



Bioinformatika és genomanalízis az orvostudományban

Biológiai adatbázisok

Cserző Miklós

2020

<https://semmelweis.zoom.us/j/96102872458?pwd=Rk1PL2tqS21sdIUwc3B4eDFCZkNKQT09>

A mai előadás

- Mi az adatbázis
- A biológia kapcsolata az adatbázisokkal
- Az adatbázisok típusai
- Adatbázis formátumok, adatbázisok szerkezete
- Néhány fontos biológiai adatbázis
- Hibák az adatbázisokban

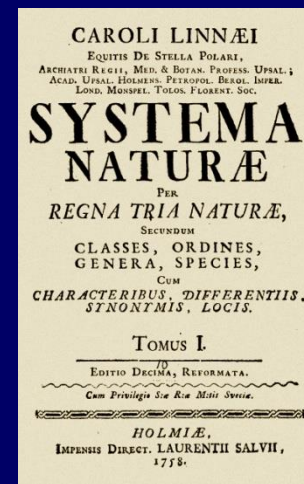
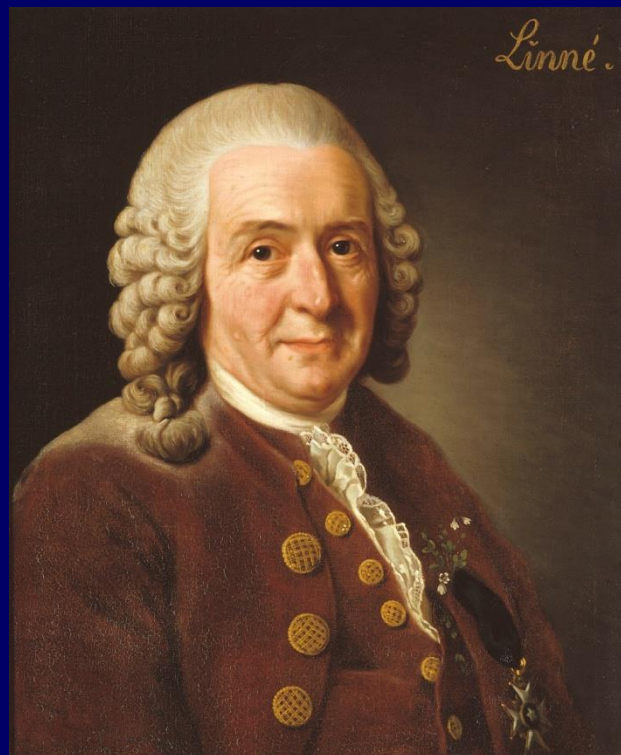
Mi az adatbázis

- Nyers adat – információ
- Adatbázis – struktúrált információ
- A struktúrának köszönhetően
 - Kereshető
 - Rendezhető
 - Szűrhető



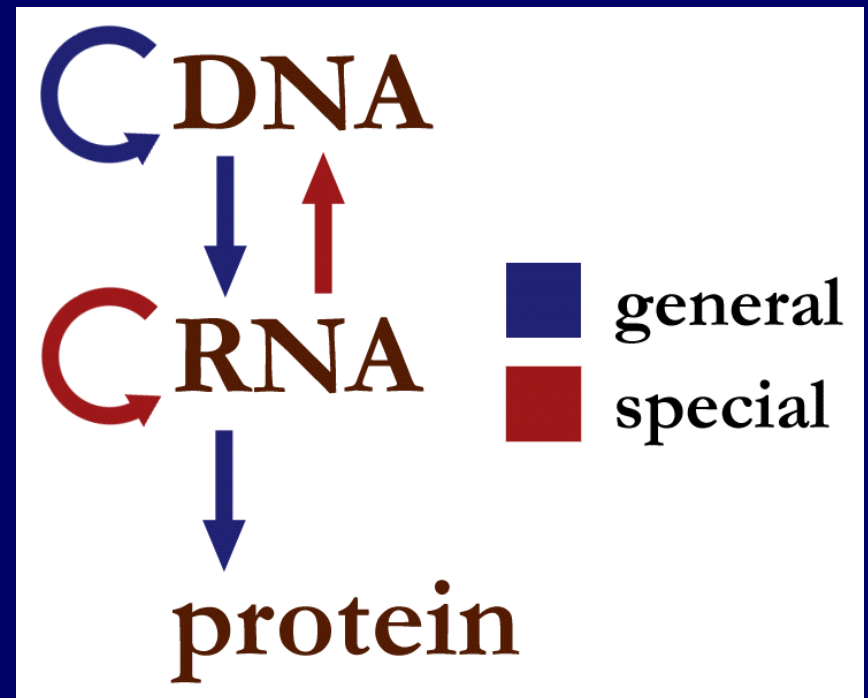
A biológia és az adatbázisok

- A XVIII. század – világutazók kora
- Rengeteg új faj felfedezése, leírása
- Rendszer nélkül áttekinthetetlen az adattömeg
- Carl von Linne rendszertana



A molekuláris biológia központi dogmája

- DNS – az információt a szekvenciájában tárolja
- RNS – az információt közvetíti
- Fehérje – a szekvenciális információ végső megjelenése, az információt használja



Browser tabs: Quick, rescue, How to, SysInf, 4 ways to, G repair, Easy T, Fixing, Free M, Repair, Buy O, VMDK, M How to, Getting sta, JGI X

Address bar: <https://gold.jgi.doe.gov>

Search:

JGI GOLD
GENOMES ONLINE DATABASE

Navigation: Home Search Distribution Graphs Biogeographical Metadata SRA Explorer Statistics GOLD Usage Policy Team Help News

Welcome to the Genomes OnLine Database
GOLD: Genomes Online Database, is a World Wide Web resource for comprehensive access to information regarding genome and metagenome sequencing projects, and their associated metadata, around the world.

GOLD Release v.7

1. Register
Register your project information and Metadata in the Genomes Online Database
[Register](#)

2. Annotate
Annotate your microbial genome or metagenome with IMG
[Annotate](#)

Studies
Metagenomic [1,763](#)
Non-Metagenomic [38,689](#)

Biosamples
[Classification](#)
Ecosystems
Host-associated [44,733](#)
Engineered [5,676](#)
Environmental [31,569](#)

Sequencing Projects
Complete Projects [19,100](#)
Permanent Drafts [193,467](#)
Incomplete Projects [101,418](#)
Targeted Projects [1,060](#)

Analysis Projects
Genome Analysis [155,594](#)
Metagenome Analysis [55,269](#)
Metagenome - Cell Enrichment [1,852](#)
Metagenome - Single Particle Sort [5,107](#)
Metagenome - Assembled Genome (MAG) [11,723](#)
Metatranscriptome Analysis [6,699](#)
Combined Assembly [276](#)
Single Cell - Screened (SAG) [2,367](#)
Single Cell - Unscreened (SAG) [1,930](#)
Transcriptome Analysis [544](#)

Special Projects
Type Strains with Projects [8,801](#)
Type Strains with projects at Genbank [6,929](#)
GEBA Projects [3,360](#)

Projects w. Genbank Data
Seq. Projects [150,426](#)
Archaeal Projects [942](#)
Bacterial Projects [136,674](#)
Eukaryal Projects [4,298](#)

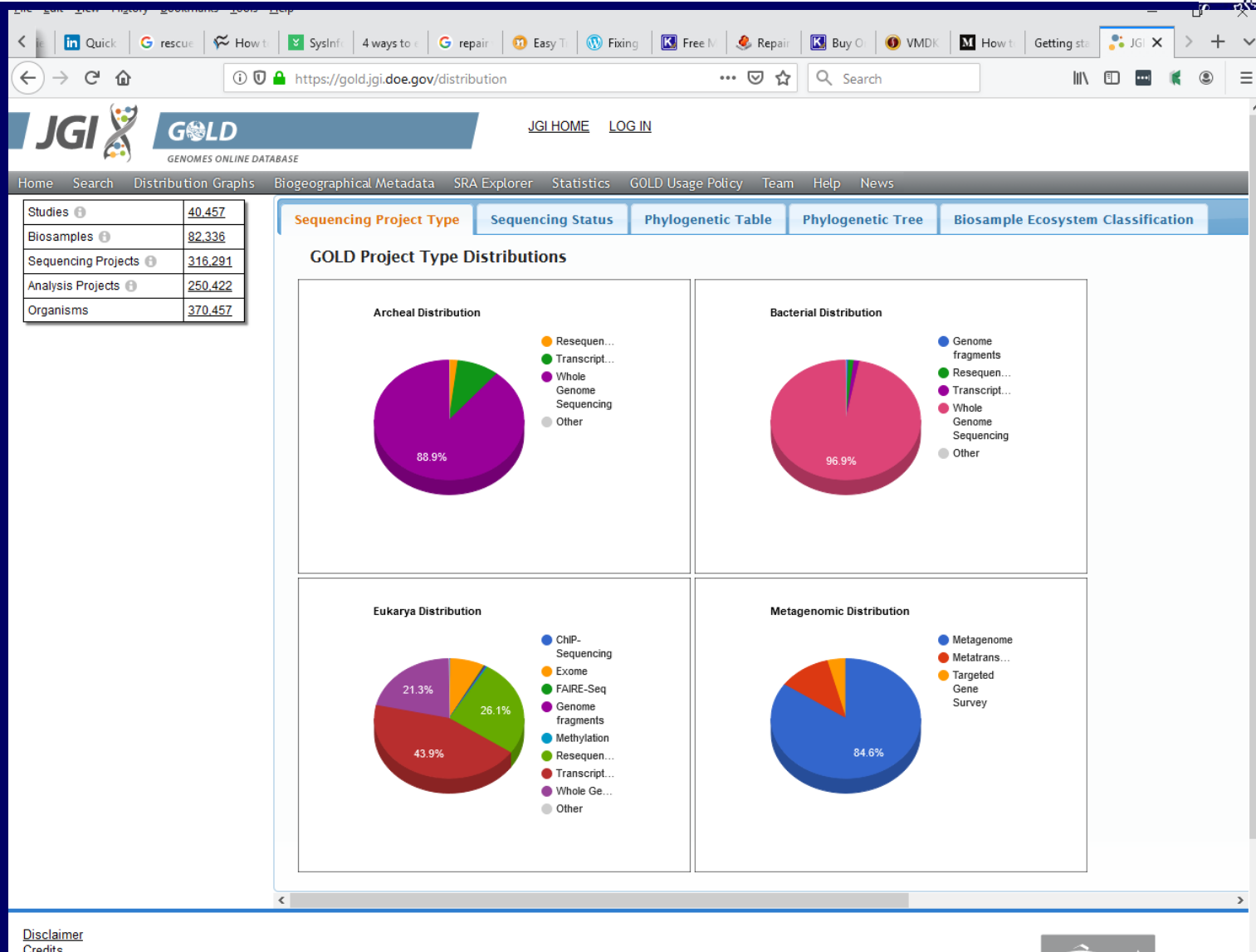
JGI Projects
JGI Studies [1,436](#)
JGI Biosamples [24,761](#)
JGI Sequencing Projects [91,911](#)
JGI Analysis Projects [46,658](#)

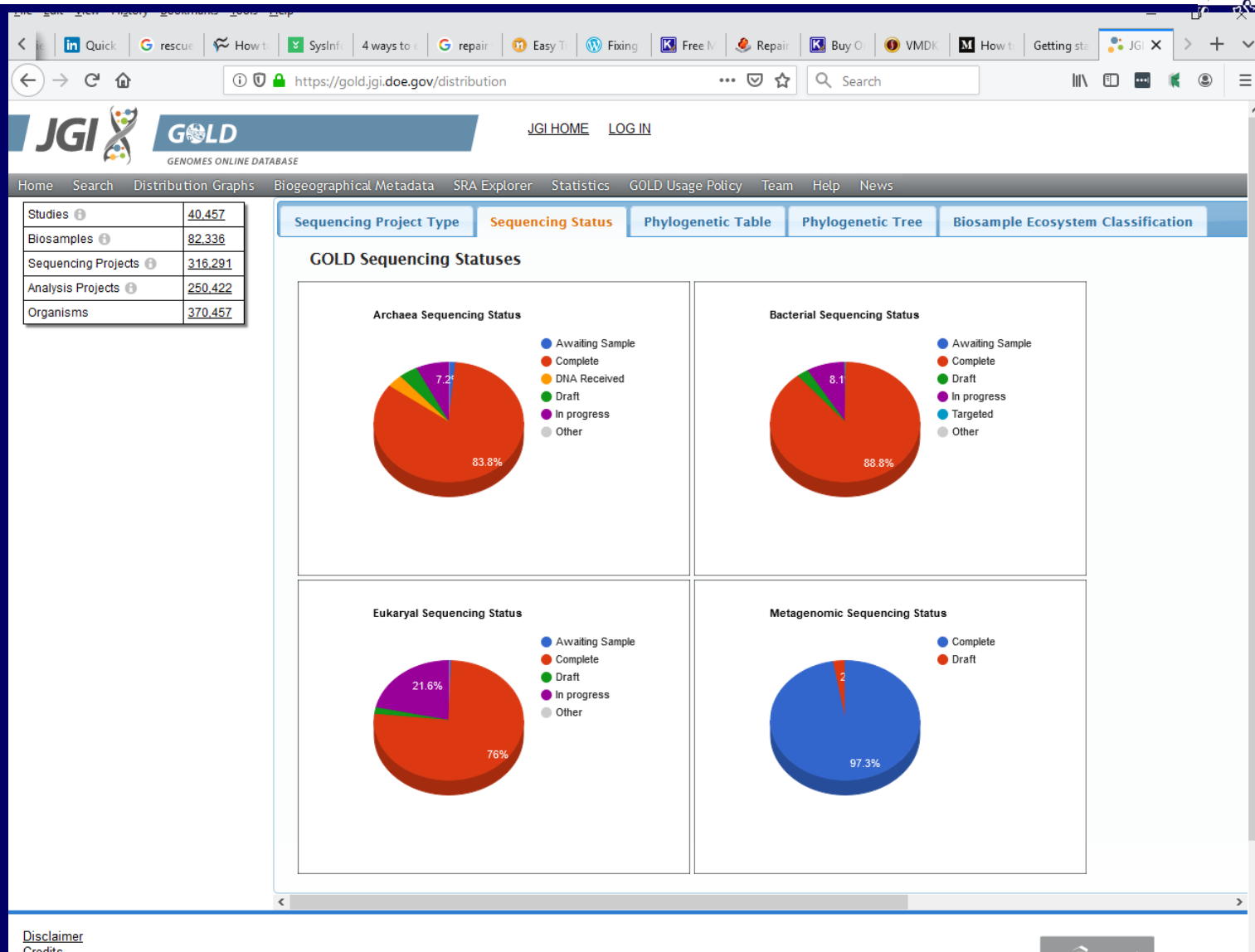
Organisms
Organisms [370,305](#)
Archaea [3,558](#)
Bacteria [326,389](#)
Eukarya [31,105](#)
Viruses [9,253](#)

NCBI Import Tracker

Category	NCBI	GOLD	IMG
Prokaryotes	~100,000	~130,000	~65,000
Viruses	~35,000	~10,000	~8,000
Eukaryotes	~10,000	~5,000	~2,000
Metagenomes	~130,000	~68,000	~5,000
Metatranscriptomes	~15,000	~5,000	~2,000

Excel Data file
File last generated: 23 Sep, 2019





Browser address bar: <https://gold.jgi.doe.gov/distribution>

JGI GOLD GENOMES ONLINE DATABASE

Navigation: Home Search Distribution Graphs Biogeographical Metadata SRA Explorer Statistics GOLD Usage Policy Team Help News

Buttons: JGI HOME LOG IN

Studies	40,457
Biosamples	82,336
Sequencing Projects	316,291
Analysis Projects	250,422
Organisms	370,457

Phylogenetic Table | **Phylogenetic Tree** | Biosample Ecosystem Classification

Bacterial Phyla

- Proteobacteria
- Firmicutes
- Actinobacteria
- Bacteroidetes
- Cyanobacteria
- Spirochaetes
- Tenericutes
- Chlamydiae
- Fusobacteria

Eukarya Phyla

- Streptophyta
- Ascomycota
- Basidiomycota
- Chordata
- Chlorophyta
- Mucoromycota
- Arthropoda
- Apicomplexa
- Chytridiomycota

Bacterial Phylogenetic Data

- Phyla [View Graph](#)
- Classes [View Graph](#)
- Orders [View Graph](#)
- Families [View Graph](#)
- Genera [View Graph](#)

Eukaryote Phylogenetic Data

- Phyla [View Graph](#)
- Classes [View Graph](#)
- Orders [View Graph](#)
- Families [View Graph](#)
- Genera [View Graph](#)

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Accessibility / Section 508 Statement
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BERKELEY LAB

Biológiai adatbázisok fajtái

- Tartalom eredete szerint:
 - Elsődleges – közvetlen, kísérletes adatok
 - Származtatott – az előbbiek feldolgozása
- Elérés szerint:
 - Szabad elérésű – nemzetközi konzorciumok
 - Előfizetési – üzleti alapú
 - Magán – gyógyszergyári, belső használatra
- Integrált adatbázisok
- Irodalmi adatbázis



Adatbázisok elérése

- Internet – első számú forrás
 - Régebben nyomtatásban, mágnes-szalagon és CD-n
- Sok szaklapnak van adatbázis szekciója
- „Nucleic Acid Research” januári száma
- „Database” Oxford University Press
- Az adatbázisokat rendszeresen frissítik
- Új adatbázisokat hoznak létre

Adatbázisok felépítése

- Az adatbázisok bejegyzésekből állnak (record)
- A bejegyzések mezőkre oszlanak (field)
- A mezők sorrendje meghatározott
- A mezők tartalma szintén
- Excell táblázat szerű, vagy sablon, vagy űrlap

Adatbázis formátumok

- „MS Word is **NOT** a database format!!!” – (EBI: FAQ)
- Az adatbázisok tipikusan egyszerű szöveg formátumúak („.txt” MS Word vagy ‘notepad’)
- Közvetlenül is olvashatók, de nem feltétlenül ebben a formában kerülnek felhasználásra
- Sok alkalmazás néhány szabványos formátumban várja a bemenő adatokat

A FASTA formátum

- Bejegyzés=szekvencia
- Első karakter:
 - ‘;’: komment, kerül
 - ‘>’: címsor, utána azonosító
- A többi a szekvencia maga
- 120 karakternél ne legyen hosszabb sor
- ‘*’-gal végződik, vagy a következő címsorral

```
;LCBO - Prolactin precursor - Bovine  
; a sample sequence in FASTA format  
MDSKGSSQKGSRLLLLIVVSNLLLCQGVVSTPVCNPGNPGNCQVSLRDLFDRAVMVSHYIHDLS  
EMFNEFDKRYAQKGFFITMALNSCHTSSLPTPEDKEQAQTHHEVLMSSLILGLLRWNPLHYHL  
VTEVRGMKGAPDAILSRRAIEIEENKRLLEGMEMIFGQVIPGAKETEPYPVWGLPSLQTKDED  
ARYSAFYNLLHCLRRDSSKIDTYLKLNCRIIYNNNC*
```

```
>MCHU - Calmodulin - Human, rabbit, bovine, rat, and chicken  
ADQLTEEQIAEFKEAFSLFDKDGDTITTKELGTVMRSLGQNPTAELODMINEVDADGNGTID  
FPEFLTMMARKMKDIDSEEEIREAFRVFDKDGNGYISAAELRHVMTNLGEKLTDDEEVDDEMIREA  
DIDGDGQVNYEEFVQMMTAK*
```

```
>gi|5524211|gb|AAD44166.1| cytochrome b [Elephas maximus maximus]  
LCLYTHIGRNIYGSYLYSETWNTGIMLLLITMATAFMGYVLPWGQMSFWGATVITNLFSAIPYIGTNLV  
EWIWWGGSVDKATLNRFFAFHFILPFTMVALAGVHLTFLHETGSNNPLGLTSDSDKIPFHPYTIKDFLG  
LLILILLLLLALLSPDMLGDPDNHMPADPLNTPHHPKPEWYFLFAYAILRSVPNKLGGVLALFLSIVIL  
GLMPFLHTSKHRSMMLRPLSQALFWTLTMDLLTLTWIGSQPVEYPYTIIGQMASILYFSIILAFPLIAGX  
IENY
```

A nukleinsav adatbázis

- International Nucleotide Sequence Database Collaboration: ENA, NCBI, DDBJ
- Elsődleges adatbázis, ingyenes
- Közös formátum
- Közös azonosító kódrendszer
- Csak az egyik helyre kell beküldeni – a többi automatikusan szinkronizál
- Honlap: <http://www.ebi.ac.uk/ena/home>

EMBL formátum

Mező azonosító

A mező tartalma:

```
ID   X64011; SV 1; linear; genomic DNA; STD; PRO; 756 BP.
XX
AC   X64011; S78972;
XX
SV   X64011.1
XX
DT   28-APR-1992 (Rel. 31, Created)
DT   30-JUN-1993 (Rel. 36, Last updated, Version 6)
XX
DE   Listeria ivanovii sod gene for superoxide dismutase
XX
KW   sod gene; superoxide dismutase.
XX
OS   Listeria ivanovii
OC   Bacteria; Firmicutes; Bacillus/Clostridium group;
OC   Bacillus/Staphylococcus group; Listeria.
XX
RN   [1]
RX   MEDLINE; 92140371.
RA   Haas A., Goebel W.;
RT   "Cloning of a superoxide dismutase gene from Listeria ivanovii by
RT   functional complementation in Escherichia coli and characterization of the
RT   gene product.";
RL   Mol. Gen. Genet. 231:313-322(1992).
XX
RN   [2]
RP   1-756
RA   Kreft J.;
RT   ;
RL   Submitted (21-APR-1992) to the EMBL/GenBank/DDBJ databases.
RL   J. Kreft, Institut f. Mikrobiologie, Universitaet Wuerzburg, Biozentrum Am
RL   Hubland, 8700 Wuerzburg, FRG
XX
```

Tulajdonságok:

A szekvencia:

Itt a vége:

```

RL   Submitted (21-APR-1992) to the EMBL/GenBank/DDBJ databases.
RL   J. Kreft, Institut f. Mikrobiologie, Universitaet Wuerzburg, Biozentrum Am
RL   Hubland, 8700 Wuerzburg, FRG
XX
FH   Key                      Location/Qualifiers
FH
FT   source                    1..756
FT                               /db_xref="taxon:1638"
FT                               /organism="Listeria ivanovii"
FT                               /strain="ATCC 19119"
FT                               /mol_type="genomic DNA"
FT   RBS                       95..100
FT                               /gene="sod"
FT   terminator                723..746
FT                               /gene="sod"
FT   CDS                       109..717
FT                               /transl_table=11
FT                               /gene="sod"
FT                               /EC_number="1.15.1.1"
FT                               /db_xref="GOA:P28763"
FT                               /db_xref="HSSP:P00448"
FT                               /db_xref="InterPro:IPR001189"
FT                               /db_xref="UniProtKB/Swiss-Prot:P28763"
FT                               /product="superoxide dismutase"
FT                               /protein_id="CAA45406.1"
FT                               /translation="MTYELPKLPYTYDALEPNFDKETMEIHYTKHHNIYVTKLNEAVSG
FT                               HAELASKPGEELVANLDSVPPEIRGAVRNHGGGHANHTLFWSSLSPNGGGAPTGNLKAA
FT                               IESEFGTDFEKFNFNAAAAARFGSGWAWLVVNNGKLEIVSTANQDSPLSEGKTPVLGL
FT                               DVWEHAYYLKFFQNRPEYIDTFWNVINWDERNKRFDAAK"
XX
SQ   Sequence 756 BP; 247 A; 136 C; 151 G; 222 T; 0 other;
      cgttatttaa ggtgttatcat agttctatgg aaataggggc tatacctttc gccttacaat   60
      gtaatttctt .....
      //
  
```

GeneBank formátum

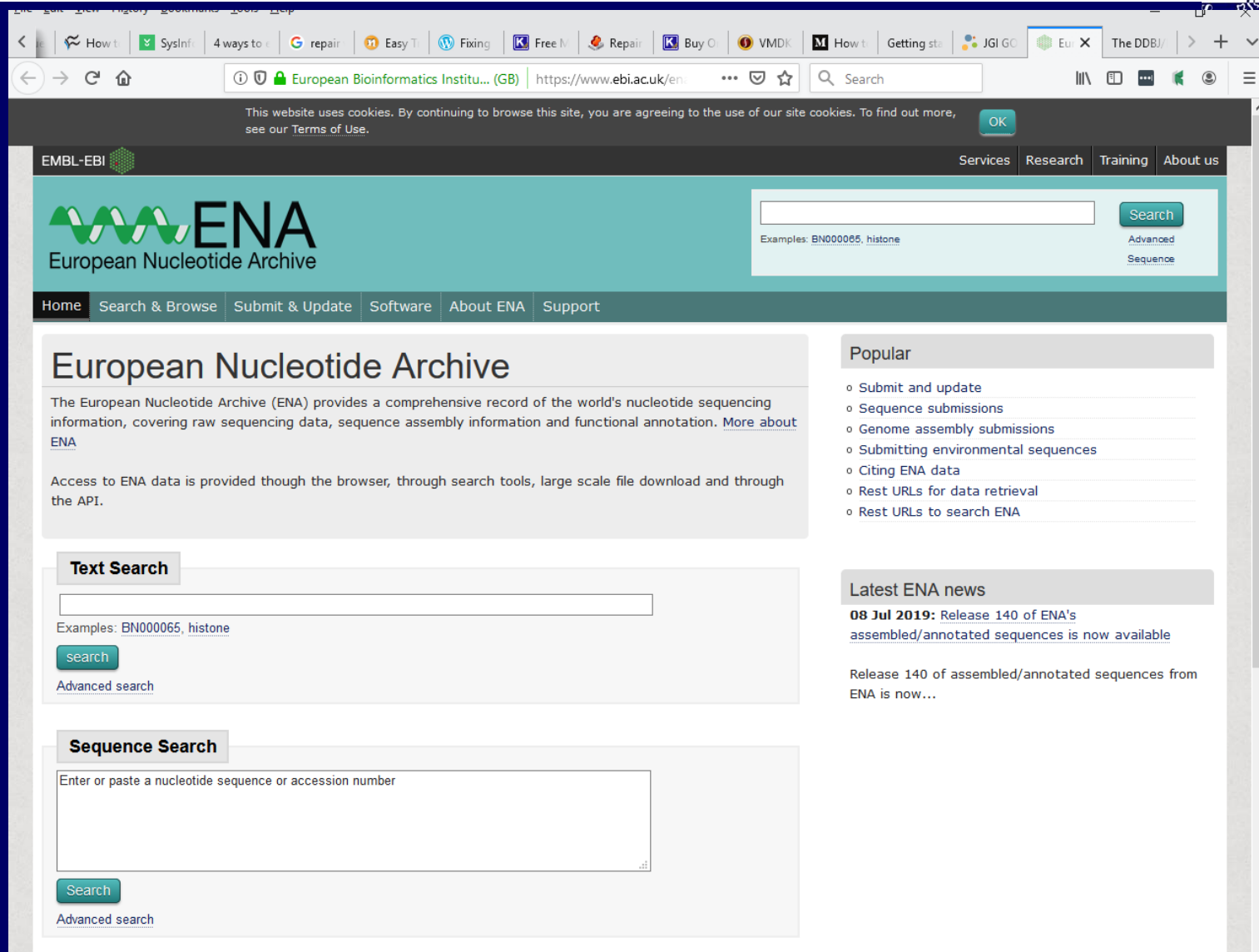
```

LOCUS       LISOD                               756 bp    DNA     linear   BCT 30-JUN-1993
DEFINITION  Listeria ivanovii sod gene for superoxide dismutase.
ACCESSION   X64011 S78972
VERSION     X64011.1   GI:44010
KEYWORDS    sod gene; superoxide dismutase.
SOURCE      Listeria ivanovii
  ORGANISM  Listeria ivanovii
            Bacteria; Firmicutes; Bacillales; Listeriaceae; Listeria.
REFERENCE   1  (bases 1 to 756)
  AUTHORS   Haas,A. and Goebel,W.
  TITLE     Cloning of a superoxide dismutase gene from Listeria ivanovii by
            functional complementation in Escherichia coli and characterization
            of the gene product
  JOURNAL   Mol. Gen. Genet. 231 (2), 313-322 (1992)
  MEDLINE   92140371
REFERENCE   2  (bases 1 to 756)
  AUTHORS   Kreft,J.
  TITLE     Direct Submission
  JOURNAL   Submitted (21-APR-1992) J. Kreft, Institut f. Mikrobiologie,
            Universitaet Wuerzburg, Biozentrum Am Hubland, 8700 Wuerzburg, FRG

FEATURES             Location/Qualifiers
     source             1..756
                        /organism="Listeria ivanovii"
                        /strain="ATCC 19119"
                        /db_xref="taxon:1638"
                        /mol_type="genomic DNA"
     RBS                 95..100
                        /gene="sod"
     gene                95..746
                        /gene="sod"
     CDS                 109..717
                        /gene="sod"
                        /EC_number="1.15.1.1"
                        /codon_start=1
                        /transl_table=11
                        /product="superoxide dismutase"
    
```

Kicsit más formátum
Könnyű átalakítani
A teljes leírás:

http://www.insdc.org/documents/feature_table.html



The screenshot shows the European Nucleotide Archive (ENA) website. The browser address bar displays the URL <https://www.ebi.ac.uk/ena/>. The website header includes the EMBL-EBI logo and navigation links for Services, Research, Training, and About us. The main banner features the ENA logo and a search bar with a search button. Below the banner, there is a navigation menu with links for Home, Search & Browse, Submit & Update, Software, About ENA, and Support.

The main content area is titled "European Nucleotide Archive" and provides a comprehensive record of the world's nucleotide sequencing information, covering raw sequencing data, sequence assembly information, and functional annotation. It includes a link to "More about ENA".

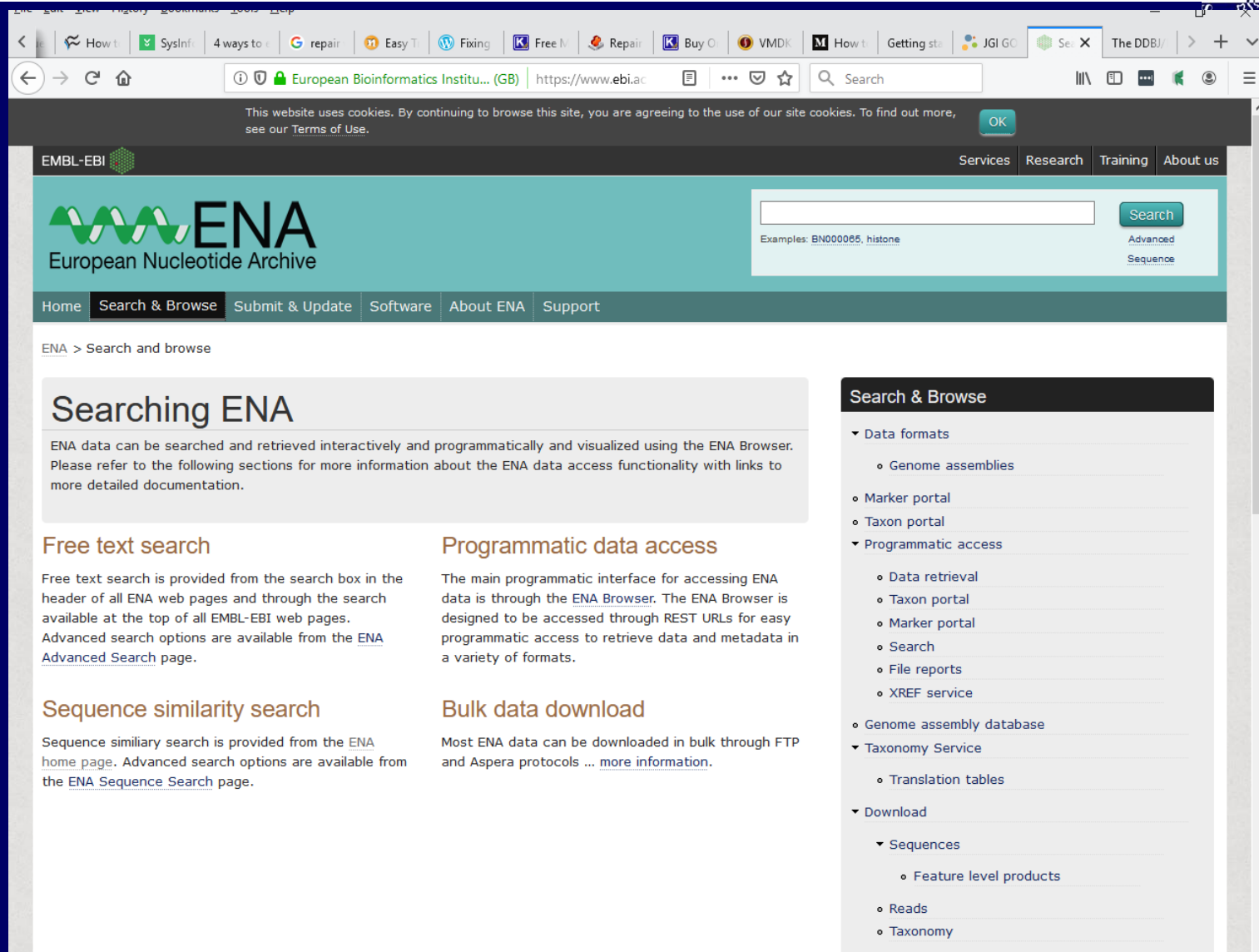
Access to ENA data is provided through the browser, through search tools, large scale file download, and through the API.

The "Text Search" section includes a search input field, a search button, and a link to "Advanced search". Examples provided are "BN000065, histone".

The "Sequence Search" section includes a search input field, a search button, and a link to "Advanced search". The input field contains the text "Enter or paste a nucleotide sequence or accession number".

The "Popular" section lists several links: Submit and update, Sequence submissions, Genome assembly submissions, Submitting environmental sequences, Citing ENA data, Rest URLs for data retrieval, and Rest URLs to search ENA.

The "Latest ENA news" section features a headline: "08 Jul 2019: Release 140 of ENA's assembled/annotated sequences is now available". Below the headline, it states: "Release 140 of assembled/annotated sequences from ENA is now..."



EMBL-EBI

Services Research Training About us

ENA
European Nucleotide Archive

Home Search & Browse Submit & Update Software About ENA Support

ENA > Search and browse

Searching ENA

ENA data can be searched and retrieved interactively and programmatically and visualized using the ENA Browser. Please refer to the following sections for more information about the ENA data access functionality with links to more detailed documentation.

Free text search

Free text search is provided from the search box in the header of all ENA web pages and through the search available at the top of all EMBL-EBI web pages. Advanced search options are available from the [ENA Advanced Search](#) page.

Sequence similarity search

Sequence similarity search is provided from the [ENA](#) home page. Advanced search options are available from the [ENA Sequence Search](#) page.

Programmatic data access

The main programmatic interface for accessing ENA data is through the [ENA Browser](#). The ENA Browser is designed to be accessed through REST URLs for easy programmatic access to retrieve data and metadata in a variety of formats.

Bulk data download

Most ENA data can be downloaded in bulk through FTP and Aspera protocols ... [more information](#).

Search & Browse

- ▼ Data formats
 - Genome assemblies
- Marker portal
- Taxon portal
- ▼ Programmatic access
 - Data retrieval
 - Taxon portal
 - Marker portal
 - Search
 - File reports
 - XREF service
- Genome assembly database
- ▼ Taxonomy Service
 - Translation tables
- ▼ Download
 - ▼ Sequences
 - Feature level products
 - Reads
 - Taxonomy

EMBL-EBI

Search results for **x64011**

Sequence (Release) (1)

Coding (Release) (1)

Sequence (Release) (1 results found)

X64011 Listeria ivanovii sod gene for superoxide dismutase
View all 1 results

Coding (Release) (1 results found)

CAA45406 Listeria ivanovii superoxide dismutase
View all 1 results

Powered by [EBI Search](#)

EMBL-EBI

News
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Intranet

Services
By topic
By name (A-Z)
Help & Support

Research
Overview
Publications
Research groups
Postdocs & PhDs

Training
Overview
Train at EBI
Train outside EBI
Train online
Contact organisers

Industry
Overview
Members Area
Workshops
SME Forum
Contact Industry programme

About us
Overview
Leadership
Funding
Background
Collaboration
Jobs
People & groups

Sequence: X64011.1

Listeria ivanovii sod gene for superoxide dismutase

View: [TEXT](#) [FASTA](#) [XML](#) Download: [XML](#) [FASTA](#) [TEXT](#)

Organism Listeria ivanovii	Molecule type genomic DNA	Topology linear	Data class STD	Taxonomic Division PRO
Sequence length 756	Sequence Version 1	First public 28-APR-1992	Last updated 26-SEP-2006	Show Version History X64011

Keywords
sod gene, superoxide dismutase.

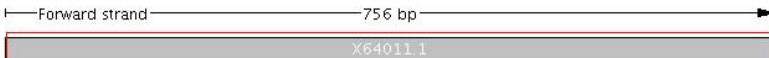
Secondary accession(s)
S78972.

Lineage
[Bacteria](#), [Firmicutes](#), [Bacilli](#), [Bacillales](#), [Listeriaceae](#), [Listeria](#)

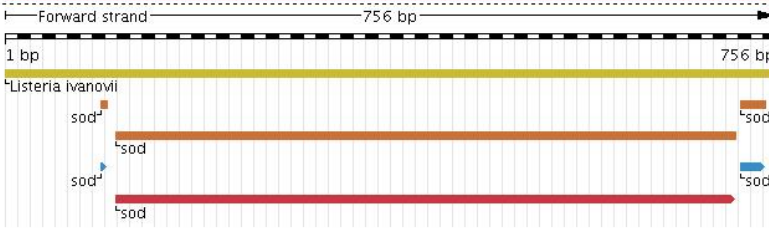
Navigation Overview **Source Feature(s)** Sequence Publications Submission Details Other Feature(s)

Base range: 1 - 756 Apply

Overview



Features



Source: Listeria ivanovii

Genes: sod⁺

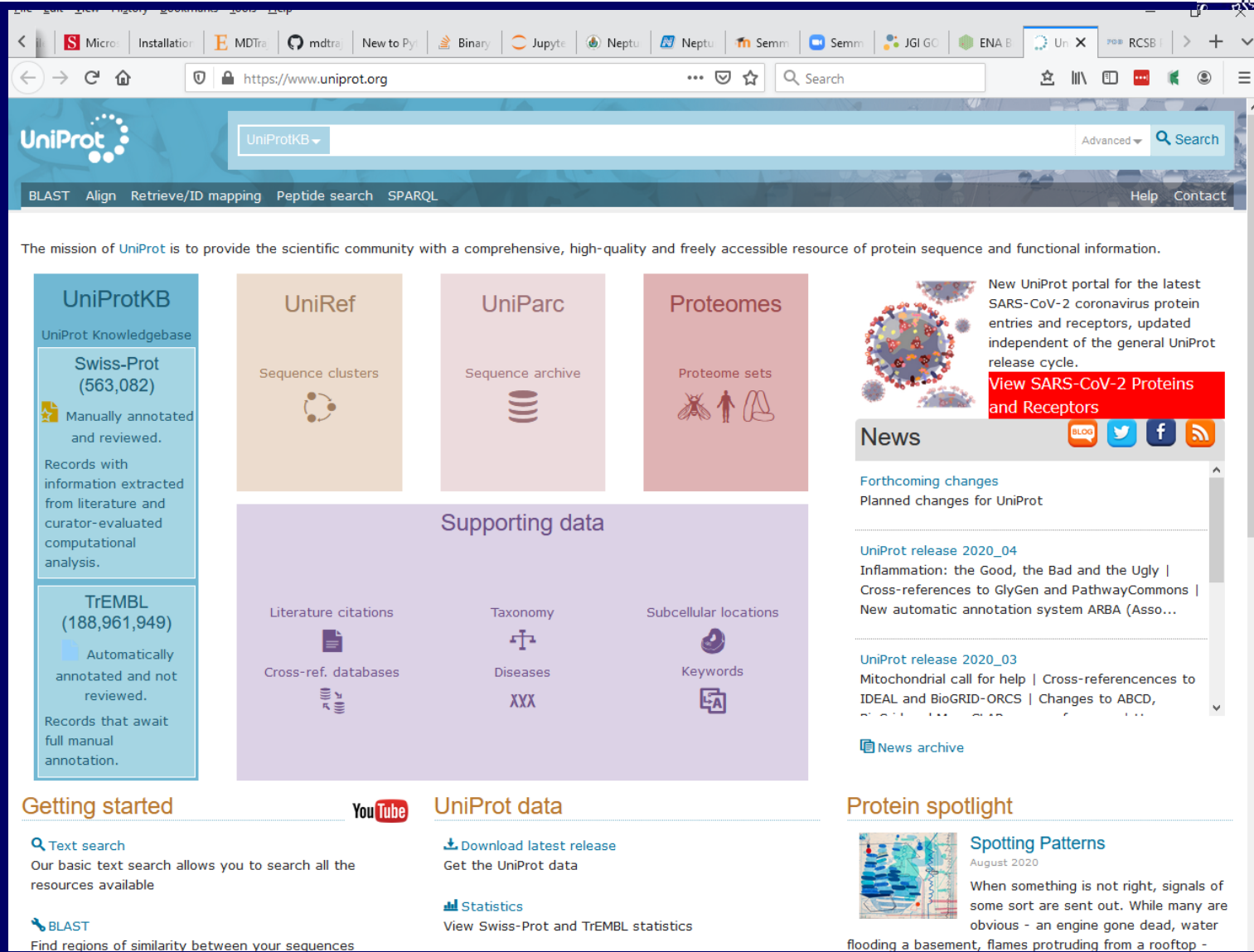
regulatory: sod⁺

CDS: sod

UniProt adatbázis

- Konzorcium üzemelteti:
- A fehérjékkel kapcsolatos információk fő forrása
- Az adatbázis nem homogén:
 - SwissProt: egyedileg annotált és ellenőrzött
 - TrEMBL: automatikusan annotált adatok
- Ingyenesen elérhető:
<http://www.uniprot.org/>





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

UniProtKB

UniProt Knowledgebase

Swiss-Prot
(563,082)

Manually annotated and reviewed.

Records with information extracted from literature and curator-evaluated computational analysis.

TrEMBL
(188,961,949)

Automatically annotated and not reviewed.

Records that await full manual annotation.

UniRef

Sequence clusters

UniParc

Sequence archive

Proteomes

Proteome sets

Supporting data

Literature citations

Cross-ref. databases

Taxonomy

Diseases

Subcellular locations

Keywords

News

View SARS-CoV-2 Proteins and Receptors

Forthcoming changes
Planned changes for UniProt

UniProt release 2020_04
Inflammation: the Good, the Bad and the Ugly | Cross-references to GlyGen and PathwayCommons | New automatic annotation system ARBA (Asso...

UniProt release 2020_03
Mitochondrial call for help | Cross-references to IDEAL and BioGRID-ORCS | Changes to ABCD, ...

[News archive](#)

Getting started

[Text search](#)
Our basic text search allows you to search all the resources available

[BLAST](#)
Find regions of similarity between your sequences

UniProt data

[Download latest release](#)
Get the UniProt data

[Statistics](#)
View Swiss-Prot and TrEMBL statistics

Protein spotlight

Spotting Patterns
August 2020

When something is not right, signals of some sort are sent out. While many are obvious - an engine gone dead, water flooding a basement, flames protruding from a rooftop -

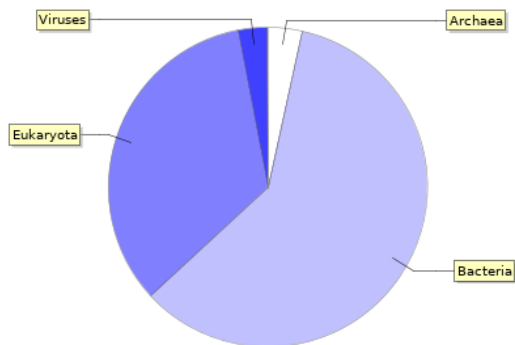
A legfrissebb változat adatai

	Number of entries
New entries	289
Updated entries	187,296
Unchanged entries	373,238
Total	560,823
Entries with updated sequences	29
With a fragmented AA sequence	9,175
With known alternative products	25,328

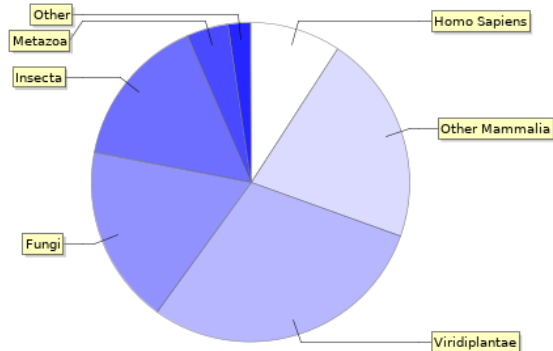
	Number of entries
New entries	4,227,499
Updated entries	20,902,200
Unchanged entries	146,371,789
Total	171,501,488
Entries with updated sequences	18,613
With a fragmented AA sequence	16,359,479
With known alternative products	0

A fehérjék megoszlása:

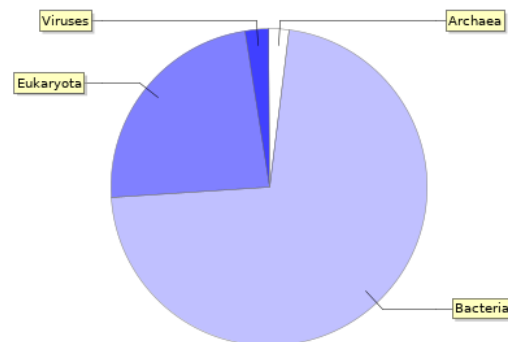
Swiss-Prot entries per taxonomic group



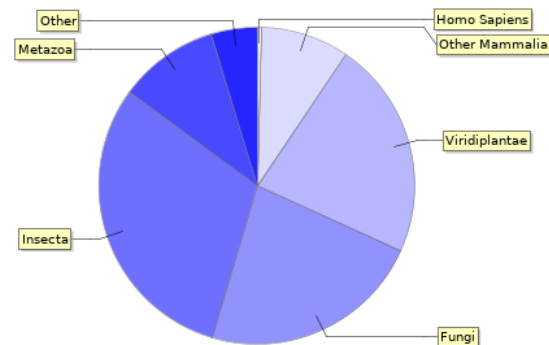
Swiss-Prot entries in Eukaryota



TrEMBL entries per taxonomic group



TrEMBL entries in Eukaryota



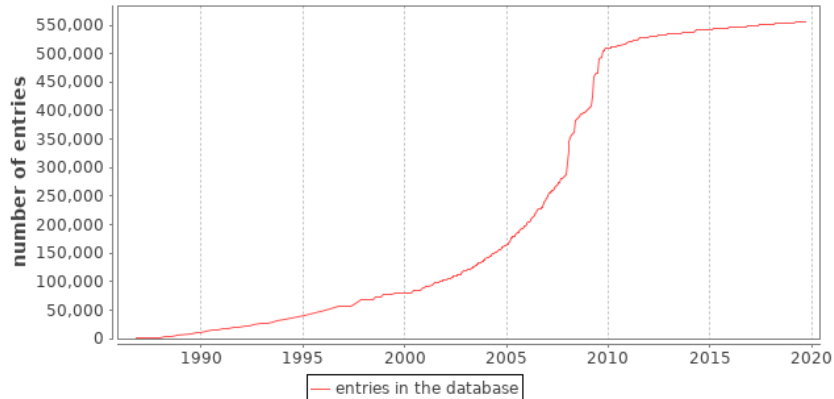


Mennyire biztos?

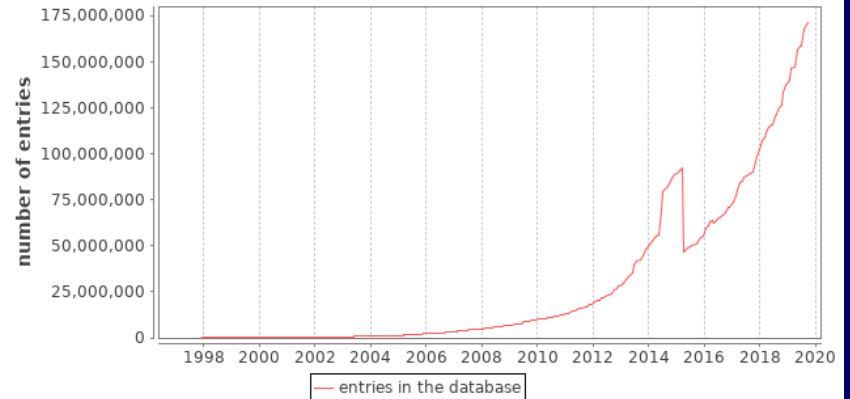
Evidence:	Swiss-Prot	TrEMBL
protein level	17.7%	0.12%
transcript level	10.3%	0.93%
from homology	69.2%	24.60%
predicted	2.4%	74.35%
uncertain	0.3%	0%

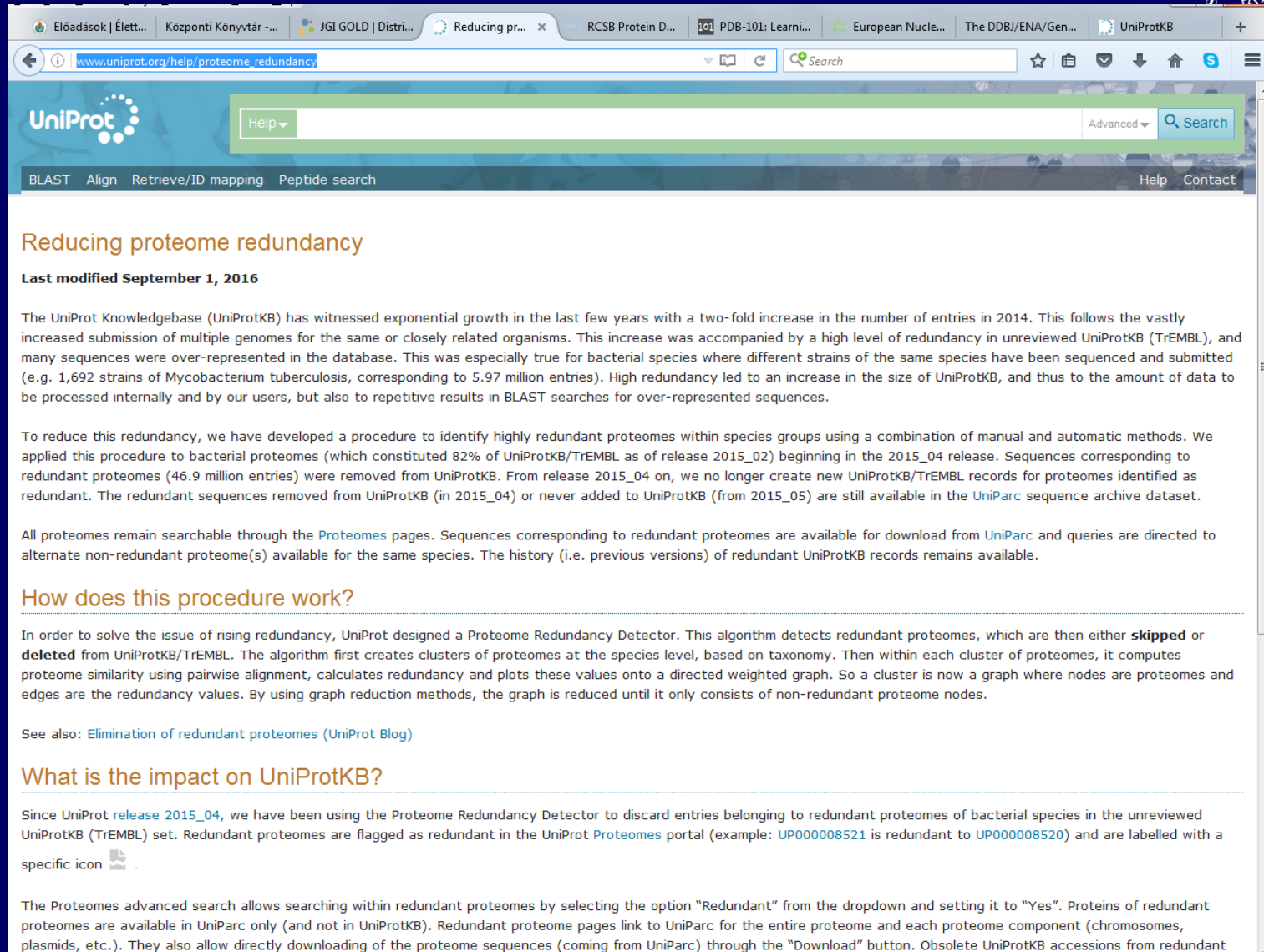
Az adatbázis gyarapodása

Number of entries in UniProtKB/Swiss-Prot over time



Number of entries in UniProtKB/TrEMBL over time





Reducing proteome redundancy

Last modified September 1, 2016

The UniProt Knowledgebase (UniProtKB) has witnessed exponential growth in the last few years with a two-fold increase in the number of entries in 2014. This follows the vastly increased submission of multiple genomes for the same or closely related organisms. This increase was accompanied by a high level of redundancy in unreviewed UniProtKB (TrEMBL), and many sequences were over-represented in the database. This was especially true for bacterial species where different strains of the same species have been sequenced and submitted (e.g. 1,692 strains of *Mycobacterium tuberculosis*, corresponding to 5.97 million entries). High redundancy led to an increase in the size of UniProtKB, and thus to the amount of data to be processed internally and by our users, but also to repetitive results in BLAST searches for over-represented sequences.

To reduce this redundancy, we have developed a procedure to identify highly redundant proteomes within species groups using a combination of manual and automatic methods. We applied this procedure to bacterial proteomes (which constituted 82% of UniProtKB/TrEMBL as of release 2015_02) beginning in the 2015_04 release. Sequences corresponding to redundant proteomes (46.9 million entries) were removed from UniProtKB. From release 2015_04 on, we no longer create new UniProtKB/TrEMBL records for proteomes identified as redundant. The redundant sequences removed from UniProtKB (in 2015_04) or never added to UniProtKB (from 2015_05) are still available in the [UniParc](#) sequence archive dataset.

All proteomes remain searchable through the [Proteomes](#) pages. Sequences corresponding to redundant proteomes are available for download from [UniParc](#) and queries are directed to alternate non-redundant proteome(s) available for the same species. The history (i.e. previous versions) of redundant UniProtKB records remains available.

How does this procedure work?

In order to solve the issue of rising redundancy, UniProt designed a Proteome Redundancy Detector. This algorithm detects redundant proteomes, which are then either **skipped** or **deleted** from UniProtKB/TrEMBL. The algorithm first creates clusters of proteomes at the species level, based on taxonomy. Then within each cluster of proteomes, it computes proteome similarity using pairwise alignment, calculates redundancy and plots these values onto a directed weighted graph. So a cluster is now a graph where nodes are proteomes and edges are the redundancy values. By using graph reduction methods, the graph is reduced until it only consists of non-redundant proteome nodes.

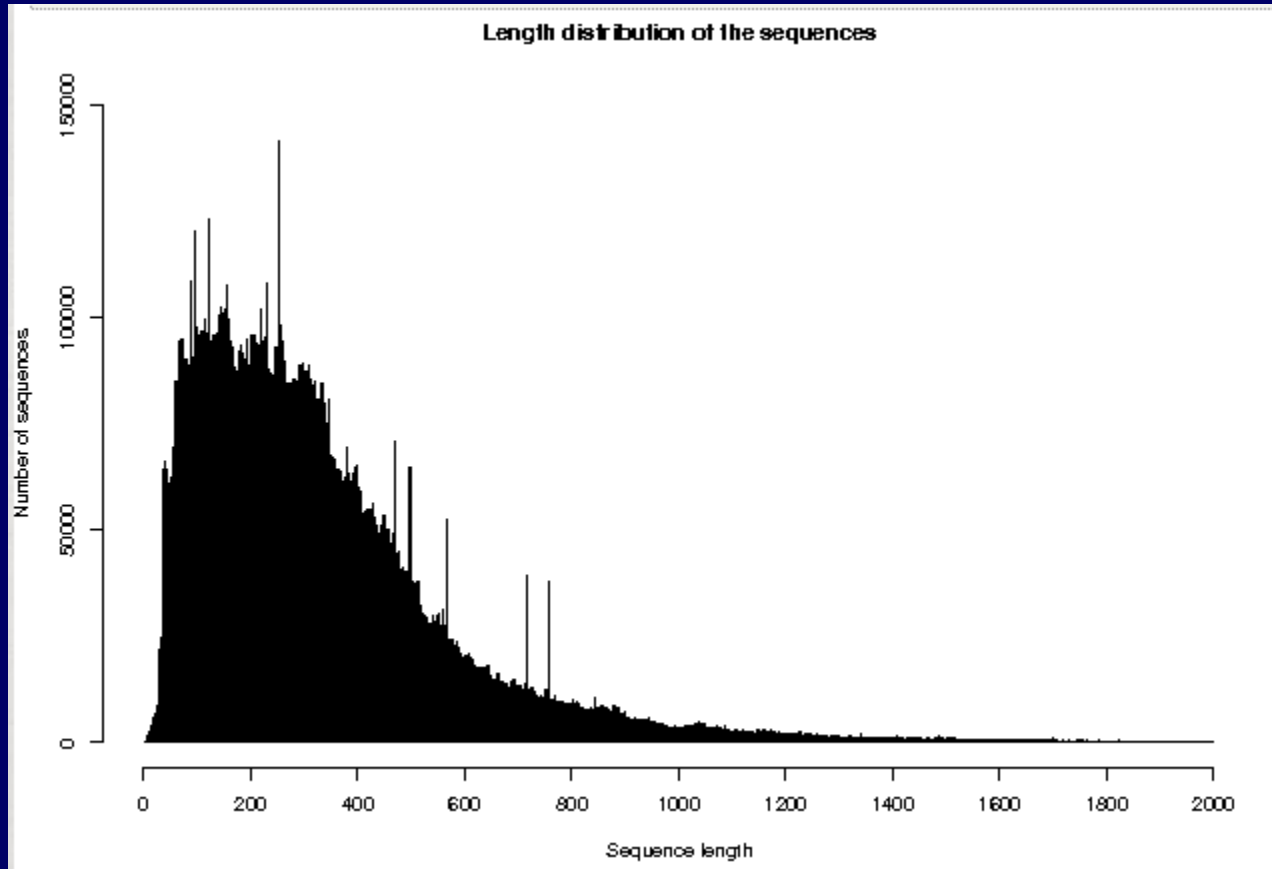
See also: [Elimination of redundant proteomes \(UniProt Blog\)](#)

What is the impact on UniProtKB?

Since UniProt [release 2015_04](#), we have been using the Proteome Redundancy Detector to discard entries belonging to redundant proteomes of bacterial species in the unreviewed UniProtKB (TrEMBL) set. Redundant proteomes are flagged as redundant in the UniProt [Proteomes](#) portal (example: [UP000008521](#) is redundant to [UP000008520](#)) and are labelled with a specific icon .

The Proteomes advanced search allows searching within redundant proteomes by selecting the option "Redundant" from the dropdown and setting it to "Yes". Proteins of redundant proteomes are available in UniParc only (and not in UniProtKB). Redundant proteome pages link to UniParc for the entire proteome and each proteome component (chromosomes, plasmids, etc.). They also allow directly downloading of the proteome sequences (coming from UniParc) through the "Download" button. Obsolete UniProtKB accessions from redundant

A fehérjék hosszának eloszlása:



Az adsatbázis formátuma:

```
ID SHH_HUMAN Reviewed: 462 AA.
AC Q15465; A4D247; Q75MC9;
DT 15-JUL-1999, integrated into UniProtKB/Swiss-Prot.
DT 01-NOV-1996, sequence version 1.
DT 27-JUL-2011, entry version 137.
DE RecName: Full=Sonic hedgehog protein;
DE Short=SHH;
DE AltName: Full=HHG-1;
DE Contains:
DE RecName: Full=Sonic hedgehog protein N-product;
DE Contains:
DE RecName: Full=Sonic hedgehog protein C-product;
DE Flags: Precursor;
GN Name=SHH;
OS Homo sapiens (Human).
OC Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi;
OC Mammalia; Eutheria; Euarchontoglires; Primates; Haplorrhini;
OC Catarrhini; Hominidae; Homo.
OX NCBI_TaxID=9606;
RN [1]
RP NUCLEOTIDE SEQUENCE [MRNA].
RC TISSUE=Fetal lung;
RX MEDLINE=96070431; PubMed=7590746; DOI=10.1006/geno.1995.1104;
RA Marigo V., Roberts D.J., Lee S.M.K., Tsukurov O., Levi T.,
RA Gastier J.M., Epstein D.J., Gilbert D.J., Copeland N.G., Seidman C.E.,
RA Jenkins N.A., Seidman J.G., McMahon A.P., Tabin C.;
RT "Cloning, expression, and chromosomal location of SHH and IHH: two
RT human homologues of the Drosophila segment polarity gene hedgehog.";
RL Genomics 28:44-51(1995).
RN [2]
RP NUCLEOTIDE SEQUENCE [GENOMIC DNA].
RA Tate G., Kishimoto K., Mitsuya T.;
RT "Expression of Sonic hedgehog and its receptor Patched/Smoothed in
RT human cancer cell lines and embryonic organs.";
RL J. Biochem. Mol. Biol. Biophys. 4:27-34(2000).
RN [3]
RP NUCLEOTIDE SEQUENCE [GENOMIC DNA].
RG NIEHS SNPs program;
RL Submitted (SEP-2003) to the EMBL/GenBank/DDBJ databases.
RN [4]
RP NUCLEOTIDE SEQUENCE [LARGE SCALE GENOMIC DNA].
RX MEDLINE=22737999; PubMed=12853948; DOI=10.1038/nature01782;
RA Hillier L.W., Fulton R.S., Fulton L.A., Graves T.A., Pepin K.H.,
RA Wagner-McPherson C., Layman D., Maas J., Jaeger S., Walker R.,
RA Wylie K., Sekhon M., Becker M.C., O'Laughlin M.D., Schaller M.E.,
RA Fewell G.A., Delehaanty K.D., Miner T.L., Nash W.E., Cordes M., Du H.,
RA Sun H., Edwards J., Bradshaw-Cordum H., Ali J., Andrews S., Isak A.,
RA Vanbrunt A., Nguyen C., Du F., Lamar B., Courtney L., Kalicki J.,
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FT /FTId=VAR_062643.
FT VARIANT 404 408 Missing (in HPE3; familial).
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FT VARIANT 405 409 Missing (in HPE3; uncertain
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FT /FTId=VAR_062645.
FT VARIANT 416 416 T -> A (in HPE3; uncertain
FT pathogenicity).
FT /FTId=VAR_062646.
FT VARIANT 424 424 P -> A (in HPE3; familial).
FT /FTId=VAR_009176.
FT VARIANT 435 435 Y -> N (in HPE3).
FT /FTId=VAR_062647.
FT VARIANT 436 436 S -> L (in HPE3; sporadic).
FT /FTId=VAR_009177.
FT VARIANT 456 456 G -> R (in HPE3; uncertain
FT pathogenicity).
FT /FTId=VAR_062648.
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FT MUTAGEN 24 24
FT STRAND 47 51
FT TURN 72 75
FT STRAND 84 86
FT HELIX 100 116
FT STRAND 122 126
FT STRAND 145 150
FT HELIX 155 157
FT HELIX 161 167
FT STRAND 172 174
FT STRAND 181 184
SQ SEQUENCE 462 AA; 49607 MW; DD687AFA582A4749 CRC64;
MLLLARCLLL VLVSSLLVCS GLACGPGRGF GKRRHPKRLT PLAYKQFIPN VAEKTLGASG
RYEGKISRNS ERFKELTPNY NPDIIFKDEE NTGADRLMTQ RCKDKLNALA ISVMNQWPGV
KLRVTEGWDE DGHHSSESLH YGRAVDITT SDRDRSKYGM LARLAVEAGF DWVYYESKAH
IHCSVKAENS VAAKSGGCFP GSAIVHLEQG GTKLVKDLSP GDRVLAADDQ GRLLYSDFLT
FLDRDDGAKK VFYVIETREP RERLLLTAAH LLFVAPHNDS ATGEPEASSG SGPPSGGALG
PRALFASVRV FGQRVYVVAE RDGDRRLLP AAVHSVTLSEE AAGAYAPLTA QGTILINRVL
ASCYAVIEEH SWAHRAFPF RLAHALLAAL APARTDRGGD SGGGDRGGGG GRVALTAPGA
ADAPGAGATA GIHWYSQLLY QIGTWLLDSE ALHPLGMVAVK SS
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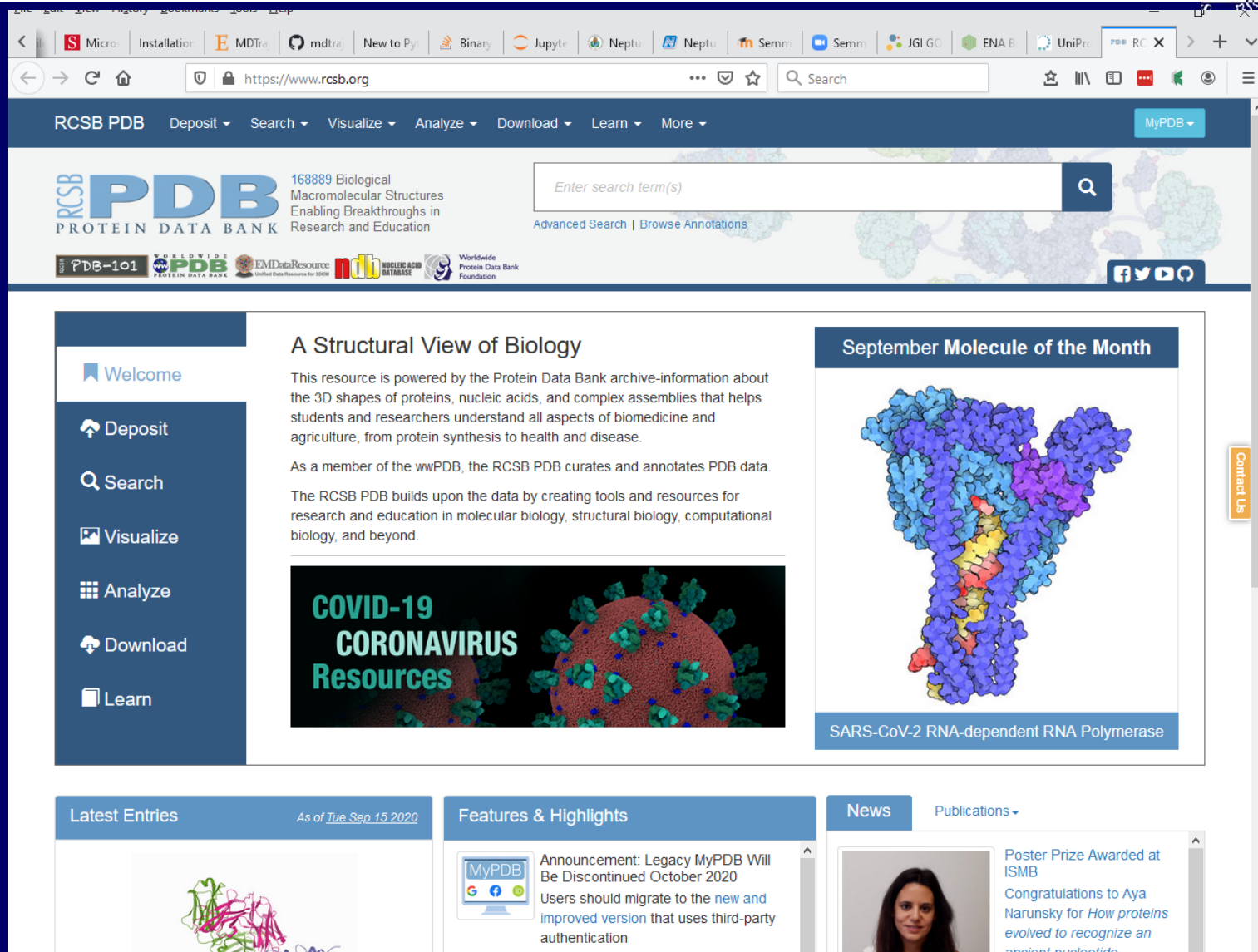
//



SZÜNET

PDB adatbázis

- Nemzetközi konzorcium üzemelteteti
 - Ingyenesen elérhető:
<http://www.rcsb.org/pdb/home/home.do>
- Elsődleges térszerkezeti adatbázis



RCSB PDB 168889 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

Enter search term(s)

Advanced Search | Browse Annotations

Welcome

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

As a member of the wwPDB, the RCSB PDB curates and annotates PDB data.

The RCSB PDB builds upon the data by creating tools and resources for research and education in molecular biology, structural biology, computational biology, and beyond.

September Molecule of the Month

SARS-CoV-2 RNA-dependent RNA Polymerase

COVID-19 CORONAVIRUS Resources

Latest Entries As of Tue Sep 15 2020

Features & Highlights

Announcement: Legacy MyPDB Will Be Discontinued October 2020

Users should migrate to the **new and improved version** that uses third-party authentication

News

Poster Prize Awarded at ISMB

Congratulations to Aya Narunsky for *How proteins evolved to recognize an ancient nucleotide*

https://www.rcsb.org/stats/summary

RCSB PDB Deposit Search Visualize Analyze Download Learn More MyPDB

RCSB PDB 156101 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

Search by PDB ID, author, macromolecule, sequence, or ligands **Go**

Advanced Search | Browse by Annotations

PDB-101 PDB EMDataResource NDB Worldwide Protein Data Bank Foundation

PDB Data Distribution by Experimental Method and Molecular Type Other Statistics

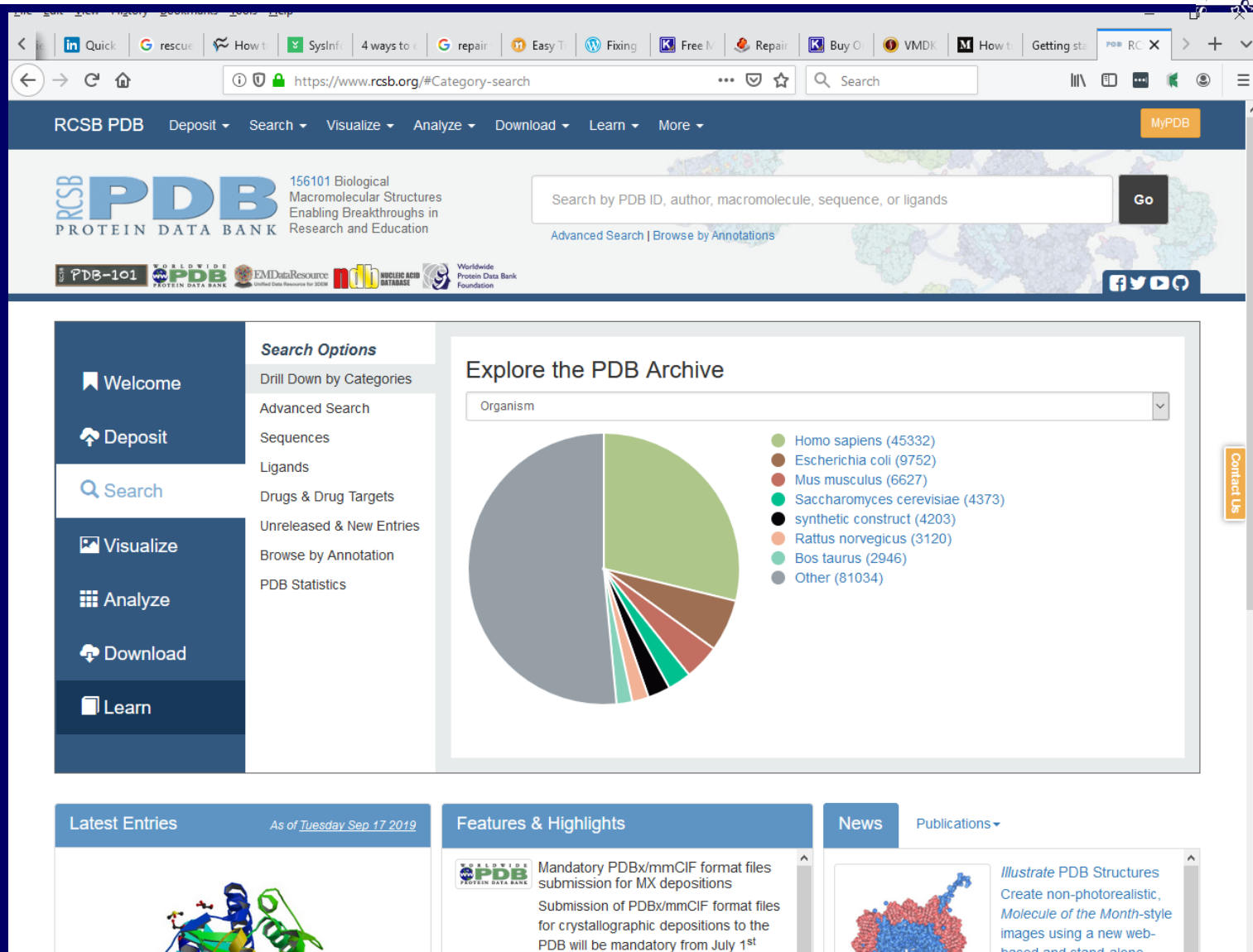
Copy CSV

Experimental Method	Proteins	Nucleic Acids	Protein/NA Complex	Other	Total
X-Ray	130354	2046	6724	8	139132
NMR	11200	1297	261	8	12766
Electron Microscopy	2758	32	965	0	3755
Other	275	4	6	13	298
Multi Method	142	5	2	1	150
Total	144729	3384	7958	30	156101

129041 structures in the PDB have a structure factor file.
 10116 structures in the PDB have an NMR restraint file.
 3868 structures in the PDB have a chemical shifts file.
 3832 structures in the PDB have a 3DEM map file.

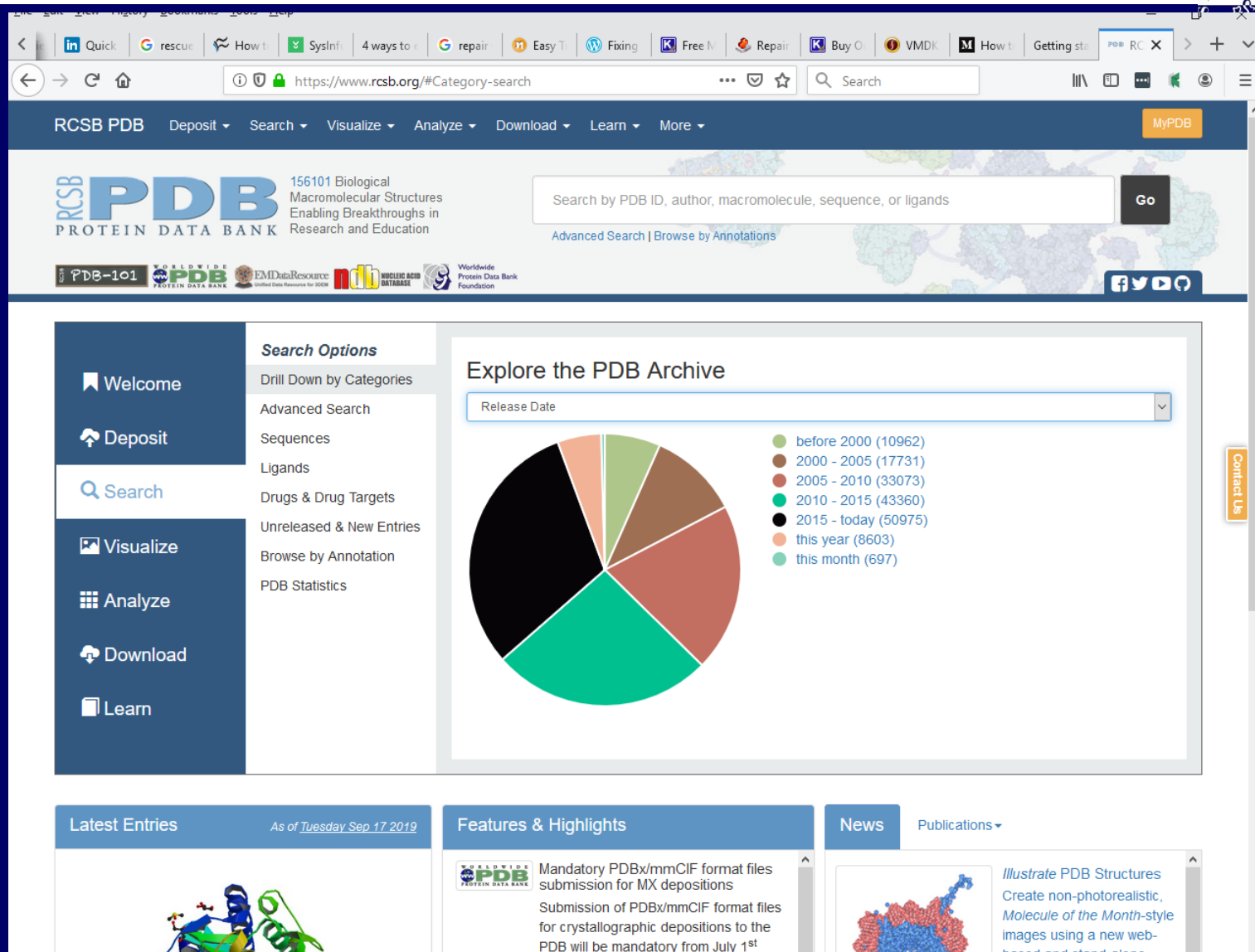
Sunburst Chart for Experimental Method and Molecular Type

Distribution by experimental method shown in yellow; molecular type in blue. Mouse over to view the statistical description of the particular section; click on a section to zoom in that particular section's statistical distribution, and then click on the center bullseye to zoom out back to the previous distribution.



The screenshot displays the RCSB PDB website interface. At the top, there's a navigation bar with links like 'RCSB PDB', 'Deposit', 'Search', 'Visualize', 'Analyze', 'Download', 'Learn', and 'More'. A search bar is prominently featured with the text 'Search by PDB ID, author, macromolecule, sequence, or ligands'. Below this, a 'Go' button is visible. The main content area is divided into several sections:

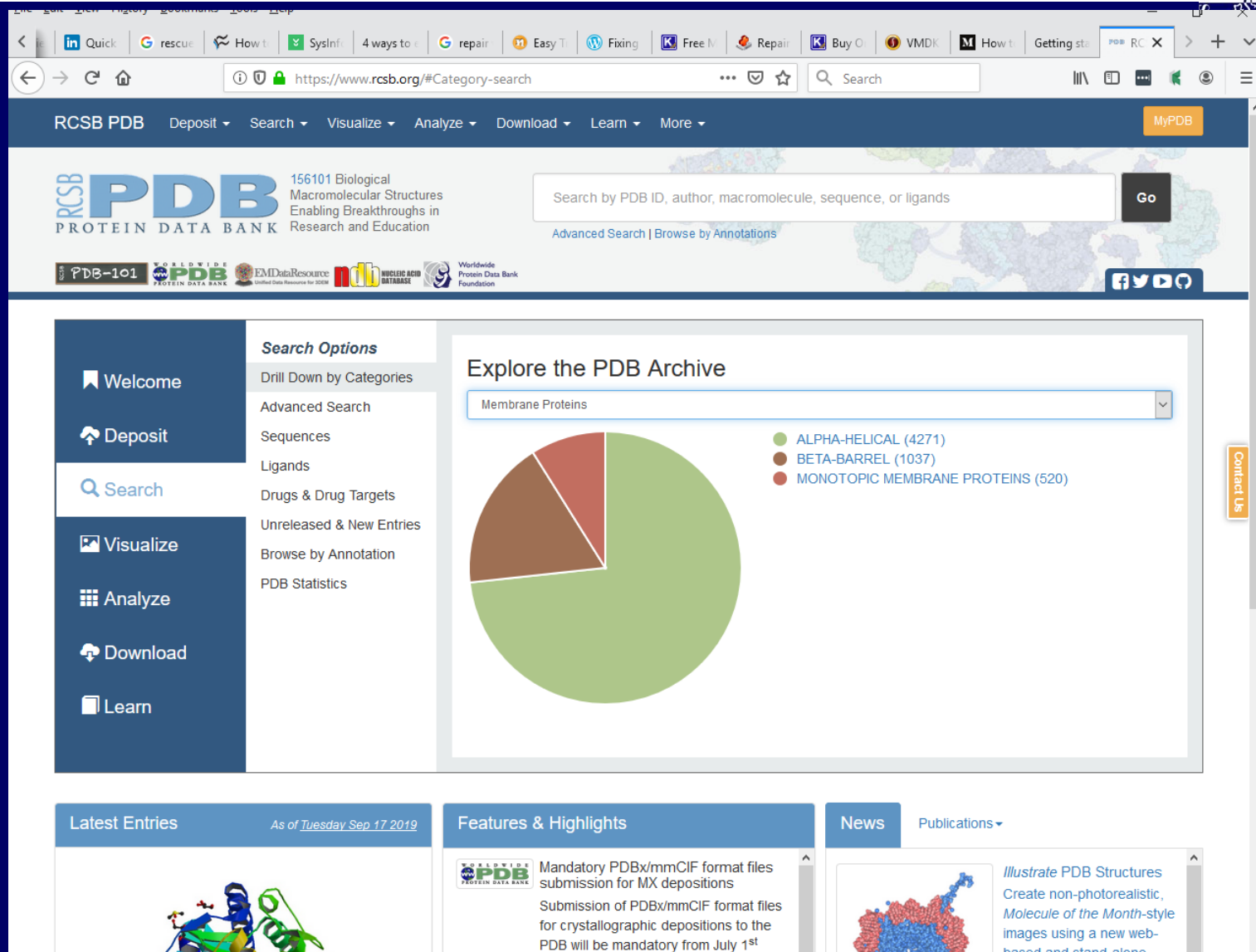
- Search Options:** A sidebar on the left lists various search and analysis tools: Welcome, Deposit, Search, Visualize, Analyze, Download, and Learn. The 'Search Options' section includes 'Drill Down by Categories', 'Advanced Search', 'Sequences', 'Ligands', 'Drugs & Drug Targets', 'Unreleased & New Entries', 'Browse by Annotation', and 'PDB Statistics'.
- Explore the PDB Archive:** A central section featuring a pie chart titled 'Explore the PDB Archive'. The chart shows the distribution of structures by organism. A legend on the right lists the organisms and their respective counts:
 - Homo sapiens (45332)
 - Escherichia coli (9752)
 - Mus musculus (6627)
 - Saccharomyces cerevisiae (4373)
 - synthetic construct (4203)
 - Rattus norvegicus (3120)
 - Bos taurus (2946)
 - Other (81034)
- Latest Entries:** A section at the bottom left showing the most recent protein structure depositions, dated 'Tuesday Sep 17 2019'.
- Features & Highlights:** A section at the bottom center highlighting important updates, such as the mandatory submission of PDBx/mmCIF format files for MX depositions starting from July 1st.
- News:** A section at the bottom right featuring a 'Molecule of the Month' style image and a link to 'Illustrate PDB Structures'.



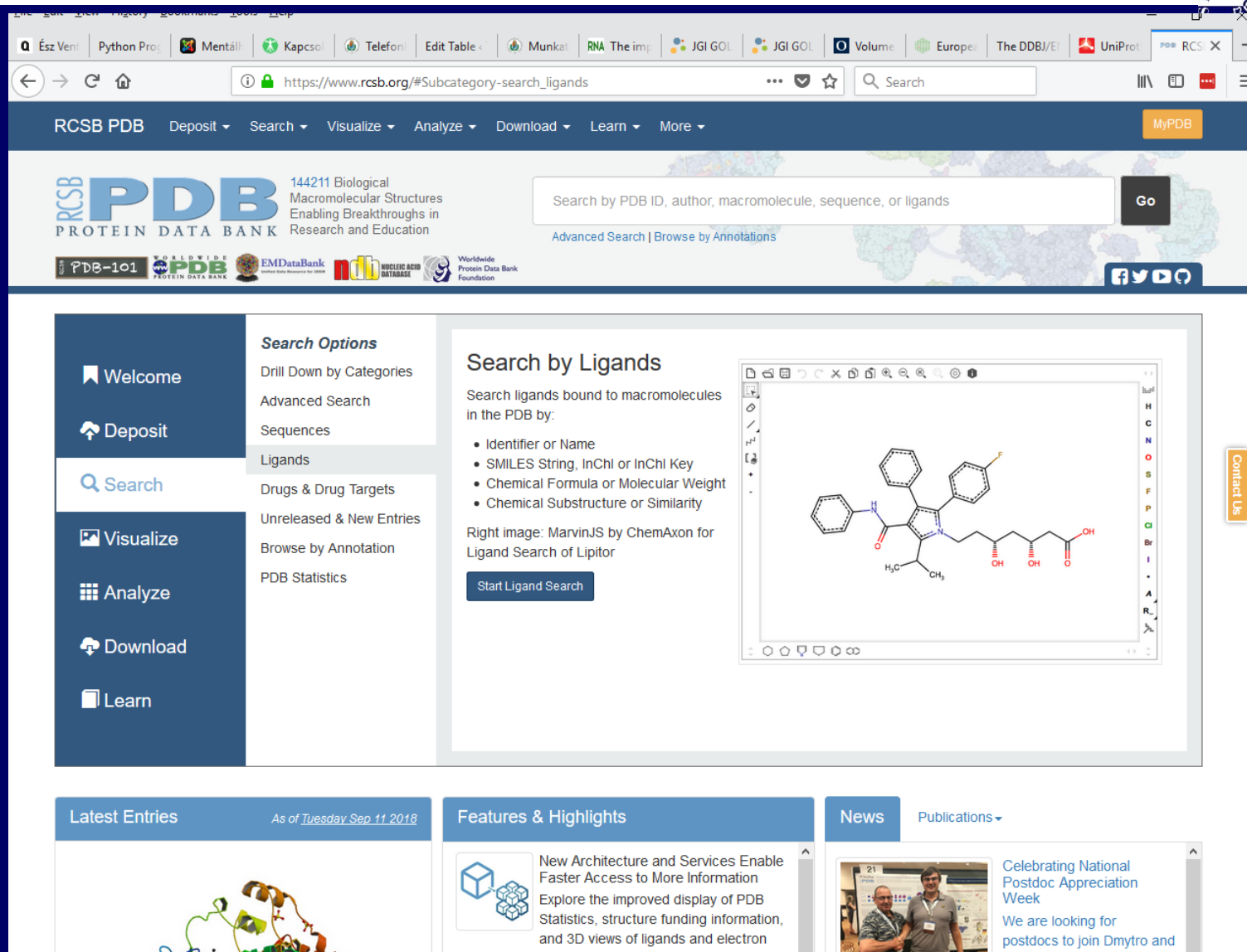
The screenshot displays the RCSB PDB website interface. At the top, there's a navigation bar with links like 'RCSB PDB', 'Deposit', 'Search', 'Visualize', 'Analyze', 'Download', 'Learn', and 'More'. A search bar is prominently featured with the text 'Search by PDB ID, author, macromolecule, sequence, or ligands'. Below the search bar, there's a section titled 'Explore the PDB Archive' which includes a pie chart showing the distribution of structures by release date. The legend for the pie chart is as follows:

Release Date	Count
before 2000	10962
2000 - 2005	17731
2005 - 2010	33073
2010 - 2015	43360
2015 - today	50975
this year	8603
this month	697

Below the pie chart, there's a section for 'Latest Entries' and 'Features & Highlights'. The 'Features & Highlights' section mentions the mandatory PDBx/mmCIF format files submission for MX depositions, effective from July 1st. The 'Latest Entries' section shows a list of recent protein structures with their corresponding 3D models.



The screenshot displays the RCSB PDB website interface. At the top, there's a navigation bar with links like 'RCSB PDB', 'Deposit', 'Search', 'Visualize', 'Analyze', 'Download', 'Learn', and 'More'. A search bar is prominently featured with the text 'Search by PDB ID, author, macromolecule, sequence, or ligands'. Below this, a 'Go' button is visible. The main content area is divided into several sections. On the left, a sidebar contains links for 'Welcome', 'Deposit', 'Search', 'Visualize', 'Analyze', 'Download', and 'Learn'. The central part of the page features a 'Search Options' section with a 'Drill Down by Categories' list including 'Advanced Search', 'Sequences', 'Ligands', 'Drugs & Drug Targets', 'Unreleased & New Entries', 'Browse by Annotation', and 'PDB Statistics'. To the right of this is a section titled 'Explore the PDB Archive' which includes a dropdown menu set to 'Membrane Proteins' and a pie chart showing the distribution of protein types: ALPHA-HELICAL (4271), BETA-BARREL (1037), and MONOTOPIC MEMBRANE PROTEINS (520). At the bottom, there are three columns: 'Latest Entries' (dated Tuesday Sep 17 2019), 'Features & Highlights' (mentioning mandatory PDBx/mmCIF format files for MX depositions), and 'News' (with a link to 'Illustrate PDB Structures').



RCSB PDB 144211 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

Search by PDB ID, author, macromolecule, sequence, or ligands **Go**

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

Search Options

- Drill Down by Categories
- Advanced Search
- Sequences
- Ligands**
- Drugs & Drug Targets
- Unreleased & New Entries
- Browse by Annotation
- PDB Statistics

Search by Ligands

Search ligands bound to macromolecules in the PDB by:

- Identifier or Name
- SMILES String, InChI or InChI Key
- Chemical Formula or Molecular Weight
- Chemical Substructure or Similarity

Right image: MarvinJS by ChemAxon for Ligand Search of Lipitor

Start Ligand Search

Latest Entries As of Tuesday Sep 11 2018

Features & Highlights

New Architecture and Services Enable Faster Access to More Information

Explore the improved display of PDB Statistics, structure funding information, and 3D views of ligands and electron

News Publications

Celebrating National Postdoc Appreciation Week

We are looking for postdocs to join Dmytro and



The screenshot displays the RCSB PDB website interface. At the top, there's a navigation bar with links like 'RCSB PDB', 'Deposit', 'Search', 'Visualize', 'Analyze', 'Download', 'Learn', and 'More'. A search bar is prominently featured with the text 'Search by PDB ID, author, macromolecule, sequence, or ligands'. Below this, a sidebar on the left lists navigation options: 'Welcome', 'Deposit', 'Search', 'Visualize', 'Analyze', 'Download', and 'Learn'. The main content area is divided into sections: 'Search Options' (listing categories like 'Drill Down by Categories', 'Advanced Search', 'Sequences', 'Ligands', etc.), 'Search PDB Statistics' (featuring a bar chart showing growth of released structures per year), 'Latest Entries' (showing a protein structure), 'Features & Highlights' (describing new architecture and services), and 'News' (announcing a postdoc appreciation week).

```

HEADER    RNA/RNA BINDING PROTEIN                12-APR-10   3MJ0
TITLE     CRYSTAL STRUCTURE OF DROSOPHILA AGO-PAZ DOMAIN IN COMPLEX WITH 3'-END
TITLE     2 2'-O-METHYLATED RNA
COMPND    MOL_ID: 1;
COMPND    2 MOLECULE: PROTEIN ARGONAUTE-2;
COMPND    3 CHAIN: A;
COMPND    4 FRAGMENT: UNP RESIDUES 601-723, PAZ DOMAIN;
COMPND    5 ENGINEERED: YES;
COMPND    6 MOL_ID: 2;
COMPND    7 MOLECULE: RNA (5'-R(*CP*GP*UP*UP*AP*CP*GP*CP*(OMU))-3');
COMPND    8 CHAIN: B;
COMPND    9 ENGINEERED: YES
SOURCE    MOL_ID: 1;
SOURCE    2 ORGANISM_SCIENTIFIC: DROSOPHILA MELANOGASTER;
SOURCE    3 ORGANISM_COMMON: FRUIT FLY;
SOURCE    4 ORGANISM_TAXID: 7227;
SOURCE    5 GENE: AGO2, CG7439;
SOURCE    6 EXPRESSION_SYSTEM: ESCHERICHIA COLI;
SOURCE    7 EXPRESSION_SYSTEM_TAXID: 562;
SOURCE    8 EXPRESSION_SYSTEM_STRAIN: BL21(DE3)GOLD;
SOURCE    9 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
SOURCE    10 EXPRESSION_SYSTEM_PLASMID: PET28-SMT3;
SOURCE    11 MOL_ID: 2;
SOURCE    12 SYNTHETIC: YES;
SOURCE    13 OTHER_DETAILS: THIS SEQUENCE WAS SYNTHESIZED.
KEYWDS    ARGONAUT, PAZ DOMAIN, 3'-END 2'-O-METHYLATED SSRNA, RNA-RNA BINDING
KEYWDS    2 PROTEIN COMPLEX
EXPDTA    X-RAY DIFFRACTION
AUTHOR    Y.HUANG,L.DING,J.MA
REVDAT    1   25-MAY-11 3MJ0      0
JRNL      AUTH  Y.HUANG,L.DING,J.MA
JRNL      TITL  CRYSTAL STRUCTURE OF DROSOPHILA AGO2 PAZ DOMAIN IN COMPLEX
JRNL      TITL  2 WITH 3'-END 2'-O-METHYLATED RNA
JRNL      REF   TO BE PUBLISHED
JRNL      REFN
REMARK    2
REMARK    2 RESOLUTION.      2.31 ANGSTROMS.
REMARK    3
REMARK    3 REFINEMENT.
REMARK    3   PROGRAM      : PHENIX (PHENIX.REFINE: 1.5_2)
REMARK    3   AUTHORS     : PAUL ADAMS,PAVEL AFONINE,VICENT CHEN,IAN
REMARK    3                  : DAVIS,KRESHNA GOPAL,RALF GROSSE-
REMARK    3                  : KUNSTLEVE,LI-WEI HUNG,ROBERT IMMORMINO,
REMARK    3                  : TOM IOERGER,AIRLIE MCCOY,ERIK MCKEE,NIGEL
REMARK    3                  : MORIARTY,REETAL PAI,RANDY READ,JANE
REMARK    3                  : RICHARDSON,DAVID RICHARDSON,TOD ROMO,JIM
REMARK    3                  : SACCHETTINI,NICHOLAS SAUTER,JACOB SMITH,
REMARK    3                  : LAURENT STORONI,TOM TERWILLIGER,PETER
REMARK    3                  : ZWART
REMARK    3
REMARK    3 REFINEMENT TARGET : MLHL
REMARK    3

```

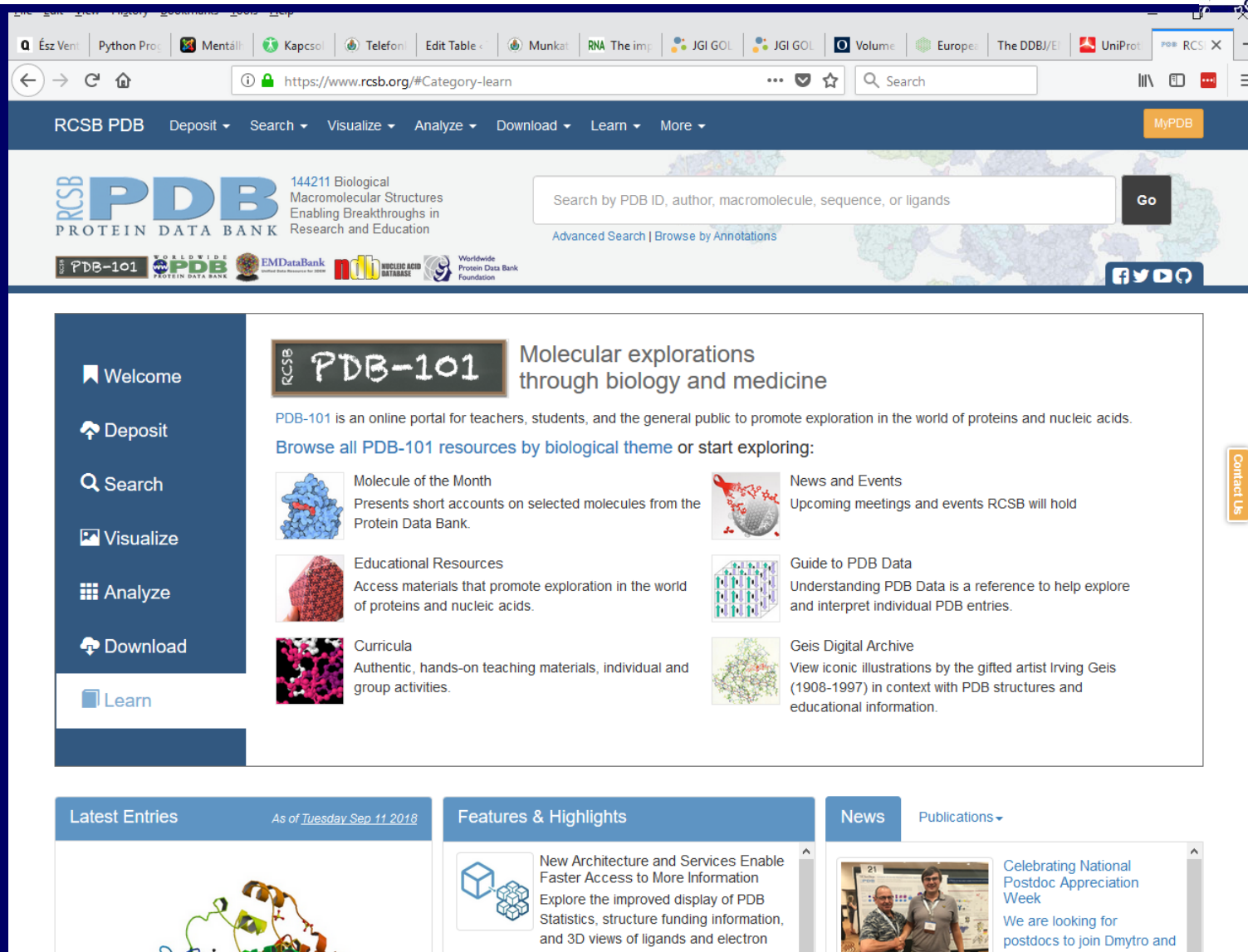
```

REMARK    280
REMARK    280 CRYSTAL
REMARK    280 SOLVENT CONTENT, VS      (%): 46.54
REMARK    280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): 2.30
REMARK    280
REMARK    280 CRYSTALLIZATION CONDITIONS: 50 MM MES, PH 5.8, 100 MM AMMONIUM
REMARK    280 SULFATE, 10 MM MGCL2, 16% PEG 8000 AND 5% GLYCEROL, VAPOR
REMARK    280 DIFFUSION, HANGING DROP, TEMPERATURE 293K
REMARK    290
REMARK    290 CRYSTALLOGRAPHIC SYMMETRY
REMARK    290 SYMMETRY OPERATORS FOR SPACE GROUP: C 2 2 21
REMARK    290
REMARK    290      SYMOP      SYMMETRY
REMARK    290      NNNMMM      OPERATOR
REMARK    290      1555      X,Y,Z
REMARK    290      2555      -X,-Y,Z+1/2
REMARK    290      3555      -X,Y,-Z+1/2
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REMARK    290      7555      -X+1/2,Y+1/2,-Z+1/2
REMARK    290      8555      X+1/2,-Y+1/2,-Z
REMARK    290
REMARK    290      WHERE NNN -> OPERATOR NUMBER
REMARK    290      MMM -> TRANSLATION VECTOR
REMARK    290
REMARK    290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK    290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK    290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK    290 RELATED MOLECULES.
REMARK    290 SMTRY1  1  1.000000  0.000000  0.000000  0.000000
REMARK    290 SMTRY2  1  0.000000  1.000000  0.000000  0.000000
REMARK    290 SMTRY3  1  0.000000  0.000000  1.000000  0.000000
REMARK    290 SMTRY1  2 -1.000000  0.000000  0.000000  0.000000
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REMARK    290 SMTRY3  3  0.000000  0.000000 -1.000000  19.33050
REMARK    290 SMTRY1  4  1.000000  0.000000  0.000000  0.000000
REMARK    290 SMTRY2  4  0.000000 -1.000000  0.000000  0.000000
REMARK    290 SMTRY3  4  0.000000  0.000000 -1.000000  0.000000
REMARK    290 SMTRY1  5  1.000000  0.000000  0.000000  34.60550
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REMARK    290 SMTRY1  6 -1.000000  0.000000  0.000000  34.60550
REMARK    290 SMTRY2  6  0.000000 -1.000000  0.000000  58.39800
REMARK    290 SMTRY3  6  0.000000  0.000000  1.000000  19.33050

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SEQRES 2 A 124 LEU LYS ALA LYS ILE ASN ASN THR THR ASN LEU ASP TYR
SEQRES 3 A 124 SER ARG ARG PHE LEU GLU PRO PHE LEU ARG GLY ILE ASN
SEQRES 4 A 124 VAL VAL TYR THR PRO PRO GLN SER PHE GLN SER ALA PRO
SEQRES 5 A 124 ARG VAL TYR ARG VAL ASN GLY LEU SER ARG ALA PRO ALA
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SEQRES 8 A 124 PHE PRO GLN LEU HIS CYS LEU ASN VAL GLY SER SER ILE
SEQRES 9 A 124 LYS SER ILE LEU LEU PRO ILE GLU LEU CYS SER ILE GLU
SEQRES 10 A 124 GLU GLY GLN ALA LEU ASN ARG
SEQRES 1 B 9 C G U U A C G C OMU
MODRES 3MJ0 OMU B 9 U O2'-METHYLURIDINE 5'-MONOPHOSPHATE
HET OMU B 9 21
HETNAM OMU O2'-METHYLURIDINE 5'-MONOPHOSPHATE
FORMUL 2 OMU C10 H15 N2 O9 P
FORMUL 3 HOH *33 (H2 O)
HELIX 1 1 MET A 604 SER A 612 1 9
HELIX 2 2 ASN A 622 TYR A 625 5 4
HELIX 3 3 SER A 626 ARG A 635 1 10
HELIX 4 4 PRO A 644 GLN A 648 5 5
HELIX 5 5 ILE A 678 SER A 684 1 7
HELIX 6 6 PRO A 709 GLU A 711 5 3
SHEET 1 A 4 SER A 601 PRO A 603 0
SHEET 2 A 4 CYS A 713 GLU A 716 -1 O ILE A 715 N MET A 602
SHEET 3 A 4 ASN A 638 TYR A 641 -1 N VAL A 640 O SER A 714
SHEET 4 A 4 ARG A 652 ARG A 655 -1 O ARG A 652 N TYR A 641
SHEET 1 B 3 GLY A 658 PRO A 663 0
SHEET 2 B 3 HIS A 695 ASN A 698 -1 O CYS A 696 N SER A 660
SHEET 3 B 3 LEU A 707 LEU A 708 -1 O LEU A 708 N LEU A 697
SHEET 1 C 2 THR A 668 GLU A 670 0
SHEET 2 C 2 LYS A 675 THR A 677 -1 O VAL A 676 N PHE A 669
LINK O3' C B 8 P OMU B 9 1555 1555 1.63
CRYST1 69.211 116.796 38.661 90.00 90.00 90.00 C 2 2 21 8
ORIGX1 1.000000 0.000000 0.000000 0.000000
ORIGX2 0.000000 1.000000 0.000000 0.000000
ORIGX3 0.000000 0.000000 1.000000 0.000000
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SCALE2 0.000000 0.008562 0.000000 0.000000
SCALE3 0.000000 0.000000 0.025866 0.000000
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ATOM	1	N	SER A 600	6.283	8.861	-8.154	1.00	65.33	N
ATOM	2	CA	SER A 600	6.119	9.334	-6.784	1.00	68.88	C
ATOM	3	C	SER A 600	7.307	8.914	-5.918	1.00	67.53	O
ATOM	4	O	SER A 600	8.330	8.478	-6.445	1.00	70.29	C
ATOM	5	CB	SER A 600	4.801	8.828	-6.187	1.00	74.92	C
ATOM	6	OG	SER A 600	4.734	7.412	-6.204	1.00	74.42	O
ATOM	7	N	SER A 601	7.163	9.037	-4.599	1.00	62.45	N
ATOM	8	CA	SER A 601	8.284	8.835	-3.687	1.00	61.77	C
ATOM	9	C	SER A 601	7.857	8.445	-2.278	1.00	65.47	C
ATOM	10	O	SER A 601	6.713	8.671	-1.876	1.00	66.71	O
ATOM	11	CB	SER A 601	9.130	10.107	-3.598	1.00	63.47	C
ATOM	12	OG	SER A 601	8.456	11.097	-2.843	1.00	60.71	O
ATOM	13	N	MET A 602	8.801	7.879	-1.525	1.00	60.84	N
ATOM	14	CA	MET A 602	8.575	7.513	-0.132	1.00	55.67	C
ATOM	15	C	MET A 602	9.552	8.232	0.804	1.00	52.46	C
ATOM	16	O	MET A 602	10.734	8.346	0.502	1.00	51.93	O
ATOM	17	CB	MET A 602	8.688	5.997	0.040	1.00	53.12	C
ATOM	18	CG	MET A 602	8.692	5.547	1.492	1.00	60.07	C
ATOM	19	SD	MET A 602	8.480	3.773	1.748	1.00	67.00	S
ATOM	20	CE	MET A 602	10.063	3.122	1.252	1.00	64.41	C
ATOM	21	N	PRO A 603	9.050	8.722	1.944	1.00	50.54	N
ATOM	22	CA	PRO A 603	9.879	9.431	2.925	1.00	48.35	C
ATOM	23	C	PRO A 603	10.992	8.549	3.437	1.00	52.20	C
ATOM	24	O	PRO A 603	10.730	7.427	3.839	1.00	58.02	O
ATOM	25	CB	PRO A 603	8.911	9.703	4.072	1.00	52.67	C
ATOM	26	CG	PRO A 603	7.553	9.661	3.455	1.00	55.93	C
ATOM	27	CD	PRO A 603	7.637	8.656	2.349	1.00	53.63	C
ATOM	28	N	MET A 604	12.215	9.057	3.441	1.00	51.47	N
ATOM	29	CA	MET A 604	13.333	8.303	3.971	1.00	52.57	C
ATOM	30	C	MET A 604	13.072	7.851	5.388	1.00	55.38	C
ATOM	31	O	MET A 604	13.595	6.829	5.819	1.00	58.51	O
ATOM	32	CB	MET A 604	14.627	9.115	3.912	1.00	51.24	C
ATOM	33	CG	MET A 604	15.308	9.073	2.547	1.00	50.14	C
ATOM	34	SD	MET A 604	15.618	7.377	1.994	1.00	53.74	S
ATOM	35	CE	MET A 604	16.596	6.758	3.344	1.00	52.26	C
ATOM	36	N	ILE A 605	12.264	8.608	6.120	1.00	54.74	N
ATOM	37	CA	ILE A 605	11.974	8.251	7.499	1.00	52.91	C
ATOM	38	C	ILE A 605	11.214	6.923	7.558	1.00	61.84	C
ATOM	39	O	ILE A 605	11.549	6.020	8.326	1.00	59.30	O
ATOM	40	CB	ILE A 605	11.154	9.335	8.189	1.00	55.89	C
ATOM	41	CG1	ILE A 605	12.020	10.575	8.434	1.00	51.55	C
ATOM	42	CG2	ILE A 605	10.608	8.809	9.504	1.00	60.92	C
ATOM	43	CD1	ILE A 605	13.120	10.358	9.463	1.00	54.08	C
ATOM	44	N	GLU A 606	10.216	6.816	6.702	1.00	59.72	N
ATOM	45	CA	GLU A 606	9.446	5.578	6.594	1.00	61.38	C
ATOM	46	C	GLU A 606	10.371	4.511	6.022	1.00	63.26	C
ATOM	47	O	GLU A 606	10.590	3.464	6.630	1.00	63.43	O



The screenshot shows the RCSB PDB website interface. At the top, there's a navigation bar with links like 'RCSB PDB', 'Deposit', 'Search', 'Visualize', 'Analyze', 'Download', 'Learn', and 'More'. Below this is a search bar with the text 'Search by PDB ID, author, macromolecule, sequence, or ligands' and a 'Go' button. The main content area is titled 'Molecular explorations through biology and medicine' and features a sidebar with links: 'Welcome', 'Deposit', 'Search', 'Visualize', 'Analyze', 'Download', and 'Learn'. The main content area lists several resources: 'Molecule of the Month', 'Educational Resources', 'Curricula', 'News and Events', 'Guide to PDB Data', and 'Geis Digital Archive'. At the bottom, there are sections for 'Latest Entries', 'Features & Highlights', and 'News'.

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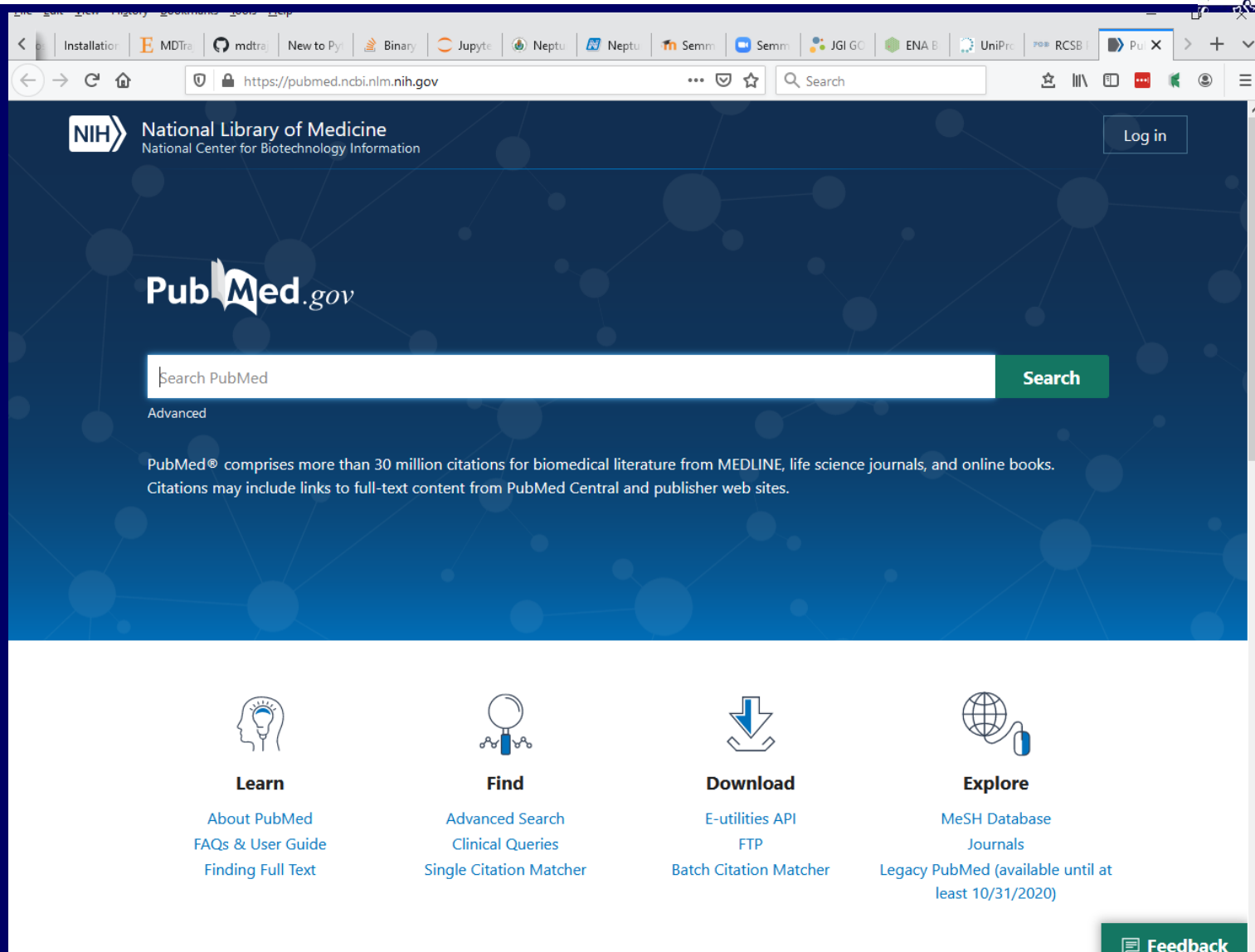
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- Integrált adatbázis: a felületen keresztül fehérje és nukleinsav adatbázisok is elérhetők



The screenshot shows the PubMed.gov website in a web browser. The browser's address bar displays the URL <https://pubmed.ncbi.nlm.nih.gov>. The page header includes the NIH logo and the text "National Library of Medicine National Center for Biotechnology Information". A "Log in" button is located in the top right corner. The main content area features the "PubMed.gov" logo, a search bar with the placeholder text "Search PubMed", and a green "Search" button. Below the search bar, the text "Advanced" is visible. A paragraph states: "PubMed® comprises more than 30 million citations for biomedical literature from MEDLINE, life science journals, and online books. Citations may include links to full-text content from PubMed Central and publisher web sites." The bottom section of the page is divided into four columns, each with an icon and a title: "Learn" (lightbulb icon), "Find" (magnifying glass icon), "Download" (download arrow icon), and "Explore" (globe icon). Each column lists several links related to its category. A green "Feedback" button is located in the bottom right corner.

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4. Taft RJ, Simons C, Nahkuri S, Oey H, Korbie DJ, Mercer TR, Holst J, Ritchie W, Wong JJ, Rasko JE, Rokhsar DS, Degnan BM, Mattick JS.
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The relationship between transcription initiation RNAs and CCCTC-binding factor (CTCF) localization.

Taft RJ, Hawkins PG, Mattick JS, Morris KV.

Department of Molecular and Experimental Medicine, The Kellogg School of Science and Technology, The Scripps Research Institute, La Jolla, CA 92037, USA. kmorris@scripps.edu.

Abstract

ABSTRACT:

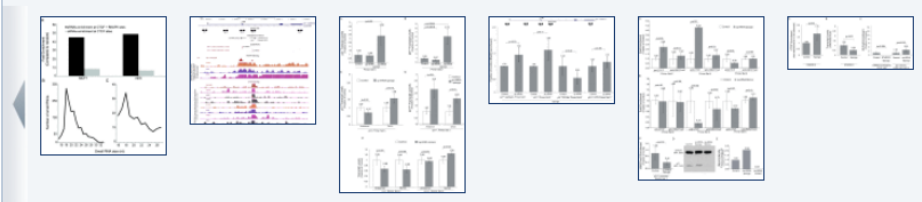
BACKGROUND: Transcription initiation RNAs (tiRNAs) are nuclear localized 18 nucleotide RNAs derived from sequences immediately downstream of RNA polymerase II (RNAPII) transcription start sites. Previous reports have shown that tiRNAs are intimately correlated with gene expression, RNA polymerase II binding and behaviors, and epigenetic marks associated with transcription initiation, but not elongation.

RESULTS: In the present work, we show that tiRNAs are commonly found at genomic CCCTC-binding factor (CTCF) binding sites in human and mouse, and that CTCF sites that colocalize with RNAPII are highly enriched for tiRNAs. To directly investigate the relationship between tiRNAs and CTCF we examined tiRNAs originating near the intronic CTCF binding site in the human tumor suppressor gene, p21 (cyclin-dependent kinase inhibitor 1A gene, also known as CDKN1A). Inhibition of CTCF-proximal tiRNAs resulted in increased CTCF localization and increased p21 expression, while overexpression of CTCF-proximal tiRNA mimics decreased CTCF localization and p21 expression. We also found that tiRNA-regulated CTCF binding influences the levels of trimethylated H3K27 at the alternate upstream p21 promoter, and affects the levels of alternate p21 (p21alt) transcripts. Extending these studies to another randomly selected locus with conserved CTCF binding we found that depletion of tiRNA alters nucleosome density proximal to sites of tiRNA biogenesis.

CONCLUSIONS: Taken together, these data suggest that tiRNAs modulate local epigenetic structure, which in turn regulates CTCF localization.

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The relationship between transcription initiation RNAs and CCTC-binding factor (CTCF) localization

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Epigenetics & Chromatin 2011, 4:13 doi:10.1186/1756-8935-4-13

The electronic version of this article is the complete one and can be found online at: <http://www.epigeneticsandchromatin.com/content/4/1/13>

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Abstract

Background
Transcription initiation RNAs (tiRNAs) are nuclear localized 18 nucleotide RNAs derived from

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 DP - 2011
 TI - The relationship between transcription initiation RNAs and CCCTC-binding factor (CTCF) localization.
 PG - 13
 AB - ABSTRACT: BACKGROUND: Transcription initiation RNAs (tiRNAs) are nuclear localized 18 nucleotide RNAs derived from sequences immediately downstream of RNA polymerase II (RNAPII) transcription start sites. Previous reports have shown that tiRNAs are intimately correlated with gene expression, RNA polymerase II binding and behaviors, and epigenetic marks associated with transcription initiation, but not elongation. RESULTS: In the present work, we show that tiRNAs are commonly found at genomic CCCTC-binding factor (CTCF) binding sites in human and mouse, and that CTCF sites that colocalize with RNAPII are highly enriched for tiRNAs. To directly investigate the relationship between tiRNAs and CTCF we examined tiRNAs originating near the intronic CTCF binding site in the human tumor suppressor gene, p21 (cyclin-dependent kinase inhibitor 1A gene, also known as CDKN1A). Inhibition of CTCF-proximal tiRNAs resulted in increased CTCF localization and increased p21 expression, while overexpression of CTCF-proximal tiRNA mimics decreased CTCF localization and p21 expression. We also found that tiRNA-regulated CTCF binding influences the levels of trimethylated H3K27 at the alternate upstream p21 promoter, and affects the levels of alternate p21 (p21alt) transcripts. Extending these studies to another randomly selected locus with conserved CTCF binding we found that depletion of tiRNA alters nucleosome density proximal to sites of tiRNA biogenesis. CONCLUSIONS: Taken together, these data suggest that tiRNAs modulate local epigenetic structure, which in turn regulates CTCF localization.
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- Az adatokat nem lehet kritika nélkül elfogadni

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 - Változik a megbízhatóság
- Hibás predikció
 - A másodlagos adatbázisok predikción alapulnak
 - 99%-os hatékonyság – az emberi genom esetén 250 gént hibásan annotálunk!
- Hiányos tudás
 - 'Aki keres az talál.' – pl. cisPro

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- Emberi beavatkozás – teljesen reménytelen
 - Túl sok az adat és vannak emberi hibák is
- Kollektív bölcsesség – wikipédia
 - Kiegyenlíti a hibákat, de új problémákat generál
- A meglévő predikciós módszerek javítása
 - Igen lassú és körülményes
- Külön hibajavító – ellenőrző módszerek kidolgozása
 - Hibajavítás szakértői rendszerrel

A MisPred adatbázis

- Patthy László nevéhez fűződik
- Elérhető: <http://mispred.com/>
- Elve: a fehérje annotáció különböző elemei közt van-e konfliktus?
 1. Extracelluláris domén van, de nincs szignál peptid
 2. Extracelluláris és citoplazmatikus domén van, de nincs transzmembrán szakasz
 3. Nukleáris és extracelluláris domén is van
 4. Domén méret jelentős eltérése a család többi tagjához képest
 5. Egy gén csak egy kromoszómán lehet jelen



The screenshot shows the MisPred website interface. At the top, there's a navigation bar with links: HOME, ABOUT MISPREP, SEARCH MISPREP, ANALYZE YOUR SEQUENCE, RECENT RESULTS, and CONTACT AND FEEDBACK. The main heading is "MisPred 8.0 (May 2014)". Below this, a paragraph describes the database as a collection of protein sequences identified as erroneous. To the left of the text are logos for the European Union and the NIH National Innovation Office. A section titled "Citing MisPred" provides references for citing the database. At the bottom, there's a footer with logos for the NIH National Innovation Office, the Hungarian Government (Új Magyarország Fejlesztési Terv), and the European Union, along with a copyright notice for 2011 by Combit Számítástechnikai Zrt.

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MisPred 8.0 (May 2014)

The MisPred database is a collection of protein sequences identified by the MisPred pipeline as erroneous (incomplete, abnormal or mispredicted). The MisPred database may be searched in various ways ([SEARCH MISPREP](#)) and you may also analyze your sequence using the MisPred pipeline to decide whether your sequence violates some basic rules of protein sequences ([ANALYZE YOUR SEQUENCE](#)).

Citing MisPred

If you find MisPred useful, please consider citing the references that describe this work:

Nagy A, Hegyi H, Farkas K, Tordai H, Kozma E, Bányai L, Patthy L. Identification and correction of abnormal, incomplete and mispredicted proteins in public databases. BMC Bioinformatics. 2008; 9:353. <http://www.ncbi.nlm.nih.gov/pubmed/18752676>

Nagy A. and Patthy L. MisPred: a resource for identification of erroneous protein sequences in public databases. Database (2013) Vol. 2013: article ID bat053; doi:10.1093/database/bat053 <http://database.oxfordjournals.org/content/2013/bat053.full>

The FixPred9 project is funded by the National Innovation Office of Hungary through grant FixPred9 "Exploiting genome information", contract number TECH_09_A1-FixPred9.

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MisPred: a resource for identification of erroneous protein sequences in public databases

Alinda Nagy and László Patthy*

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Abstract

Correct prediction of the structure of protein-coding genes of higher eukaryotes is still a difficult task; therefore, public databases are heavily contaminated with mispredicted sequences. The high rate of misprediction has serious consequences because it significantly affects the conclusions that may be drawn from genome-scale sequence analyses of eukaryotic genomes. Here we present the MisPred database and computational pipeline that provide efficient means for the identification of erroneous sequences in public databases. The MisPred database contains a collection of abnormal, incomplete and mispredicted protein sequences from 19 metazoan species identified as erroneous by MisPred quality control tools in the UniProtKB/Swiss-Prot, UniProtKB/TrEMBL, NCBI/RefSeq and Ensembl databases. Major releases of the database are automatically generated and updated regularly. The database (<http://www.mispred.com>) is easily accessible through a simple web interface coupled to a powerful query engine and a standard web service. The content is completely or partially downloadable in a variety of formats.

Database URL: <http://www.mispred.com>

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7070-7084 *Nucleic Acids Research*, 2018, Vol. 46, No. 14
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Loose ends: almost one in five human genes still have unresolved coding status

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ABSTRACT

Seventeen years after the sequencing of the human genome, the human proteome is still under revision. One in eight of the 22 210 coding genes listed by the Ensembl/GENCODE, RefSeq and UniProtKB reference databases are annotated differently across the three sets. We have carried out an in-depth investigation on the 2764 genes classified as coding by one or more sets of manual curators and not coding by others. Data from large-scale genetic variation analyses suggests that most are not under protein-like puri-

to 100 000 genes (2,3). However, the accumulation of experimental data has progressively brought this estimate down. The 'finished' version of the human genome revised the estimates to between 20 000 and 25 000 coding genes (4).

The gradual downward trend of the human protein gene count has been mirrored in the reference human gene set. The annotation of human coding genes began with the Ensembl project (5) and the initial release included more than 24 000 coding genes. This number soon decreased to 22 000 as the genome assembly improved and automatic predictions were refined (6). Until recently there were still gene loci in the reference set defined as coding based on the ini-

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