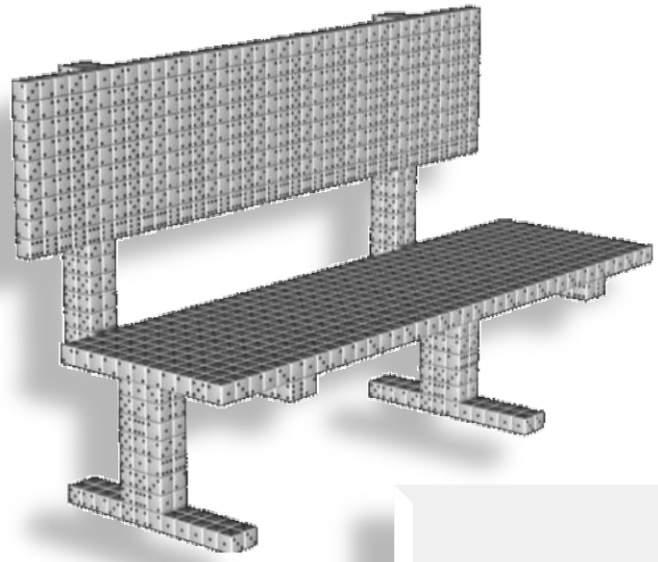
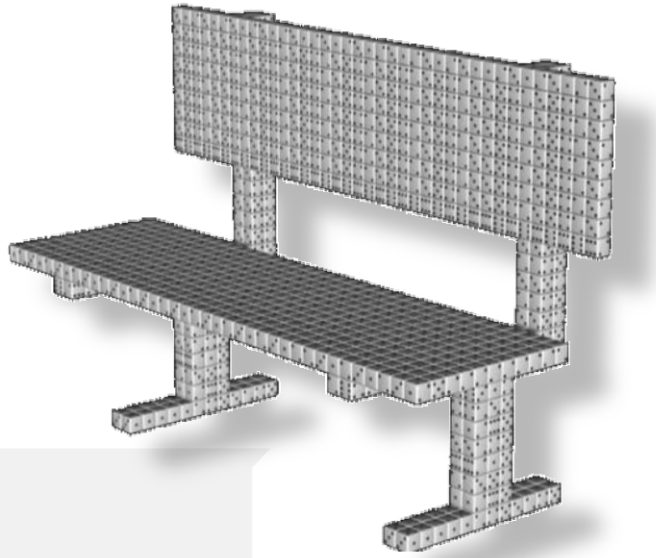




Bancos de Dados de Informação Estrutural

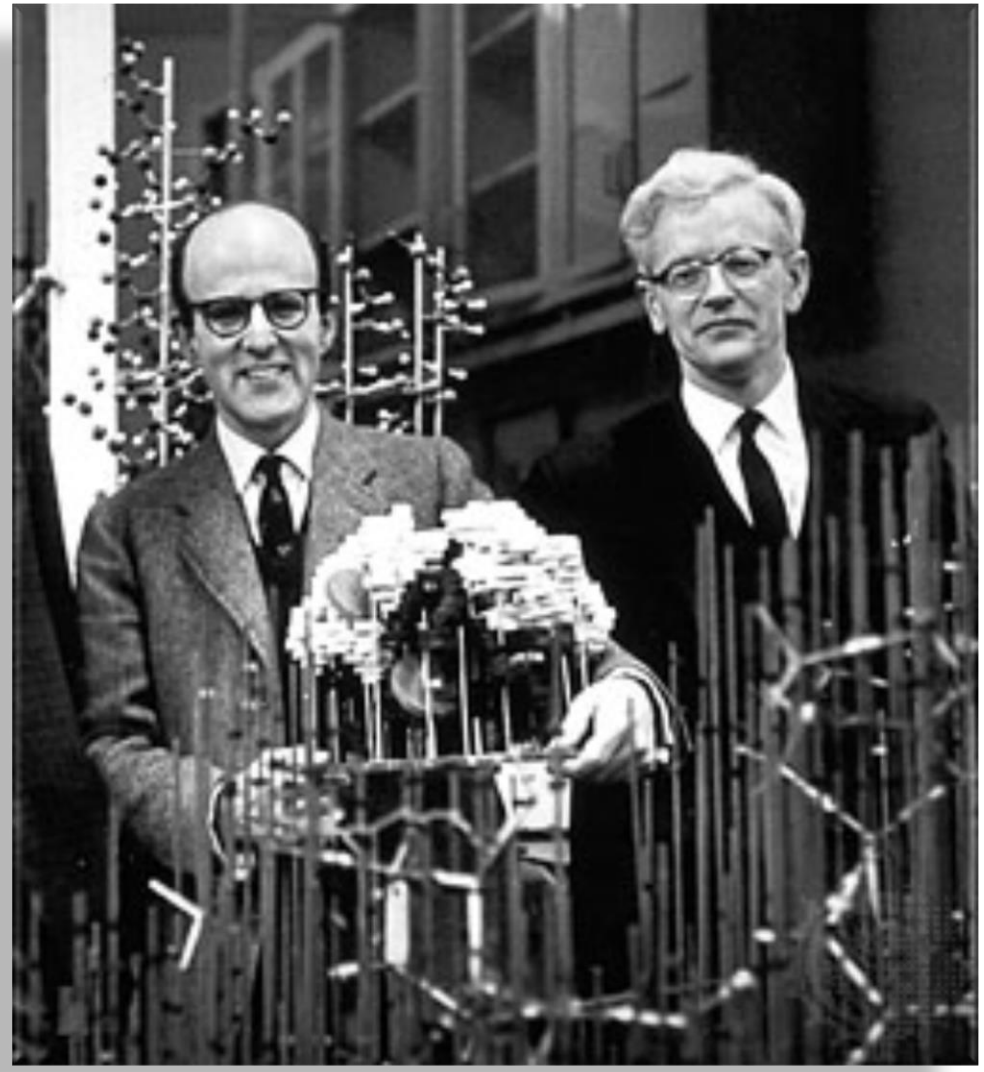
Ignez Caracelli

BioMat – DF

Julio Zukerman Schpector

LaCrEMM – DQ – UFSCar

1as Estruturas 3D



Prêmio Nobel em 1962.

Perutz ⇨
Hemoglobina

1957:
baixa resolução 5.5 Å
1968:
alta resolução 2 Å

Kendrew ⇨
Mioglobina

1957:
baixa resolução 6 Å
1959:
alta resolução 2 Å

Um pouco de história

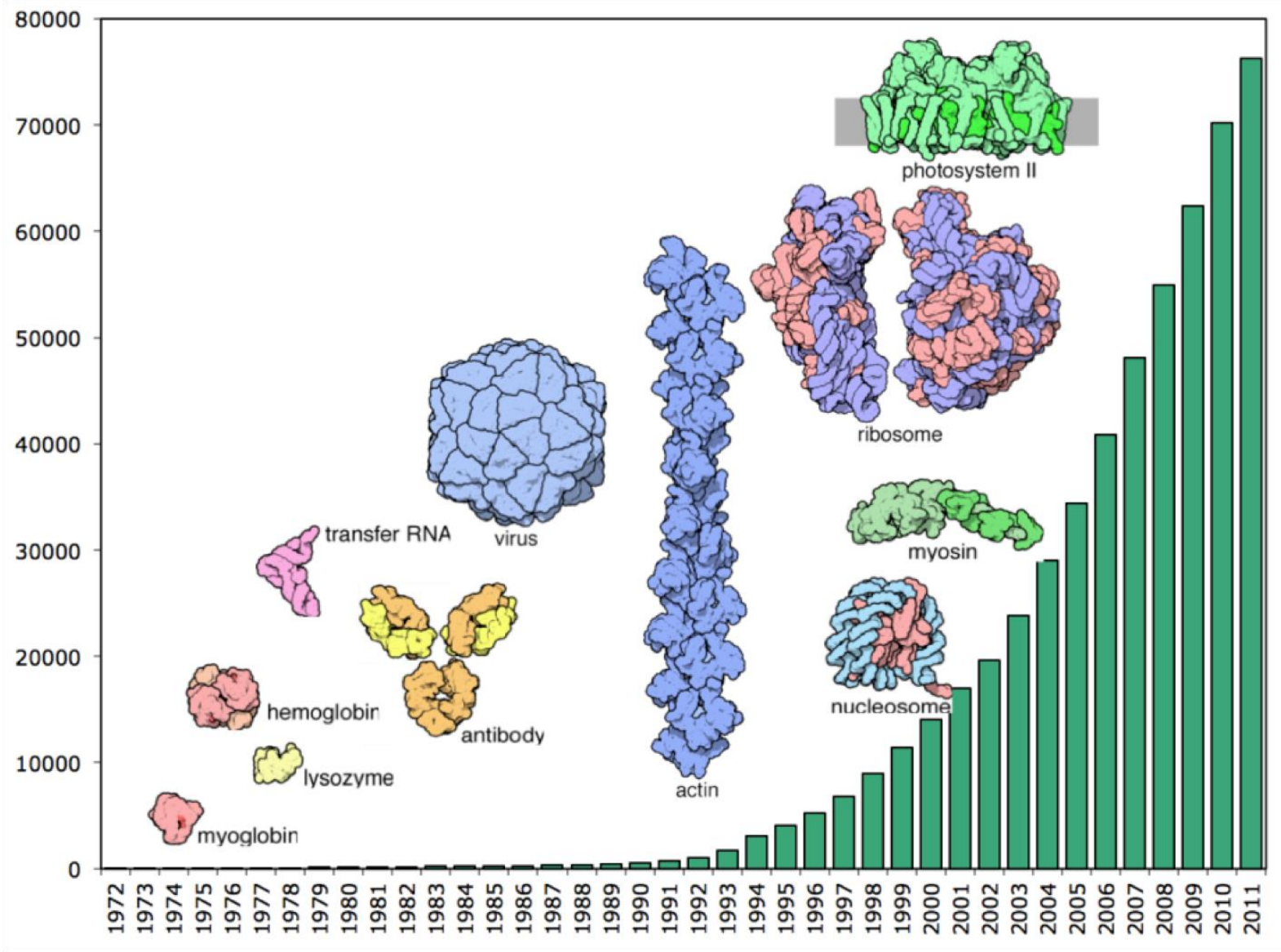
anos 1970

um grupo de jovens cristalógrafos, Edgar Meyer, Gerson Cohen e Helen Berman, reuniu esforços no sentido de estabelecer uma central de coordenadas de estruturas cristalográficas de moléculas biológicas

Protein **D**ata **B**ank

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

RCSB PDB
PROTEIN DATA BANK


80000
70000
60000
50000
40000
30000
20000
10000
0
1972
1973
1974
1975
1976
1977
1978
1979
1980
1981
1982
1983
1984
1985
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1987
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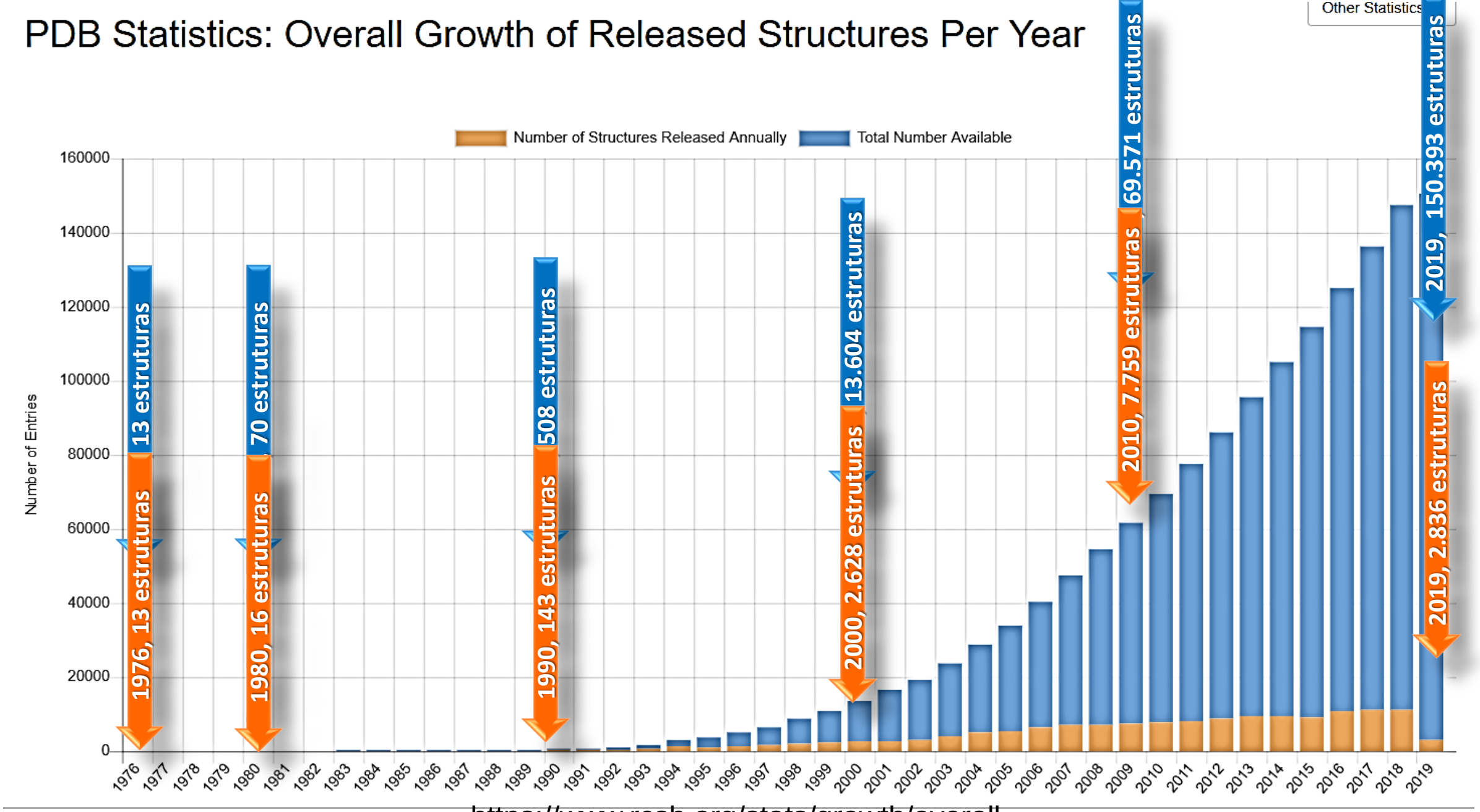
1989
1990
1991
1992
1993
1994
1995
1996
1997
1998
1999
2000
2001
2002
2003
2004
2005
2006
2007
2008
2009
2010
2011
photosystem II
ribosome
virus
transfer RNA
myosin
hemoglobin
antibody
nucleosome
lysozyme
actin
myoglobin

PDB Statistics: Overall Growth of Released Structures Per Year



https://www.rcsb.org/stats/growth/overall

Métodos Experimentais & Sistemas Estudados

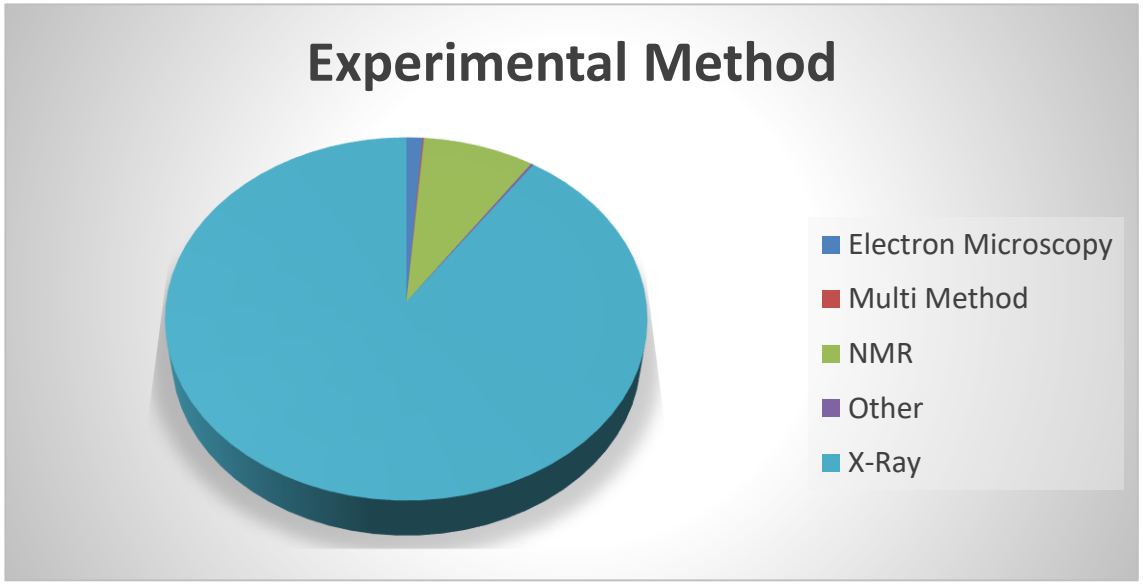
PDB Data Distribution by Experimental Method and Molecular Type

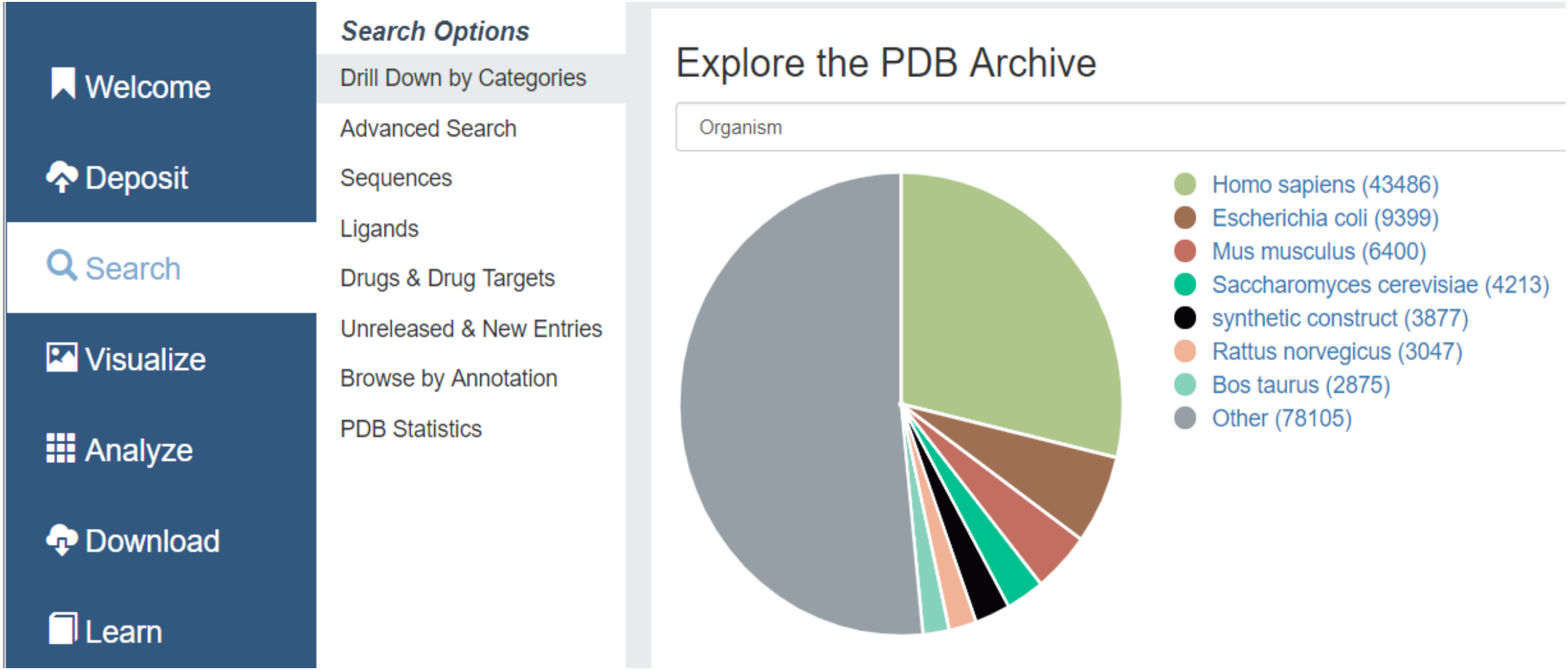
Copy | CSV

Experimental	Proteins	Nucleic Acids	Protein/NA Complex	Other	Total
X-Ray	125909	1999	6509	8	134425
NMR	11031	1277	259	8	12575
Electron Microscopy	2181	31	771	0	2983
Other	252	4	6	13	275
Multi Method	127	5	2	1	135
Total	139500	3316	7547	30	150393

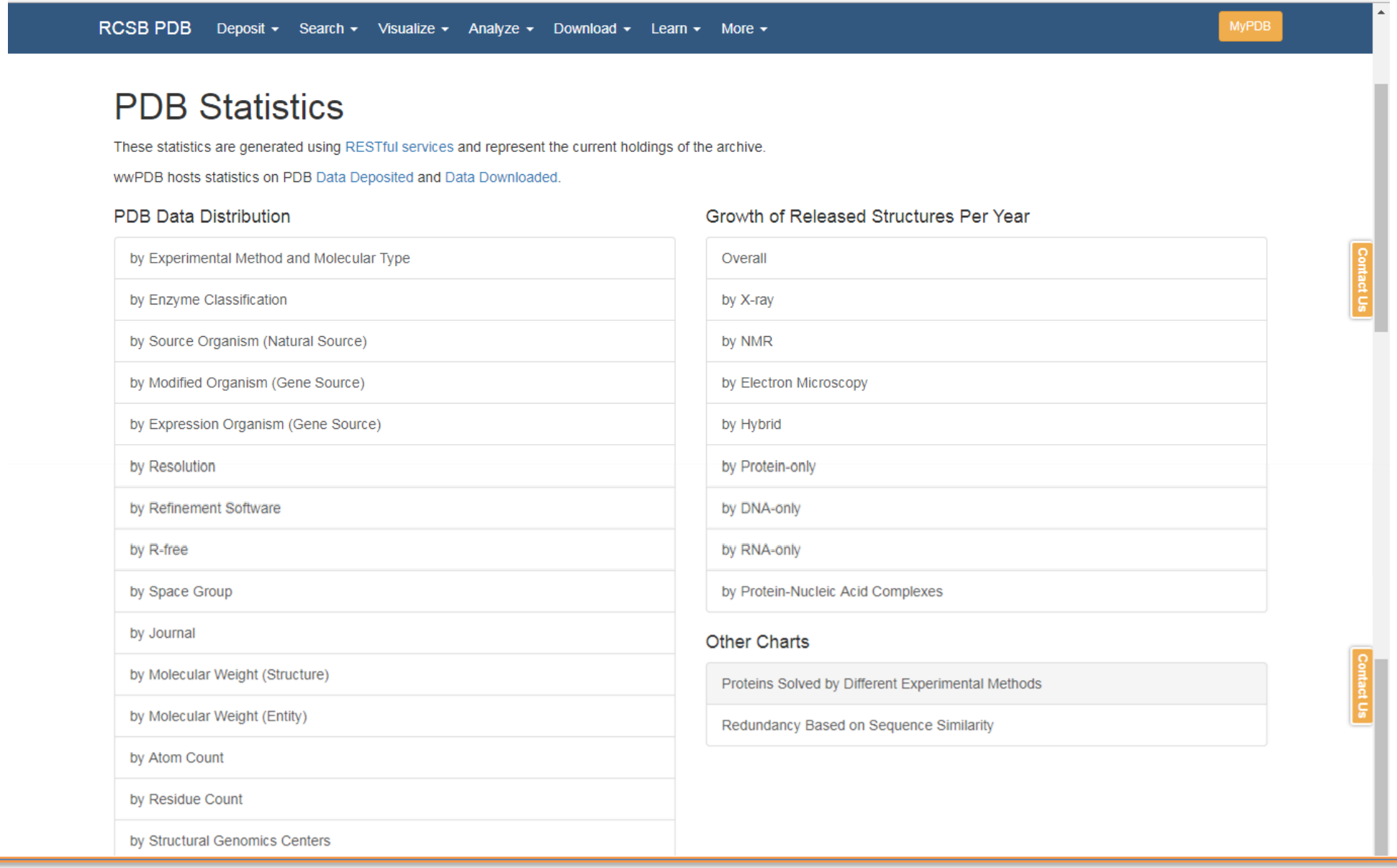
91% X-Ray

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




Welcome
Deposit
Search
Visualize
Analyze
Download
Learn
Search Options
Drill Down by Categories
Advanced Search
Sequences
Ligands
Drugs & Drug Targets
Unreleased & New Entries
Browse by Annotation
PDB Statistics
Explore the PDB Archive
Organism
Homo sapiens (43486)
Escherichia coli (9399)
Mus musculus (6400)
Saccharomyces cerevisiae (4213)
synthetic construct (3877)
Rattus norvegicus (3047)
Bos taurus (2875)
Other (78105)

Estatísticas



Estatísticas

PDB Statistics

These statistics are generated using RESTful services and represent the current holdings of the archive.

wwPDB hosts statistics on PDB Data Deposited and Data Downloaded.

PDB Data Distribution

- by Experimental Method and Molecular Type
- by Enzyme Classification
- by Source Organism (Natural Source)
- by Modified Organism (Gene Source)
- by Expression Organism (Gene Source)
- by Resolution
- by Refinement Software
- by R-free
- by Space Group
- by Journal
- by Molecular Weight (Structure)
- by Molecular Weight (Entity)
- by Atom Count
- by Residue Count
- by Structural Genomics Centers

Growth of Released Structures Per Year

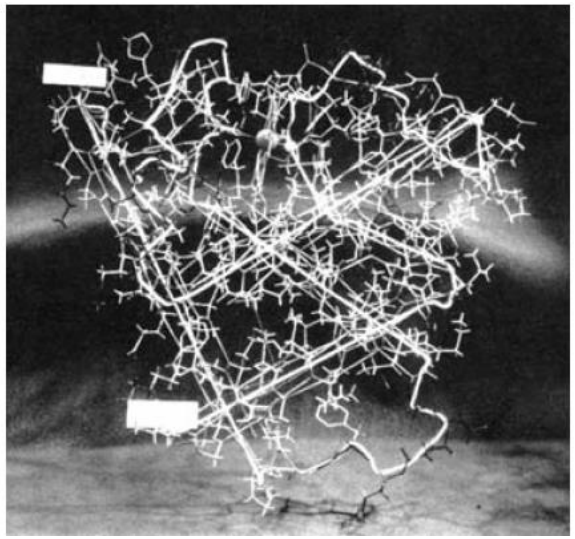
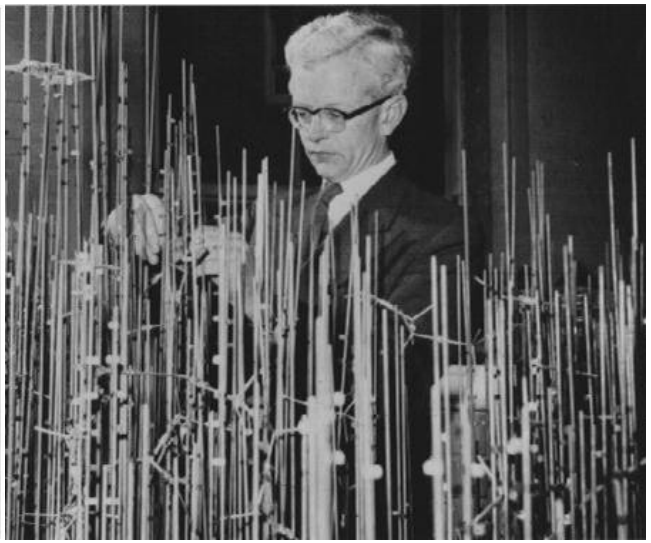
- Overall
- by X-ray
- by NMR
- by Electron Microscopy
- by Hybrid
- by Protein-only
- by DNA-only
- by RNA-only
- by Protein-Nucleic Acid Complexes

Other Charts

- Proteins Solved by Different Experimental Methods
- Redundancy Based on Sequence Similarity

https://www.rcsb.org/stats

Moléculas e representação

coordenadas

obter dados

visualizar

armazenar

PDBSum

PDBsum foi criado em 1995 no University College London.

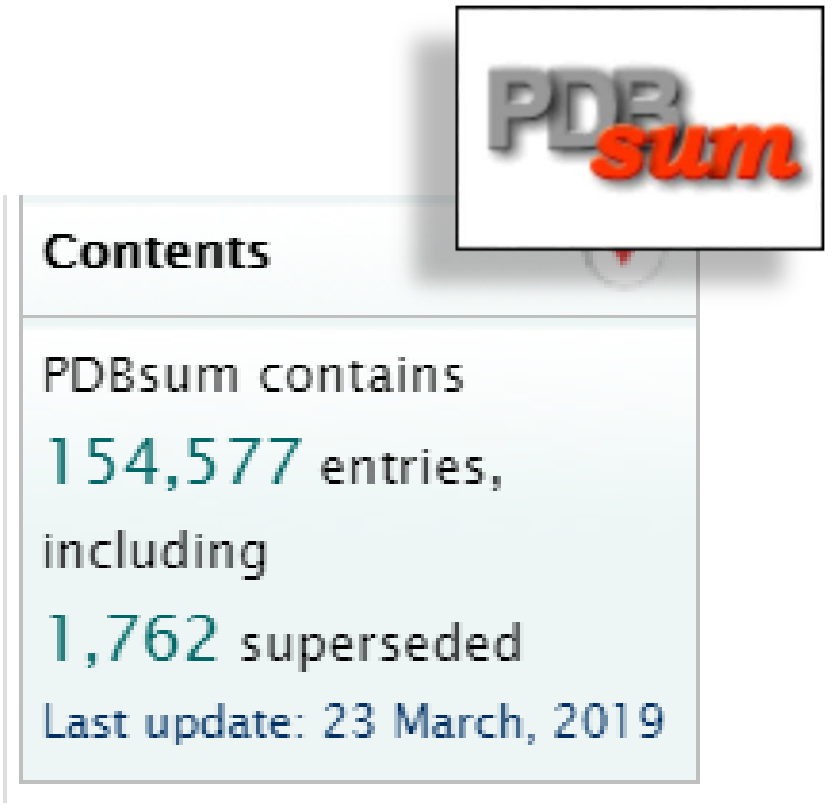
http://www.ebi.ac.uk/pdbsum/

O PDBSum foi construído com uma forma mais resumida e com uma visualização gráfica mais imediata, permitindo consultar os resultados a uma simples vista

RCSB PDB PROTEIN DATA BANK

150393 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

03/19/2019



NDB

Nucleic **A**cid **D**atabase - NDB , é um repositório de informações sobre ácidos nucléicos.

Em 27-Mar-2019 contém **10.103 estruturas**, envolvendo o DNA, RNA, DNA-RNA e complexos de DNA com proteínas, vírus e outras moléculas.

http://ndbserver.rutgers.edu/

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

NUCLEIC ACID DATABASE

A Portal for Three-dimensional Structural Information about Nucleic Acids

As of 27-Mar-2019 number of released structures: 10103

Search DNA | Search RNA | Advanced Search

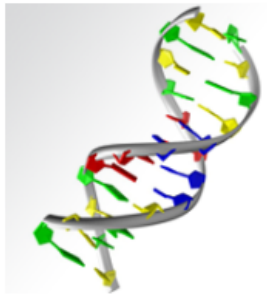
Enter an NDB ID or PDB ID

Search for released structures

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

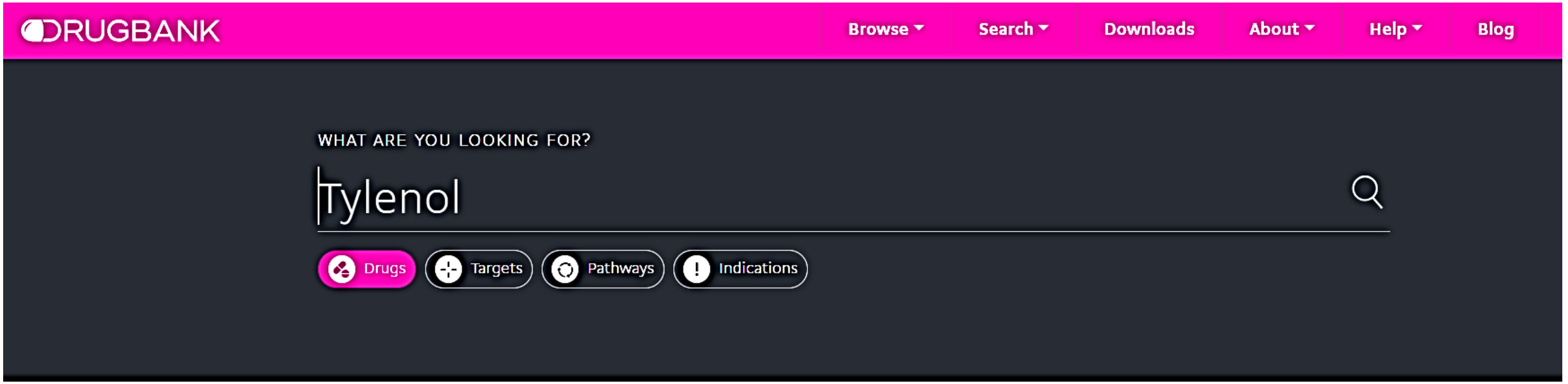
R3D Align, an application for detailed nucleotide to nucleotide alignments of RNA 3D structures

DrugBank

DrugBank

The DrugBank database is a unique bioinformatics and cheminformatics resource that combines detailed drug (i.e. chemical, pharmacological and pharmaceutical) data with comprehensive drug target (i.e. sequence, structure, and pathway) information.

http://www.drugbank.ca/



DRUGBANK

The DrugBank database is a unique bioinformatics and cheminformatics resource that combines detailed drug data with comprehensive drug target information.

> The latest release of DrugBank (version 5.1.2, released 2018-12-20) contains 12,112 drug entries including 2,556 approved small molecule drugs, 1,280 approved biotech (protein/peptide) drugs, 130 nutraceuticals and over 5,842 experimental drugs. Additionally, 5,161 non-redundant protein (i.e. drug target/enzyme/transporter/carrier) sequences are linked to these drug entries. Each DrugCard entry