 - 723	Jmol AstexViewer SPICE
			B	392 - 723	Jmol AstexViewer SPICE
		3kar	A	392 - 723	Jmol AstexViewer SPICE
KI13B_HUMAN	11 - 352	3gbj	A	11 - 352	Jmol AstexViewer SPICE
			B	11 - 352	Jmol AstexViewer SPICE
			C	11 - 352	Jmol AstexViewer SPICE
		1ii6	A	24 - 359	Jmol AstexViewer SPICE
			B	24 - 359	Jmol AstexViewer SPICE
		1q0b	A	24 - 359	Jmol AstexViewer SPICE
			B	24 - 359	Jmol AstexViewer SPICE
		1x88	A	24 - 359	Jmol AstexViewer SPICE
			B	24 - 359	Jmol AstexViewer SPICE
			A	24 - 359	Jmol AstexViewer SPICE

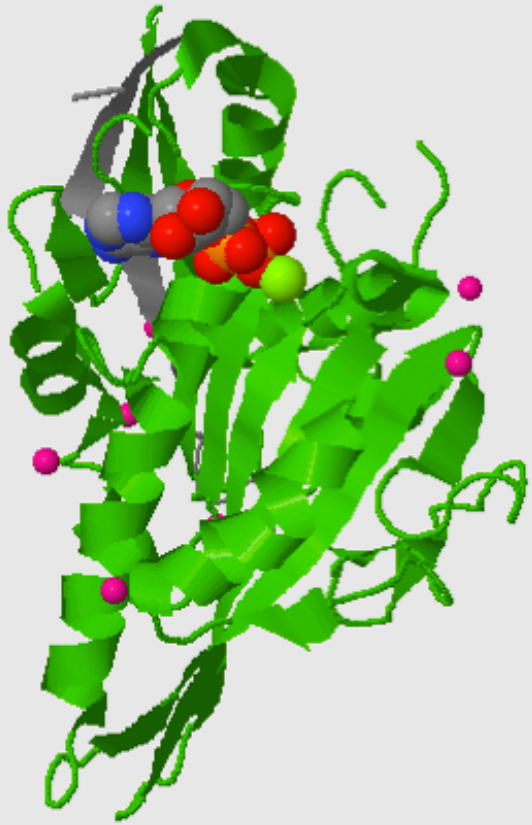
Pfam: Jmol

http://pfam.janelia.org/structure/viewer?viewer=jmol&id=3bfn

Pfam: Family: Kinesin (PF00225) | Pfam: Jmol

wellcome trust sanger institute

PDB entry 3bfn



Jmol

Your turn:
What can you find out about "eg5"

PDB			UniProt			Pfam family	Colour
Chain	Start	End	ID	Start	End		
A	49	368	KIF22_HUMAN	49	368	Kinesin (PF00225)	

Close window

SUMMARY

- Bioinformatics is computer aided biology.
- Bioinformatics deals with the collection, archiving, organization, and interpretation of a wide range of biological data.
- There are a large number of primary, secondary and tertiary bioinformatics databases.
- The NCBI and EBI are major online bioinformatics service providers.
- Introduced Gene, UniProt, PDB databases as well as a number of ‘boutique’ databases including PFAM and OMIM.
- Introduced the notion of *controlled vocabularies* and *ontologies.*

HOMEWORK

https://bioboot.github.io/bggn213_f17/lectures/#1

- ☑ Complete the **initial course questionnaire**:
- ☑ Check out the "**Background Reading**" material online:
- ☑ Complete the **lecture 1 homework questions**: