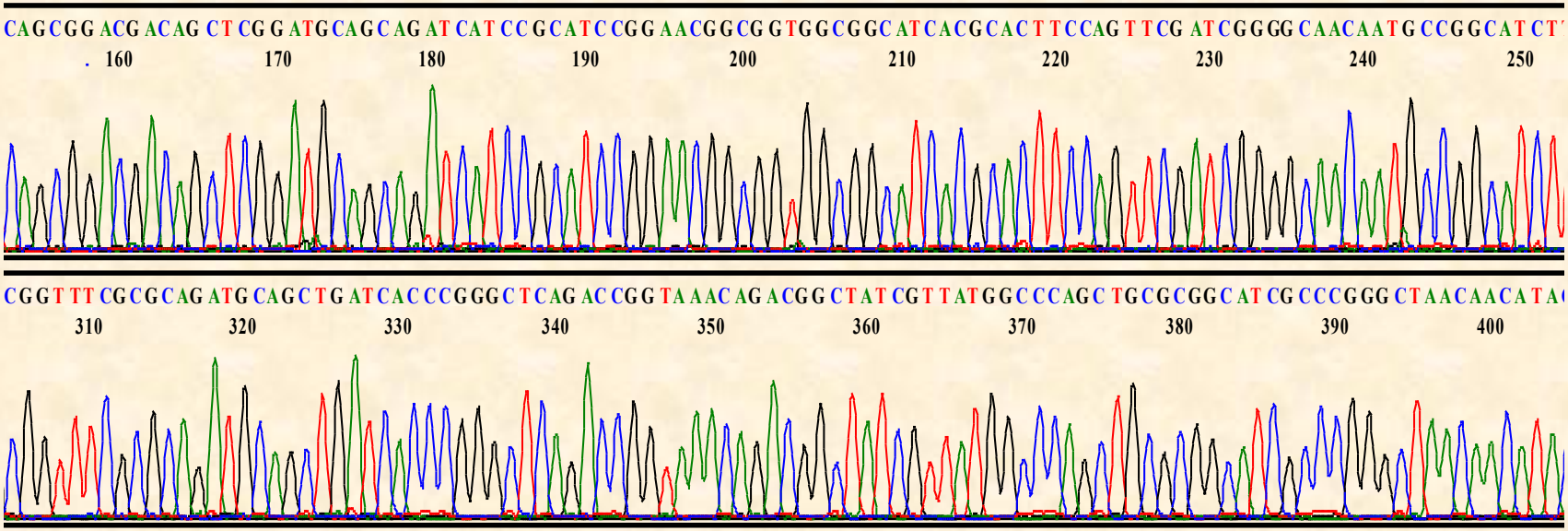
Molekulárně biologické databáze

Pro zajímavost…

Důležité…

Molekulárně biologická data



GATAGCGTAATGATCGGCTGGCTGCCGCATTTCATGCTGGTTTCCCAACGAAAATAACCGCTCACGGTGCCATCACGATCGCACACCGCAAAATCGGCGG

TACAGGTGGTCGCGCCCGCCGCCAGCACATCGCTGCGCCAATAATGATCTTTCAGCGGACGACAGCTCGGATGCAGCAGATCATCCGCATCCGGAACGGC

GGTGGCGGCATCACGCACTTCCAGTTCGATCGGGGCAACAATGCCGGCATCTTTCAGGGCAAAGCGAATAAACAGCACGCTCACTTCCGCGCGCAGCGCC

AGCGCGGTTTCGCGCAGATGCAGCTGATCACCCGGGCTCAGACCGGTAAACAGACGGCTATCGTTATGGCCCAGCTGCGCGGCATCGCCCGGGCTAACAA

CATACAGGTGGCGACCATCAATCACGGTCGGGGCGGCCGGATCACGGCTGGCTTCCGGATAGGCGCTCAGCAGGGTAACGGCATCCACAATCACCAGCAT

Molekulárně biologická data

MALDI-TOF

Identifikace proteinů

Sekvenace proteinů

MDRNGNFSLPPNTAFKAIFYANAADRQDLK

LFIDDAPEPAATFVGNSEDGVRLFTLNSKG

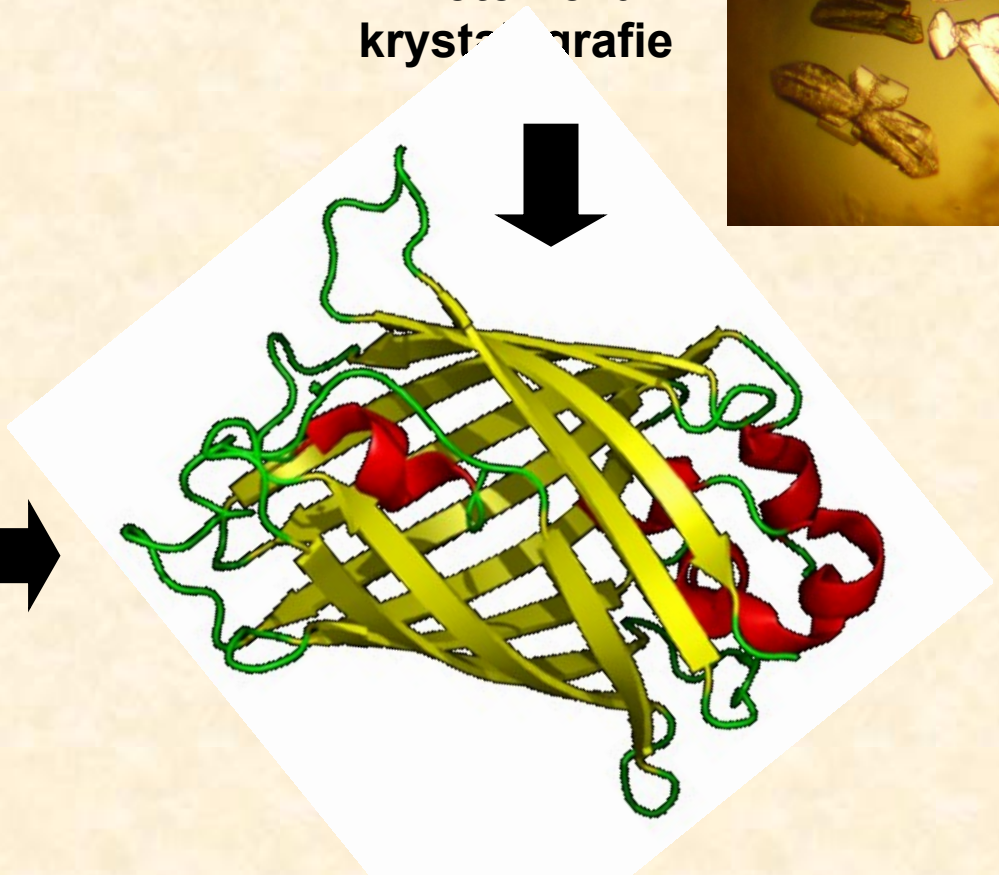
GKIRIEASANGRQSATDARLAPLSAGDTVW

LGWLGAEDGADADYNDGIVILQWPIT

Molekulárně biologická data

NMR spektroskopie

Proteinová krystalografie



Molekulárně biologická data

- **Výkonné technologie:**

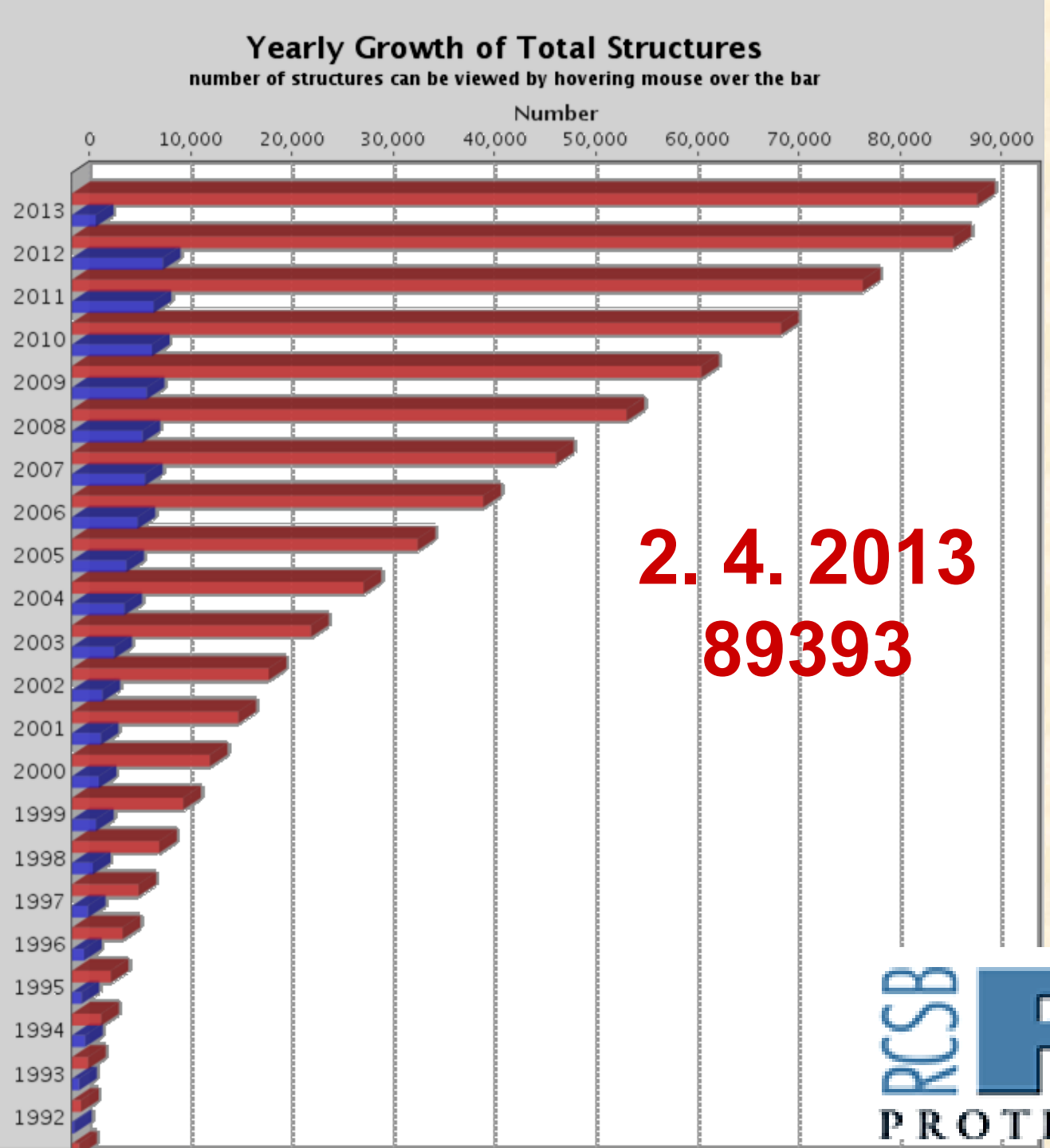
  Automatické sekvencování

  MALDI-TOF

  NMR spektroskopie

  Proteinová krystalografie

Výrazný nárůst množství biologických dat.

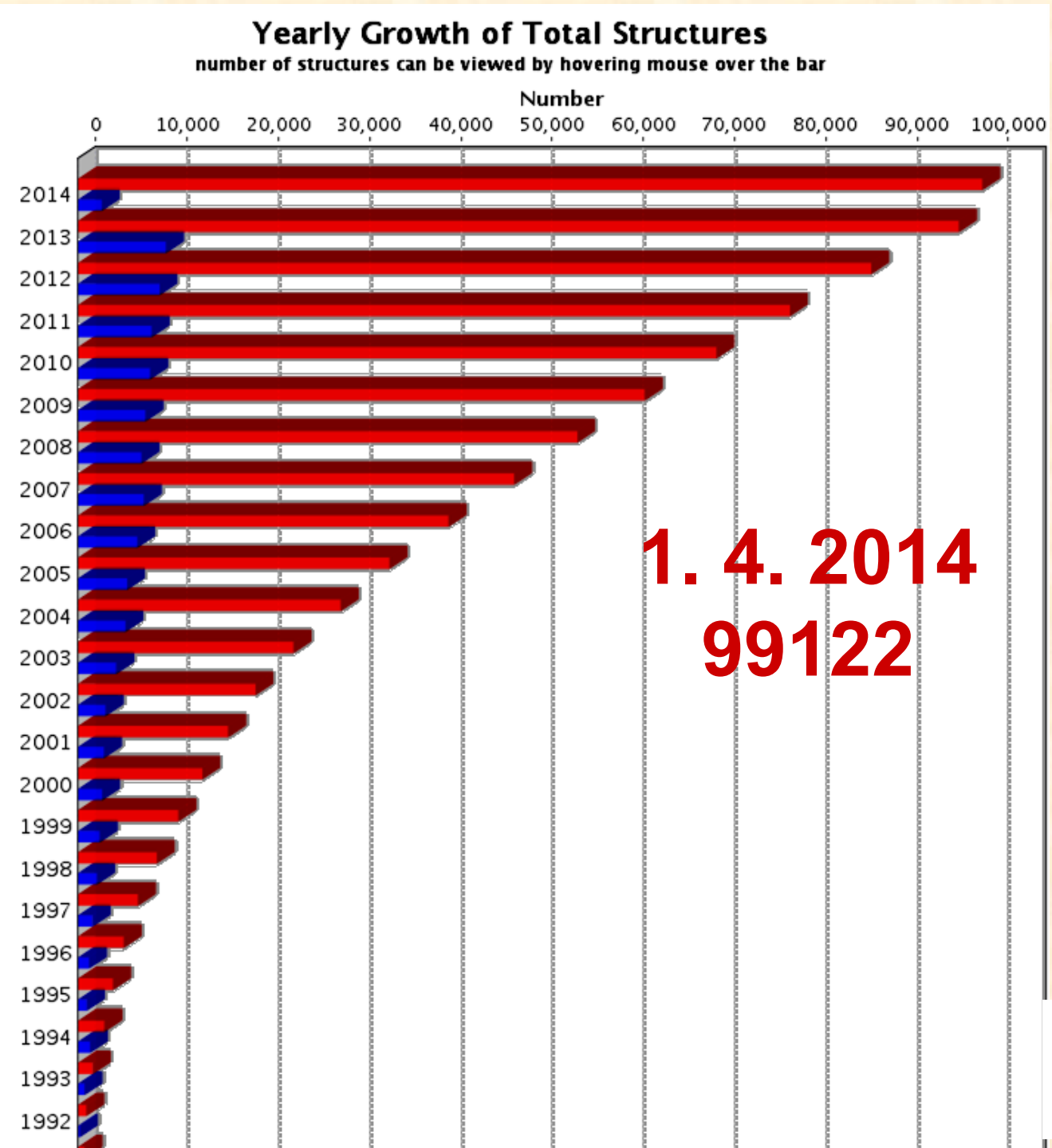


2. 4. 2013

89393

RCSB PDB

PROTEIN DATA BANK



1. 4. 2014

99122

RCSB PDB
PROTEIN DATA BANK

Éra reverzní genetiky

Klasická genetika

GATAGCGTAATGATCGGCTGGCTGCCGCATTTC

TACAGGTGGTCGCGCCCGCCGCCAGCACATCGC

GGTGGCGGCATCACGCACTTCCAGTTCGATCGG

AGCGCGGTTTCGCGCAGATGCAGCTGATCACCC

Fenotyp → **Genotyp**

Éra reverzní genetiky

Klasická genetika

GATAGCGTAATGATCGGCTGGCTGCCGCATTTC

TACAGGTGGTCGCGCCCGCCGCCAGCACATCGC

GGTGGCGGCATCACGCACTTCCAGTTCGATCGG

AGCGCGGTTTCGCGCAGATGCAGCTGATCACCC

Fenotyp → Genotyp

Reverzní genetika

Automatické DNA sekvencování

Produkce velkého množství dat

GATAGCGTAATGATCGGCTGGCTGCCGCAT

TACAGGTGGTCGCGCCCGCCGCCAGCACAT

Genotyp → Fenotyp

Molekulárně biologická data

- **Nutnost organizovaného ukládání a skladování dat.**

Databáze je určitá uspořádaná množina informací (dat) uložená na paměťovém médiu.

Molekulárně biologická data

- **Nutnost organizovaného ukládání a skladování dat.**
- **Nutnost prohlížení a analyzování uložených dat.**

Databáze je určitá uspořádaná množina informací (dat) uložená na paměťovém médiu.

V širším smyslu jsou součástí databáze i softwarové prostředky, které umožňují manipulaci s uloženými daty a přístup k nim.

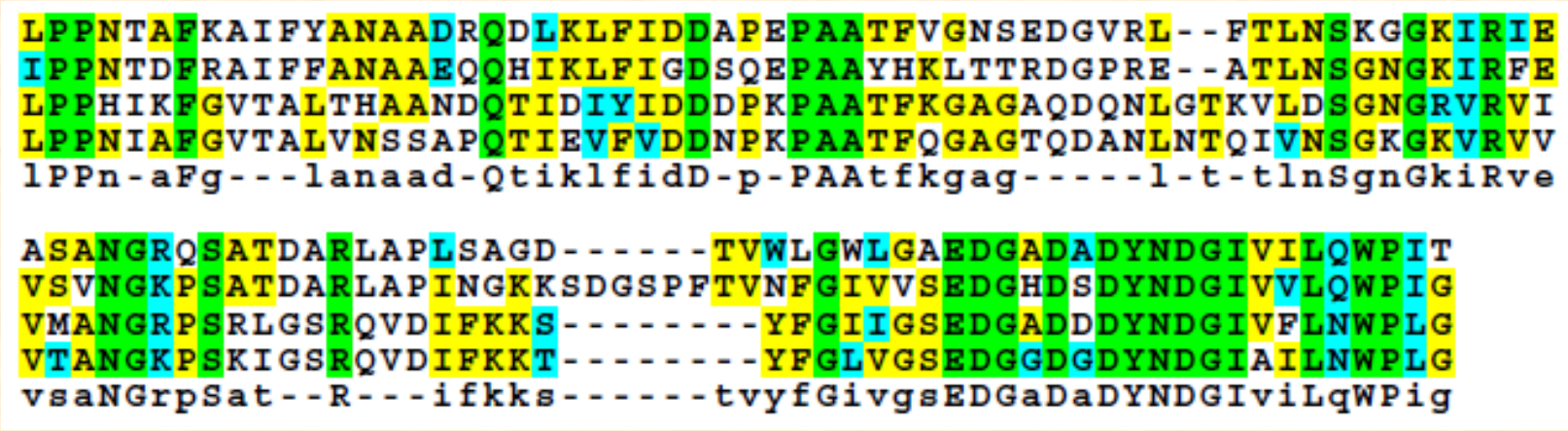
Analytické nástroje

- **Vyhledávácí software**

  Nutnost snadného, rychlého a specifického vyhledání informací.

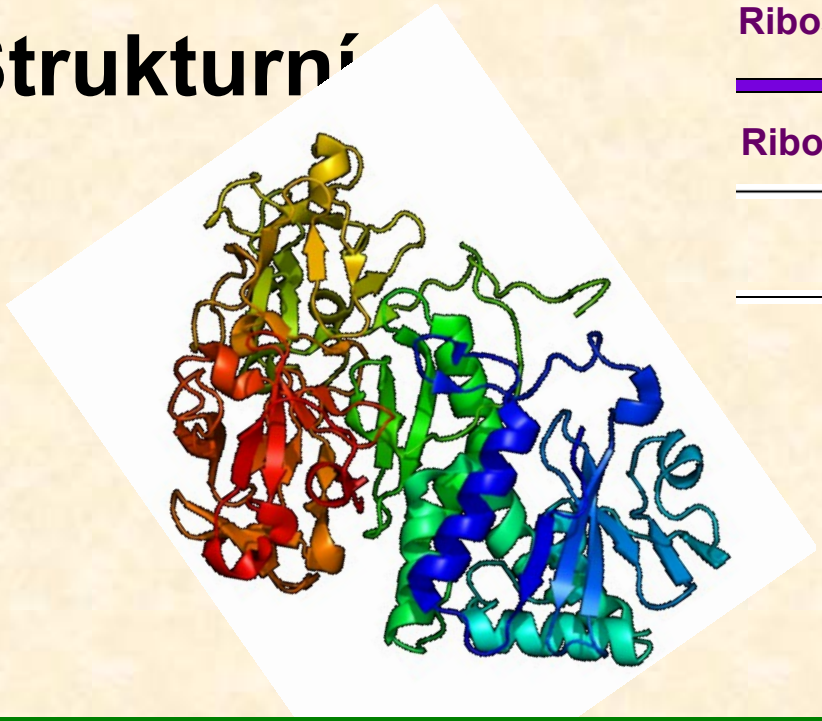
- **Srovnávání dat (sekvencí)**

  Sequence alignment – „seřazení“ sekvencí.



Rozdělení molekulárně biologických databází

- **Databáze:**
  - Primární
  - Sekundární
  - Strukturní



```
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LPFYGTYGDLERWAHQSRQQIPLGLQALTHGISFFRSGGNDNEEKARTLIVII
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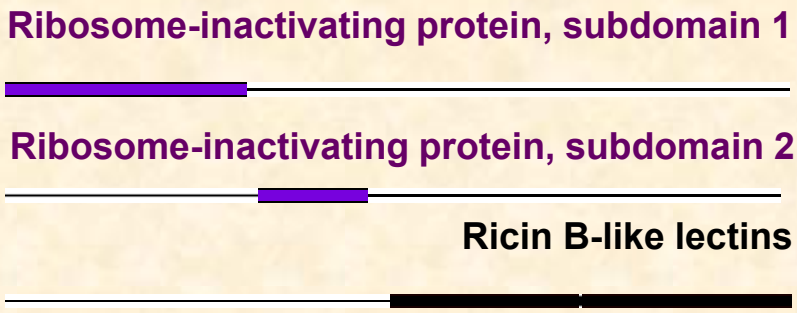
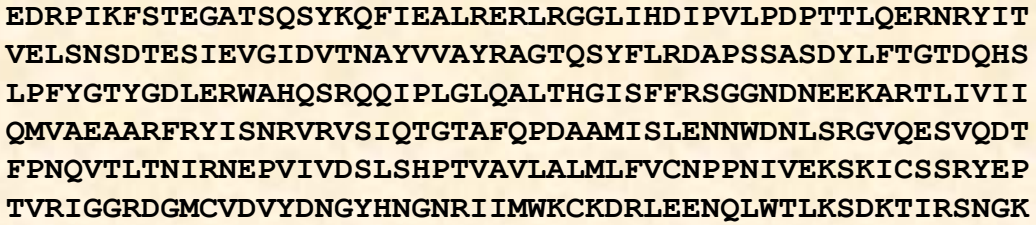


Rozdělení molekulárně biologických databází

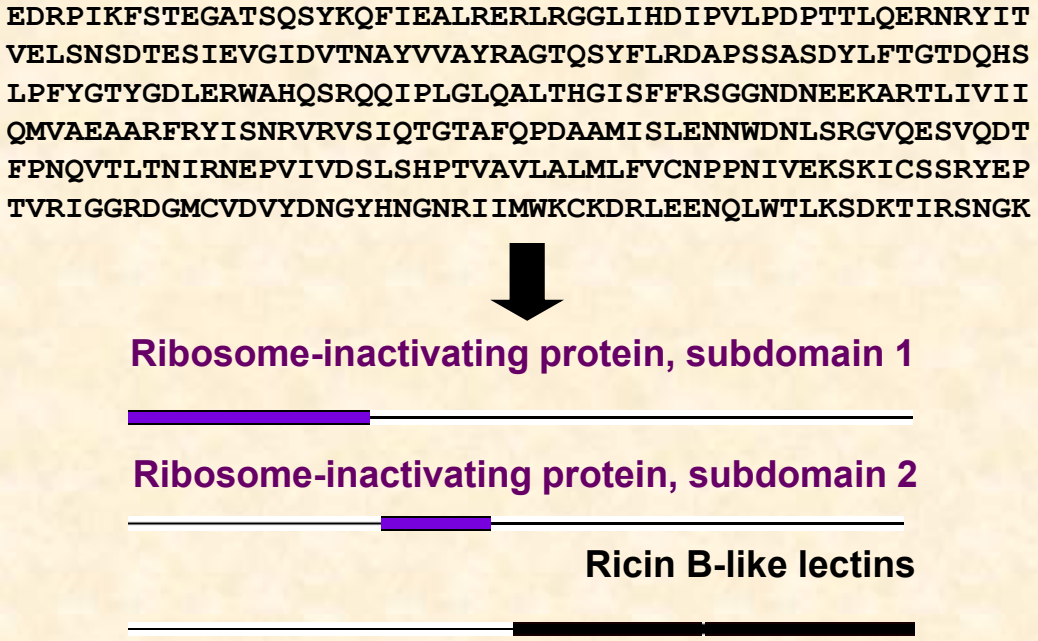
- **Databáze:**
  Primární
  Sekundární
  Strukturní



Primární databáze obsahují anotované sekvence NA nebo proteinů.

Rozdělení molekulárně biologických databází

- **Databáze:**
  - Primární
  - **Sekundární**
  - Strukturní



Sekundární databáze obsahují informace odvozené z primárních databází ve formě charakteristických vzorů sekvencí, tj. funkčních nebo strukturních motivů získaných srovnáním primárních dat (sekvencí).

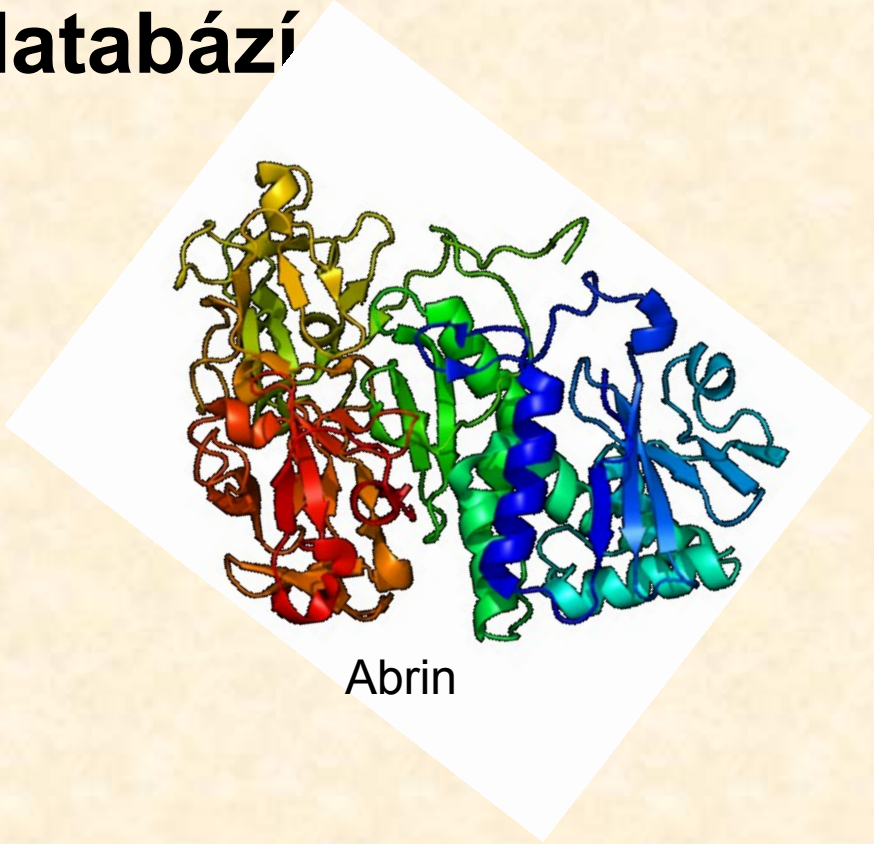
Rozdělení molekulárně biologických databází

- **Databáze:**

  Primární

  Sekundární

  Strukturní



Abrin

Obsahují struktury proteinů (nukleových kyselin) a jejich anotace.

Rozdělení molekulárně biologických databází

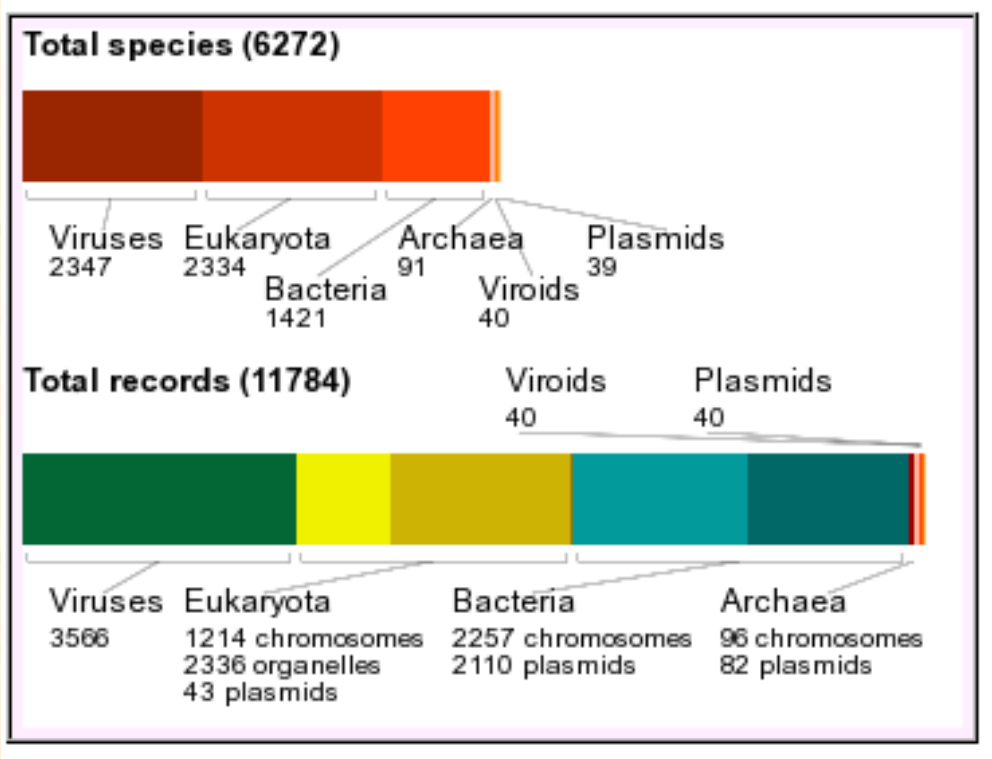
- **Databáze:**

  Primární

  Sekundární

  Strukturní

Genomové zdroje



Rozdělení molekulárně biologických databází

- **Databáze:**

  Specializované

  Univerzální

Rozdělení molekulárně biologických databází

- **Databáze:**

  Specializované

  Univerzální

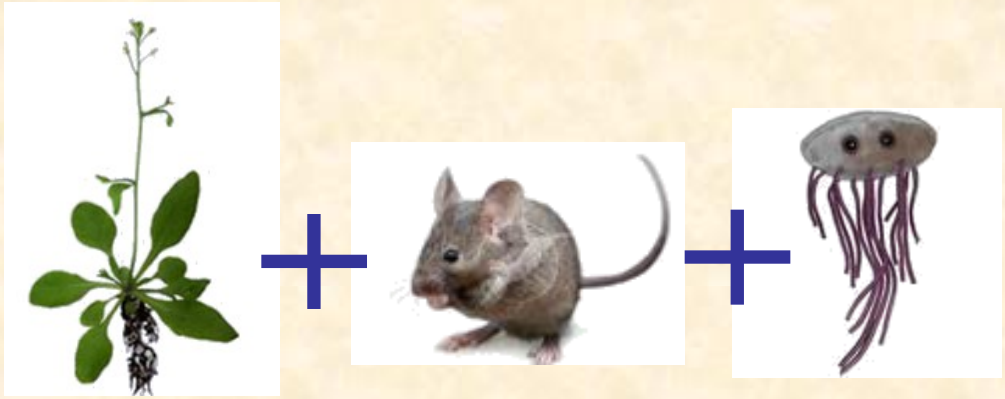
Specializované databáze obsahují informace o určité proteinové rodině nebo skupině proteinů, případně o určitém organismu.

Rozdělení molekulárně biologických databází

- **Databáze:**

  Specializované

  Univerzální



Univerzální databáze obsahují informace o proteinech (NA) ze všech organismů.

Rozdělení univerzálních proteinových databází

- **Univerzální databáze:**

  „Skladiště“ sekvencí – sequence repository

  „Manuálně“ spravovaná – curated database

Rozdělení univerzálních proteinových databází

- **„Skladiště“ sekvencí – sequence repository**

  Kromě sekvencí obsahují málo nebo žádné dodatečné informace.

  Záznamy generovány automaticky.

  Proteiny mohou být zastoupeny několika různými záznamy (sekvencemi) = „nadbytečnost“ (redundance) sekvencí.

Rozdělení univerzálních proteinových databází

- **Manuálně spravované – curated databases**

  Záznamy obsahují dodatečné informace.

  Informace jsou před vložením do databáze validovány experty.

  Všechny záznamy o stejné proteinové sekvenci jsou sdružovány do jediného = non-redundant dataset.

Rozdělení molekulárně biologických databází

- **Databáze:**

  Primární

  Sekundární

  Strukturní

  Genomové zdroje

  Složené databáze

Složené databáze

- **Složené (composite) databáze:**

  Slučují data z několika primárních databází.

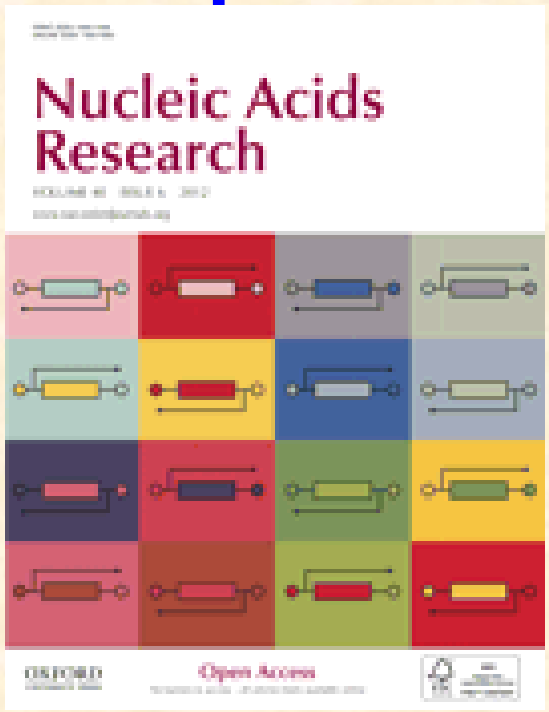
  Eliminace redundantních dat.

  Různá priorita zdrojových databází podle kvality validace a anotace (eliminace redundantních dat z databáze s nižší prioritou).

Molekulárně biologické databáze

Nucleic Acids Research

http://www3.oup.co.uk/nar/database/a/



Nucleotide Sequence Databases
International Nucleotide Sequence Database Collaboration
Coding and non-coding DNA
Gene structure, introns and exons, splice sites
Transcriptional regulator sites and transcription factors
RNA sequence databases
Protein sequence databases
Structure Databases

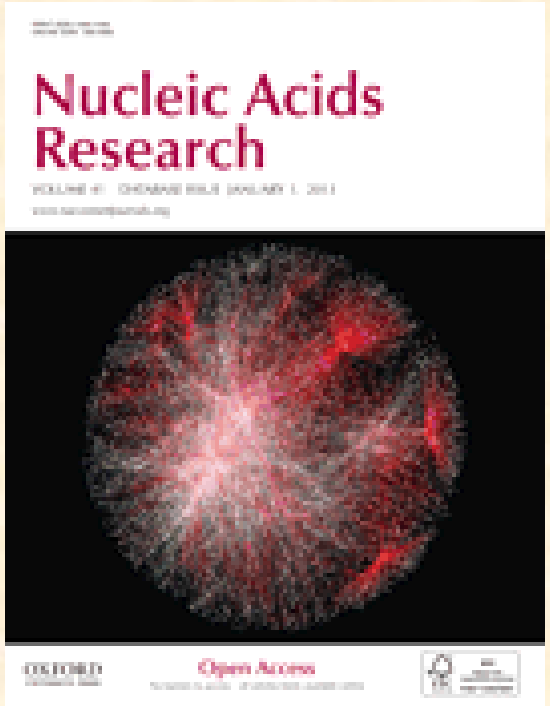
Genomics Databases (non-vertebrate)
Metabolic and Signaling Pathways
Human and other Vertebrate Genomes
Human Genes and Diseases
Microarray Data and other Gene Expression Databases
Proteomics Resources
Other Molecular Biology Databases
Organelle databases
Plant databases
Immunological databases

2012: 1380 databází

Molekulárně biologické databáze

Nucleic Acids Research

http://www3.oup.co.uk/nar/database/a/



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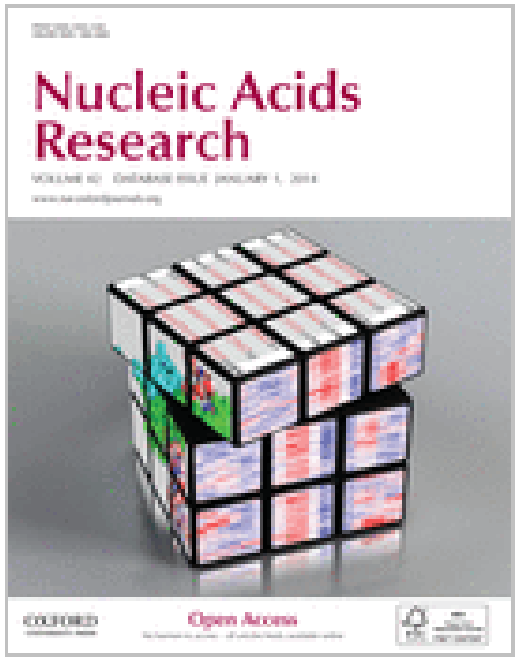
Immunological databases

2013: 1512 databází

Molekulárně biologické databáze

Nucleic Acids Research

http://www3.oup.co.uk/nar/database/a/



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Organelle databases
Plant databases
Immunological databases

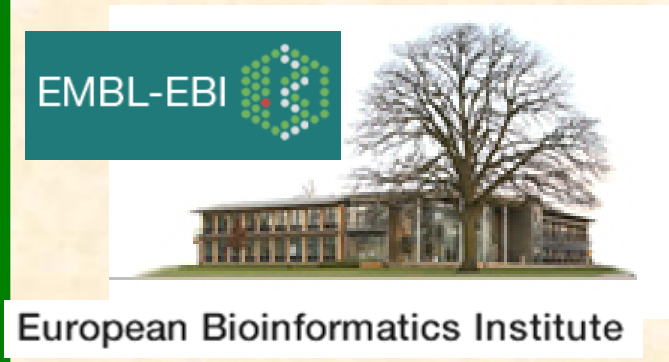
2014: 1552 databází

EBI/NCBI/CIB

Instituce zabývající se shromažďováním, správou a poskytováním dat a informací a vývojem analytických nástrojů.

EBI

Evropský institut pro bioinformatiku



NCBI

Národní centrum pro biotechnologické informace

CIB

National Center for Biotechnology Information

Center for Information Biology

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

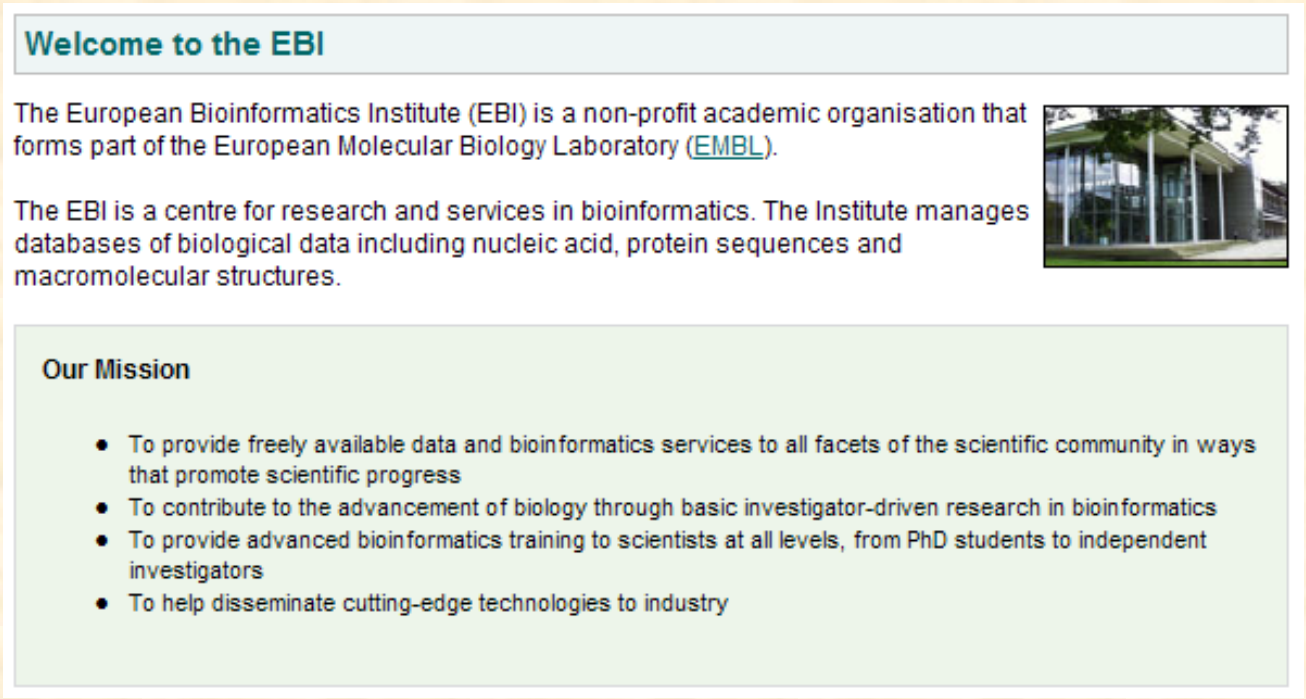
http://www.ncbi.nlm.nih.gov/

http://www.nig.ac.jp/

EBI – Evropský institut pro bioinformatiku

European Bioinformatics Institute

- **Založen roku 1992 jako součást European Molecular Biology Laboratory - EMBL.**
- **Sídlo v Hinxtonu ve Velké Británii.**



Welcome to the EBI

The European Bioinformatics Institute (EBI) is a non-profit academic organisation that forms part of the European Molecular Biology Laboratory (EMBL).

The EBI is a centre for research and services in bioinformatics. The Institute manages databases of biological data including nucleic acid, protein sequences and macromolecular structures.

Our Mission

- To provide freely available data and bioinformatics services to all facets of the scientific community in ways that promote scientific progress
- To contribute to the advancement of biology through basic investigator-driven research in bioinformatics
- To provide advanced bioinformatics training to scientists at all levels, from PhD students to independent investigators
- To help disseminate cutting-edge technologies to industry

NCBI - Národní centrum pro biotechnologické informace

NCBI

National Center for Biotechnology Information

National Library of Medicine National Institutes of Health

- **Založeno v roce 1988 jako oddělení Národní lékařské knihovny (National Library of Medicine – NLM) v USA.**
- **Součást National Institutes of Hea**

What does NCBI do?

Established in 1988 as a national resource for molecular biology information, NCBI creates public databases, conducts research in computational biology, develops software tools for analyzing genome data, and disseminates biomedical information - all for the better understanding of molecular processes affecting human health and disease.

CIB – Centrum pro informační biologii

- Založeno jako oddělení Národního institutu genetiky (国立遺伝学研究所, NIG) v Japonsku.

Research Organization of Information and Systems
National Institute of Genetics

http://www.nig.ac.jp/

Information/Database

- DNA Data Bank of Japan
- National BioResource Project - Information Site
- WFCC-MIRCEN World Data Centre for Microorganisms
- Genetic Resources Database (SHIGEN)
- Nematode Gene Expression Database
- Mouse Microsatellite Database
- Rice Genome Database (Oryzabase)
- E.coli Genome Database (PEC)

Virtual Museum of Genetics(Japanese)
DNA Data Bank of Japan
National BioResource Project
Genome Netwaork Project

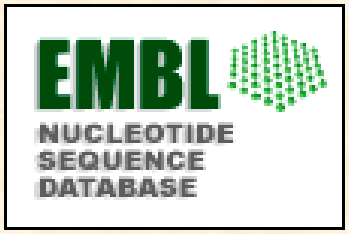
Primární databáze NA

- **EMBL - Evropský institut pro bioinformatiku**

- **GenBank - Národní centrum pro biotechnologické informace**

- **DDBJ - Národní genetický institut (NIG)**

EMBL



- **EMBL Nucleotide Sequence Database (EMBL-Bank) byla založena roku 1980 jako první databáze nukleotidových sekvencí.**
- **Obsahuje sekvence RNA a DNA.**
- **Zdroje sekvencí: vloženy přímo autory, genomové projekty, patenty**

This week the EMBL Database contained
301,588,430,608 nucleotides in 199,575,971 entries

This week = 20.4.2011

EMBL-EBI

EMBL

ENA
European Nucleotide Archive

- **EMBL Nucleotide Sequence Database (EMBL-Bank) – součást ENA (European Nucleotide Archive).**

About the European Nucleotide Archive

The European Nucleotide Archive (ENA) captures and presents information relating to experimental workflows that are based around nucleotide sequencing. A typical workflow includes the isolation and preparation of material for sequencing, a run of a sequencing machine in which sequencing data are produced and a subsequent bioinformatic analysis pipeline. ENA records this information in a data model that covers input information (sample, experimental setup, machine configuration), output machine data (sequence traces, reads and quality scores) and interpreted information (assembly, mapping, functional annotation).

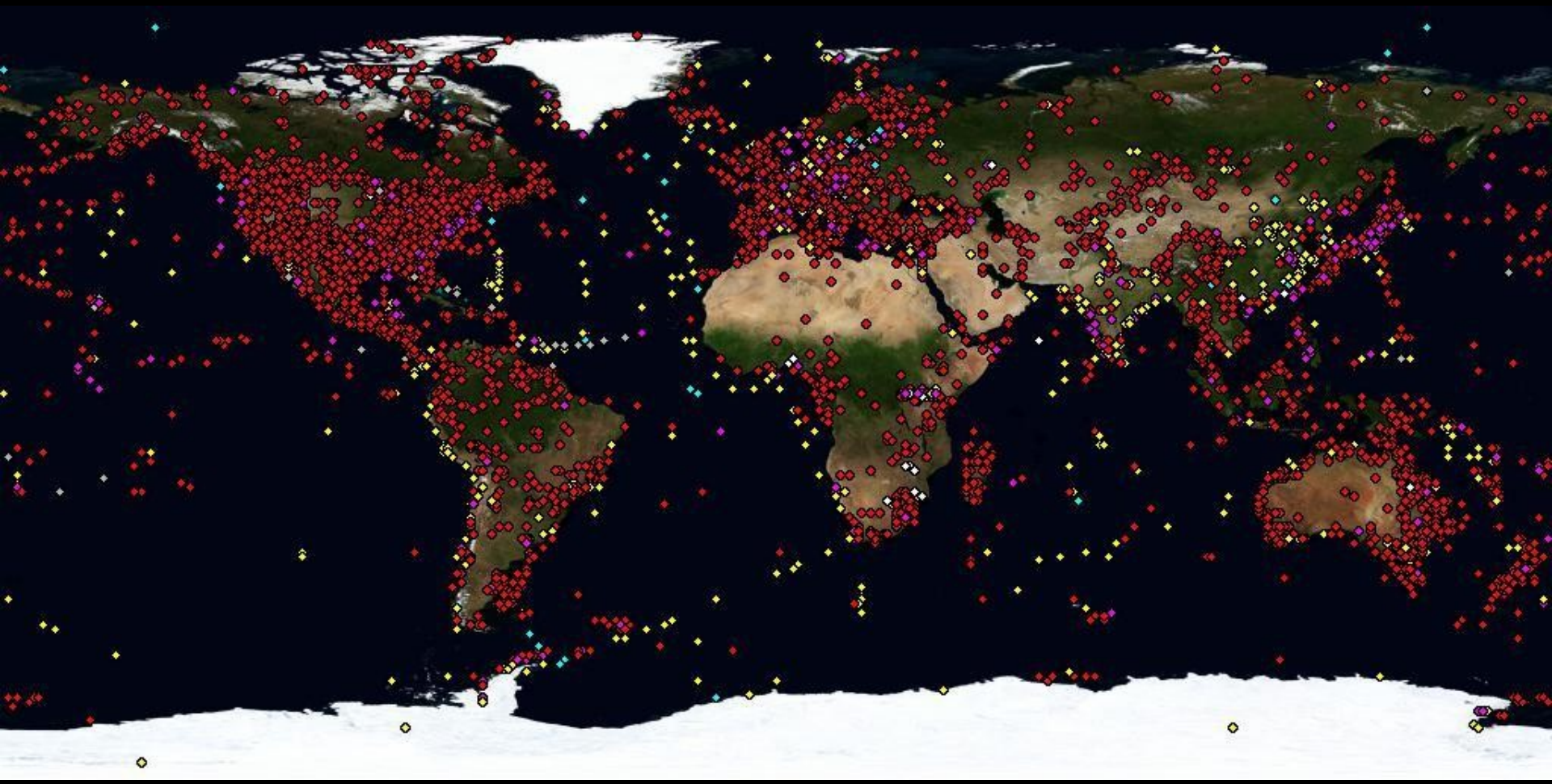
Data arrive at ENA from a variety of sources. These include submissions of raw data, assembled sequences and annotation from small-scale sequencing efforts, data provision from the major European sequencing centres and routine and comprehensive exchange with our partners in the International Nucleotide Sequence Database Collaboration (INSDC).

Provision of nucleotide sequence data to ENA or its INSDC partners has become a central and mandatory step in the dissemination of research findings to the scientific community. ENA works with publishers of scientific literature and funding bodies to ensure compliance with these principles and to provide optimal submission systems and data access tools that work seamlessly with the published literature.

ENA is made up of a number of distinct databases that includes EMBL-Bank, the newly established Sequence Read Archive (SRA) and the Trace Archive each with their own data formats and standards. ENA data classes and formats are described here.

http://www.ebi.ac.uk/ena/home

The map shows 18,628,656 entries distributed over 57,974 locations.

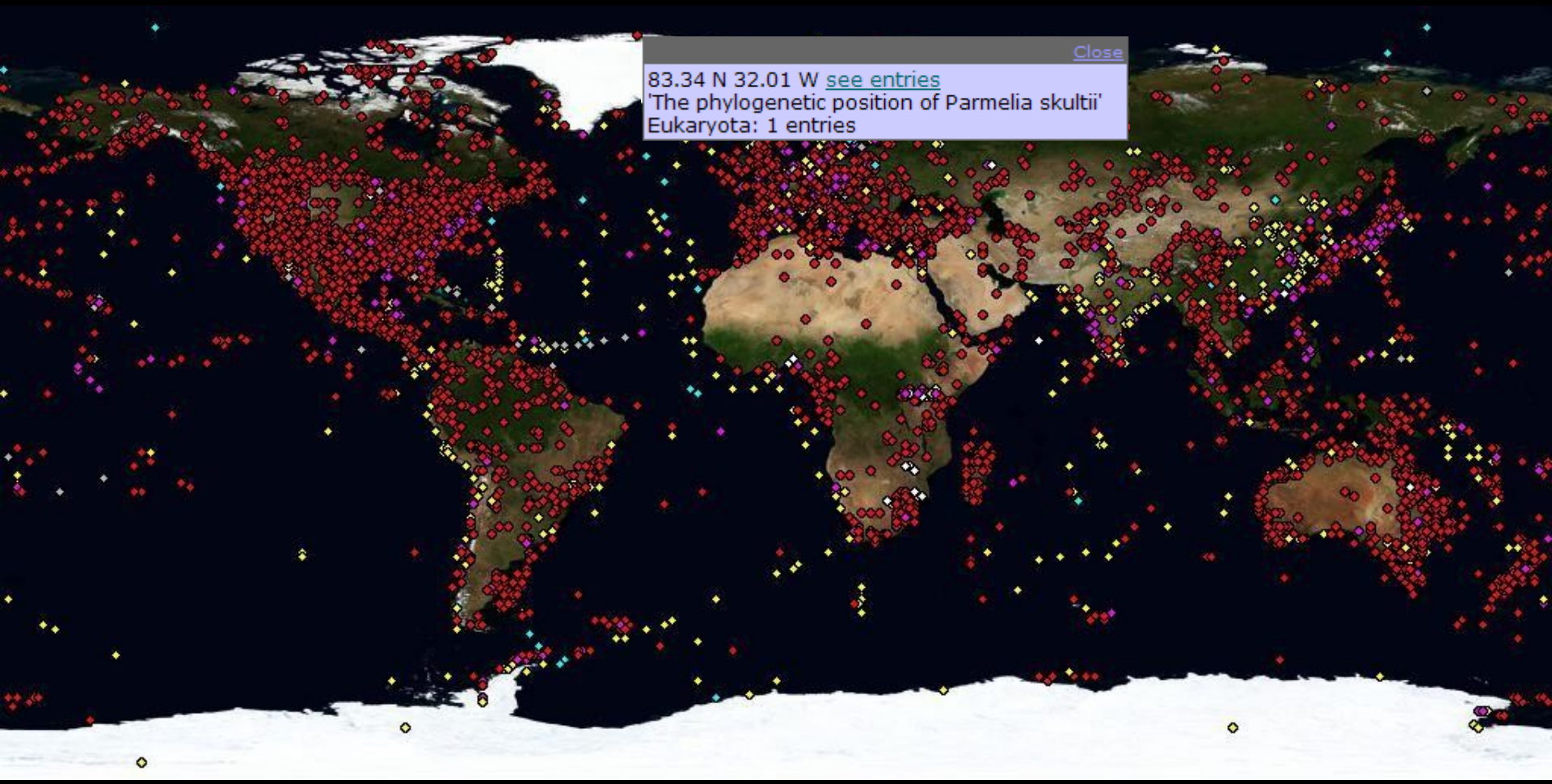


The dots on the map have different colours according to the taxonomy of the specimens:

Eukaryota Bacteria Archaea Other Mixed

2010

The map shows 18,628,656 entries distributed over 57,974 locations.

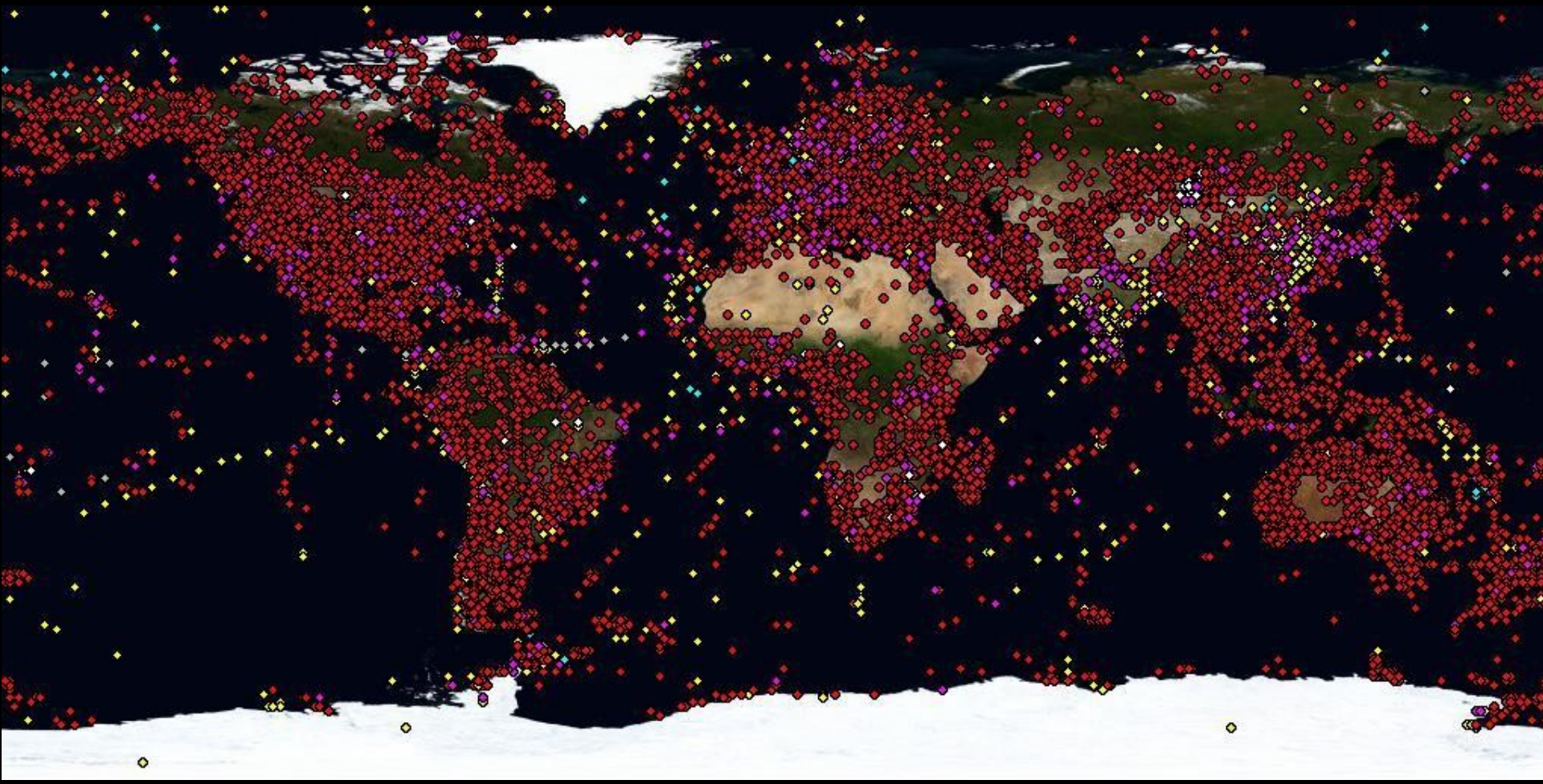


The dots on the map have different colours according to the taxonomy of the specimens:

Eukaryota **Bacteria** **Archaea** **Other** **Mixed**

2010

The map shows 18,710,024 entries distributed over 62,882 locations.



The dots on the map have different colours according to the taxonomy of the specimens:

Eukaryota Bacteria Archaea Other Mixed

2012

EMBL „entry“

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ID   X56734; SV 1; linear; mRNA; STD; PLN; 1859 BP.
XX
AC   X56734; S46826;
XX
DT   12-SEP-1991 (Rel. 29, Created)
DT   25-NOV-2005 (Rel. 85, Last updated, Version 11)
XX
DE   Trifolium repens mRNA for non-cyanogenic beta-glucosidase
XX
KW   beta-glucosidase.
XX
OS   Trifolium repens (white clover)
OC   Eukaryota; Viridiplantae; Streptophyta; Embryophyta; Tracheophyta;
OC   Spermatophyta; Magnoliophyta; eudicotyledons; core eudicotyledons; rosids;
OC   eurosids I; Fabales; Fabaceae; Papilionoideae; Trifolieae; Trifolium.
XX
RN   [5]
RP   1-1859
RX   PUBMED; 1907511.
RA   Oxtoby E., Dunn M.A., Pancoro A., Hughes M.A.;
RT   "Nucleotide and derived amino acid sequence of the cyanogenic
RT   beta-glucosidase (linamarase) from white clover (Trifolium repens L.)";
RL   Plant Mol. Biol. 17(2):209-219(1991).
XX
RN   [6]
RP   1-1859
RA   Hughes M.A.;
RT   ;
RL   Submitted (19-NOV-1990) to the EMBL/GenBank/DDBJ databases.
RL   Hughes M.A., University of Newcastle Upon Tyne, Medical School, Newcastle
RL   Upon Tyne, NE2 4HH, UK
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FT                   VLEDEYGGFLNSGVINDFRDYTDLCFKEFGDRVRYWSTLNEPWVFSNSGYALGTNAPGR
FT                   CSASNVAKPGDSGTGPYIVTHNQILAHAEAVHVYKTKYQAYQKGKIGITLVSNWLMPLD
FT                   DNSIPDIKAAERSLDFQFGLFMEQLTTGDYSKSMRRIVKNRLPKFSKFESSLVNGSFDF
FT                   IGINYYSSSYISNAPSHGNAKPSYSTNPMTNISFEKHGIPLGPRAASIWIYVYPYMFIQ
FT                   EDFEIFCYILKINITILQFSITENGMNEFNDATLPVEEALLNTYRIDYYYRHLYYIRSA
FT                   IRAGSNVKGFYAWSFLDCNEWFAGFTVRFGLNFVD"
FT   mRNA            1..1859
FT                   /experiment="experimental evidence, no additional details
FT                   recorded"
XX
SQ   Sequence 1859 BP; 609 A; 314 C; 355 G; 581 T; 0 other;
aaacaaacca aatatggatt ttattgtagc catatttgct ctgtttgtta ttagctcatt        60
cacaattact tccacaaatg cagttgaagc ttctactctt cttgacatag gtaacctgag       120
tcggagcagt tttcctcgtg gcttcatctt tggtgctgga tcttcagcat accaatttga       180
aggtgcagta aacgaaggcg gtagaggacc aagtatttgg gataccttca cccataaata       240
tccagaaaaa ataagggatg gaagcaatgc agacatcacg gttgaccaat atcaccgcta       300
caaggaagat gttgggatta tgaaggatca aaatatggat tcgtatagat tctcaatctc       360
ttggccaaga atactcccaa aggggaaagtt gagcggaggc ataaatcacg aaggaatcaa      420
```

Translation =
***proteinová* databáze**

Formát EMBL databáze

```
ID - identification                (begins each entry; 1 per entry)
AC - accession number              (>=1 per entry)
PR - project identifier            (0 or 1 per entry)
DT - date                          (2 per entry)
DE - description                   (>=1 per entry)
KW - keyword                       (>=1 per entry)
OS - organism species              (>=1 per entry)
OC - organism classification       (>=1 per entry)
OG - organelle                     (0 or 1 per entry)
RN - reference number              (>=1 per entry)
RC - reference comment             (>=0 per entry)
RP - reference positions           (>=1 per entry)
RX - reference cross-reference     (>=0 per entry)
RG - reference group               (>=0 per entry)
RA - reference author(s)           (>=0 per entry)
RT - reference title               (>=1 per entry)
RL - reference location            (>=1 per entry)
DR - database cross-reference      (>=0 per entry)
CC - comments or notes             (>=0 per entry)
AH - assembly header               (0 or 1 per entry)
AS - assembly information          (0 or >=1 per entry)
FH - feature table header          (2 per entry)
FT - feature table data            (>=2 per entry)
XX - spacer line                   (many per entry)
SQ - sequence header               (1 per entry)
CO - contig/construct line         (0 or >=1 per entry)
bb - (blanks) sequence data        (>=1 per entry)
// - termination line              (ends each entry; 1 per entry)
```

Formát EMBL databáze

```
ID   <1>; SV <2>; <3>; <4>; <5>; <6>; <7> BP.
```

The tokens represent:

1. Primary accession number
2. Sequence version number
3. Topology: 'circular' or 'linear'
4. Molecule type
5. Data class
6. Taxonomic division
7. Sequence length

```
ID   CD789012; SV 4; linear; genomic DNA; HTG; MAM; 500 BP.
```

ftp://ftp.ebi.ac.uk/pub/databases/embl/doc/usrman.txt

Formát EMBL databáze

Class	Definition
CON	Entry constructed from segment entry sequences, drawing annotation from segment entries
ANN	Entry constructed from segment entry sequences with its own annotation
PAT	Patent
EST	Expressed Sequence Tag
GSS	Genome Survey Sequence
HTC	High Thoughput CDNA sequencing
HTG	High Thoughput Genome sequencing
MGA	Mass Genome Annotation
WGS	Whole Genome Shotgun
TPA	Third Party Annotation
STS	Sequence Tagged Site
STD	Standard (all entries not classified as above)

ftp://ftp.ebi.ac.uk/pub/databases/embl/doc/usrman.txt

Formát EMBL databáze

Division	Code
Bacteriophage	PHG
Environmental Sample	ENV
Fungal	FUN
Human	HUM
Invertebrate	INV
Other Mammal	MAM
Other Vertebrate	VRT
Mus musculus	MUS
Plant	PLN
Prokaryote	PRO
Other Rodent	ROD
Synthetic	SYN
Transgenic	TGN
Unclassified	UNC
Viral	VRL

ftp://ftp.ebi.ac.uk/pub/databases/embl/doc/usrman.txt

Sequence: AB849925.1 : Ipomoea nil GAPDH mRNA for glyceraldehyde-3-phosphate dehydrogenase, complete cds, cultivar: Violet.

View: TEXT FASTA XML
Overview Source Feature(s) Other Features References Sequence

Download: TEXT FASTA XML
Send Feedback

Organism	Molecule type	Topology	Data class	Taxonomic Division
Ipomoea nil	mRNA	linear	STD	PLN

Sequence length	Sequence Version	First public	Last updated	Show Version History
1,343	1	01-APR-2014	01-APR-2014	AB849925

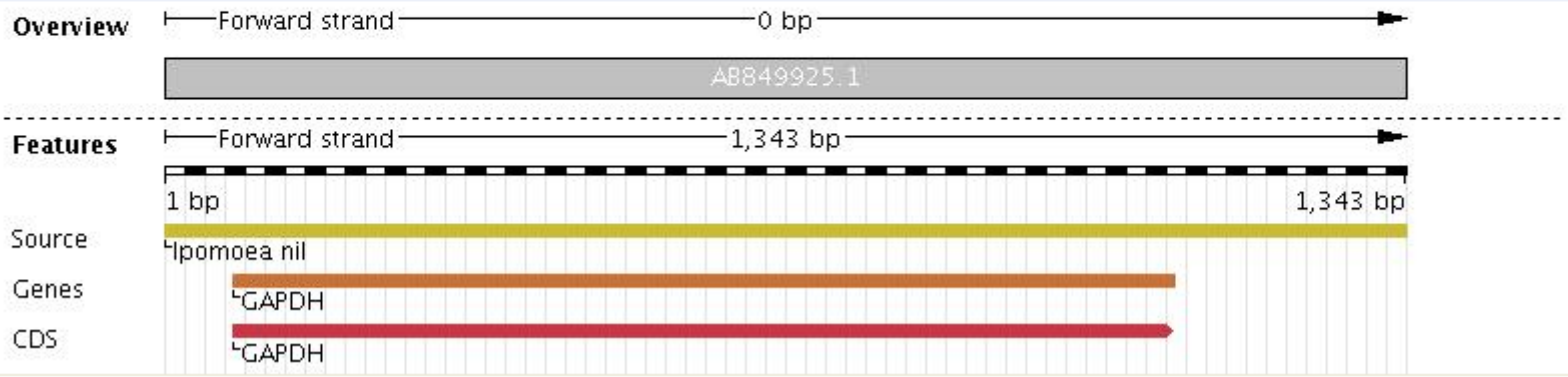
Lineage
Eukaryota, Viridiplantae, Streptophyta, Embryophyta, Tracheophyta, Spermatophyta, Magnoliophyta, eudicotyledons, Gunneridae, Pentapetalae, asterids, lamiids, Solanales, Convolvulaceae, Ipomoeeae, Ipomoea

Navigation Top

Taxon: Taxon:35883

Overview Top

Base range: 1 - 1343 Apply



GenBank

- **Založena roku 1982 v rámci institutu NCBI.**

GenBank® is the NIH genetic sequence database, an annotated collection of all publicly available DNA sequences (*Nucleic Acids Research*, 2008 Jan;36(Database issue):D25-30). There are approximately 85,759,586,764 bases in 82,853,685 sequence records in the traditional GenBank divisions and 108,635,736,141 bases in 27,439,206 sequence records in the WGS division as of February 2008.

NCBI Sample GenBank Record

http://www.ncbi.nlm.nih.gov/Sitemap/samplerecord.html

Sample GenBank Record

```
LOCUS       SCU49845     5028 bp    DNA             PLN       21-JUN-1999
DEFINITION  Saccharomyces cerevisiae TCP1-beta gene, partial cds, and Axl2p
            (AXL2) and Rev7p (REV7) genes, complete cds.
ACCESSION   U49845
VERSION     U49845.1  GI:1293613
KEYWORDS    .
SOURCE      Saccharomyces cerevisiae (baker's yeast)
  ORGANISM  Saccharomyces cerevisiae
            Eukaryota; Fungi; Ascomycota; Saccharomycotina; Saccharomycetes;
            Saccharomycetales; Saccharomycetaceae; Saccharomyces.
REFERENCE   1  (bases 1 to 5028)
  AUTHORS   Torpey,L.E., Gibbs,P.E., Nelson,J. and Lawrence,C.W.
  TITLE     Cloning and sequence of REV7, a gene whose function is required for
            DNA damage-induced mutagenesis in Saccharomyces cerevisiae
  JOURNAL   Yeast 10 (11), 1503-1509 (1994)
  PUBMED    7871890
REFERENCE   2  (bases 1 to 5028)
  AUTHORS   Roemer,T., Madden,K., Chang,J. and Snyder,M.
  TITLE     Selection of axial growth sites in yeast requires Axl2p, a novel
            plasma membrane glycoprotein
  JOURNAL   Genes Dev. 10 (7), 777-793 (1996)
  PUBMED    8846915
REFERENCE   3  (bases 1 to 5028)
  AUTHORS   Roemer,T.
  TITLE     Direct Submission
  JOURNAL   Submitted (22-FEB-1996) Terry Roemer, Biology, Yale University, New
            Haven, CT, USA
```

http://www.ncbi.nlm.nih.gov/Sitemap/samplerecord.html

Sample GenBank Record

```
LOCUS       SCU49845     5028 bp    DNA             PLN       21-JUN-1999
DEFINITION  Saccharomyces cerevisiae TCP1-beta gene, partial cds, and Axl2p
            (AXL2) and Rev7p (REV7) genes, complete cds.
ACCESSION   U49845
VERSION     U49845.1  GI:1293613
KEYWORDS    .
SOURCE      Saccharomyces cerevi
  ORGANISM  Saccharomyces cerevi
            Eukaryota; Fungi; As
            Saccharomycetales; S
REFERENCE   1  (bases 1 to 5028)
  AUTHORS   Torpey,L.E., Gibbs,P
  TITLE     Cloning and sequence
            DNA damage-induced m
  JOURNAL   Yeast 10 (11), 1503-
  PUBMED    7871890
REFERENCE   2  (bases 1 to 5028)
  AUTHORS   Roemer,T., Madden,K.
  TITLE     Selection of axial g
            plasma membrane glyc
  JOURNAL   Genes Dev. 10 (7), 7
  PUBMED    8846915
REFERENCE   3  (bases 1 to 5028)
  AUTHORS   Roemer,T.
  TITLE     Direct Submission
  JOURNAL   Submitted (22-FEB-19
            Haven, CT, USA
```

GenBank Division

The GenBank division to which a record belongs is indicated with a three letter abbreviation. In this example, GenBank division is PLN.

The GenBank database is divided into 18 divisions:

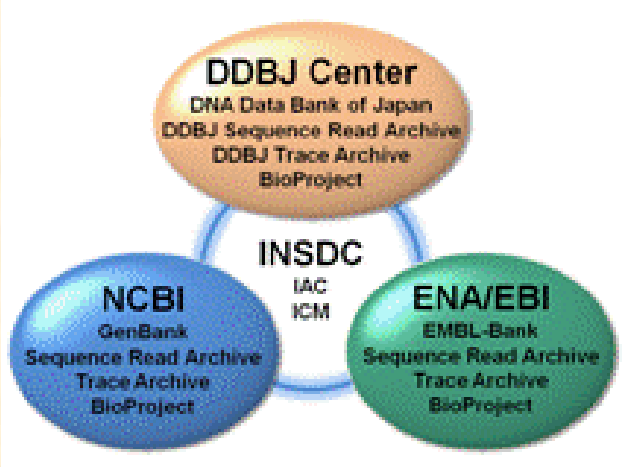
1. PRI - primate sequences
2. ROD - rodent sequences
3. MAM - other mammalian sequences
4. VRT - other vertebrate sequences
5. INV - invertebrate sequences
6. PLN - plant, fungal, and algal sequences
7. BCT - bacterial sequences
8. VRL - viral sequences
9. PHG - bacteriophage sequences
10. SYN - synthetic sequences
11. UNA - unannotated sequences
12. EST - EST sequences (expressed sequence tags)
13. PAT - patent sequences
14. STS - STS sequences (sequence tagged sites)
15. GSS - GSS sequences (genome survey sequences)
16. HTG - HTG sequences (high-throughput genomic sequences)
17. HTC - unfinished high-throughput cDNA sequencing
18. ENV - environmental sampling sequences

http://www.ncbi.nlm.nih.gov/Sitemap/samplerecord.html

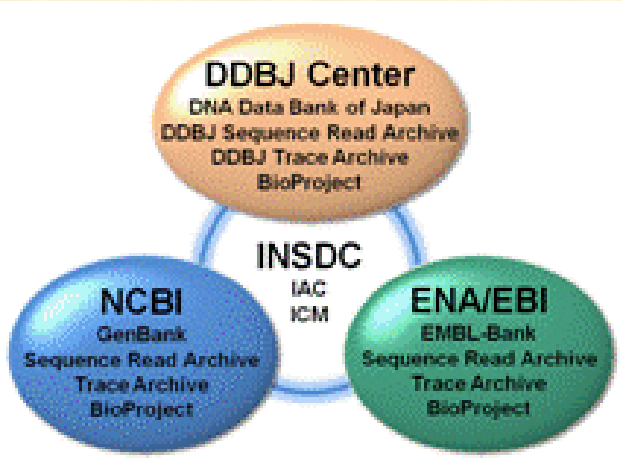
DDBJ
DNA Data Bank of Japan

The DNA Data Bank of Japan

- Původně zahrnovala data především z japonských výzkumů.
- V současnosti úzká spolupráce s ostatními databázemi.



INSDC International Nucleotide Sequence Database Collaboration



http://www.insdc.org/

DDBJ: DNA Data Bank of Japan
CIB-DDBJ: Center for Information Biology and DNA Data Bank of Japan
NIG: National Institute of Genetics

EBI: European Bioinformatics Institute
EMBL: European Molecular Biology Laboratory

NCBI: National Center for Biotechnology Information
NLM: National Library of Medicine

IAC: International Advisory Committee
ICM: International Collaborative Meeting

http://www.insdc.org/documents/feature-table#7.1.1

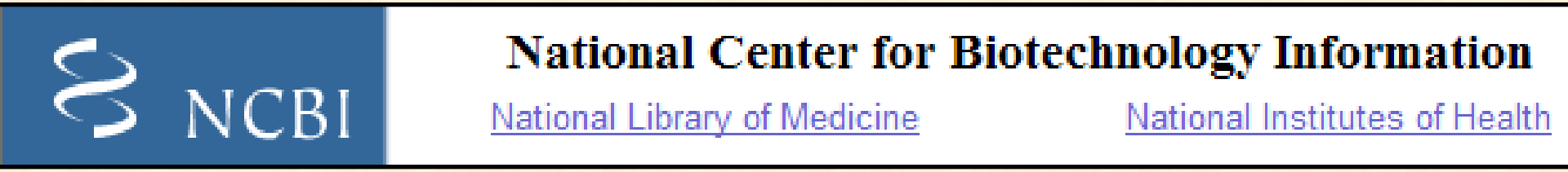
Primární databáze proteinů

- **Univerzální databáze:**

  „Skladiště“ sekvencí – sequence repository

  Manuálně spravovaná – curated database

Příklad: **GenBank *versus* RefSeq**



Primární databáze proteinů

GenBank	RefSeq
Not curated	Curated
Author submits	NCBI creates from existing data
Only author can revise	NCBI revises as new data emerge
Multiple records for same loci common	Single records for each molecule of major organisms
Records can contradict each other	
No limit to species included	Limited to model organisms
Data exchanged among INSDC members	Exclusive NCBI database
Akin to primary literature	Akin to review articles
Proteins identified and linked	Proteins and transcripts identified and linked
Access via NCBI Nucleotide databases	Access via Nucleotide & Protein databases

GenPept - GenBank Gene Products Data Bank
RefSeq - Reference Sequence

Swiss-PROT + TrEMBL

- **Swiss-Prot -** „Curated“ databáze založená na Univerzitě v Ženevě v roce 1986. Spravovaná Švýcarským institutem pro bioinformatiku (**SIB - Swiss Institute of Bioinformatics**).

- Vysoká úroveň anotace → vkládáno více sekvencí než je možno manuálně anotovat a zařadit do databáze.

- **TrEMBL –** Počítačově anotovaná data, odvozená z kódujících úseku sekvencí v DDBJ/EMBL/GenBank, která **ZATÍM** nejsou zařazena v Swiss-Prot.

Swiss-PROT + TrEMBL

- **Anotace:** Funkce
  Katalytická aktivita
  Podjednotky
  Domény
  Biotechnologické využití
  Sekvenční homologie
  Posttranslační modifikace
  Reference atd.

http://www.expasy.org/sprot/

Složené databáze

- **Databáze:**

  Primární

  Sekundární

  Strukturní

  Genomové zdroje

  Složené databáze

Složené databáze

- **Složené (composite) databáze:**

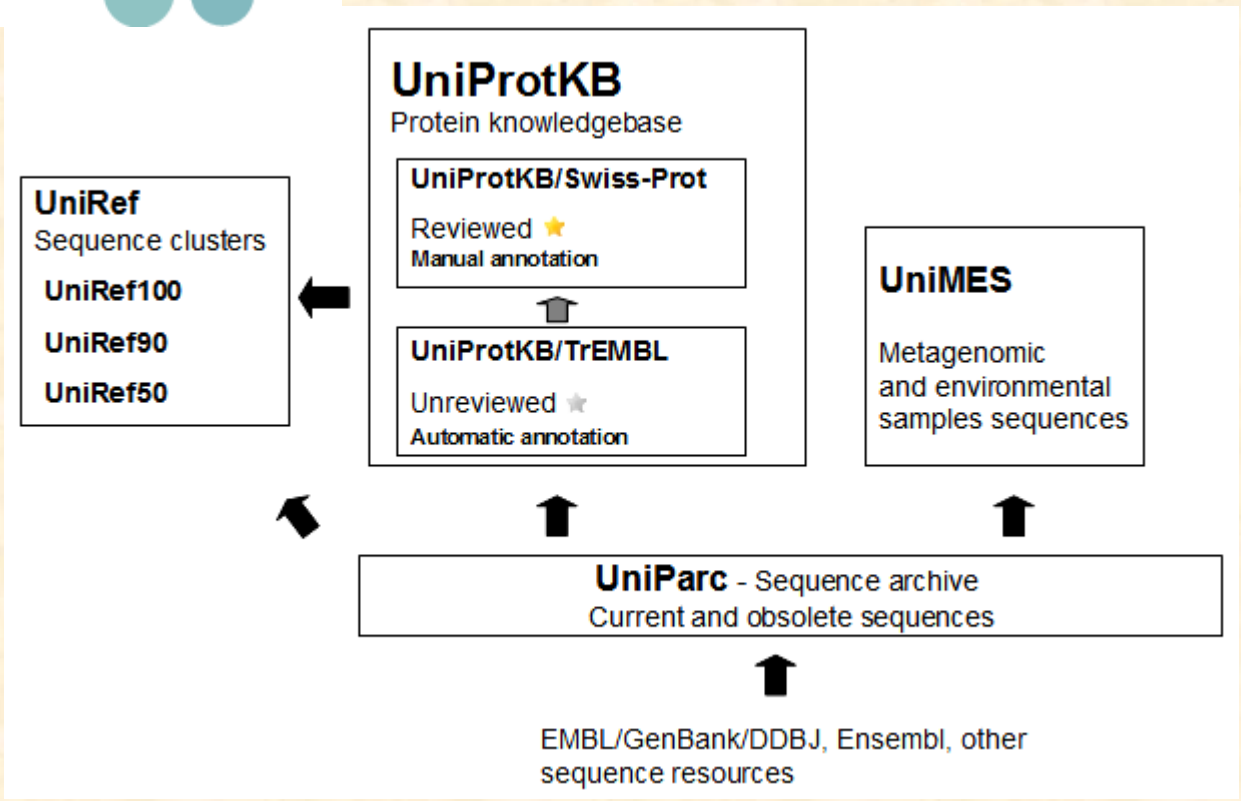
  Slučují data z několika primárních databází.

  Eliminace redundantních dat.

  Různá priorita zdrojových databází podle kvality validace a anotace (eliminace redundantních dat z databáze s nižší prioritou).

Swiss-PROT + TrEMBL

UniProt



2002- spolupráce mezi EBI, SIB a PIR

http:/www.uniprot.org

Sekundární databáze NA a proteinů

Sekundární databáze obsahují informace odvozené z primárních databází ve formě charakteristických vzorů sekvencí, tj. funkčních nebo strukturních motivů získaných srovnáním primárních dat (sekvencí).

- **Vyhledávání „vzoru“ charakteristického pro určitou skupinu proteinů.**
- **Možnost predikce funkce proteinů.**

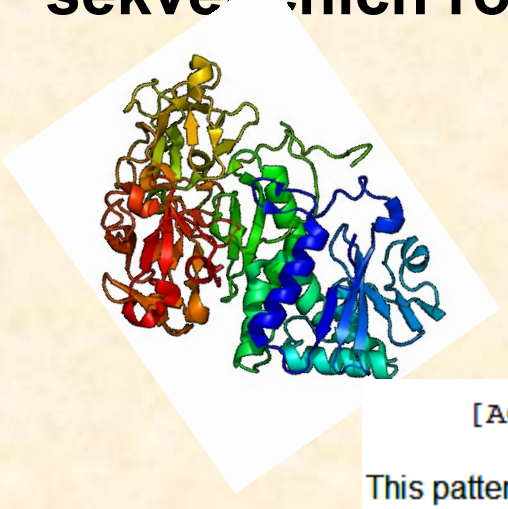
Sekundární databáze NA a proteinů

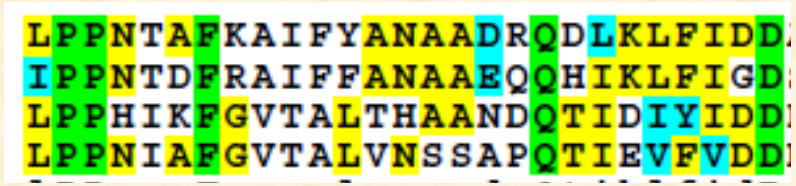
- **Databáze mohou obsahovat:**

  Proteinové DOMÉNY odvozené ze známých struktur

  Proteinové sekvence seřazené do SEKVENČNÍCH RODIN

  CHARAKTERISTICKÉ MOTIVY odvozené z těchto sekvenčních rodin.






```
[AC]-x-V-x(4)-{ED}.
```

This pattern is translated as: [Ala or Cys]-any-Val-any-any-any-any-{any but Glu or Asp}

Sekundární databáze NA a proteinů

- **Sekundární proteinové databáze:**

  PROSITE, Pfam, PRINTS, ProDom, SMART, TIGRFAMS

  V současné době sdruženy do integrované klasifikační databáze proteinů InterPro

http://www.ebi.ac.uk/interpro/

Table View | Raw Output | XML Output | Original Sequences | SUBMIT ANOTHER JOB

SEQUENCE: Sequence_1 CRC64: B08AB341813AD2EE LENGTH: 382 aa

InterPro IPR000772 Domain

Ricin B lectin

PF00652		Ricin_B_lectin
SM00458		RICIN
PS50231		RICIN_B_LECTIN

InterPro IPR001574 Family

Ribosome-inactivating protein

PF00161		RIP
SSF56371		Ribosome_inactivat_prot

InterPro IPR008997 Domain

Ricin B-related lectin

SSF50370		RicinB_like

InterPro IPR016139 Domain

Ribosome-inactivating protein, subdomain 2

G3DSA:4.10.470.10		Ribosome_inactivat_prot_sub2

InterPro IPR017989 Family

Ribosome-inactivating protein subgroup

PR00396		SHIGARICIN

Sekundární databáze NA a proteinů

- **Sekundární proteinové databáze:**

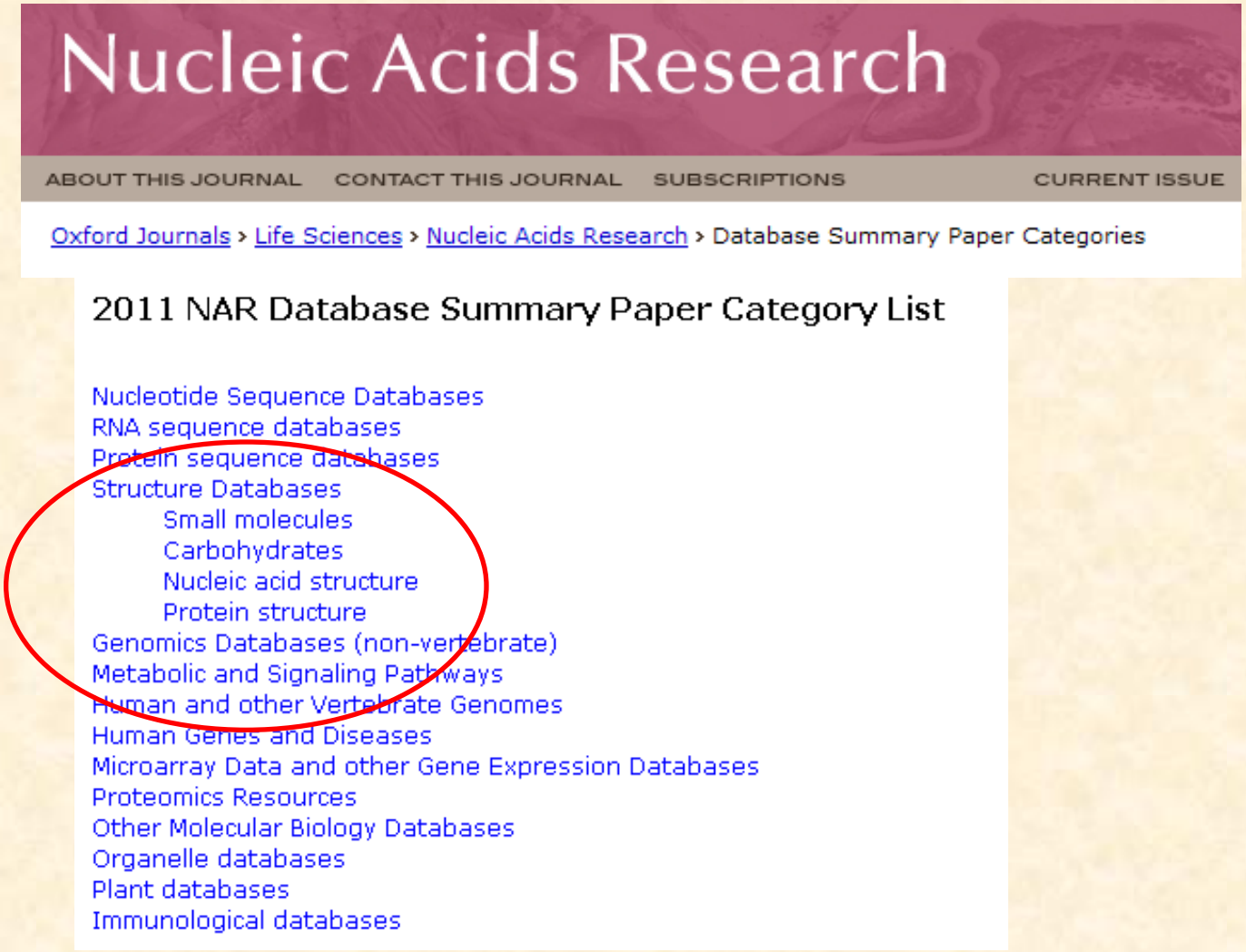
  PROSITE, Pfam, PRINTS, ProDom, SMART, TIGRFAMS

  V současné době sdruženy do integrované klasifikační databáze proteinů InterPro

  http://www.ebi.ac.uk/Tools/pfa/iprscan/

- **Sekundární databáze NA**
  TRANSFAC

Strukturní databáze



http://www3.oup.co.uk/nar/database/a/

Strukturní databáze proteinů

2011 NAR Database Summary Paper Category List

- Nucleotide Sequence Databases
- RNA sequence databases
- Protein sequence databases
- Structure Databases
  - Small molecules
  - Carbohydrates
  - Nucleic acid structure
  - Protein structure
    - 3D-Genomics
    - 3DID - 3D interacting domains
    - ArchDB
    - AS-ALPS
    - ASTRAL
    - AutoPSI
    - BANMOKI
    - BioMagResBank
    - CADB - Conformational Angles DataBase of Proteins
    - CATH
    - CC+
    - CE
    - CoC Central
    - ColiSNP
    - Columba
    - ConSurf-DB
    - CPDB
    - CSA - Catalytic Site Atlas
    - DisProt - Database of Protein Disorder
    - DMAPS
    - Dockground
    - DomIns - Database of Domain Insertions
    - DSDBASE - Disulfide Database
    - DSMM - a Database of Simulated Molecular Motions
    - E-MSD - EBI-Macromolecular Structure Database
    - eF-site - Electrostatic surface of Functional site
    - EzCatDB
    - FireDB
    - FSN
    - Gene3D
    - Genomic Threading Database
    - GTOP - Genomes To Protein structures
    - HOMSTRAD - Homologous Structure Alignment Database
    - HotSprint
    - IMGT/3Dstructure-DB
    - IMOTdb
    - JAIL
    - Jenalib: Jena Library of Biological Macromolecules
    - KineticDB
    - LPFC
    - MALISAM
    - MegaMotifbase
    - MMDB
    - ModBase
    - MolMovDB - Database of Macromolecular Movements
    - PASS2
    - PDB
    - PDB-REPRDB
    - PDBselect
    - PDBsum

RCSB PDB PROTEIN DATA BANK - Protein Data Bank

A MEMBER OF THE PDB | EMDataBank

An Information Portal to Biological Macromolecular Structures

As of Tuesday Apr 08, 2014 at 5 PM PDT there are 99293 Structures | PDB Statistics

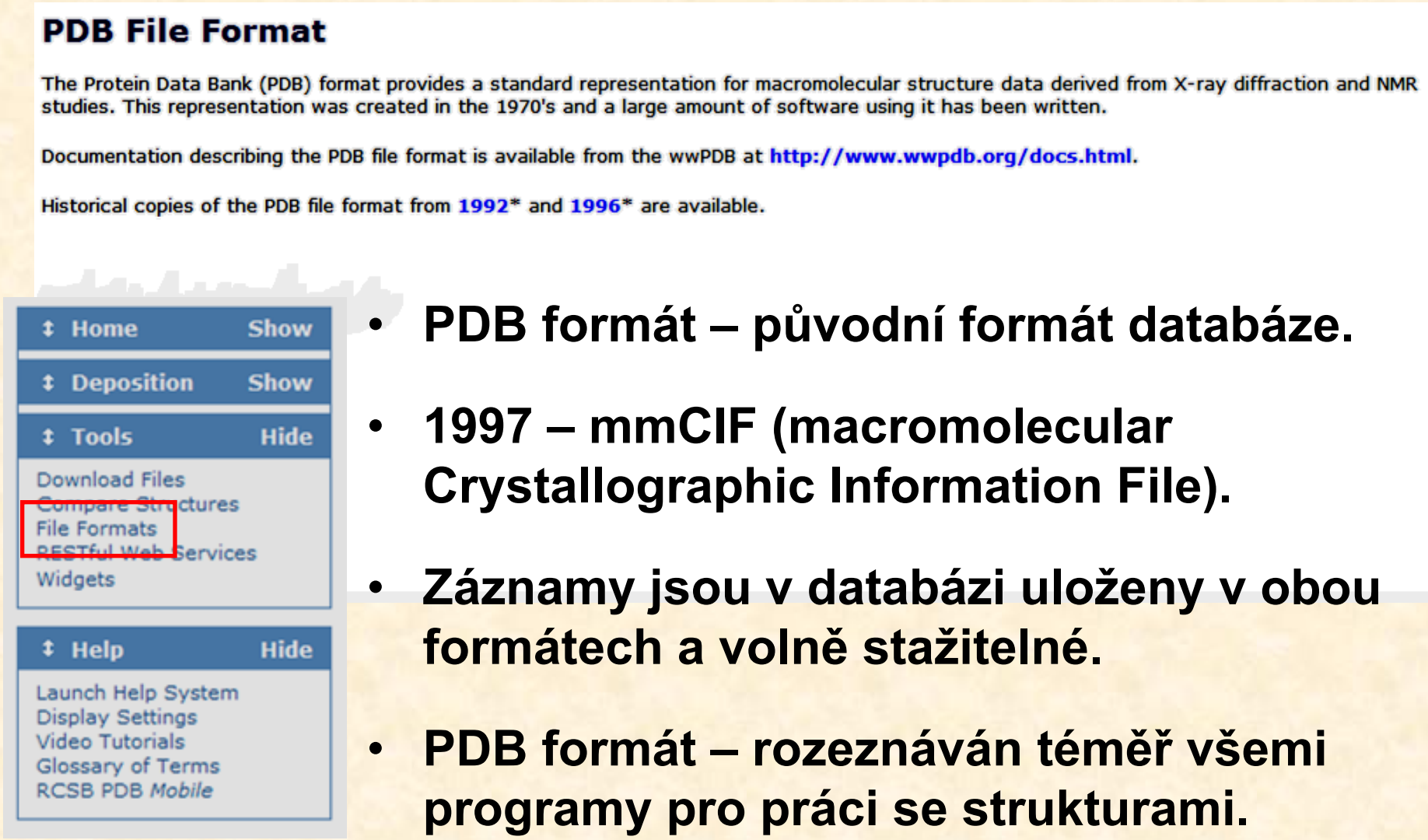
- Databáze obsahuje experimentálně získané struktury proteinů, nukleových kyselin a komplexů informačních biomakromolekul.

PDB Current Holdings Breakdown

Exp.Method	Proteins	Nucleic Acids	Protein/NA Complexes	Other	Total
X-RAY	82121	1516	4267	4	87908
NMR	9104	1079	206	7	10396
ELECTRON MICROSCOPY	521	52	173	0	746
HYBRID	59	3	2	1	65
other	155	4	6	13	178
Total	91960	2654	4654	25	99293

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

PDB formát



- **PDB formát – původní formát databáze.**
- **1997 – mmCIF (macromolecular Crystallographic Information File).**
- **Záznamy jsou v databázi uloženy v obou formátech a volně stažitelné.**
- **PDB formát – rozeznáván téměř všemi programy pro práci se strukturami.**

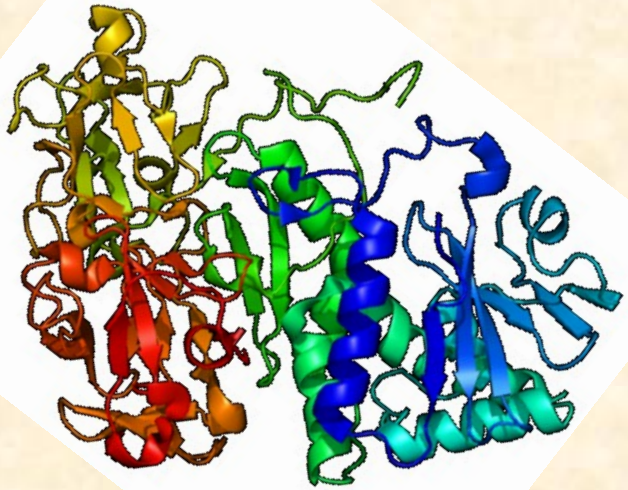
PDB formát

The ATOM records present the atomic coordinates for standard amino acids and nucleotides. They also present the occupancy and temperature factor for each atom. Non-polymer chemical coordinates use the HETATM record type. The element symbol is always present on each ATOM record; charge is optional.

Changes in ATOM/HETATM records result from the standardization atom and residue nomenclature. This nomenclature is described in the Chemical Component Dictionary (ftp://ftp.wwpdb.org/pub/pdb/data/monomers).

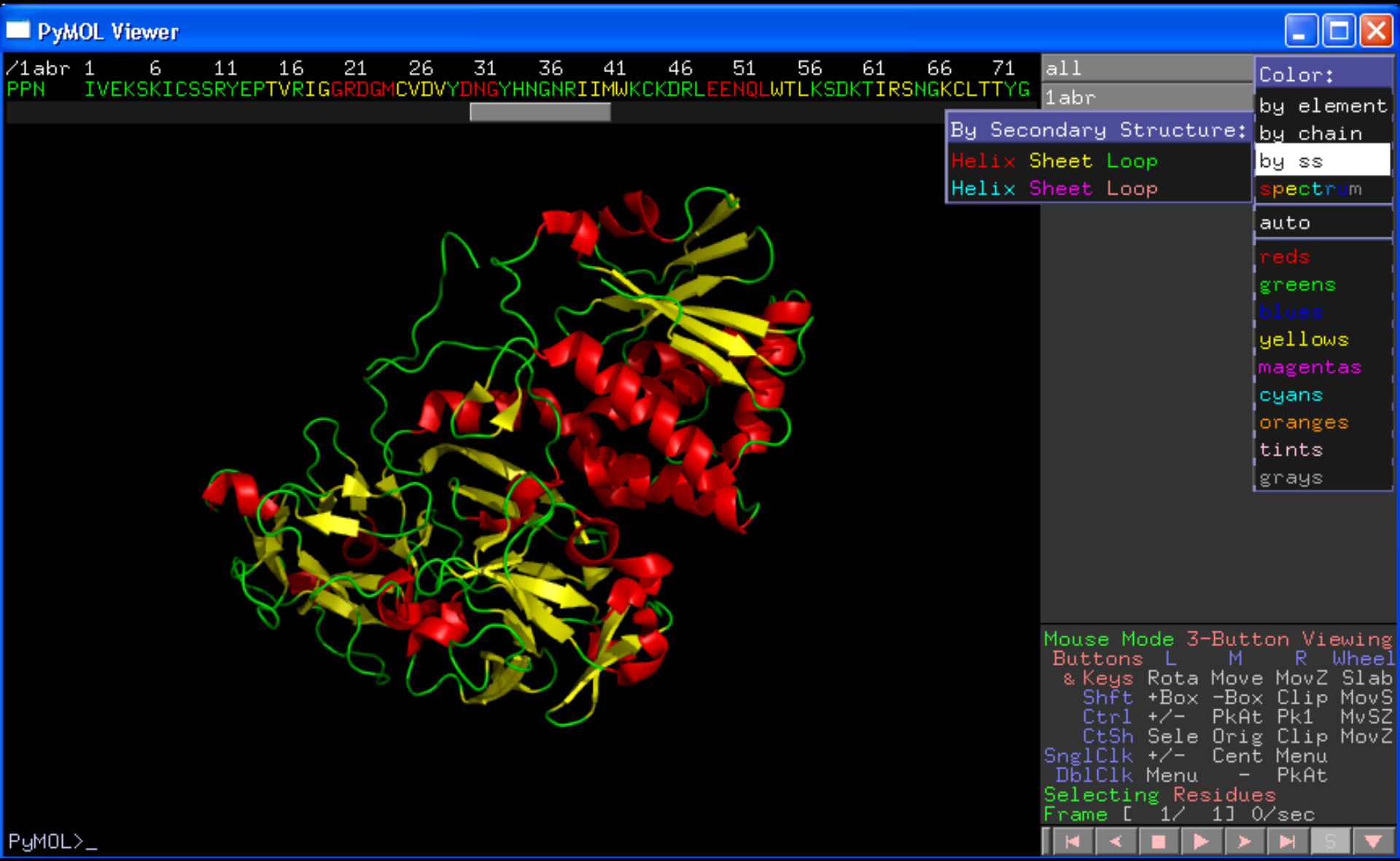
Record Format

COLUMNS	DATA TYPE	FIELD	DEFINITION
1 - 6	Record name	"ATOM "	
7 - 11	Integer	serial	Atom serial number.
13 - 16	Atom	name	Atom name.
17	Character	altLoc	Alternate location indicator.
18 - 20	Residue name	resName	Residue name.
22	Character	chainID	Chain identifier.
23 - 26	Integer	resSeq	Residue sequence number.
27	AChar	iCode	Code for insertion of residues.
31 - 38	Real(8.3)	x	Orthogonal coordinates for X in Angstroms.
39 - 46	Real(8.3)	y	Ortho
47 - 54	Real(8.3)	z	Ortho
55 - 60	Real(6.2)	occupancy	Occup
61 - 66	Real(6.2)	tempFactor	Tempe
77 - 78	LString(2)	element	Eleme
79 - 80	LString(2)	charge	Charg



Abrin

```
ATOM      2  CA  GLU A   1      64.373  11.709  60.583  1.00 79.99           C
ATOM      3  C   GLU A   1      63.512  10.438  60.597  1.00 79.31           C
ATOM      4  O   GLU A   1      63.540   9.685  61.574  1.00 79.23           O
ATOM      5  CB  GLU A   1      63.805  12.754  59.603  1.00 79.36           C
ATOM      6  CG  GLU A   1      62.880  13.819  60.228  1.00 78.52           C
ATOM      7  CD  GLU A   1      61.525  13.275  60.676  1.00 78.50           C
ATOM      8  OE1 GLU A   1      60.915  12.482  59.923  1.00 77.14           O
ATOM      9  OE2 GLU A   1      61.064  13.659  61.776  1.00 77.48           O
ATOM     10  H1  GLU A   1      66.078  10.648  60.914  1.00 20.00           H
ATOM     11  H2  GLU A   1      65.776  10.893  59.265  1.00 20.00           H
ATOM     12  H3  GLU A   1      66.387  12.177  60.222  1.00 20.00           H
```


PyMOL Viewer
/1abr 1 6 11 16 21 26 31 36 41 46 51 56 61 66 71
PPN IVEKSKICSSRYEPTVRIGGRDGMCVDVYDNGYHNGNRIIMWKCKDRLEENQLWTLKSDKTIRSNGKCLTTYG
all
1abr
By Secondary Structure:
Helix Sheet Loop
Helix Sheet Loop
Color:
by element
by chain
by ss
spectrum
auto
reds
greens
blues
yellows
magentas
cyans
oranges
tints
grays
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl +/- PkAt Pk1 MvSZ
CtSh Sele Orig Clip MovZ
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues
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PyMOL>_

A MEMBER OF THE PDB | EMDataBank

An Information Portal to Biological Macromolecular Structures

As of **Tuesday Apr 08, 2014 at 5 PM PDT** there are **99293** Structures | **PDB Statistics**

2014-04-09 : 2293 EMDB map entries, 785 PDB coordinate entries

EMDataBank

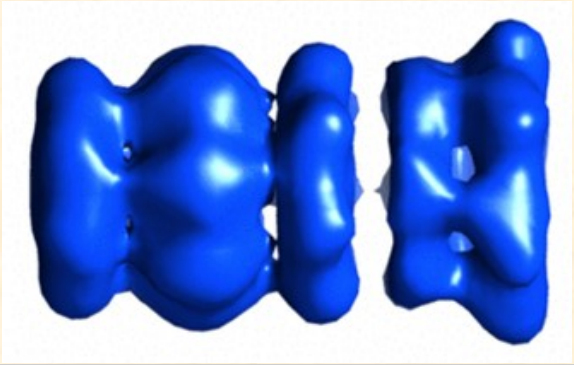
Unified Data Resource for 3DEM

http://emdatabank.org/

One-stop shop for 3DEM deposition and retrieval

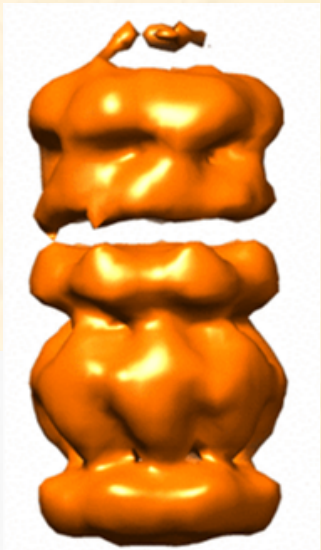
Unified Data Resource for 3-Dimensional Electron Microscopy

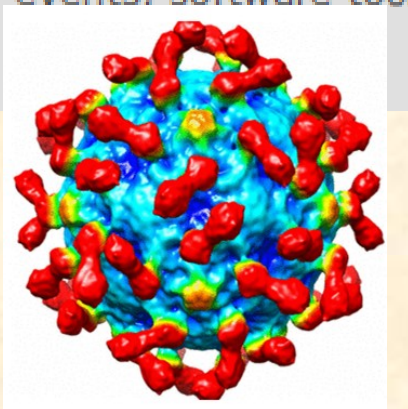
EMDataBank is a unified global portal for deposition and retrieval of 3DEM density maps, atomic models, and associated metadata, as well as a resource for news, events, software tools, data standards, validation methods for the 3DEM community.



March 13, 2014 RELEASED ON April 9, 2014 singleParticle 42.0Å **NEW**

Architecture and assembly of the archaeal Cdc48-20S proteasome





March 19, 2014 RELEASED ON April 9, 2014 singleParticle 9.0Å **NEW**

Kinetic and Structural Analysis of Coxsackievirus B3 Receptor Interactions and Formation of the A-particle

Strukturní databáze NA

Nucleic Acids Research

ABOUT THIS JOURNAL CONTACT THIS JOURNAL SUBSCRIPTIONS CURRENT ISSUE

Oxford Journals › Life Sciences › Nucleic Acids Research › Database Summary Paper

2011 NAR Database Summary Paper

Nucleotide Sequence Databases
RNA sequence databases
Protein sequence databases
Structure Databases
- Small molecules
- Carbohydrates
- Nucleic acid structure
  - 3DNALandscapes
  - Greglist
  - GRSDB
  - ITS2
  - MeRNA
  - NCIR - Non-Canonical Interactions in RNA
  - NDB
  - NNDB
  - non-B DB
  - NTDB
  - QuadBase
  - Rfam
  - RNA FRABASE
  - RNA SSTRAND
  - RNAJunction
  - SARS-CoV RNA SSS
  - SCOR - Structural Classification Of RNA
  - Vir-Mir db

NDB - Nucleic Acid Database

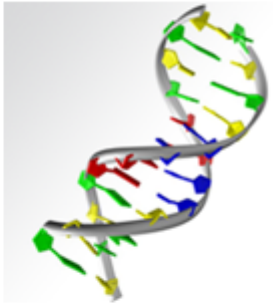
NUCLEIC ACID DATABASE

A Portal for Three-dimensional Structural Information about Nucleic Acids
As of 02-Apr-2014 number of released structures: 7113

Welcome to the NDB

The NDB contains information about experimentally-determined nucleic acids and complex assemblies.
Use the NDB to perform searches based on annotations relating to sequence, structure and function, and to download, analyze, and learn about nucleic acids.

Search Structures



Search DNA
Search DNA and its complexes

Search RNA
Search for RNA structures in the NDB archive or in the Non-Redundant list

Advanced Search
Search for structures based on structural features, chemical features, binding modes, citation and experimental information

Featured Tools

RNA 3D Motif Atlas, a representative collection of RNA 3D internal and hairpin loop motifs

Non-redundant Lists of RNA-containing 3D structures

RNA Base Triple Atlas, a collection of motifs consisting of two RNA basepairs

WebFR3D, a webserver for symbolic and geometric searching of RNA 3D structures

R3D Align, an application for detailed nucleotide to nucleotide alignments of RNA 3D structures

http://ndbserver.rutgers.edu/

NUCLEIC ACID DATABASE

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About NDB | Standards | Education | Tools | Software | Download

- Introduction to Nucleic Acids
- Definition of terms
- NA Highlights from PDB-101
- Paper Models
- Musical Atlas
- Links

INTRODUCTION

DNA can be represented in a variety of ways, which can provide different visual perspectives of molecular structure.

DNA can also be aurally represented when a correspondence is created between the bases and musical notes, as seen in Dr. David Deamer's earlier work DNA Suite (1983).

This Musical Atlas presents an aural representation of the B-DNA molecules without mismatches, drugs, or modifiers that were contained in the NDB as of July 25, 1996.

This atlas follows a newly created pattern. For each structure, there is a "Plain Melody," which follows a simple algorithm to highlight the structure's sequence, and a "Composition," which follows a more complicated algorithm that features the base pairing of the structure.

These algorithms contain rules for determining the meter and rhythm for each piece.

In each case, the notes are assigned to each base as follows:

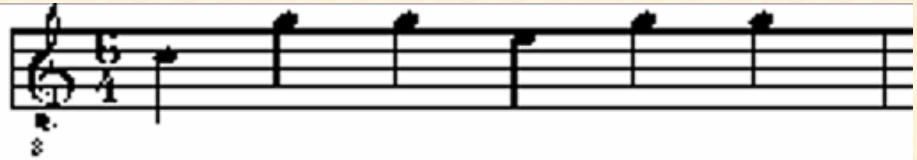
Adenine	A	Cytosine	C
Thymine	E	Guanine	G

These are found within the range a to g^1.

Each base of the asymmetric strand is given one note. The strand is read 5' to 3'.

Thymine was assigned to E so that the four bases would fall into an a minor seventh chord.

The Plain Melody for BDF062, Strand A (C G C T G G)



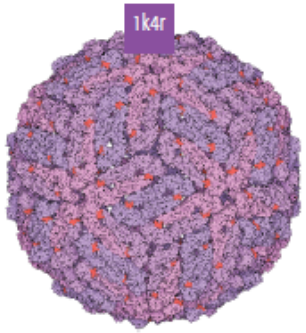
http://ndbserver.rutgers.edu/

DNA

Download this **PDF** to build one complete turn of a DNA double helix, with the major and minor grooves labeled. Choose from a schematic model with space to fill in the names of the bases and a detailed model that shows all the atoms in each nucleotide.

RCSB PDB-101
www.rcsb.org • info@rcsb.org

Build a Paper Model of Dengue Virus



This paper model of PDB entry 1k4r shows the virus magnified by 1,500,000 times. The RNA genome, which contains 10,649 nucleotides, can be modeled using a piece of string approximately 5.4 meters long and placed inside of the structure.

To build the dengue virus, cut out the protein structure below and fold along the dotted lines. Then tape or glue the flaps into place to form an icosahedron.

For more information about dengue virus, see the RCSB PDB's *Molecule of the Month* at dx.doi.org/10.2210/rcsb_pdb/mom_2008_7

To learn about dengue fever, see the National Institute of Allergy and Infectious Diseases' site at www.niaid.nih.gov/topics/denguefever/

Genomové zdroje

Nucleic Acids Research

ABOUT THIS JOURNAL CONTACT THIS JOURNAL SUBSCRIPTIONS CURRENT ISSUE

Oxford Journals › Life Sciences › Nucleic Acids Research › Database Summary Paper Categories

2011 NAR Database Summary Paper Category List

Nucleotide Sequence Databases
RNA sequence databases
Protein sequence databases
Structure Databases
Genomics Databases (non-vertebrate)
MGD - Mouse Genome Database
TIGR Gene Indices
Genome annotation terms, ontologies and nomenclature
Taxonomy and identification
General genomics databases
Viral genome databases
Prokaryotic genome databases
Unicellular eukaryotes genome databases
Fungal genome databases
Invertebrate genome databases

EBI, NCBI – genomové databáze

Vyhledávací systémy

- **Nutnost organizovaného ukládání a skladování dat.**
- **Nutnost prohlížení a analyzování uložených dat.**

Databáze je určitá uspořádaná množina informací (dat) uložená na paměťovém médiu.

V širším smyslu jsou součástí databáze i softwarové prostředky, které umožňují manipulaci s uloženými daty a přístup k nim.

Vyhledávací systémy

- **Textové vyhledávání v databázích NCBI – Entrez**

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

Entrez is the integrated, text-based search and retrieval system used at NCBI for the major databases, including PubMed, Nucleotide and Protein Sequences, Protein Structures, Complete Genomes, Taxonomy, and others.

http://www.ncbi.nlm.nih.gov/books/NBK3837/

Search NCBI databases

dengue virus

Search

Literature

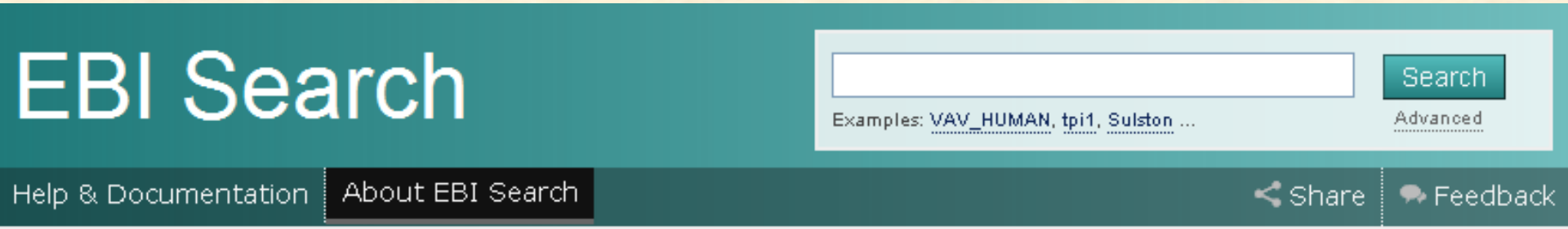
7599	**PubMed**: scientific & medical abstracts/citations	13	**MeSH**: ontology used for PubMed indexing
1041[illegible]5	**PubMed Central**: full-text journal articles	273	**Books**: books and reports
50	**NLM Catalog**: books, journals and more in the NLM Collections	26	**Site Search**: NCBI web and FTP site index

Health

18	**PubMed Health**: clinical effectiveness, disease and drug reports	1	**ClinVar**: human variations of clinical significance
3	**MedGen**: medical genetics literature and links	12	**OMIM**: online mendelian inheritance in man
(none)	GTR: genetic testing registry	(none)	OMIA: online mendelian inheritance in animals
426	**dbGaP**: genotype/phenotype interaction studies		

Organisms

1	**Taxonomy**: taxonomic classification and nomenclature catalog



About EBI Search

The EBI Search engine, also known as EB-eye, is a scalable text search engine that provides easy and uniform access to the biological data resources hosted at the EMBL-EBI.

The data resources represented in the EBI Search engine include: nucleotide and protein sequences at both the genomic and proteomic levels, structures ranging from chemicals to macro-molecular complexes, gene-expression experiments, binary level molecular interactions as well as reaction maps and pathway models, functional classifications, biological ontologies, and comprehensive literature libraries covering the biomedical sciences and related intellectual property.

The EBI Search presents search results that are up-to-date with the data resources and provides an easy inter-domain navigation via a network of cross-references.

http://www.ebi.ac.uk/ebisearch/

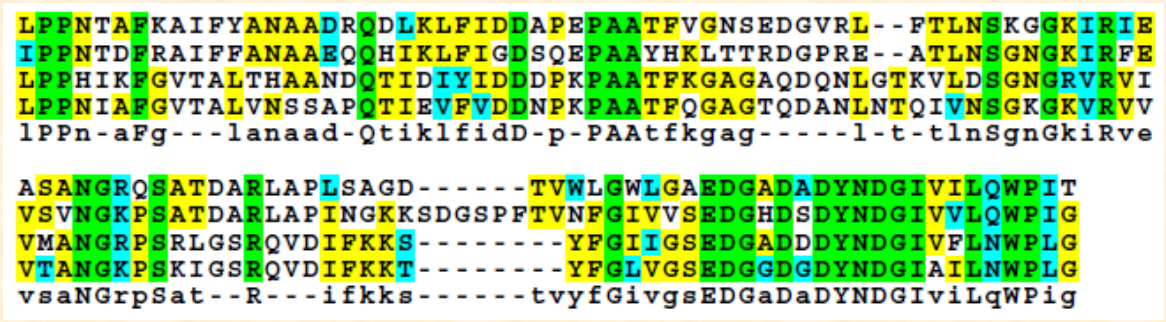
Vyhledávací systémy

- **Vyhledávání podobností sekvencí**

  Textové vyhledávání může selhat (nedostatečná anotace).

  Vyskytuje se shodná nebo podobná sekvence v databázi? (Identifikace možné funkce na základě homologie.)

- **Specializované nástroje (algoritmy) pro „seřazení“ (alignment) sekvencí.**



Shrnutí

- Výrazný nárůst množství biologických dat vede k nutnosti jejich organizovaného skladování a analyzování (databáze).
- Instituce pro správu dat a vývoj nástrojů pro analýzu: EBI/NCBI/CIB
- Základní rozdělení databází: primární/sekundární/strukturní databáze
- Textové vyhledávací systémy/ alignment