Chapter-02. 重要生物信息资源

本章内容

- 2.1 引言
- 2.2 NCBI系列数据库及数据资源
- 2.3 UCSC基因组浏览器与数据资源
- 2.4 EMBL-EBI数据库与数据资源
- 2.5 其他重要生物信息学资源
- 2.6 数据批量获取方法

第1节：引言----数据是源头、软件是手段

重要知识点

- ✓ Database and Biological database
- ✓ Database language and tool
- ✓ Primary and secondary databases
- ✓ NCBI, EMBL, DDBJ
- ✓ Software, tools

❖ 1.1 关于生物信息学数据库

1). 数据库（Database）

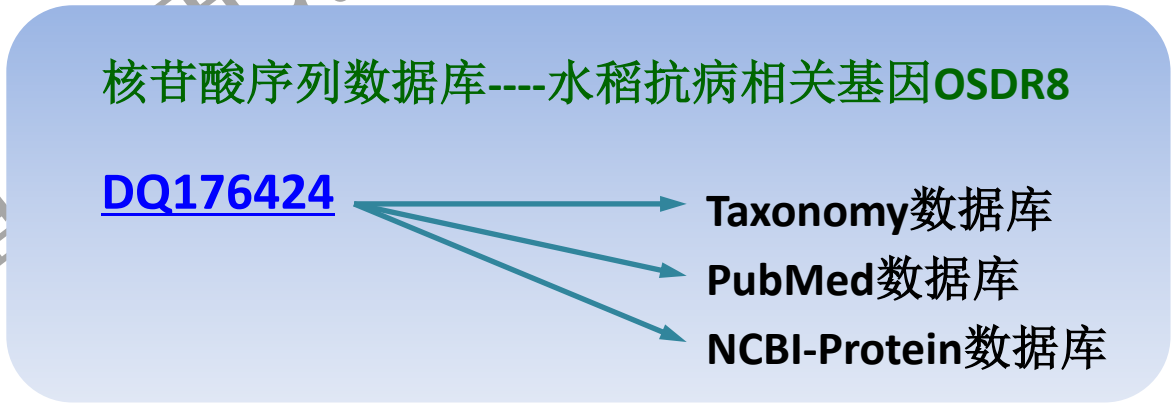
用于收集、整理、储存、加工、发布和检索数据的系统。

A. 不同层次的数据库

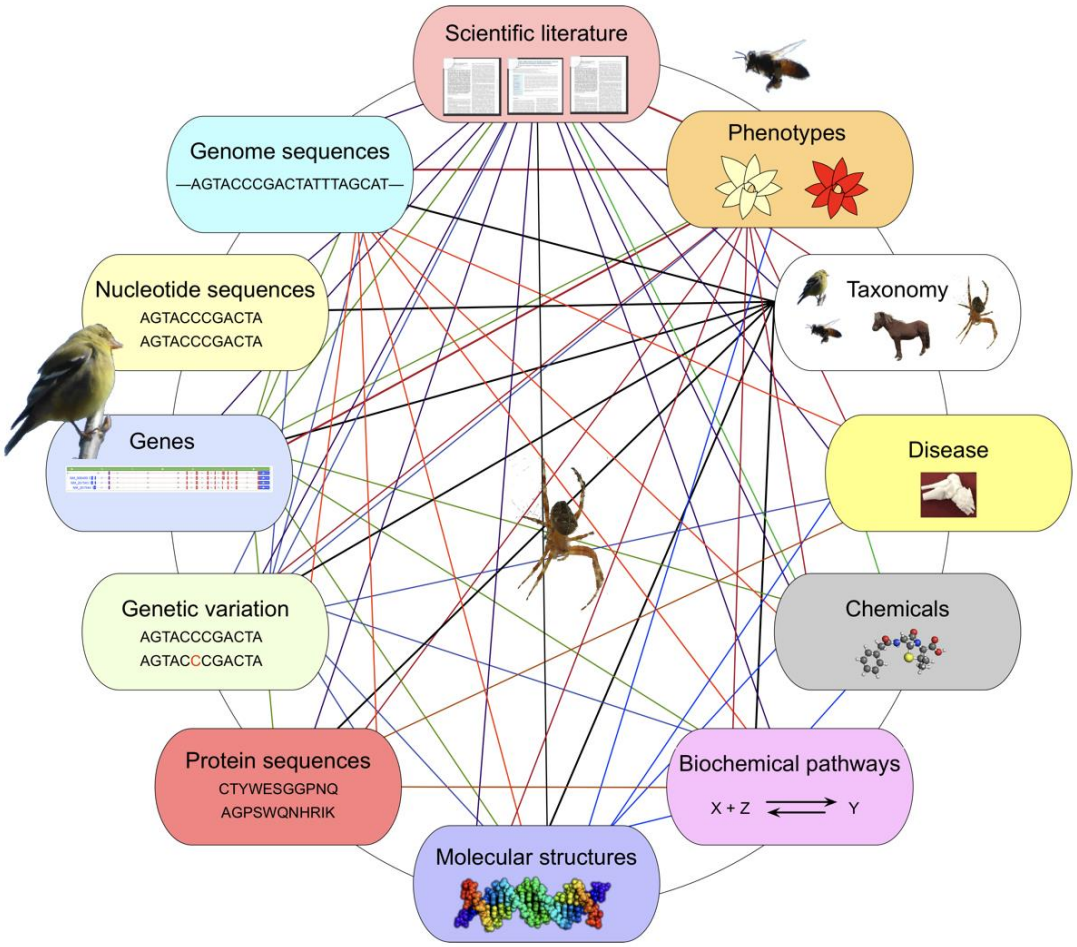
B. 通过互联网访问数据库

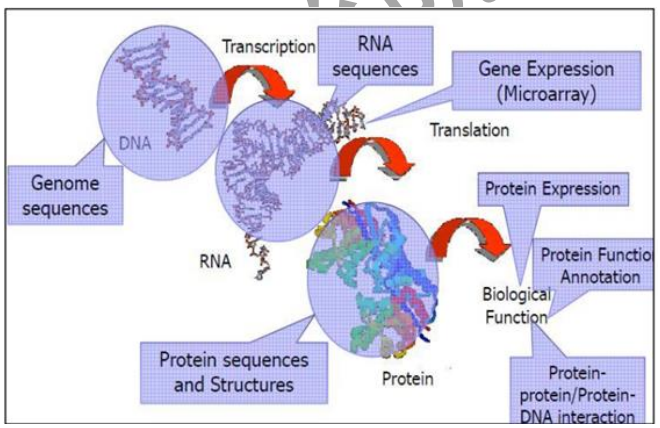
2). 数据库工具

- ✓ SQL（结构化查询语言）-世界上最流行的标准化的数据库语言，能快速存储记录文件和图像等。
- ✓ Access，Oracle等
- ✓ 生物类的数据库种类很多（序列、结构、分子间的互作等）。
- ✓ 文章投稿之前，需要先将各种核酸和蛋白质序列提交至特定的公开数据库中。
- ✓ 数据库的记录，通常包括两部分：原始数据 + 注释
- ✓ 一个数据库，通常会链接到多个相关的数据库。



Many kinds of bioinformatics databases





These are the biological data types

- nucleotide sequences
- gene level or expression data
- protein sequences
- proteins sequence patterns or motifs
- macromolecular 3D structure
- metabolic pathways

常见的生物信息学数据库

- 基因组数据库，如

  Human（https://www.ncbi.nlm.nih.gov/genome/guide/human/）

  MGD（http://www.informatics.jax.org）

  Wormbase （http://www.wormbase.org）

  Flybase（http://flybase.net）

- 核酸序列数据库，如

  GenBank（https://www.ncbi.nlm.nih.gov/genbank/）

- 蛋白质序列数据库，**如PIR-PSD、Swiss-Prot、TrEMBL、UniProt等**

  Uniprot（http://www. uniprot.org）

- 生物大分子三维结构数据库

- 其他二次专业数据库，**如药物靶点数据库TTD等**

3).Biomolecular Data Resources:

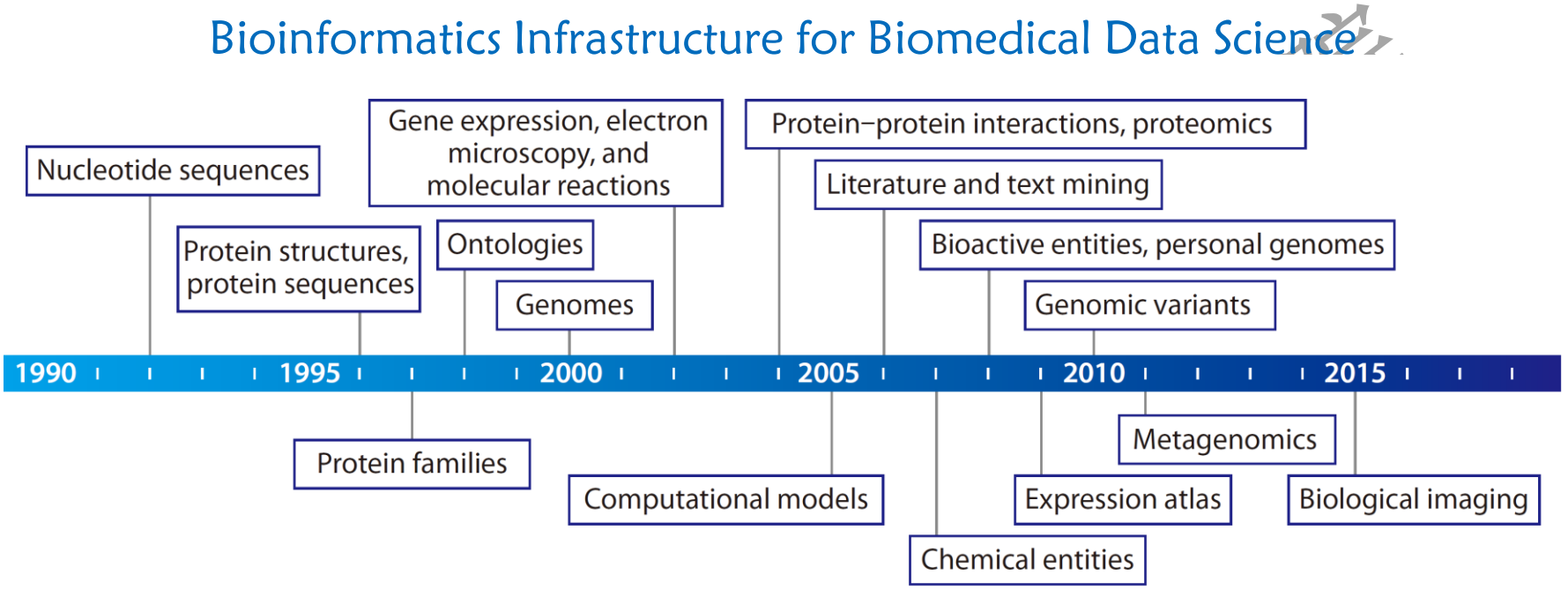


Figure 1

Time line of biomolecular data types and the establishment of data resources. From the emergence of the first shotgun nucleotide sequencing reads, advances in various types of technologies have resulted in the subsequent development of several types of data resources at the European Bioinformatics Institute of the European Molecular Biology Laboratory (EMBL-EBI). These include both archival and added-value data resources, as well as cross-supporting resources such as ontologies and literature resources.

Annu. Rev. Biomed. Data Sci. 2019. 2:199–222

❖ 1.3 国际三大核苷酸序列数据库

- ✓ **International Nucleotide Sequence Database Collaboration (INSDC，国际核苷酸序列数据库联盟)**

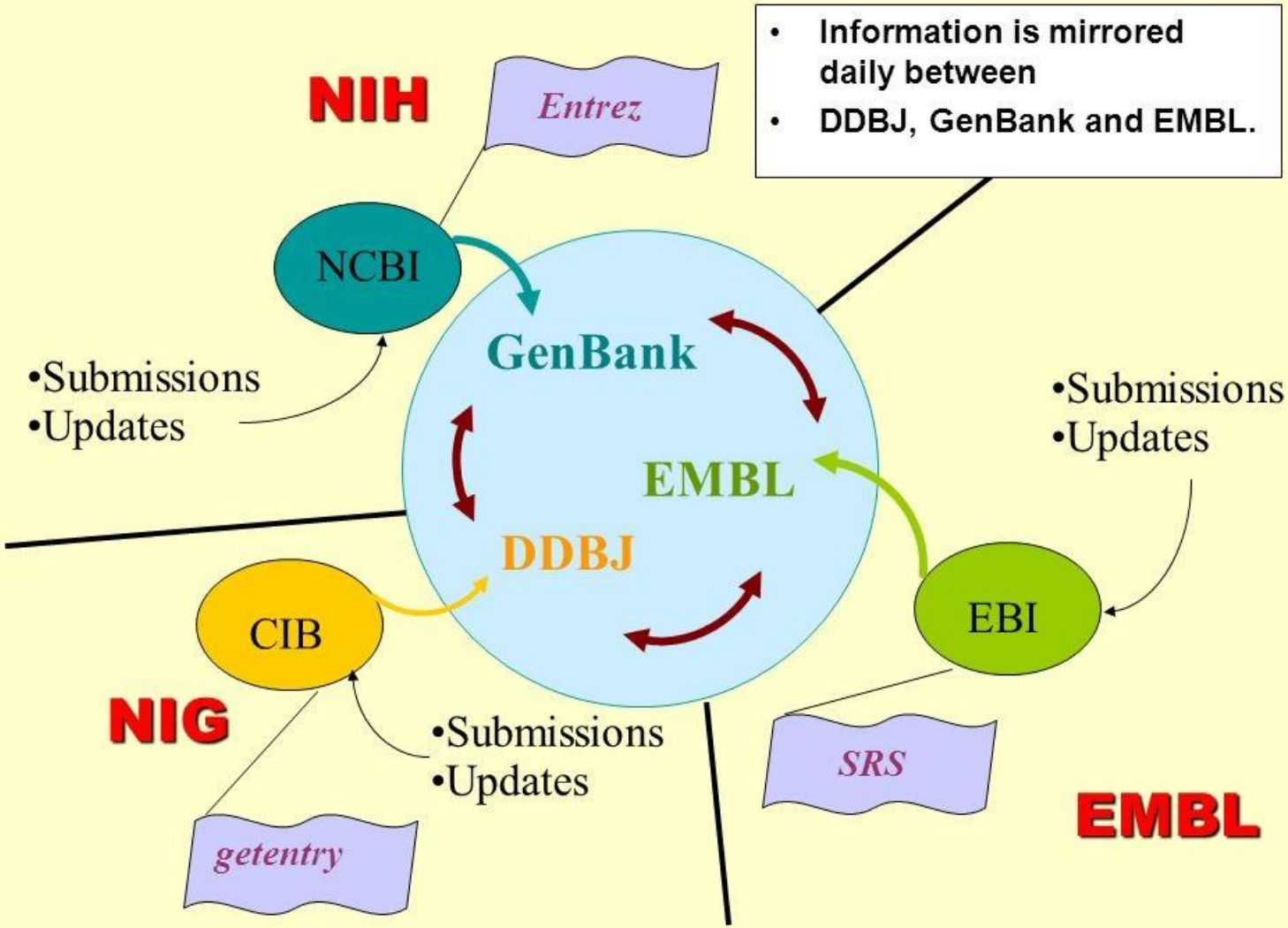
  GenBank [美] http://www.ncbi.nlm.nih.gov/Genbank

  EMBL [欧] http://www.ebi.ac.uk/embl/

  DDBJ [日] http://www.ddbj.nig.ac.jp/

- ✓ **每天这三个数据库作数据同步操作**
- ✓ 在任何一个数据库操作(查找、投递数据等)是等效的。

4). 三大核酸数据库


• Information is mirrored daily between
• DDBJ, GenBank and EMBL.
NIH
Entrez
NCBI
•Submissions
•Updates
GenBank
EMBL
DDBJ
•Submissions
•Updates
EBI
CIB
NIG
•Submissions
•Updates
SRS
EMBL
getentry

5). NIG

- 日本国立遗传学研究所(National Institute of Genetics)
- 创立于1949年7月1日,属文部省管辖
- 信息服务始于1984年
- 维护管理着*DDBJ*
  - 1987年1月发行DDBJ第一版
- http://www.nig.ac.jp

Research Highlights

2019/09/11 New
A new homologous recombination factor, HROB, controls the MCM8-MCM9 pathway

2019/09/05 New
Neural signatures of sleep in zebrafish

2019/08/30 New Press release
Glia-neuron interactions underlie state transitions to generalized seizures

2019/08/28 New Press release
The making of 'Fancy Mouse': Study reveals true cause of colorful hair on popular East Asian pet mice

2019/08/21 New
DFAST: Prokaryotic genome annotation pipeline for data submission to DDBJ

More

Seminar・Meetings

2019/09/20 13:30-14:30
Patterning chromatin with histone variants controls transcription

2019/09/24 11:00-12:00
Genetic basis of nervous-system response to stress and injury

2019/09/27 10:00-11:00
Cell-type-specific patterned activities specify gene expression patterns for olfactory circuit formation

2019/09/27 15:30-16:30
細胞内部の分子レベルイメージングを目指して
(Towards Molecular-level Imaging in Whole Cell)

Seminar Meetings

Information

2019/09/09 New
Message From NIGINTERN 2019

2019/07/10
Summer Holiday (Aug. 15,16)

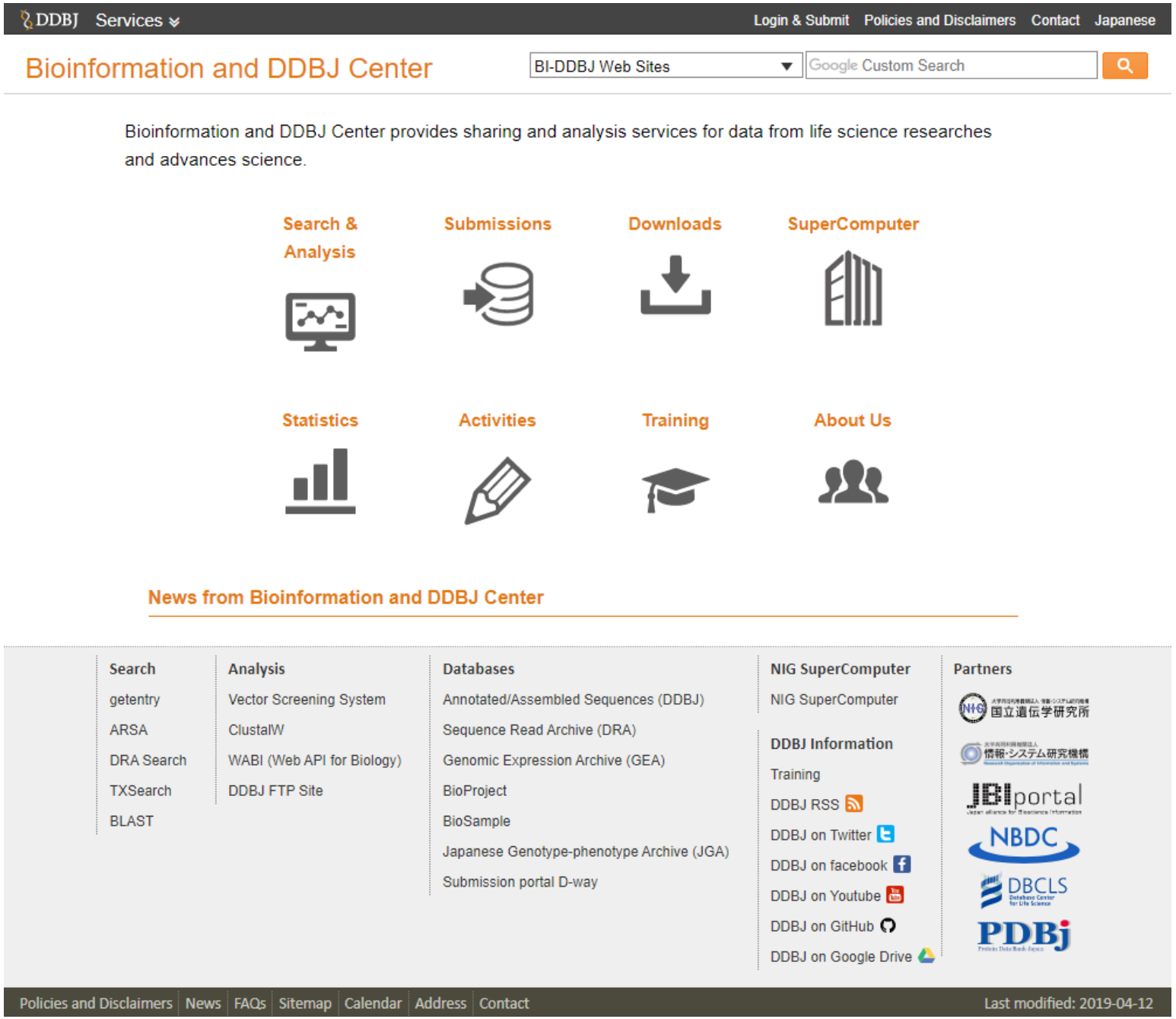
2019/07/01
Faculty member SHIMAMOTO at the Center for Frontier Research has been awarded tenure

2019/06/27 Recruitment
NIG-GS (NIG Global Scholar) selection

2019/04/26 Post
Assistant Professor (Cell Dynamics and Signaling Laboratory)

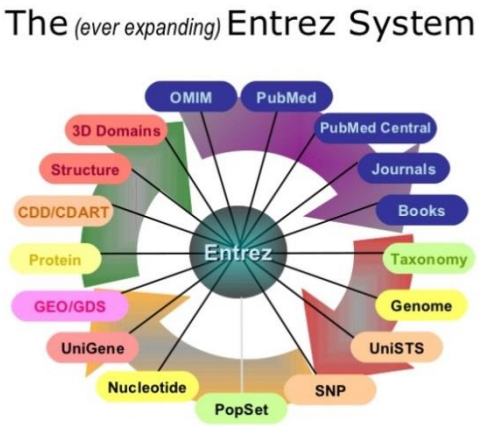
More

6).DDBJ homepage



第2节：NCBI数据库与数据资源

- **NCBI是由美国国立卫生研究院、国家医学图书馆（NLM）发起的，旨在推动分子生物学、生化、遗传学知识储存和文献整理。**
- **1988年NCBI建立,1992年GenBank成立，随后有PubMed（生物医学文献公共检索和分析平台）、OMIM（人类孟德尔遗传在线）、MMDB（3D蛋白结构分子模型数据库）、UniGene（特有人类基因序列集）、CGAP（癌症基因组剖析计划）等二级数据库。**

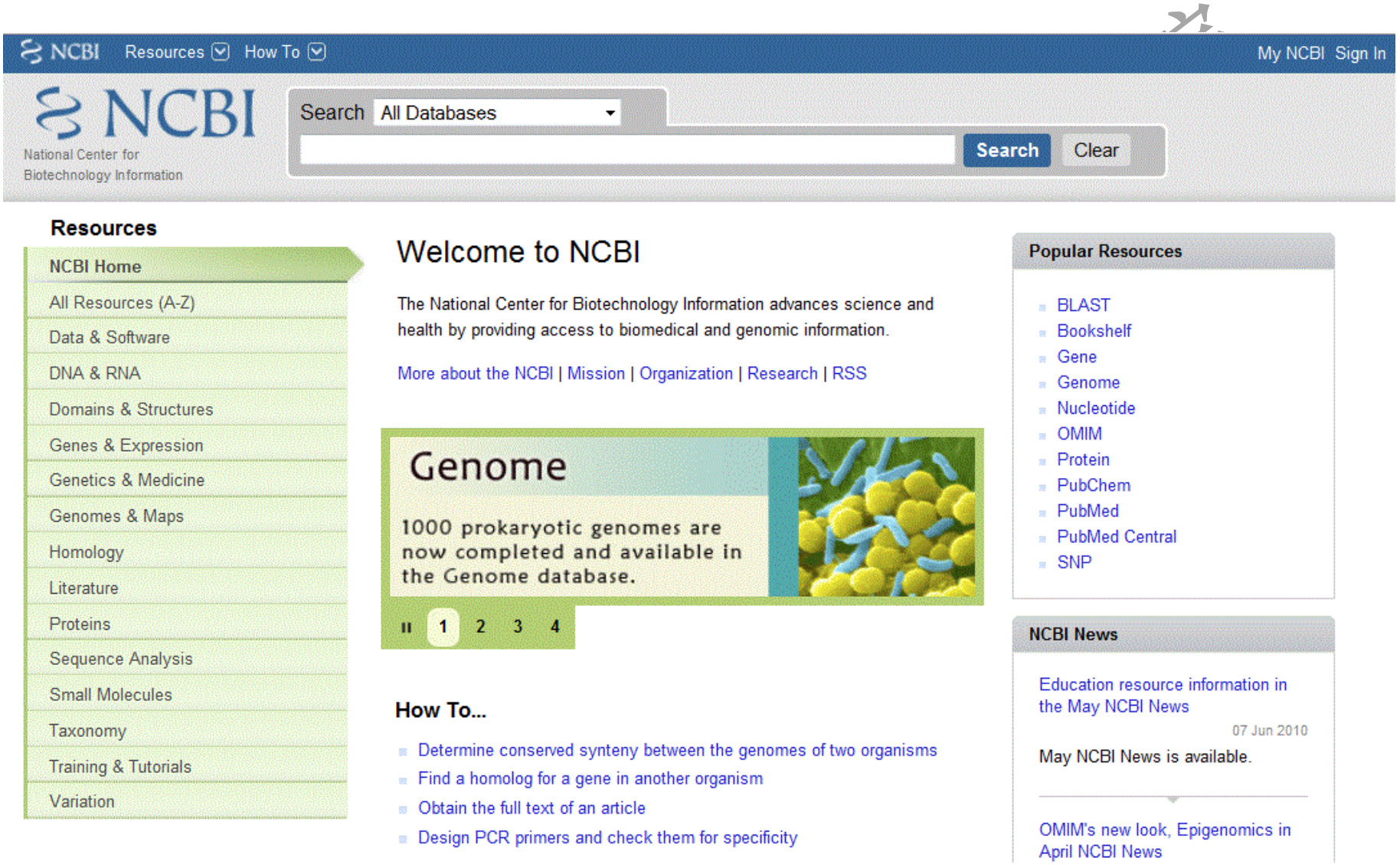


❖ 2.1 关于NCBI

美国国立生物技术信息中心

- 美国国家生物技术信息中心(National Center for Biotechnology Information)
- 前身是NIH所属的一个计算生物学研究室，1988年独立为NCBI，形式上属于国家医学图书馆(National Library of Medicine/NLM)
- 管理着许多著名数据库，如*GenBank*、PubMed、Medline、dbSNP、COG、OMIM等
- 提供Entrez、BLAST等服务
- 地址：http://www.ncbi.nlm.nih.gov

美国国立生物技术信息中心



❖ 2.2 NCBI旗下的生物信息学相关数据库

数据库名称	生物学功能分类
EST (Expressed Sequence Tag)	cDNA和cDNA特征序列
Nucleotide	核酸序列数据库
GSS (Genome Survey Sequence)	测序起始阶段的各种短reads（用于序列示踪、重复序列和基因数量预判等）
GEO	基因表达谱数据库
GenBank	公开可获得的已注释DNA序列（包括Nucleotide、GSS和EST三个子库）
RefSeq	在GenBank基础上给予每个基因一个可靠的注释条目，构成该数据库
Gene	收录全部已测序物种的基因注释信息，是目前最权威的基因注解数据库，标识码问Entrez ID
Genome	完整的基因组数据库
遗传多态数据库（dbSNP、dbVar、dbGap和ClinVar）	分别收录所有物种中发现的短序列多态和突变信息、较大规模的基因组变异、以遗传多态为分子标记物的基因型和表型关联性研究数据，以及临床上发现啊或报道的有证据支持的与人类健康有关的变异位点
蛋白质数据库（Protein Cluster、Structure等）	蛋白质分类、三维结构等信息
Unigene	针对每个基因建立一个独立的数据体系，分别将不同来源的基因序列、蛋白相似性、表达、定位等信息罗列和比较，提供一个整合的数据资源

Table 1. The Entrez Databases (as of 9 September 2020)

Database	Records	Description
Literature		
PubMed	31 471 600	scientific and medical abstracts/citations
PubMed Central	6 447 271	full-text journal articles
NLM catalog	1 619 856	index of NLM collections
Books	825 385	books and reports
MeSH	300 500	ontology used for PubMed indexing
Genomes		
Nucleotide	429 731 711	DNA and RNA sequences
BioSample	14 628 076	descriptions of biological source materials
SRA	11 807 161	high-throughput DNA and RNA sequence read archive
Taxonomy	2 401 136	taxonomic classification and nomenclature catalog
Assembly	837 406	genome assembly information
BioProject	458 893	biological projects providing data to NCBI
Genome	55 580	genome sequencing projects by organism
BioCollections	8 138	museum, herbaria and other biorepository collections
Genes		
GEO Profiles	128 414 055	gene expression and molecular abundance profiles
Gene	28 377 759	collected information about gene loci
GEO datasets	4 002 373	functional genomics studies
PopSet	350 627	sequence sets from phylogenetic and population studies
HomoloGene	141 268	homologous gene sets for selected organisms
Genetics		
SNP	720 643 623	short genetic variations
dbVar	6 030 887	genome structural variation studies
ClinVar	845 008	human variations of clinical significance
MedGen	335 277	medical genetics literature and links
GTR	76 814	genetic testing registry
dbGaP	1 397	genotype/phenotype interaction studies
Proteins		
Protein	874 272 642	protein sequences
Identical protein groups	329 946 078	protein sequences grouped by identity
Protein clusters	1 137 329	sequence similarity-based protein clusters
Structure	167 650	experimentally-determined biomolecular structures
Sparcle	149 462	conserved domain architectures
Conserved domains	59 951	conserved protein domains
Chemicals		
PubChem substance	285 048 146	deposited substance and chemical information
PubChem compound	111 325 418	chemical information with structures, information and links
PubChem BioAssay	1 229 071	bioactivity screening studies
BioSystems	983 968	molecular pathways with links to genes, proteins and chemicals

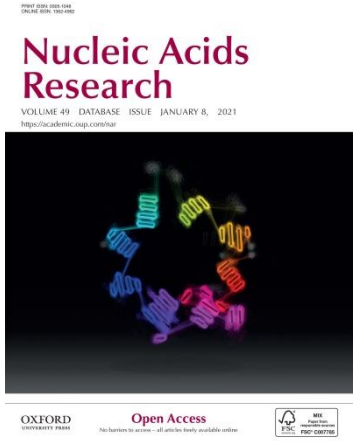


Fig. *Landing page for the new NCBI Datasets product* (*https://www.ncbi.nlm.nih.gov/datasets/*) *that provides packaged downloads of genomic datasets using either a web interface, an API, or a LINUX command-line tool.*

Welcome to NCBI Datasets BETA

NCBI Datasets is an experimental resource for finding and building datasets - and we're just getting started! Our web interface allows you to download genome sequence and annotation for eukaryotic organisms and our recently added SARS-CoV-2 genome and protein datasets. ... more

Programmatic access

Bacterial and viral data are not yet supported for online browsing. For access to data for all organisms, including bacteria and viruses, use our command line tool and RESTful APIs.

Command-line

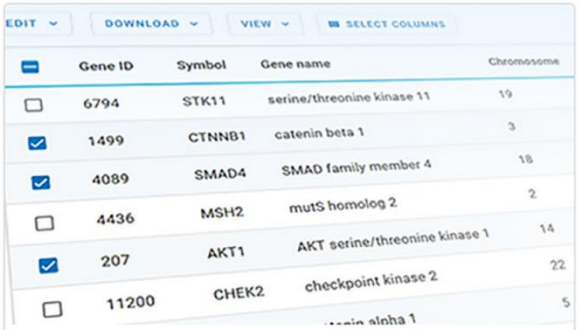
Our Datasets command-line tool, is available for Windows, Mac, and Linux.

GitHub

Explore Datasets with our Python library and Jupyter notebooks.

Datasets API

Use our RESTful APIs to add functionality to your applications.



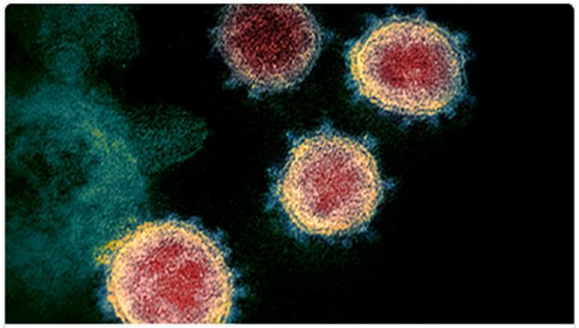
Data tables

Build a table of genes or transcripts and choose from a variety of custom columns.

GET STARTED

Browsing genome datasets

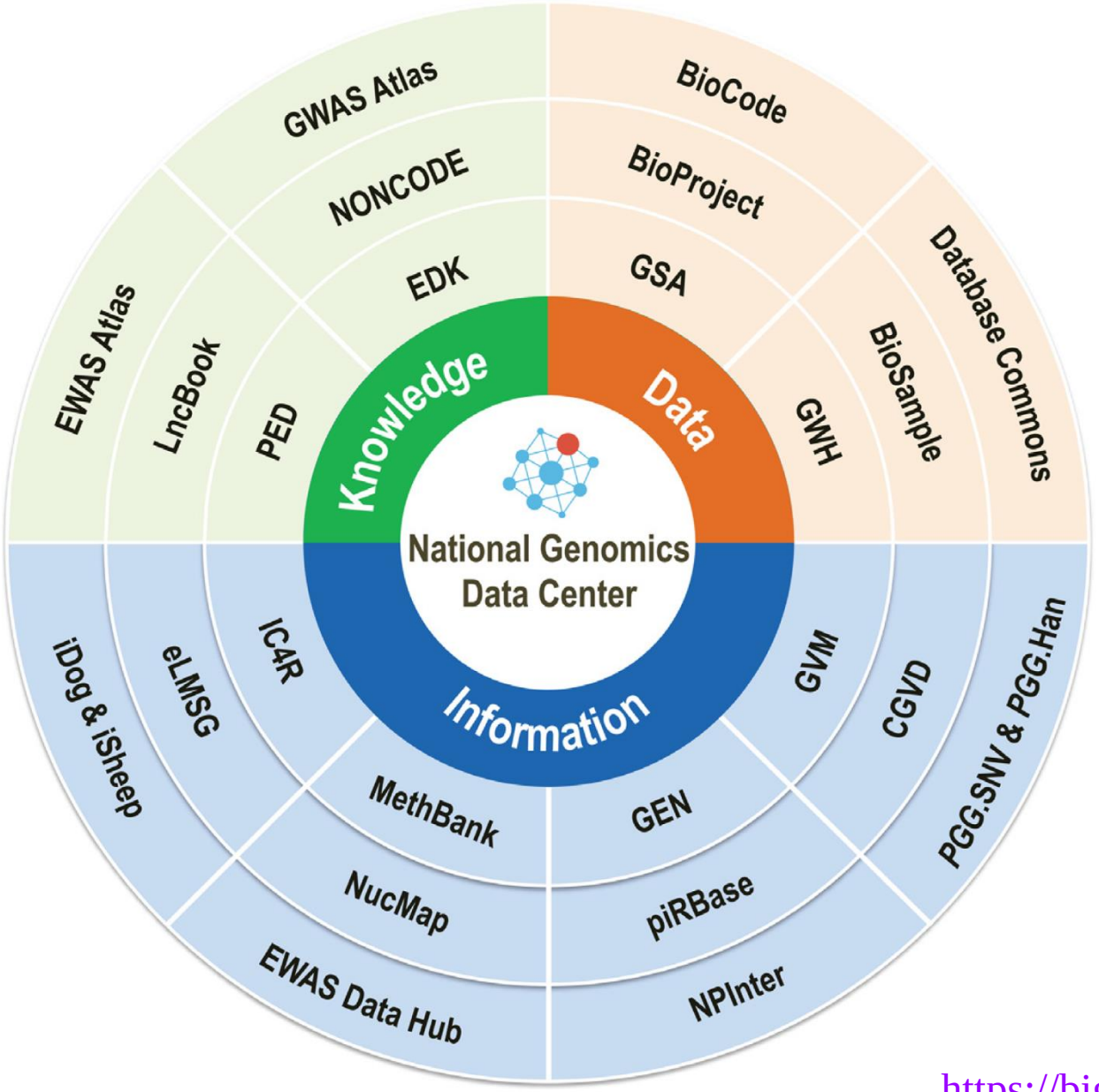
Homo sapiens human	129 assemblies
Mus musculus house mouse	22 assemblies
Arabidopsis thaliana thale cress	30 assemblies



Coronavirus datasets

Download SARS-CoV-2 genome and protein sequences, annotation and a data report for all complete genomes.

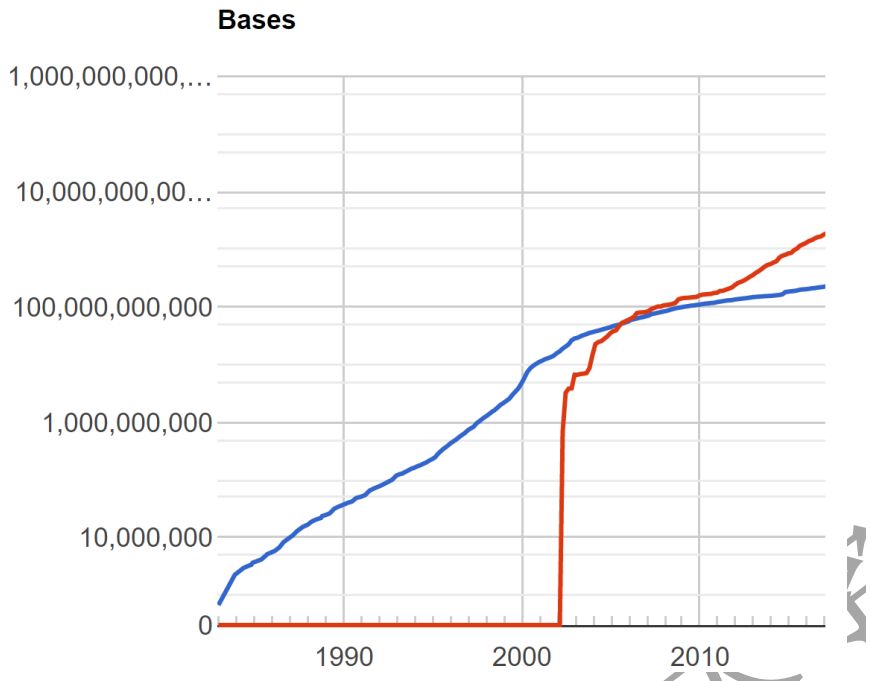
GET DATA

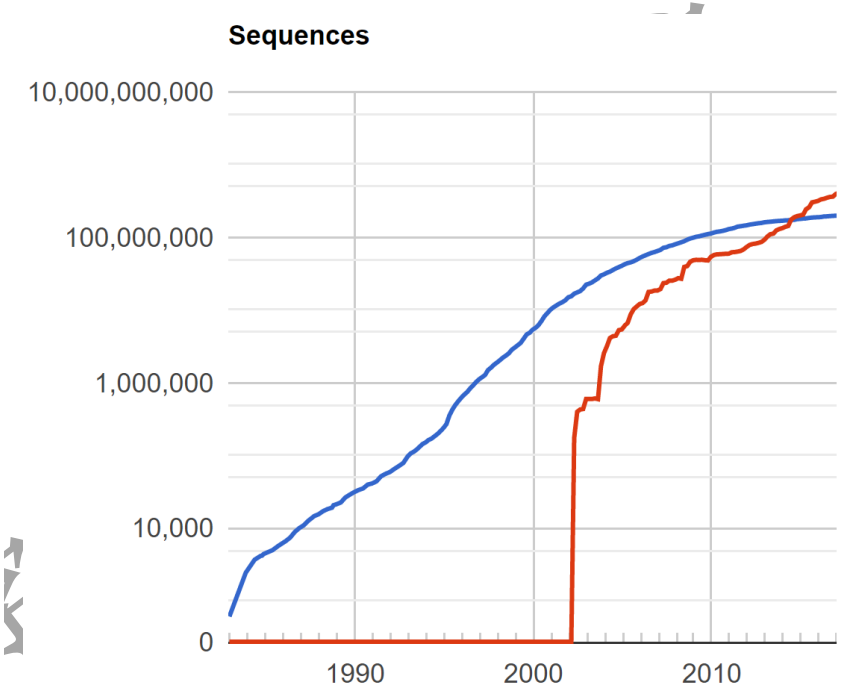


https://bigd.big.ac.cn/

Fig. The National Genomics Data Center's core data resources.

GenBank statistics





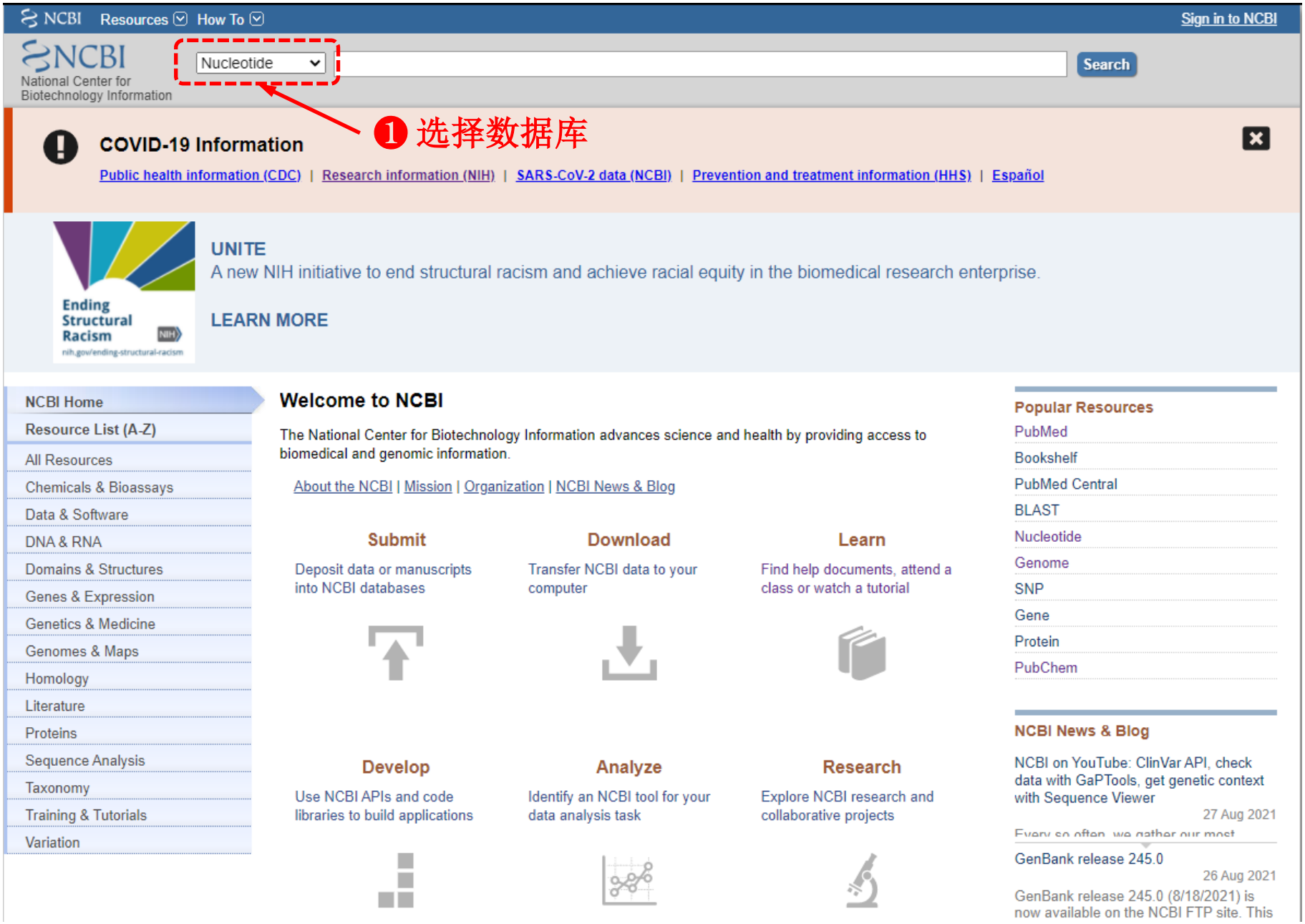
Above figures showed that the number of bases and the number of sequence records in each release of GenBank, beginning with Release 3 in 1982. CON-division records are not represented in these statistics: because they are constructed from the non-CON records in the database, their inclusion here would be a form of double-counting. From 1982 to the present, **the number of bases in GenBank has doubled approximately every 18 months**.

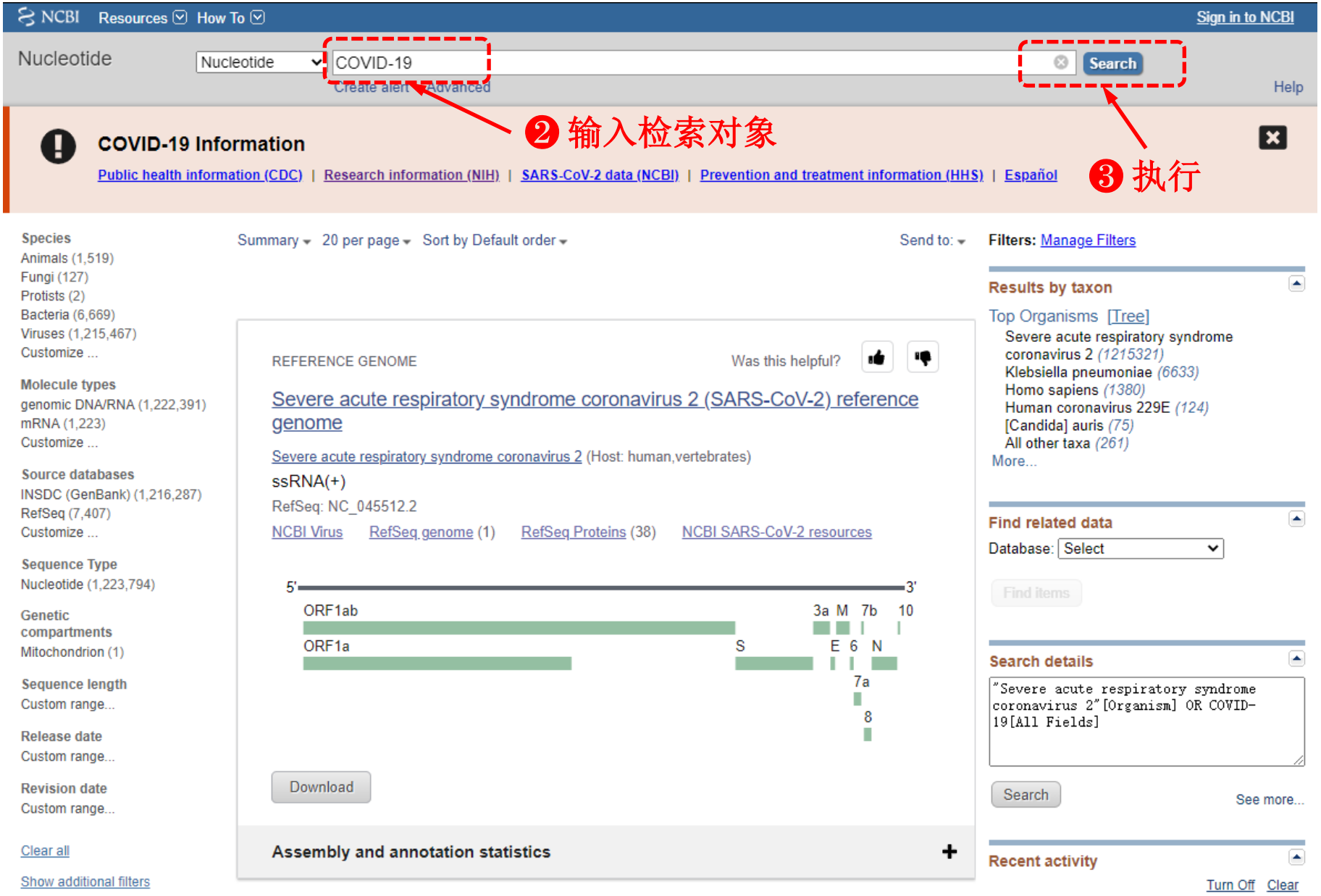
❖ 2.3 生物信息学数据库的使用实例

【实例1】

查询引起2019冠状病毒病（COVID-19）的病原体的全基因组序列，并了解其基因组的基本结构。

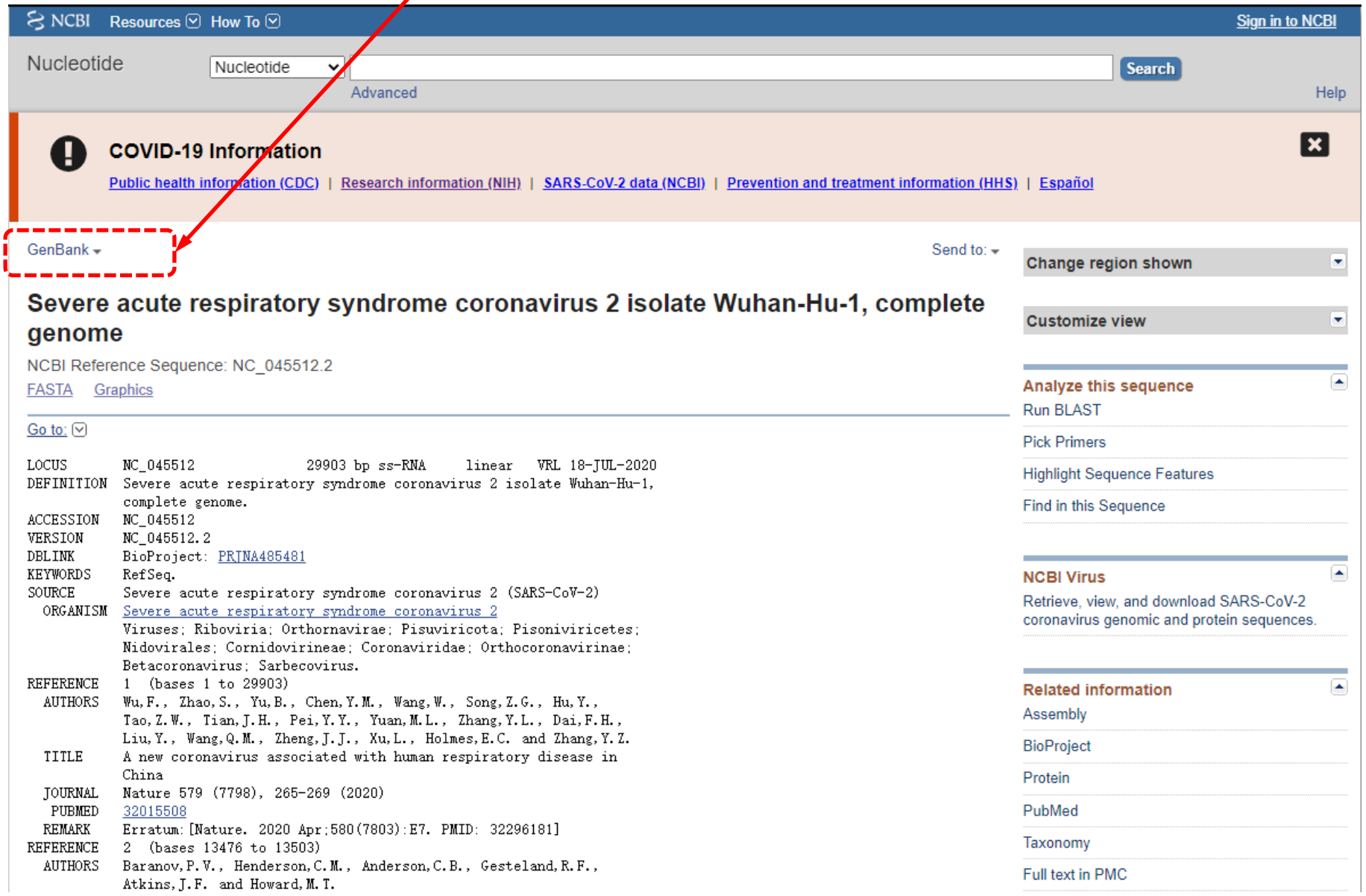
人类新型冠状病毒：***SARS-CoV-2***


NCBI Resources How To
Sign in to NCBI
NCBI
National Center for Biotechnology Information
Nucleotide
Search
❶ 选择数据库
COVID-19 Information
Public health information (CDC) | Research information (NIH) | SARS-CoV-2 data (NCBI) | Prevention and treatment information (HHS) | Español
Ending Structural Racism
nih.gov/ending-structural-racism
UNITE
A new NIH initiative to end structural racism and achieve racial equity in the biomedical research enterprise.
LEARN MORE
NCBI Home
Resource List (A-Z)
All Resources
Chemicals & Bioassays
Data & Software
DNA & RNA
Domains & Structures
Genes & Expression
Genetics & Medicine
Genomes & Maps
Homology
Literature
Proteins
Sequence Analysis
Taxonomy
Training & Tutorials
Variation
Welcome to NCBI
The National Center for Biotechnology Information advances science and health by providing access to biomedical and genomic information.
About the NCBI | Mission | Organization | NCBI News & Blog
Submit
Deposit data or manuscripts into NCBI databases
Download
Transfer NCBI data to your computer
Learn
Find help documents, attend a class or watch a tutorial
Develop
Use NCBI APIs and code libraries to build applications
Analyze
Identify an NCBI tool for your data analysis task
Research
Explore NCBI research and collaborative projects
Popular Resources
PubMed
Bookshelf
PubMed Central
BLAST
Nucleotide
Genome
SNP
Gene
Protein
PubChem
NCBI News & Blog
NCBI on YouTube: ClinVar API, check data with GaPTools, get genetic context with Sequence Viewer
27 Aug 2021
GenBank release 245.0
26 Aug 2021
GenBank release 245.0 (8/18/2021) is now available on the NCBI FTP site. This



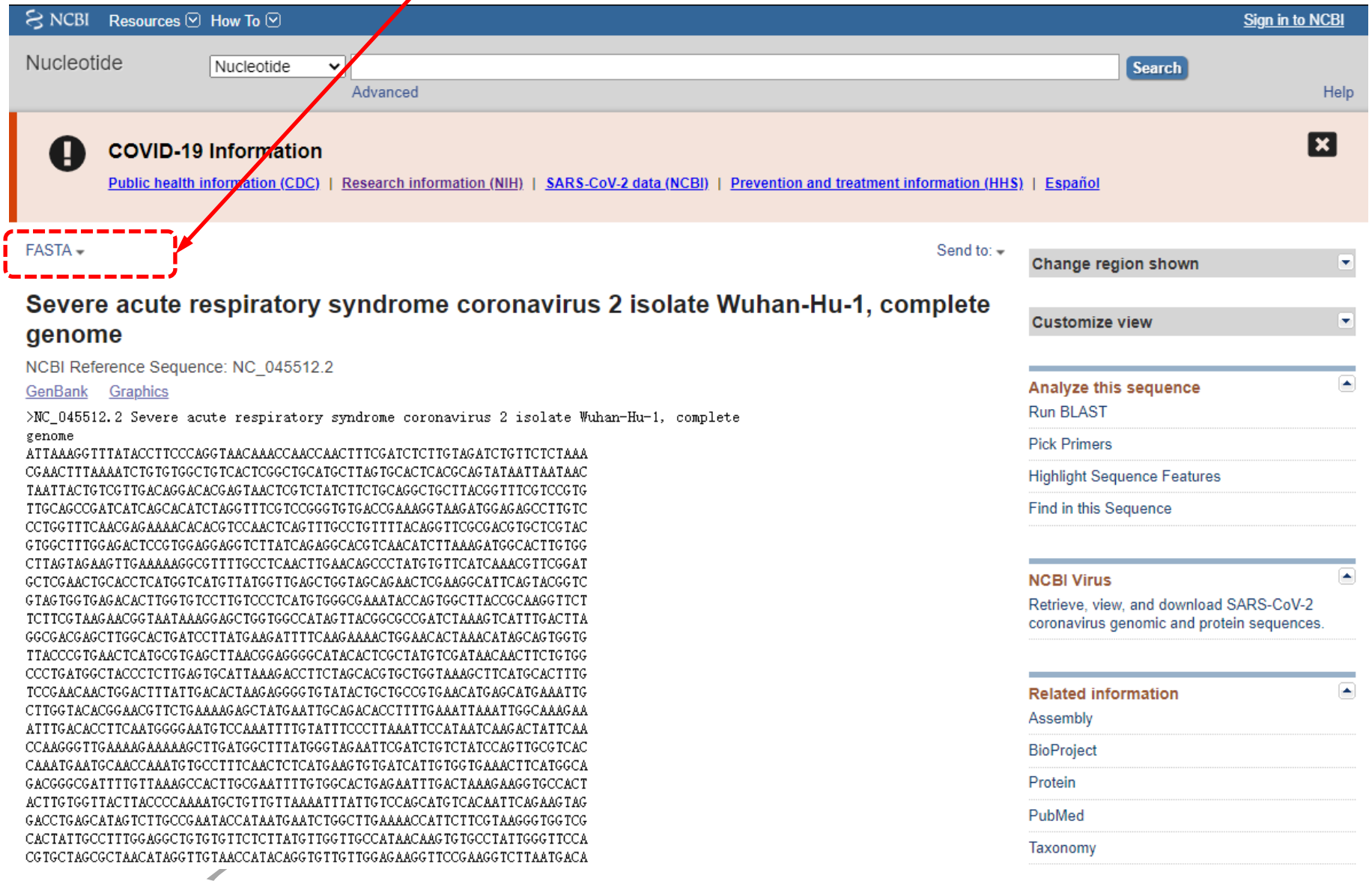
❹ 结果呈现 https://www.ncbi.nlm.nih.gov/nuccore/?term=COVID-19

❺ 展示COVID-19的全基因组序列（ GenBank格式）



https://www.ncbi.nlm.nih.gov/nuccore/1798174254

❻ 展示COVID-19的全基因组序列（ FASTA格式）



❼ 展示COVID-19的全基因组序列（ Graphics格式）

Graphics

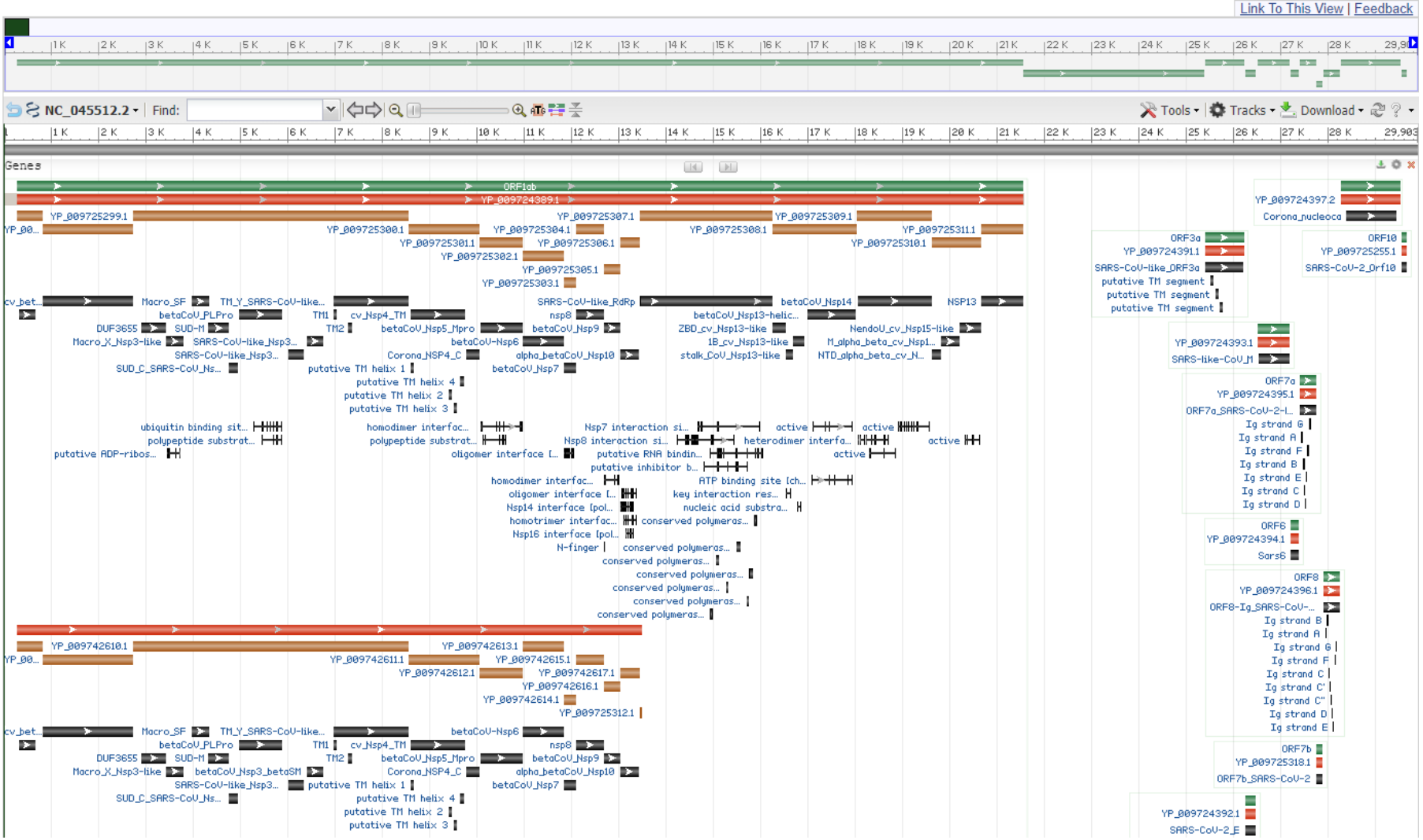
Send to:

Severe acute respiratory syndrome coronavirus 2 isolate Wuhan-Hu-1, complete genome

NCBI Reference Sequence: NC_045512.2

GenBank FASTA

Link To This View | Feedback



【实例2 】

对“人类beta-珠蛋白cDNA序列”进行相似性分析。

（提示：NM_000518.5;工具：在线BLAST）

步骤：

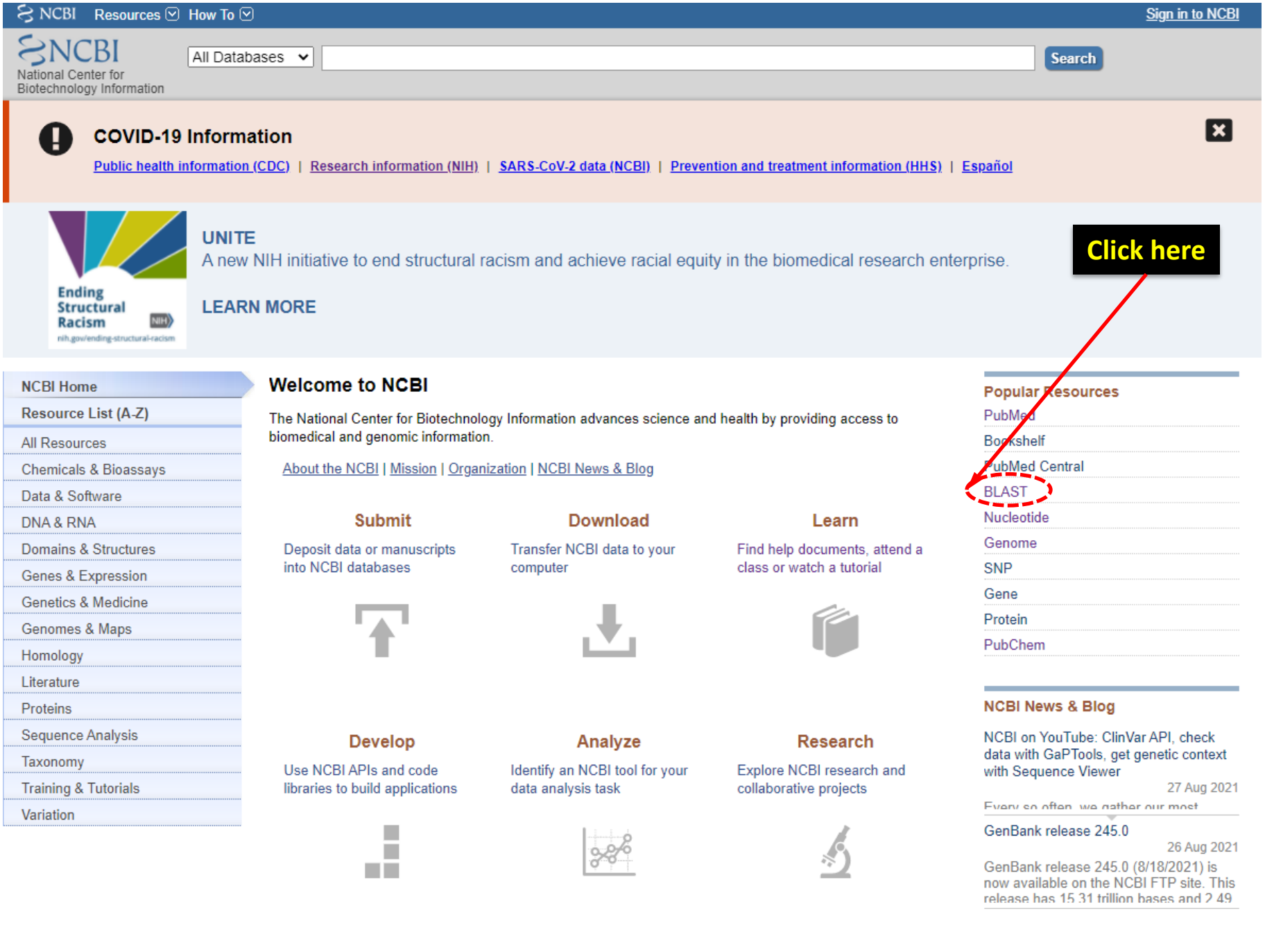
1、先检索出cDNA核苷酸序列

2、用FASTA格式显示

3、将FASTA格式全选后黏贴与BLAST检索框内

4、选择分析所用的数据库

5、点击BLAST按钮进行分析


NCBI Resources How To
Sign in to NCBI
NCBI
National Center for Biotechnology Information
All Databases
Search
COVID-19 Information
Public health information (CDC) | Research information (NIH) | SARS-CoV-2 data (NCBI) | Prevention and treatment information (HHS) | Español
Ending Structural Racism
nih.gov/ending-structural-racism
UNITE
A new NIH initiative to end structural racism and achieve racial equity in the biomedical research enterprise.
LEARN MORE
Click here
NCBI Home
Resource List (A-Z)
All Resources
Chemicals & Bioassays
Data & Software
DNA & RNA
Domains & Structures
Genes & Expression
Genetics & Medicine
Genomes & Maps
Homology
Literature
Proteins
Sequence Analysis
Taxonomy
Training & Tutorials
Variation
Welcome to NCBI
The National Center for Biotechnology Information advances science and health by providing access to biomedical and genomic information.
About the NCBI | Mission | Organization | NCBI News & Blog
Submit
Deposit data or manuscripts into NCBI databases
Download
Transfer NCBI data to your computer
Learn
Find help documents, attend a class or watch a tutorial
Develop
Use NCBI APIs and code libraries to build applications
Analyze
Identify an NCBI tool for your data analysis task
Research
Explore NCBI research and collaborative projects
Popular Resources
PubMed
Bookshelf
PubMed Central
BLAST
Nucleotide
Genome
SNP
Gene
Protein
PubChem
NCBI News & Blog
NCBI on YouTube: ClinVar API, check data with GaPTools, get genetic context with Sequence Viewer
27 Aug 2021
GenBank release 245.0
26 Aug 2021
GenBank release 245.0 (8/18/2021) is now available on the NCBI FTP site. This release has 15.31 trillion bases and 2.49

Basic Local Alignment Search Tool

BLAST finds regions of similarity between biological sequences. The program compares nucleotide or protein sequences to sequence databases and calculates the statistical significance. Learn more

NEWS

BLAST+ 2.12.0 is here!

We have made some improvements to how BLAST multi-threads and the amount of memory required by makeblastdb.

Tue, 13 Jul 2021 12:00:00 EST

More BLAST news...

Web BLAST

Nucleotide BLAST
nucleotide ▶ nucleotide

blastx
translated nucleotide ▶ protein

tblastn
protein ▶ translated nucleotide

Protein BLAST
protein ▶ protein

BLAST Genomes

Enter organism common name, scientific name, or tax id

Search

Human Mouse Rat Microbes

Standalone and API BLAST

Download BLAST
Get BLAST databases and executables

Use BLAST API
Call BLAST from your application

Use BLAST in the cloud
Start an instance at a cloud provider

BLAST® » blastn suite

Home

Standard Nucleotide BLAST

blastn | blastp | blastx | tblastn | tblastx

BLASTN programs search nucleotide databases using a nucleotide query. more...

Enter Query Sequence

Enter accession number(s), gi(s), or FASTA sequence(s) Clear

Query subrange

From

To

Or, upload file 选择文件 sequence.fasta

Job Title

Enter a descriptive title for your BLAST search

Align two or more sequences

Choose Search Set

Database: Standard databases (nr etc.): rRNA/ITS databases Genomic + transcript databases Betacoronavirus

Nucleotide collection (nr/nt)

Organism Optional: Enter organism name or id--completions will be suggested exclude Add organism

Enter organism common name, binomial, or tax id. Only 20 top taxa will be shown

Exclude Optional: Models (XM/XP) Uncultured/environmental sample sequences

Limit to Optional: Sequences from type material

Entrez Query Optional: YouTube Create custom database

Enter an Entrez query to limit search

Program Selection

Optimize for:

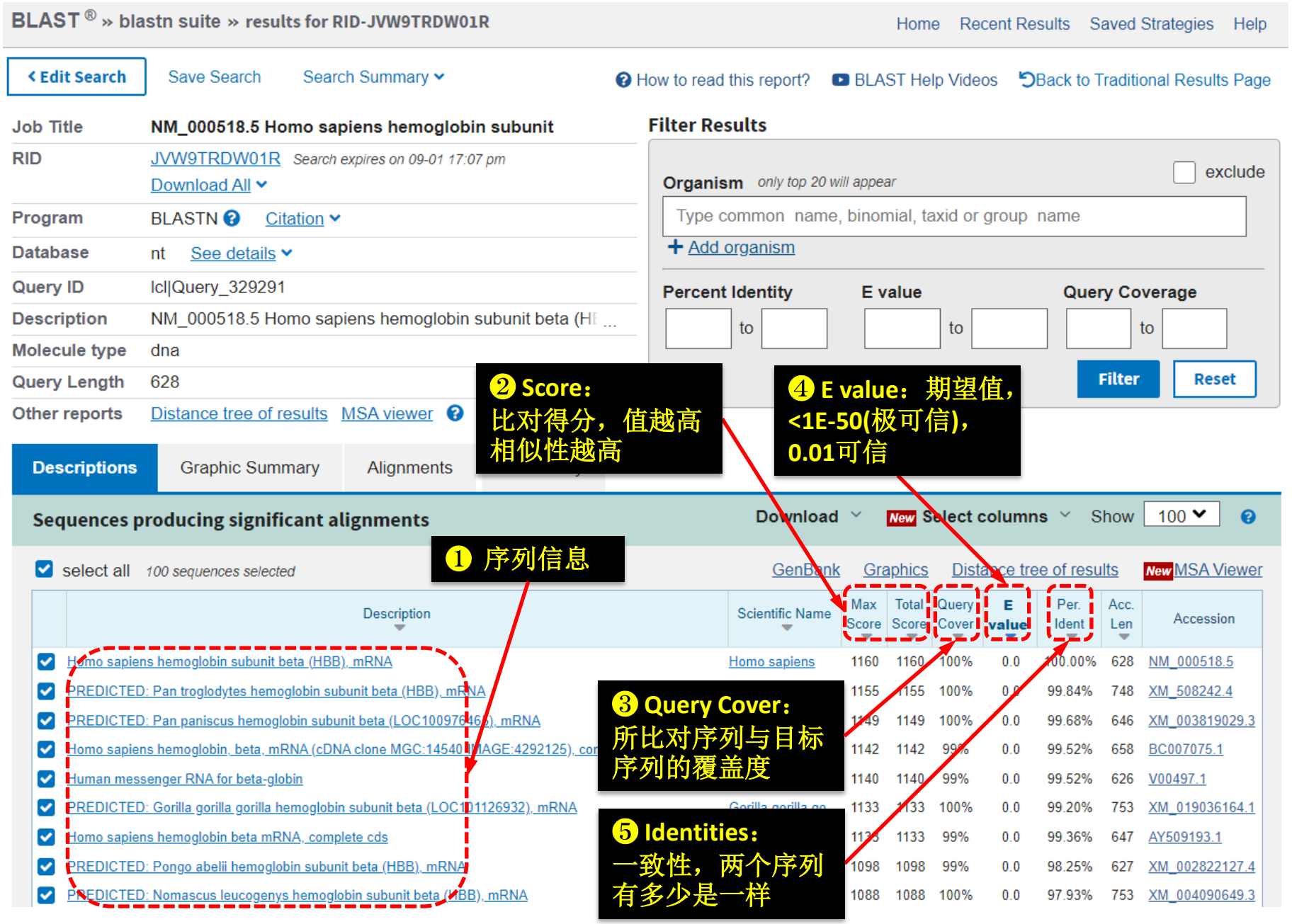
- Highly similar sequences (megablast)
- More dissimilar sequences (discontiguous megablast)
- Somewhat similar sequences (blastn)

Choose a BLAST algorithm

BLAST

Search database Nucleotide collection (nr/nt) using Megablast (Optimize for highly similar sequences)

Show results in a new window


BLAST® » blastn suite » results for RID-JVW9TRDW01R
Home
Recent Results
Saved Strategies
Help
Edit Search
Save Search
Search Summary
How to read this report?
BLAST Help Videos
Back to Traditional Results Page
Job Title
NM_000518.5 Homo sapiens hemoglobin subunit
RID
JVW9TRDW01R
Search expires on 09-01 17:07 pm
Download All
Program
BLASTN
Citation
Database
nt
See details
Query ID
lcl|Query_329291
Description
NM_000518.5 Homo sapiens hemoglobin subunit beta (H
Molecule type
dna
Query Length
628
Other reports
Distance tree of results
MSA viewer
Filter Results
Organism
only top 20 will appear
exclude
Type common name, binomial, taxid or group name
Add organism
Percent Identity
E value
Query Coverage
to
Filter
Reset
Descriptions
Graphic Summary
Alignments
Sequences producing significant alignments
Download
New
Select columns
Show
100
select all
100 sequences selected
GenBank
Graphics
Distance tree of results
New
MSA Viewer
Description
Scientific Name
Max Score
Total Score
Query Cover
E value
Per. Ident
Acc. Len
Accession
Homo sapiens hemoglobin subunit beta (HBB), mRNA
Homo sapiens
1160
1160
100%
0.0
100.00%
628
NM_000518.5
PREDICTED: Pan troglodytes hemoglobin subunit beta (HBB), mRNA
1155
1155
100%
0.0
99.84%
748
XM_508242.4
PREDICTED: Pan paniscus hemoglobin subunit beta (LOC100976469), mRNA
1149
1149
100%
0.0
99.68%
646
XM_003819029.3
Homo sapiens hemoglobin, beta, mRNA (cDNA clone MGC:14540 IMAGE:4292125), cor
1142
1142
99%
0.0
99.52%
658
BC007075.1
Human messenger RNA for beta-globin
1140
1140
99%
0.0
99.52%
626
V00497.1
PREDICTED: Gorilla gorilla gorilla hemoglobin subunit beta (LOC101126932), mRNA
1133
1133
100%
0.0
99.20%
753
XM_019036164.1
Homo sapiens hemoglobin beta mRNA, complete cds
1133
1133
99%
0.0
99.36%
647
AY509193.1
PREDICTED: Pongo abelii hemoglobin subunit beta (HBB), mRNA
1098
1098
99%
0.0
98.25%
627
XM_002822127.4
PREDICTED: Nomascus leucogenys hemoglobin subunit beta (HBB), mRNA
1088
1088
100%
0.0
97.93%
753
XM_004090649.3
❶ 序列信息
❷ Score：
比对得分，值越高
相似性越高
❸ Query Cover：
所比对序列与目标
序列的覆盖度
❹ E value：期望值，
<1E-50(极可信)，
0.01可信
❺ Identities：
一致性，两个序列
有多少是一样

< Edit Search | Save Search | Search Summary

How to read this report? | BLAST Help Videos | Back to Traditional Results Page

Job Title	NM_000518.5 Homo sapiens hemoglobin subunit
RID	JVW9TRDW01R *Search expires on 09-01 17:07 pm* Download All
Program	BLASTN Citation
Database	nt See details
Query ID	lcl|Query_329291
Description	NM_000518.5 Homo sapiens hemoglobin subunit beta (HE ...
Molecule type	dna
Query Length	628
Other reports	Distance tree of results MSA viewer

Filter Results

Organism *only top 20 will appear* exclude

Type common name, binomial, taxid or group name

+ Add organism

Percent Identity to

E value to

Query Coverage to

Filter Reset

Descriptions | Graphic Summary | **Alignments** | Taxonomy

Alignment view: Pairwise | CDS feature | Restore defaults | Download

100 sequences selected

Download GenBank Graphics ▼ Next ▲ Previous ◀ Descriptions

Homo sapiens hemoglobin subunit beta (HBB), mRNA

Sequence ID: NM_000518.5 **Length:** 628 **Number of Matches:** 1

Range 1: 1 to 628 GenBank Graphics ▼ Next Match ▲ Previous Match

Score	Expect	Identities	Gaps	Strand
1160 bits(628)	0.0	628/628(100%)	0/628(0%)	Plus/Plus

```
Query  1    ACATTTGCTTCTGACACAACTGTGTTCACTAGCAACCTCAAACAGACACCATGGTGCATC  60
            ||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||
Sbjct  1    ACATTTGCTTCTGACACAACTGTGTTCACTAGCAACCTCAAACAGACACCATGGTGCATC  60

Query  61   TGACTCCTGAGGAGAAGTCTGCCGTTACTGCCCTGTGGGGCAAGGTGAACGTGGATGAAG  120
            ||||||||||||||||||||||||||||||||||||||||||||||||||||||||||||
Sbjct  61   TGACTCCTGAGGAGAAGTCTGCCGTTACTGCCCTGTGGGGCAAGGTGAACGTGGATGAAG  120
```

Related Information

Gene - associated gene details

PubChem BioAssay - bioactivity screening

Genome Data Viewer - aligned genomic context

Synthetic construct Homo sapiens clone IMAGE:100002185 for hypothetical protein (HBB gene)	synthetic construct	811	811	70%	0.0	99.55%	483	AM393351.1
Human ORFeome Gateway entry vector pENTR223-HBB, complete sequence	Human ORFeo…	809	809	70%	0.0	99.55%	3231	LT736709.1
Synthetic construct Homo sapiens clone ccsbBroadEn_06353 HBB gene, encodes complete protein	synthetic construct	809	809	70%	0.0	99.55%	573	KJ896959.1
Homo sapiens full open reading frame cDNA clone RZPDo834E0633D for gene HBB, hemoglobin, beta; co…	Homo sapiens	809	809	70%	0.0	99.77%	441	CR541913.1
Synthetic construct Homo sapiens clone FLH028849.01X hemoglobin beta (HBB) mRNA, complete cds	synthetic construct	809	809	70%	0.0	99.55%	444	AY890157.1
Synthetic construct Homo sapiens clone FLH130860.01L hemoglobin beta (HBB) mRNA, partial cds	synthetic construct	809	809	70%	0.0	99.77%	444	AY894014.1
Synthetic construct Homo sapiens clone FLH028845.01L hemoglobin beta (HBB) mRNA, partial cds	synthetic construct	806	806	70%	0.0	99.55%	444	AY892640.1
Synthetic construct Homo sapiens clone CCSBHm_00010626 HBB (HBB) mRNA, encodes complete protein	synthetic construct	804	804	70%	0.0	99.32%	573	KR710229.1
Synthetic construct Homo sapiens clone CCSBHm_00010601 HBB (HBB) mRNA, encodes complete protein	synthetic construct	804	804	70%	0.0	99.32%	573	KR710228.1
Synthetic construct Homo sapiens clone CCSBHm_00010525 HBB (HBB) mRNA, encodes complete protein	synthetic construct	804	804	70%	0.0	99.32%	573	KR710227.1
Synthetic construct Homo sapiens clone CCSBHm_00010498 HBB (HBB) mRNA, encodes complete protein	synthetic construct	804	804	70%	0.0	99.32%	573	KR710226.1
PREDICTED: Mandrillus leucophaeus hemoglobin subunit beta (LOC105535916), transcript variant X1, mR…	Mandrillus leuco…	791	1027	99%	0.0	95.90%	756	XM_011975165.1
Symphalangus syndactylus hemoglobin subunit beta (HBB) gene, complete cds	Symphalangus …	782	782	70%	0.0	98.42%	444	MH382900.1
PREDICTED: Theropithecus gelada hemoglobin subunit beta (LOC112607021), transcript variant X1, mRNA	Theropithecus g…	780	999	99%	0.0	95.50%	756	XM_025358025.1
TPA: Pongo abelii GLNA1 gene for globin A1	Pongo abelii	776	776	70%	0.0	98.20%	444	LT548116.1
Macaca mulatta hemoglobin subunit beta (HBB), mRNA	Macaca mulatta	771	771	75%	0.0	96.19%	471	NM_001164428.1
PREDICTED: Carlito syrichta hemoglobin subunit beta (LOC103254684), mRNA	Carlito syrichta	769	769	99%	0.0	88.94%	750	XM_008052701.1
Cercopithecus wolfi hemoglobin subunit beta (HBB) gene, complete cds	Cercopithecus …	749	749	70%	0.0	97.08%	444	MH382906.1
Erythrocebus patas hemoglobin subunit beta (HBB) gene, complete cds	Erythrocebus pa…	749	749	70%	0.0	97.08%	444	MH382898.1
PREDICTED: Hylobates moloch hemoglobin subunit delta (HBD), mRNA	Hylobates moloch	745	745	77%	0.0	94.26%	785	XM_032166807.1
PREDICTED: Nomascus leucogenys hemoglobin subunit delta (LOC100580435), mRNA	Nomascus leuc…	745	745	77%	0.0	94.26%	765	XM_003254822.3
Allenopithecus nigroviridis hemoglobin subunit beta (HBB) gene, complete cds	Allenopithecus n…	743	743	70%	0.0	96.85%	444	MH382901.1
Miopithecus talapoin hemoglobin subunit beta (HBB) gene, complete cds	Miopithecus tala…	732	732	70%	0.0	96.40%	444	MH382902.1
Homo sapiens hemoglobin subunit delta (HBD), mRNA	Homo sapiens	723	723	77%	0.0	93.44%	620	NM_000519.4
Cercocebus atys hemoglobin subunit beta (LOC105578869), mRNA	Cercocebus atys	723	723	71%	0.0	95.77%	448	NM_001305959.1
Homo sapiens hemoglobin, delta, mRNA (cDNA clone MGC:88275 IMAGE:30418964), complete cds	Homo sapiens	723	723	77%	0.0	93.44%	644	BC070282.1
Homo sapiens hemoglobin, delta, mRNA (cDNA clone MGC:96894 IMAGE:7262103), complete cds	Homo sapiens	723	723	77%	0.0	93.44%	544	BC069307.1

重要概念辨析（identity, similarity, homology）

- 同源性是定性推断（表示序列同源与否！），而一致性进而相似性则是数量推断，用于描述序列的相关性程度。
- 一致性用以表示两条氨基酸（或核苷酸）序列发生变化的程度，常用百分比表示。
- 相似性是指两条蛋白质（或核苷酸）序列中相同和相似残基对所占的百分比之和。
- 基本假定：*如果两条DNA（或蛋白质）序列的比对结果分数较高，那么它们就被定义为同源DNA（或蛋白质）。*
- 几点特别说明：

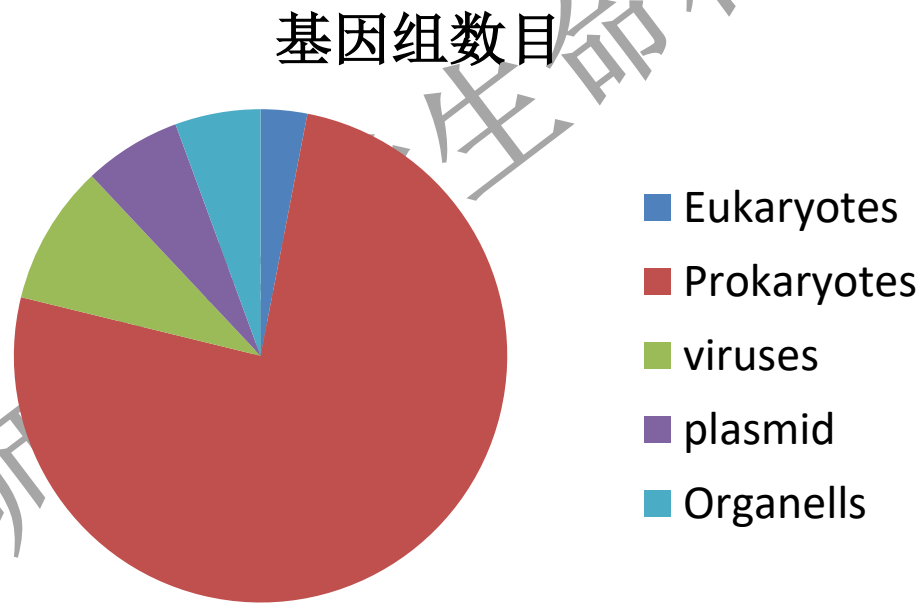
① 当两条序列同源时，它们的序列之间常常有显著的相似性；同源蛋白质几乎总是在三维结构上具有显著的相似性。

② 两个分子即使没有统计学上显著的氨基酸或核苷酸，它们也可能是同源的。

③ 对蛋白质而言，考虑一致性比相似性更有用，因为相似性的计算取决于不同氨基酸残基之间相似程度的定义方式。

【实例3 】基因组数据库展示

在NCBI genome数据库中，目前共收录了大量已公开的物种基因组序列等信息。



NCBI

ENTREZ Genome Project

connection information discovery

All Databases | PubMed | Nucleotide | Protein | Genome | Structure | PMC

Search Genome Project for [ ] Go Clear

Limits | Preview/Index | History | Clipboard | Details

New!

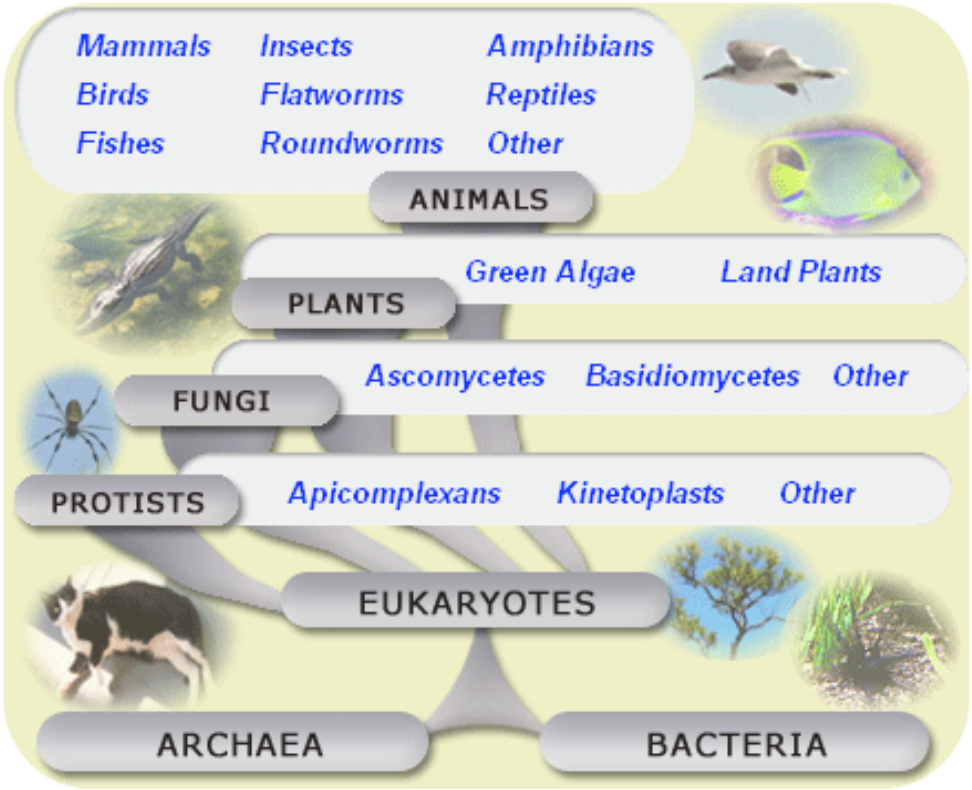
About Entrez

Entrez Genome Project
Home
Overview
Help
Statistics
Sequencing Centers

Submitting
Project Submissions
Project Instructions
General Genome Submissions
Feature Tables
Bacterial Genome Submissions
Whole Genome Shotgun Sequences

Related Resources
DOE Projects
DOE SAI Survey
Genome News Network
Genomes OnLine Database
IntlGenome
NHGRI Projects
NIAID Projects

Welcome to the NCBI Entrez Genome Project database.
This searchable database is a collection of complete and incomplete large-scale sequencing, assembly, annotation, and mapping projects for cellular organisms. The database is organized into organism-specific overviews that function as portals from which all projects in the database pertaining to that organism can be browsed and retrieved. Read more...



NCBI Res...

Entrez Gene
gene-related information

Entrez Genome
sequence and map data from whole genomes

Environmental Projects
metagenomic-specific genome projects

Eukaryotic Projects
eukaryotic-specific genome projects

Genomic Biology
organism-specific links

Prokaryotic Projects
prokaryotic-specific genome projects

Organellar Genomes
organellar reference sequences and tools

Plant Genomes
major plant genome projects

RefSeq
the reference sequence project

Viral Genomes
viral reference sequences and tools

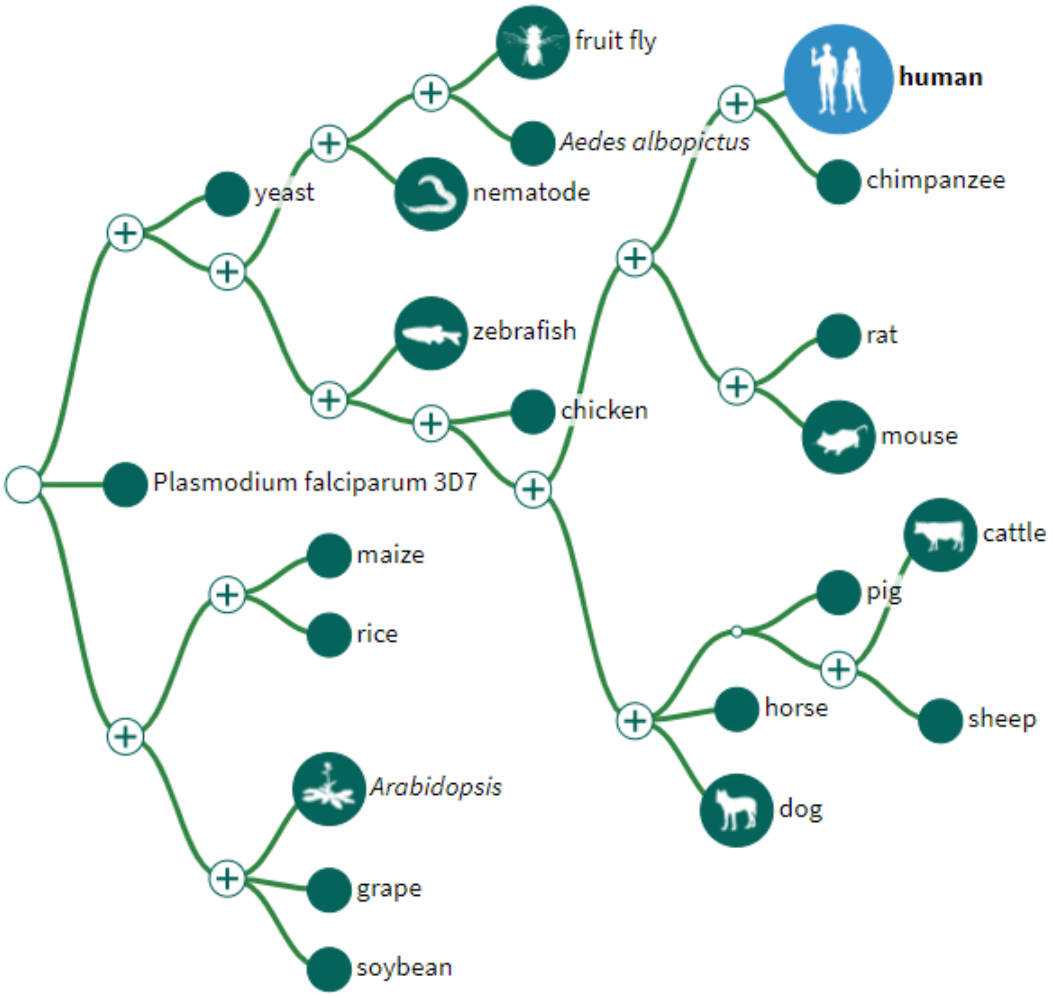
WGS Sequences
whole genome shotgun sequences

Genome Data Viewer

Switch view

Search organisms

Homo sapiens (human)



Homo sapiens (human)

Search in genome

Location, gene or phenotype

Examples: TXLNA, chr1:32178000-32200000, DNA repair

Assembly

GRCh38.p13

Browse genome | BLAST genome

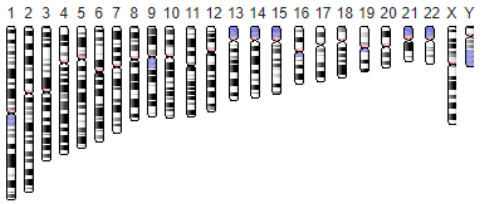
Download via NCBI Datasets

Assembly details

Name	GRCh38.p13
RefSeq accession	GCF_000001405.39
GenBank accession	GCA_000001405.28
Submitter	Genome Reference Consortium
Level	Chromosome
Category	Reference genome
Replaced by	GCF_000001405.25

Annotation details

Annotation Release	109
Release date	May 16, 2021



https://www.ncbi.nlm.nih.gov/genome/gdv/

Genome Projects

Properties of Eukaryotic Genome Sequencing Projects

Organism info | Complete genomes | Genomes in progress

organism group: – All –

Tools legend: T - TaxTable; P - ProtTable; C - COG Table; D - 3-D neighbors; L - BLAST; S - CDD search; F - FTP; R - Publications.

* size is estimated, otherwise genome size is calculated based on existing sequences

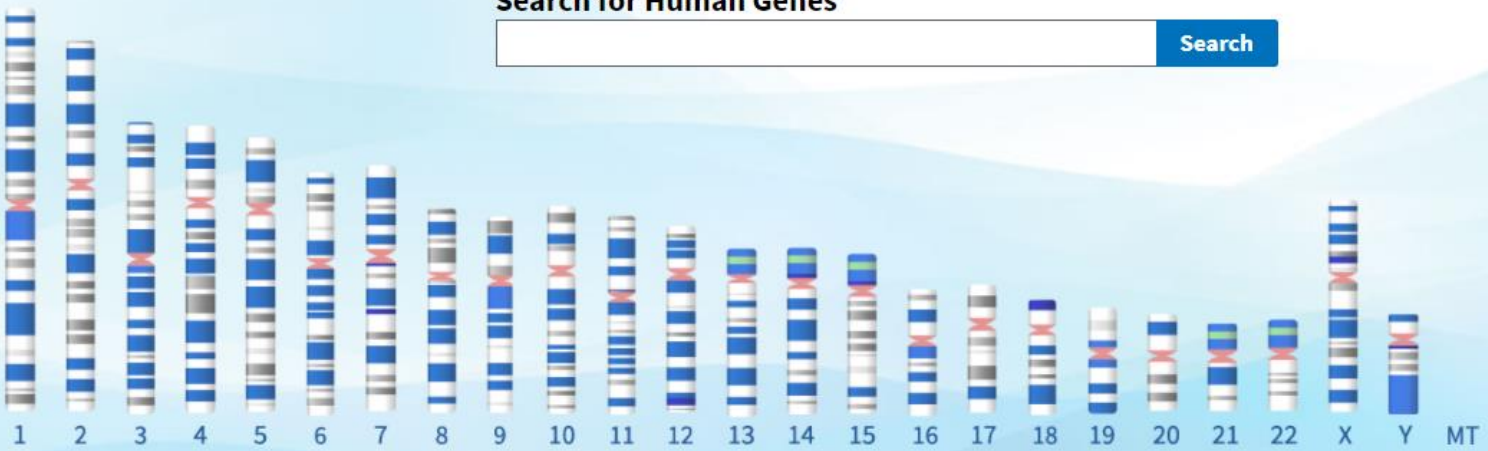
294 Complete Microbial Genomes selected: [A] - 25, [B] - 269 save

Organism	King	Group	* Size	GC	#chr	#plsm	GenBank	RefSeq	Released	Center	Tools
Acinetobacter sp. ADP1	B	Gammaproteobacteria	3.6	40.4	1		CR543861	NC_005966	10/30/2004	Genoscope	T P C D L S F R
Aeropyrum pernix K1	A	Crenarchaeota	1.67	67	1		BA000002	NC_000854	06/26/1999	NITE	T P C D L S F R
Agrobacterium tumefaciens str. C58	B	Alphaproteobacteria	5.67	59	2	2	AE008688	NC_003304	12/18/2001	University of Washington	T P C D L S F R
Agrobacterium tumefaciens str. C58	B	Alphaproteobacteria	5.67	59	2	2	AE007869	NC_003062	12/18/2001	Cereon	T P C D L S F R
Anabaena variabilis ATCC 29413	B	Cyanobacteria	7.07	41.4	1	3	CP000117	NC_007413	03/10/2004	DOE Joint Genome Institute	T P D L S F
Anaplasma marginale str. St. Maries	B	Alphaproteobacteria	1.2	49.8	1		CP000030	NC_004842	12/08/2004	Washington State University	T P C D L S F R
Aquifex aeolicus VF5	B	Aquificae	1.59	43	1	1	AE000657	NC_000918	04/16/1998	DIVERSA	T P C D L S F R
Archaeoglobus fulgidus DSM 4304	A	Euryarchaeota	2.18	46	1		AE000782	NC_000917	12/06/1997	TIGR	T P C D L S F R
Azoarcus sp. EbN1	B	Betaproteobacteria	4.73	65.1	1	2	CR555306	NC_006513	11/20/2004	Max Planck Institute	T P C D L S F R
Bacillus anthracis str. 'Ames Ancestor'	B	Firmicutes	5.5	35.2	1	2	AE017334	NC_007530	05/20/2004	TIGR	T P C D L S F
Bacillus anthracis str. Ames	B	Firmicutes	5.23	35	1		AE016879	NC_003997	05/02/2003	TIGR	T P C D L S F R
Bacillus anthracis str. Sterne	B	Firmicutes	5.23	35.4	1		AE017225	NC_005945	06/24/2004	DOE Joint Genome Institute	T P C D L S F
Bacillus cereus ATCC 10987	B	Firmicutes	5.43	38	1	1	AE017194	NC_003909	02/13/2004	TIGR	T P C D L S F R
Bacillus cereus ATCC 14579	B	Firmicutes	5.43	38	1	1	AE016877	NC_004722	05/02/2003	Institut National de la Recherche Agronomique (INRA)	T P C D L S F R
Bacillus cereus E33L	B	Firmicutes	5.84	35.4	1	5	CP000001	NC_006274	09/16/2004	DOE Joint Genome Institute	T P C D L S F

Human Genome Resources at NCBI

Search for Human Genes

Search



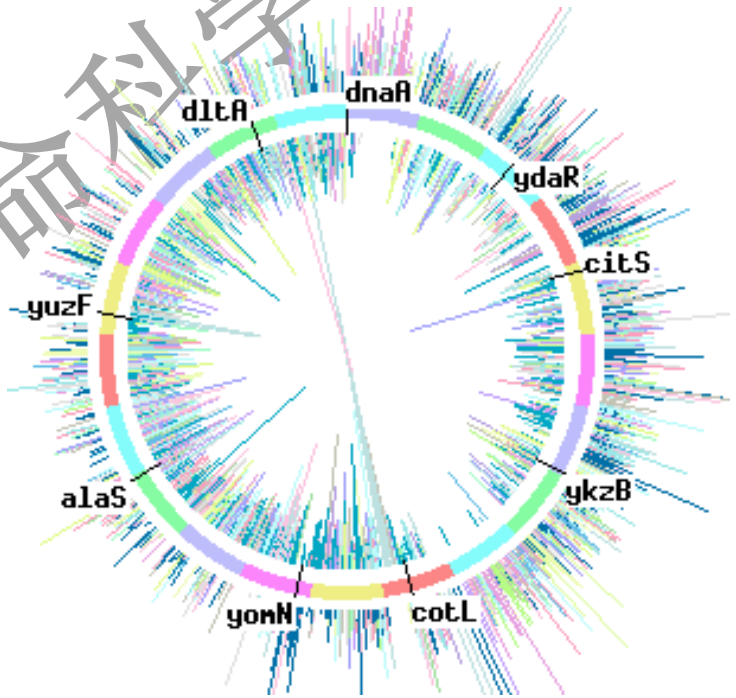
Select a chromosome to access the Genome Data Viewer

Download

	GRCh38	GRCh37
Reference Genome Sequence	Fasta	Fasta
RefSeq Reference Genome Annotation	gff3	gff3
RefSeq Transcripts	Fasta	Fasta
RefSeq Proteins	Fasta	Fasta

Simple Genomes

- **Full chromosomal sequences are provided**
- **Genes are annotated**
- **The annotation can be shown graphically and linked to sequence records**



Complex Genomes

- **Sequences are provided complete or we help assemble**
- **Heavy annotation: Genes, transcript regions & ORFs, sequence variations & markers, clones, ESTs, etc.**
- **The annotation can be shown graphically and linked to other databases using the MapViewer**

A database for retrieval and analysis of karyotype data:
Cancer Chromosomes

以昆虫基因组序列为例，目前已经公开全基因序列的有538种，其中组装到染色体、Contig和Scaffold的分别有42、52和444种。

Overview (39517); **Eukaryotes (6572)**; Prokaryotes (163344); Viruses (19778); Plasmids (13790); Organelles (12082)

Filters 1

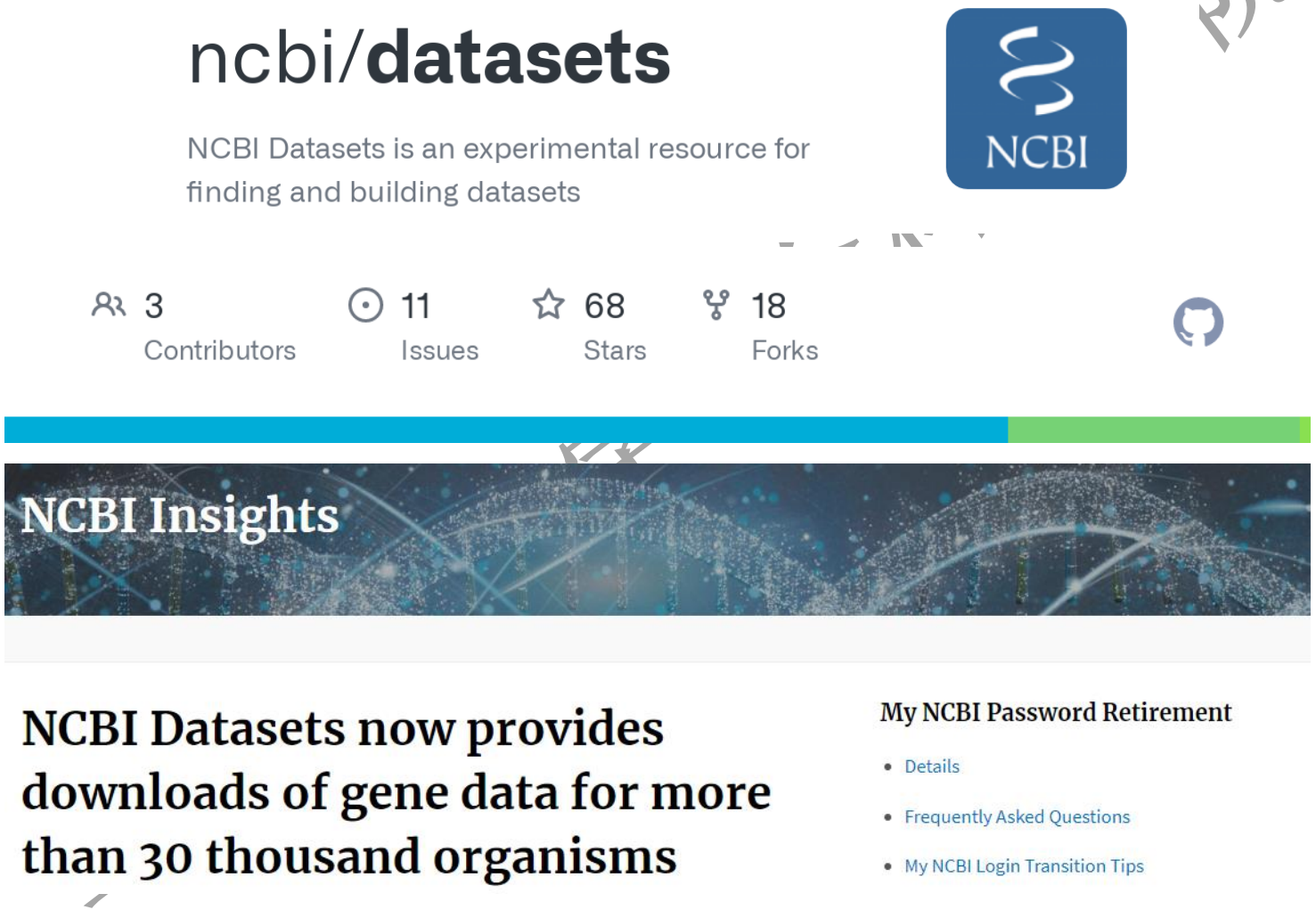
Group	Animals (538)
Subgroup	Amphibians (7) Apicomplexans (211) Ascomycetes (2,633) Basidiomycetes (682) Birds (145) Fishes (224) Flatworms (32) Green Algae (57) Insects (538) Kinetoplasts (87) more
Assembly level	Chromosome (42) Contig (52) Scaffold (444)
Partial	All (538) Exclude partial (527) Include partial only (11)
Anomalous	All (538) Exclude anomalous (538)
Host	plants (5)
RefSeq category	reference (1) representative (311)
Organism Name	filter by Scientific Name

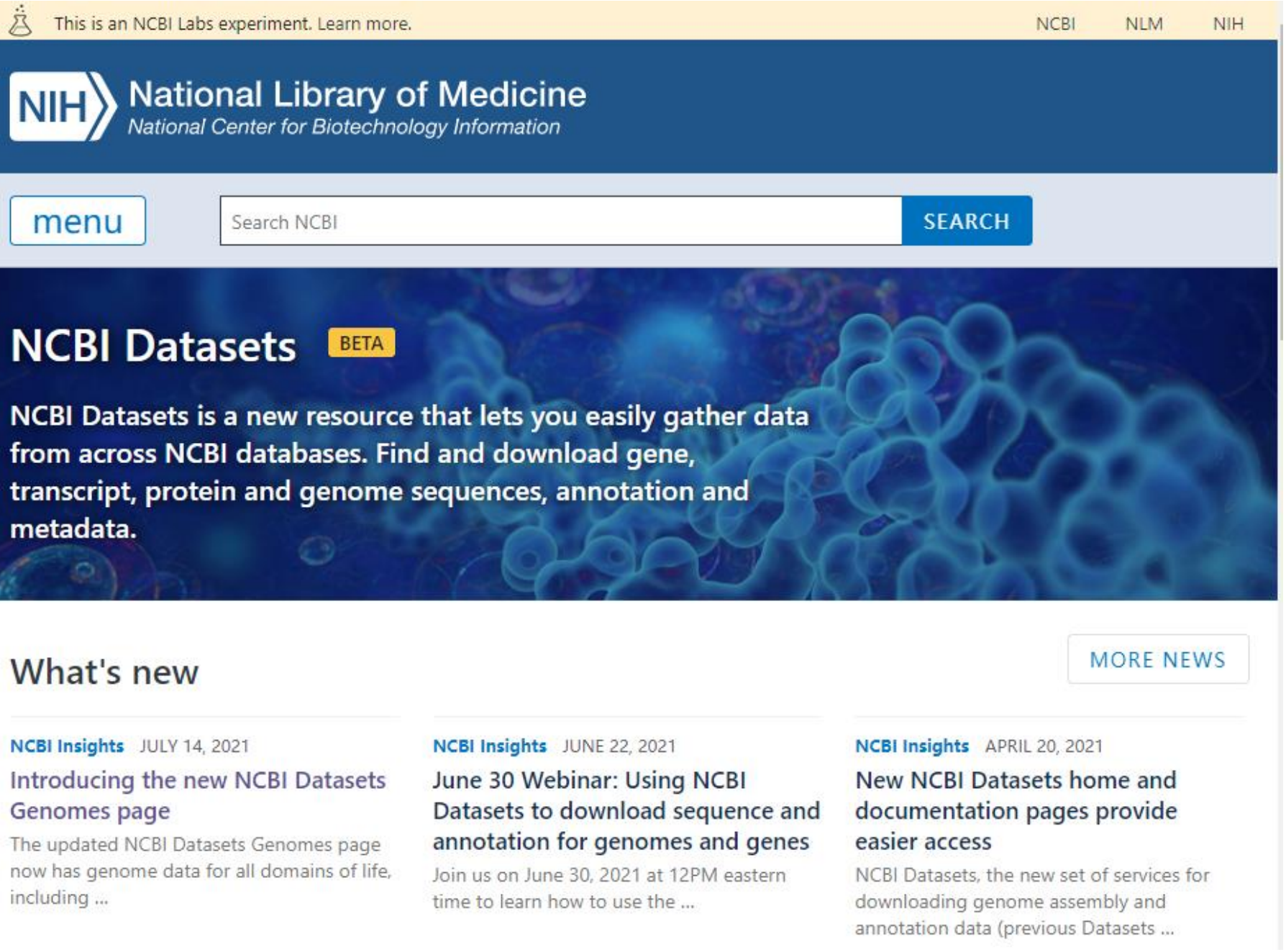
Download

Choose Columns Page 1 of 11 50 View 1 - 50 of 538

#	Organism Name	Organism Groups	Strain	BioSample	BioProjec	Assembly	Leve	Size(Mb)	GC%	Replicons	WGS	Scaffolc	CDS	Release Da	FTP
1	Achalarus lyciades	Eukaryota;Animals;Insects		SAMN05958461	PRJNA35192	GCA_002930495.1		566.83	18.10	mitochondrion MT: CM009487.1	MOOZ01	47,369		14-Feb-2018	G
2	Acromyrmex echinatior	Eukaryota;Animals;Insects		SAMN02953789	PRJNA62733	GCA_000204515.1		295.94	34.00		AEVX01	4,339	20,241	14-Apr-2011	R G
3	Acyrthosiphon pisum	Eukaryota;Animals;Insects	LSR1	SAMN00000061	PRJNA13657	GCA_000142985.2		541.69	31.20	mitochondrion MT: NC_011594.1 /FJ411411.1	ABLF02	23,925	27,999	01-Apr-2008	R G
4	Aedes aegypti	Eukaryota;Animals;Insects	LVP_AGWG	SAMN07177802	PRJNA392114	GCA_002204515.1		1,278.73	38.17	chromosome 1: NC_035107.1 /CM008043.1 chromosome 2: NC_035108.1 /CM008044.1 chromosome 3: NC_035109.1 /CM008045.1 Show all 4 replicons	NIGP01	2,310	28,317	15-Jun-2017	R G
5	Aedes aegypti	Eukaryota;Animals;Insects	Liverpool	SAMN02953616	PRJNA12434	GCA_000004015.3		1,383.97	38.80	mitochondrion MT: EU352212.1	AAGE02	4,757	17,400	11-Feb-2005	R G
6	Aedes aegypti	Eukaryota;Animals;Insects	BV_Aedes	SAMN03284760	PRJNA26839	GCA_001014885.1		744.60	28.00		JXPU01	223,039		28-May-2015	G
7	Aedes albopictus	Eukaryota;Animals;Insects	C6/36	SAMN05908721	PRJNA357111	GCA_001876365.2		2,247.31	40.40	mitochondrion MT: NC_006817.1 /AY072044.1	MNAF02	2,435	42,912	10-Nov-2016	R G
8	Aedes albopictus	Eukaryota;Animals;Insects	Foshan	SAMN03265380	PRJNA27027	GCA_001444175.2		1,923.48	40.70		JXUM01	154,782	17,146	29-Sep-2015	G
9	Aedes albopictus	Eukaryota;Animals;Insects	Rimini	SAMN03853745	PRJNA28946	GCA_001574995.1		1,341.04	40.40		LMAV01	3,342,920		22-Dec-2015	G
10	Aethina tumida	Eukaryota;Animals;Insects	BRL-Maryland	SAMN06036204	PRJNA36127	GCA_001937115.1		234.34	30.00		MRBJ01	3,063	17,463	05-Jan-2017	R G
11	Agrilus planipennis	Eukaryota;Animals;Insects	EAB-ADULT	SAMN02439909	PRJNA34347	GCA_000699045.2		353.07	36.00	mitochondrion MT: NC_030758.1 /KT363854.1	JENH02	3,613	22,159	06-Jun-2014	G
12	Aleochara bilineata	Eukaryota;Animals;Insects	Rennes	SAMN06611084	PRJNA37816	GCA_003054995.1		85.90	-		NBZA01	33,003		17-Apr-2018	G
13	Amphinemura sulcicollis	Eukaryota;Animals;Insects	Dwyryd	SAMN04568201	PRJNA31568	GCA_001676325.1		271.93	41.80		LVVV01	432,491		24-Jun-2016	G
14	Amyelois transitella	Eukaryota;Animals;Insects	UIUC subculture of SPIRL-1966	SAMN03009087	PRJNA29202	GCA_001186105.1		406.47	37.60		LACK01	7,301	18,472	21-Jul-2015	R G
15	Anopheles albimanus	Eukaryota;Animals;Insects	ALBI9_A	SAMN02953839	PRJNA19156	GCA_000349125.2		173.34	49.25	chromosome 2L: CM008152.1 chromosome 2R: CM008153.1 chromosome 3L: CM008154.1 Show all 5 replicons	APCK01	236		25-Mar-2013	G
16	Anopheles aquasalis	Eukaryota;Animals;Insects	PFPP-2014	SAMN07206858	PRJNA38975	GCA_002846955.1		162.94	-		NJHH01	16,504		21-Dec-2017	G
17	Anopheles arabiensis	Eukaryota;Animals;Insects	DONG5_A	SAMN02953842	PRJNA19156	GCA_000349185.1		246.57	45.30		APCN01	1,214		25-Mar-2013	G
18	Anopheles atroparvus	Eukaryota;Animals;Insects	EBRO	SAMN01087926	PRJNA67233	GCA_000473505.1		224.29	46.80		AXCP01	1,371		30-Sep-2013	G
19	Anopheles christyi	Eukaryota;Animals;Insects	ACHKN1017	SAMN02953841	PRJNA19156	GCA_000349165.1		172.66	42.80		APCM01	30,369		25-Mar-2013	G

【实例4】了解NCBI新发布的数据库Datasets




This is an NCBI Labs experiment. Learn more.
NCBI
NLM
NIH
National Library of Medicine
National Center for Biotechnology Information
menu
Search NCBI
SEARCH
NCBI Datasets
BETA
NCBI Datasets is a new resource that lets you easily gather data from across NCBI databases. Find and download gene, transcript, protein and genome sequences, annotation and metadata.
What's new
MORE NEWS
NCBI Insights JULY 14, 2021
Introducing the new NCBI Datasets Genomes page
The updated NCBI Datasets Genomes page now has genome data for all domains of life, including ...
NCBI Insights JUNE 22, 2021
June 30 Webinar: Using NCBI Datasets to download sequence and annotation for genomes and genes
Join us on June 30, 2021 at 12PM eastern time to learn how to use the ...
NCBI Insights APRIL 20, 2021
New NCBI Datasets home and documentation pages provide easier access
NCBI Datasets, the new set of services for downloading genome assembly and annotation data (previous Datasets ...

Datasets数据库重构了基因组数据的部署方式

Genomes Quickstart

Browse and download genome data using our Genome page. Genome data is also available using our command-line tool and API. Genome data includes genome, transcript and protein sequences, genome annotation and metadata.

BROWSE GENOMES

Popular species

Homo sapiens
human

Mus musculus
mouse

Arabidopsis thaliana
thale cress

Rattus norvegicus
rat

Drosophila melanogaster
fruit fly

Danio rerio
zebrafish

Bos taurus
cow

Gallus gallus
chicken

Oryza sativa
rice

How to

Get genome metadata

Download a genome data package

Download large genome data packages

menu MENU

Search NCBI SEARCH

Genomes – NCBI Datasets BETA

Download a genome dataset including genome, transcript and protein sequence, annotation and a data report

TAXONOMIC NAME

search

Please enter a taxon name or select from popular species

Homo sapiens
human

Arabidopsis thaliana
thale cress

Drosophila melanogaster
fruit fly

Bos taurus
cow

Oryza sativa
rice

Mus musculus
mouse

Rattus norvegicus
rat

Danio rerio
zebrafish

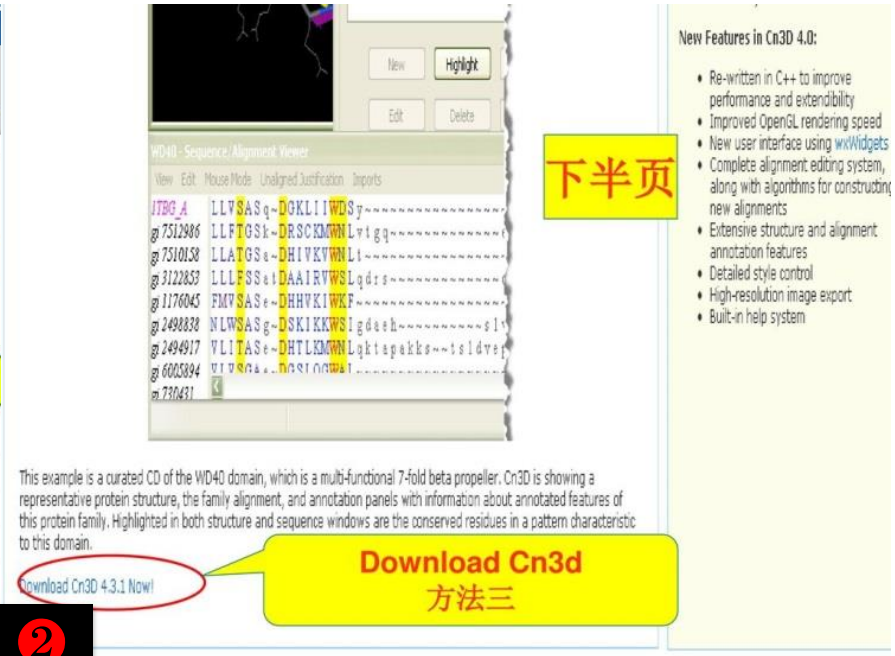
Gallus gallus
chicken


❶ 命令行下载
❷ 压缩格式的数据包
NIH National Library of Medicine
National Center for Biotechnology Information
Documentation
Quickstart guides
Command line
How-to guides
Data packages
Programming languages
Python
R
Reference
Documentation / Programming languages
Supported programming languages
Datasets supports all languages via its RESTful API, accessible using the OpenAPI v3 spec .
Python
Python-related resources for NCBI Datasets
R
R-related resources for NCBI Datasets
Generated August 30, 2021
❸ 集成化的编程语言接口

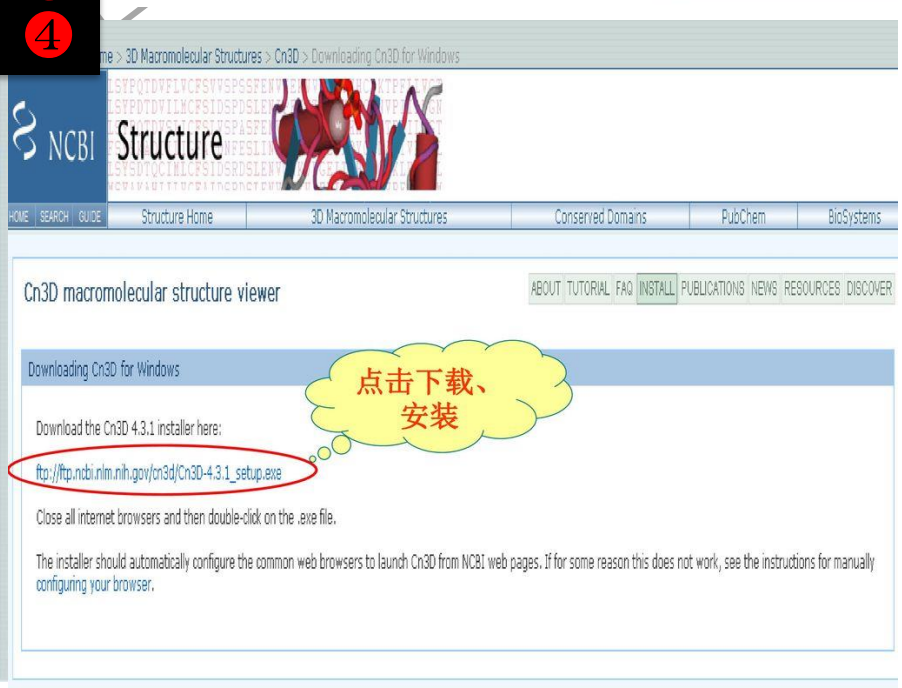
【实例5 】Structure数据库展示

NCBI Structure数据库即生物大分子三维数据库（MMDB），包含来自X-ray晶体学和三维结构的实验数据。MMDB的数据从蛋白质结构数据库PDB获得，但对结构的阐述较PDB更为详细，更多的是比较结构的相似性及亲缘关系。


NCBI Resources How To
Sign in to NCBI
Structure
Search
Advanced
Help
Structure
Three dimensional structures provide a wealth of information on the biological function and the evolutionary history of macromolecules. They can be used to examine sequence-structure-function relationships, interactions, active sites, and more.
Using Structure
使用帮助等
Structure Tools
本库工具
More Resources
其他资源
Search
How to (Quick Start) Guides
Help
News
FTP
Publications
Discover
Macromolecular Resources Overview
CBLAST
Cn3D
IBIS
VAST
PDB
Protein
CDD
PubChem
NCBI Structure Group Resources & Research
Cn3d
阅读器


下半页
New Features in Cn3D 4.0:
Re-written in C++ to improve performance and extendibility
Improved OpenGL rendering speed
New user interface using wxWidgets
Complete alignment editing system, along with algorithms for constructing new alignments
Extensive structure and alignment annotation features
Detailed style control
High-resolution image export
Built-in help system
This example is a curated CD of the WD40 domain, which is a multi-functional 7-fold beta propeller. Cn3D is showing a representative protein structure, the family alignment, and annotation panels with information about annotated features of this protein family. Highlighted in both structure and sequence windows are the conserved residues in a pattern characteristic to this domain.
Download Cn3d 4.3.1 Now!
Download Cn3d
方法三

NCBI > Structure Home > 3D Macromolecular Structures > Cn3D
NCBI Structure
Structure Home
3D Macromolecular Structures
Conserved Domains
PubChem
BioSystems
Cn3D macromolecular structure viewer
ABOUT TUTORIAL FAQ INSTALL PUBLICATIONS NEWS RESOURCES DISCOVER
Install
安装方法一
Windows
安装方法二
Tutorial
学习指南
About Cn3D
Highlights
Cn3D ("see in 3D") is a helper application for your web browser that allows you to view 3-dimensional molecular structures in the Entrez Structure database. Cn3D is provided for Windows and Macintosh, and can be compiled for Unix. Cn3D displays structure, sequence, and alignment, and now has powerful annotation and alignment editing features.
Below is a relatively simple sample of what Cn3D can do. There are many more examples in the Tutorial, along with instructions to help new users get started!
New Features in Cn3D 4.3.1:
View superpositions of structures that have similar molecular complexes, as identified by the newly released VAST+ (an enhanced version of the existing Vector Alignment Search Tool). The VAST+ help document provides additional details about the tool and examples of how it can be used to learn more about proteins.
Cn3D 4.3.1 uses the MIME type: application/vnd.ncbi.cn3d. (Up to version 4.3, Cn3D used the MIME type chemical/ncbi-asn1-binary.)
New Features in Cn3D 4.3:
View biological units and crystallographic symmetry from MMDB


NCBI > 3D Macromolecular Structures > Cn3D > Downloading Cn3D for Windows
NCBI Structure
Structure Home
3D Macromolecular Structures
Conserved Domains
PubChem
BioSystems
Cn3D macromolecular structure viewer
ABOUT TUTORIAL FAQ INSTALL PUBLICATIONS NEWS RESOURCES DISCOVER
Downloading Cn3D for Windows
Download the Cn3D 4.3.1 installer here:
ftp://ftp.ncbi.nlm.nih.gov/cn3d/Cn3D-4.3.1_setup.exe
点击下载、安装
Close all internet browsers and then double-click on the .exe file.
The installer should automatically configure the common web browsers to launch Cn3D from NCBI web pages. If for some reason this does not work, see the instructions for manually configuring your browser.

蛋白质结构与药物设计研究的利器--PDB数据库

RCSB PDB Deposit Search Visualize Analyze Download Learn More Documentation Careers MyPDB

RCSB PDB PROTEIN DATA BANK

181535 Biological Macromolecular Structures Enabling Breakthroughs in Research and Education

Enter search terms or PDB ID(s).

Advanced Search | Browse Annotations Help

PDB-101 Worldwide PDB EMDataResource Nucleic Acid Database Worldwide Protein Data Bank Foundation

Celebrating YEARS OF Protein Data Bank

Developers: Join the RCSB PDB Team Explore Open Positions

Welcome
Deposit
Search
Visualize
Analyze
Download
Learn

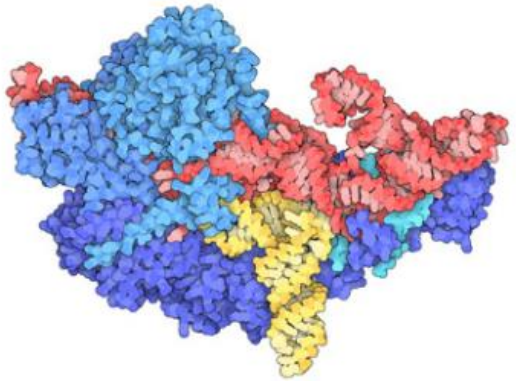
A Structural View of Biology

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.

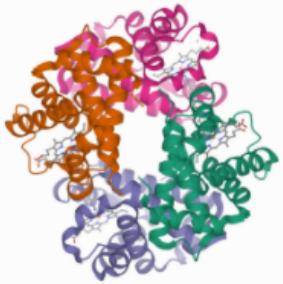
August **Molecule of the Month**



Ribonuclease P

https://www.rcsb.org/

RCSB PDB | Deposit | Search | Visualize | Analyze | Download | Learn | More | Documentation | Careers | MyPDB



3D View

2DN2

Download File | View File

1.25A resolution crystal structure of human hemoglobin in the deoxy form

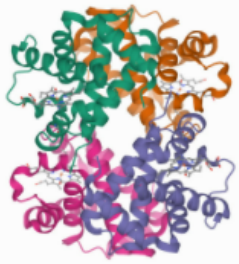
Park, S.-Y., Yokoyama, T., Shibayama, N., Shiro, Y., Tame, J.R.

(2006) J Mol Biol **360**: 690-701

Released	2006-05-09
Method	X-RAY DIFFRACTION 1.25 Å
Organisms	Homo sapiens
Macromolecule	Hemoglobin alpha subunit (protein)
	Hemoglobin beta subunit (protein)
Unique Ligands	HEM

直接下载文件

在线浏览及下载



3D View

2DN3

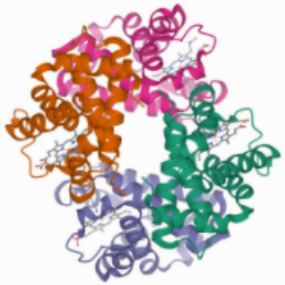
Download File | View File

1.25A resolution crystal structure of human hemoglobin in the carbonmonoxy form

Park, S.-Y., Yokoyama, T., Shibayama, N., Shiro, Y., Tame, J.R.

(2006) J Mol Biol **360**: 690-701

Released	2006-05-09
Method	X-RAY DIFFRACTION 1.25 Å
Organisms	Homo sapiens
Macromolecule	Hemoglobin alpha subunit (protein)
	Hemoglobin beta subunit (protein)
Unique Ligands	CMO, HEM



3D View

2HHE

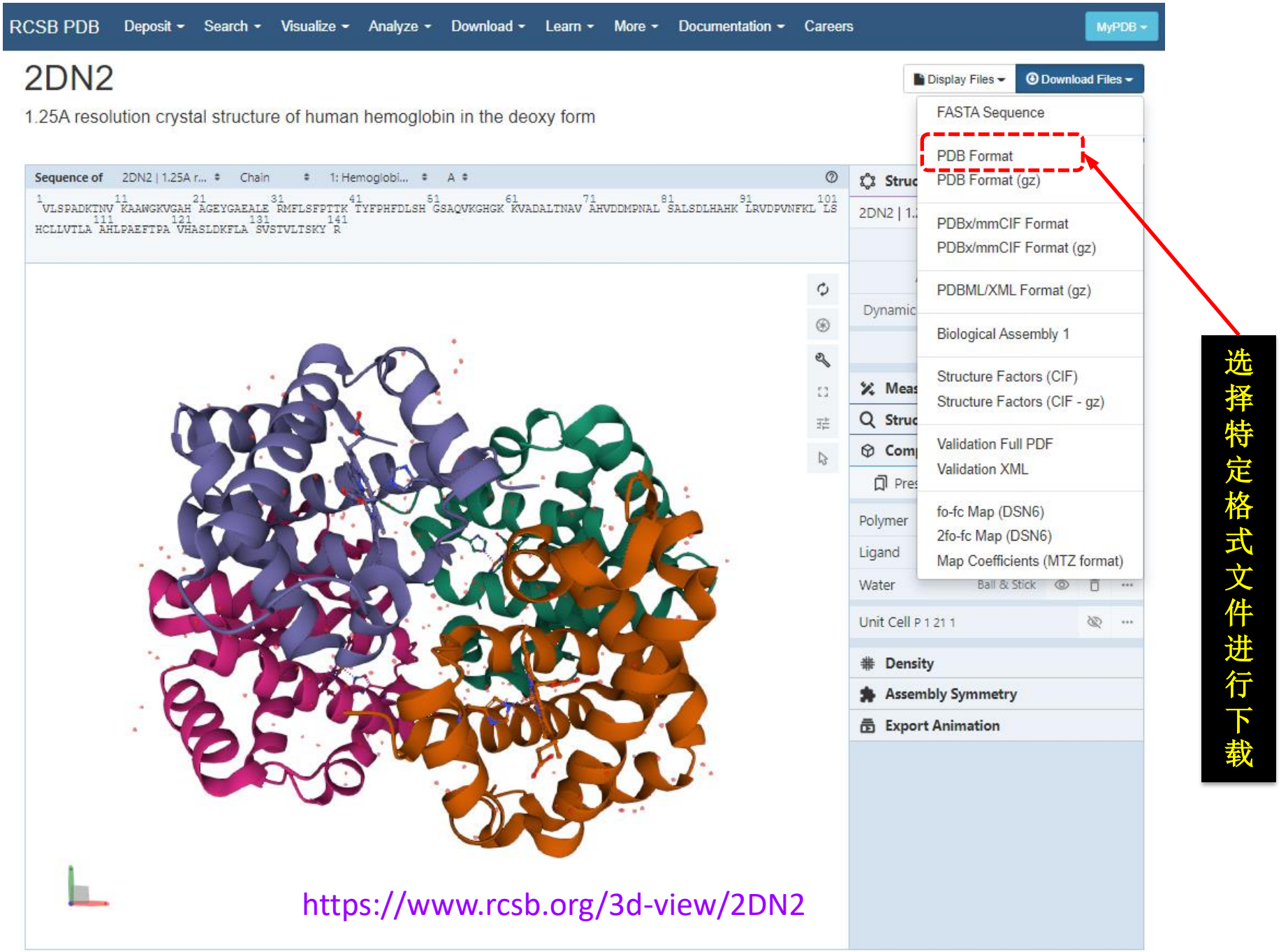
Download File | View File

OXYGEN AFFINITY MODULATION BY THE N-TERMINI OF THE BETA CHAINS IN HUMAN AND BOVINE HEMOGLOBIN

Gilliland, G.L., Pechik, I., Fronticelli, C., Ji, X.

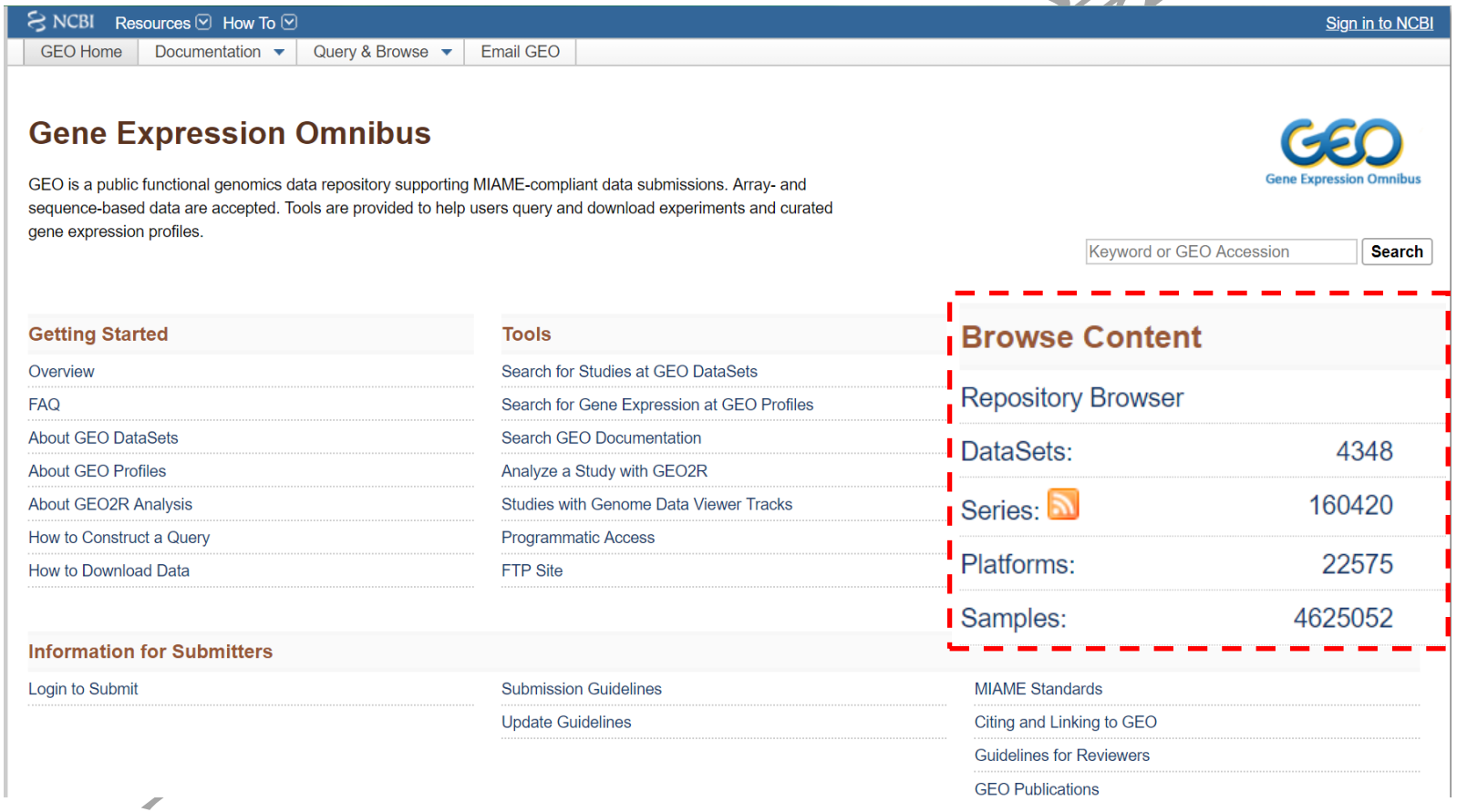
(1994) J Biol Chem **269**: 23965-23969

Released	1995-01-26
Method	X-RAY DIFFRACTION 2.2 Å
Organisms	Homo sapiens
Macromolecule	HEMOGLOBIN (DEOXY) (ALPHA CHAIN) (protein)
	HEMOGLOBIN (DEOXY) (BETA CHAIN) (protein)
Unique Ligands	HEM

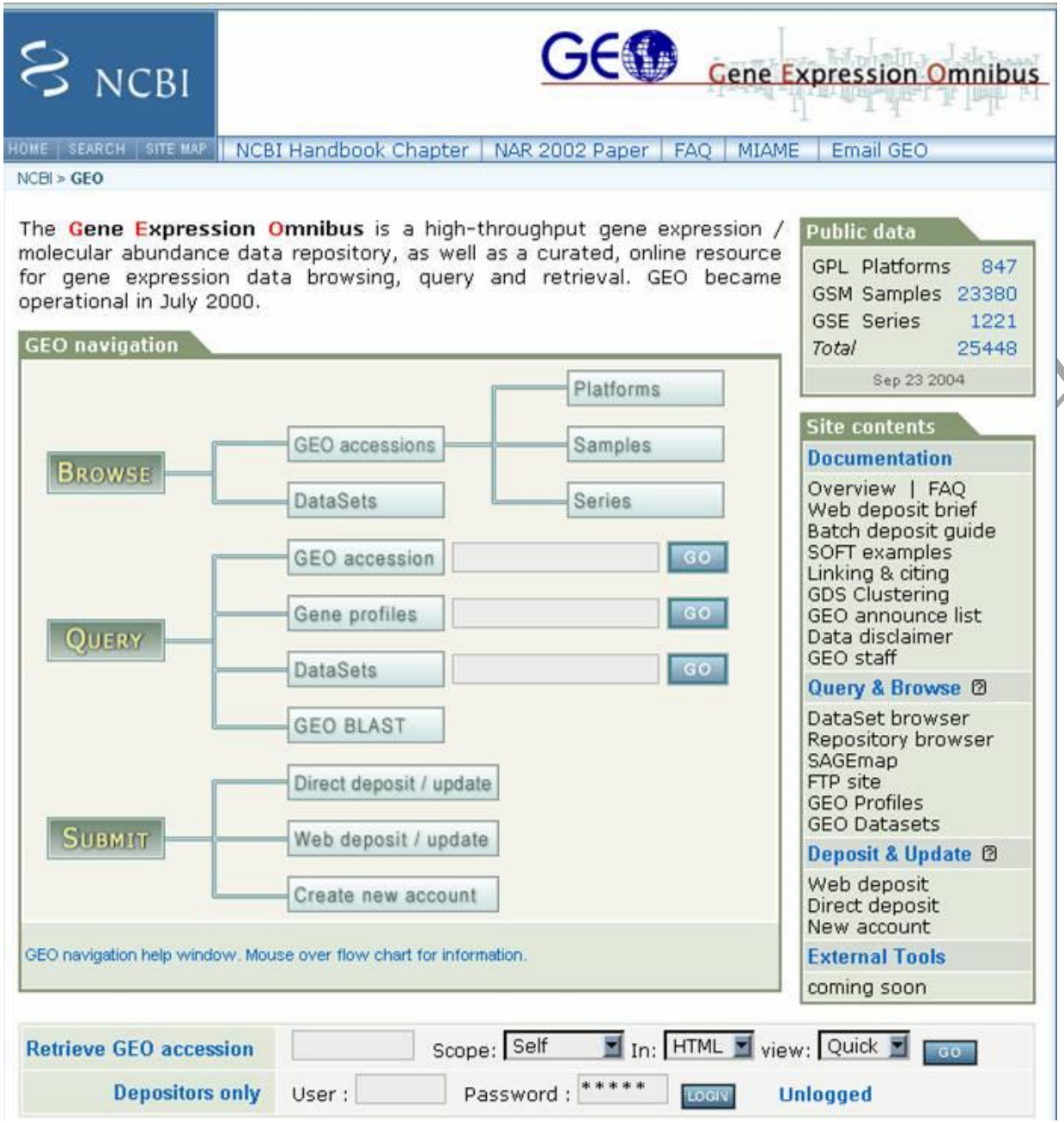

RCSB PDB
Deposit
Search
Visualize
Analyze
Download
Learn
More
Documentation
Careers
MyPDB
2DN2
1.25A resolution crystal structure of human hemoglobin in the deoxy form
Display Files
Download Files
FASTA Sequence
PDB Format
PDB Format (gz)
PDBx/mmCIF Format
PDBx/mmCIF Format (gz)
PDBML/XML Format (gz)
Biological Assembly 1
Structure Factors (CIF)
Structure Factors (CIF - gz)
Validation Full PDF
Validation XML
fo-fc Map (DSN6)
2fo-fc Map (DSN6)
Map Coefficients (MTZ format)
Sequence of
2DN2 | 1.25A r...
Chain
1: Hemoglobi...
A
VLSPADKTNV KAAWGKVGAH AGEYGAEALE RMFLSFPTTK TYFPHFDLSH GSAQVKGHGK KVADALTNAV AHVDDMPNAL SALSDLHAHK LRVDPVNFKL LS
HCLLVTLA AHLPAEFTPA VHASLDKFLA SVSTVLTSKY R
Polymer
Ligand
Water
Ball & Stick
Unit Cell P 1 21 1
Density
Assembly Symmetry
Export Animation
https://www.rcsb.org/3d-view/2DN2
选择特定格式文件进行下载

【实例6 】GEO数据库展示

在NCBI GEO数据库中，目前共收录了大量已公开的基因表达谱数据（RNA表达水平数据）。



截止2022/01/01的统计数据



Submit and update data

Query the database:

- gene identifiers
- field information
- sequence

Browse datasets

Download data

Gene Expression Omnibus

Submitted by Experimentalists

*Submitted by Manufacturer**

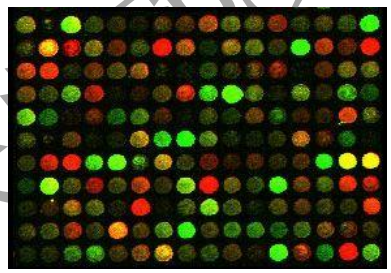
Curated by NCBI

GPL

Platform descriptions

GSM

Raw/processed spot intensities from a single slide/chip

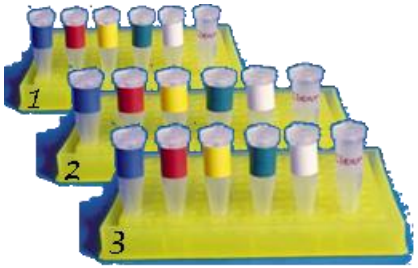


GSE

Grouping of slide/chip data "a single experiment"

GDS

Grouping of experiments



Entrez GEO

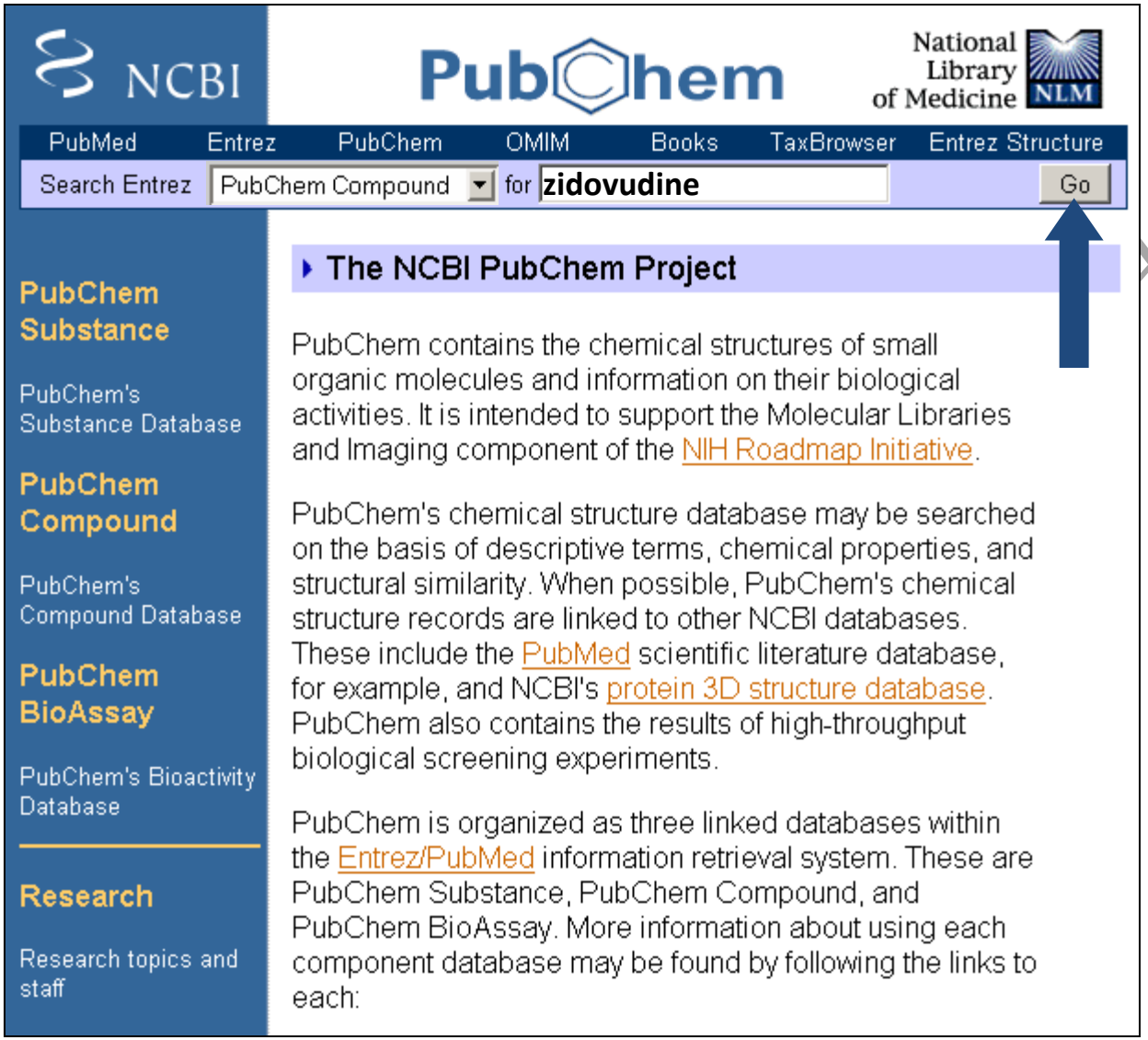
Entrez GEO Datasets

Common Species in GEO database

Organism	Series	Platforms	Samples
Homo sapiens	70,455	5,897	2,383,630
Mus musculus	49,767	2,576	1,321,462
Rattus norvegicus	4,669	638	112,170
Drosophila melanogaster	4,220	391	100,249
Arabidopsis thaliana	4,850	405	74,384
Saccharomyces cerevisiae	3,256	625	73,025
Macaca mulatta	595	73	25,881
Sus scrofa	1,021	158	23,852
Caenorhabditis elegans	1,992	215	21,441
Bos taurus	1,081	204	19,847
Gallus gallus	894	150	14,827
Oryza sativa	953	203	14,242
Zea mays	532	120	14,407
Escherichia coli	890	176	9,873
Glycine max	318	58	8,938
Xenopus laevis	242	38	2,872

【实例7】化合物数据资源

Entrez **PubChem**



PC Compound

Derived database of known chemicals from PC Substance records

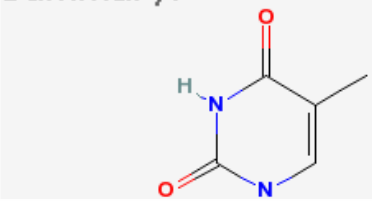
PC Substance

Primary database of chemical samples

PC BioAssay

Primary database of bioactivity screens of samples in PC Substance

Compound Summary:



CID: 35370

Substances:
All: 238 Links
Same: 33 Links
Mixture: 205 Links

BioActivity: 4 Links

Medical Subject Annotations: (Total:4) Display: Next 1 | All

Zidovudine
A dideoxynucleoside compound in which the 3'-hydroxy group on the sugar moiety has been replaced by an azido group. This modification prevents the formation of phosphodiester linkages which are needed for the completion of nucleic acid chains. The compound is a potent inhibitor of HIV replication, acting as a chain-terminator of viral DNA during reverse transcription. It improves immunologic function, partially reverses the HIV-induced neurological dysfunction, and improves certain other clinical abnormalities associated with AIDS. Its principal toxic effect is dose-dependent suppression of bo

Show MeSH Tree Structure

Pharmacological Action:
Antimetabolites
Reverse Transcriptase Inhibitors
Anti-HIV Agents

Depositor-Supplied Synonyms: (Total: 144)

Display: Next 10 | All | Sort: Weight

zidovudine
Retrovir
Azidothymidine
Combivir
Trizivir
Compound S
Propolis+AZT
Retrovir (TN)
Zidovudinum [Latin]
Zidovudina [Spanish]

Properties Computed from Structure:

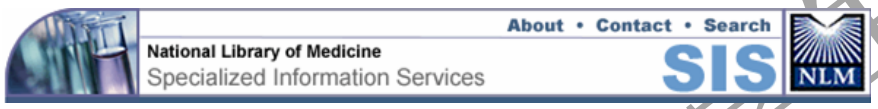
Molecular Weight: 267.242 g/mol
Molecular Formula: $C_{10}H_{13}N_5O_4$

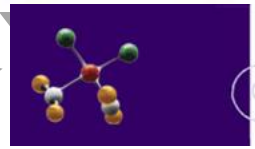
Hydrogen Bond Donor Count: 2
Hydrogen Bond Acceptor Count: 6
Rotatable Bond Count: 3
Tautomer Count: 3

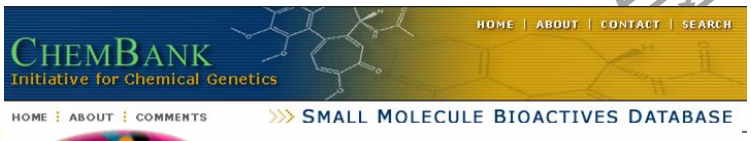
Descriptors Computed from Structure:

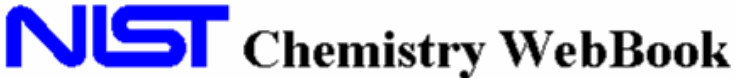
IUPAC Name: 1-[4-azido-5-(hydroxymethyl)oxolan-2-yl]-5-methyl-pyrimidine-2,4-dione
Isomeric SMILES: CC1=CN(C(=O)NC1=O)[C@H]2C[C@@H]([C@H](O2)CO)N=[N+]=[N-]
Canonical SMILES: CC1=CN(C(=O)NC1=O)C2CC(C(O2)CO)N=[N+]=[N-]
InChI: InChI=1/C10H13N5O4/c1-5-3-15(10(18)12-9(5)17)8-2-6(13-14-11)7(4-16)19-8/h3,6-8,16H,2,4H2,1H3,(H,12,17,18)/t6-,7+,8+/m0/s1/f/h12H

PubChem:
Compound, Substance, BioAssay



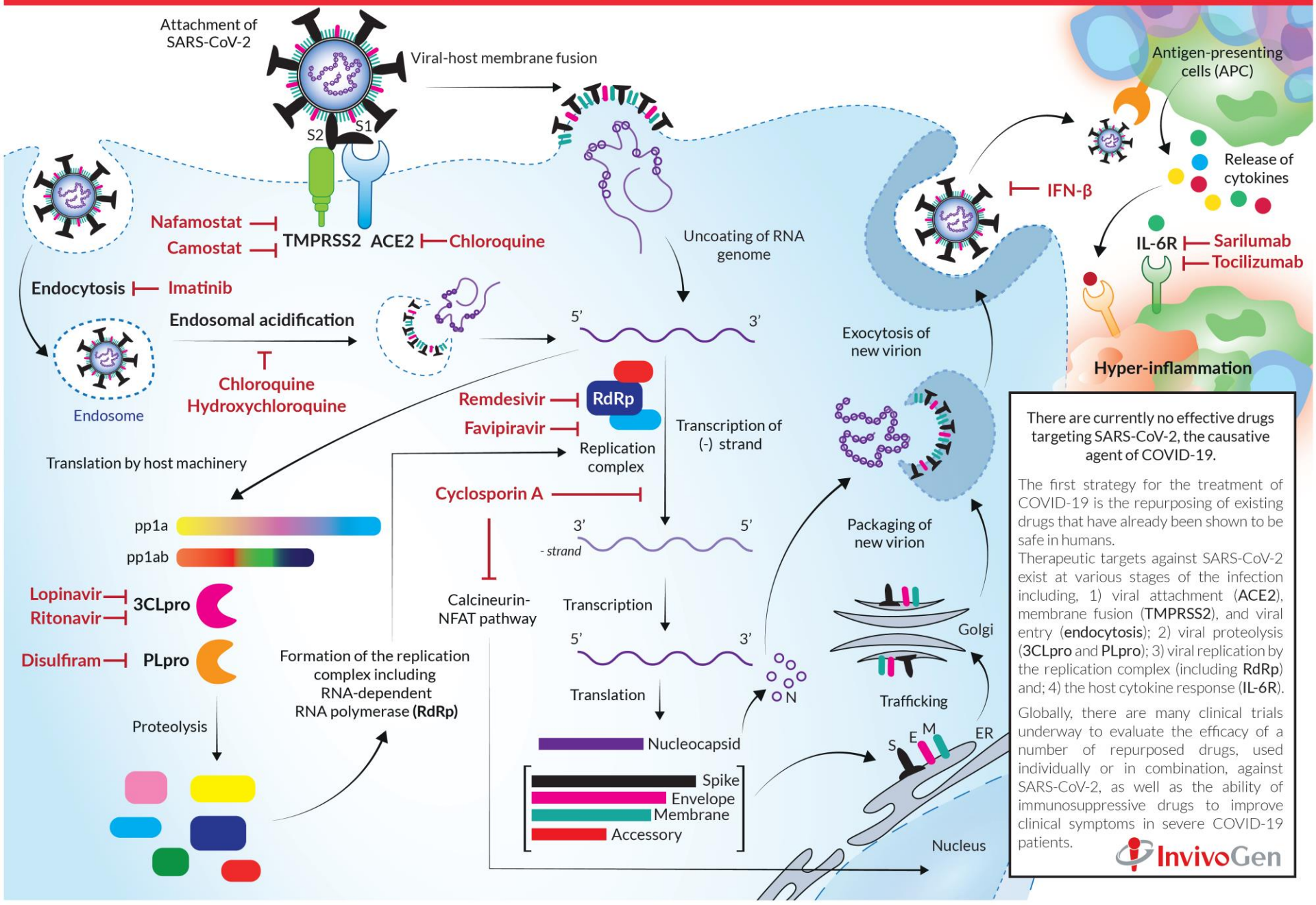






and more….

Repurposing approved drugs for targeting SARS-CoV-2



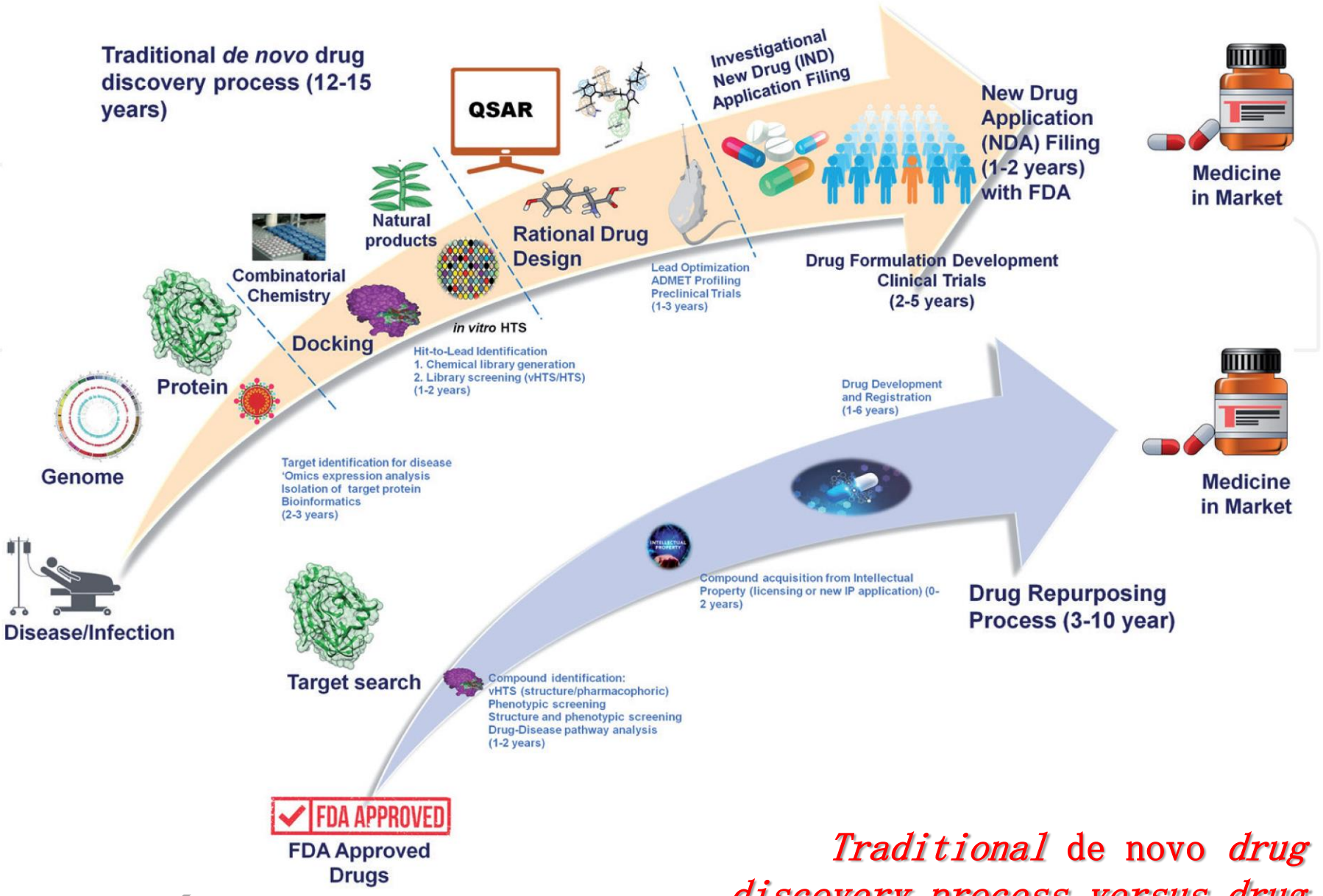
There are currently no effective drugs targeting SARS-CoV-2, the causative agent of COVID-19.

The first strategy for the treatment of COVID-19 is the repurposing of existing drugs that have already been shown to be safe in humans.

Therapeutic targets against SARS-CoV-2 exist at various stages of the infection including, 1) viral attachment (**ACE2**), membrane fusion (**TMPRSS2**), and viral entry (**endocytosis**); 2) viral proteolysis (**3CLpro** and **PLpro**); 3) viral replication by the replication complex (including **RdRp**) and; 4) the host cytokine response (**IL-6R**).

Globally, there are many clinical trials underway to evaluate the efficacy of a number of repurposed drugs, used individually or in combination, against SARS-CoV-2, as well as the ability of immunosuppressive drugs to improve clinical symptoms in severe COVID-19 patients.

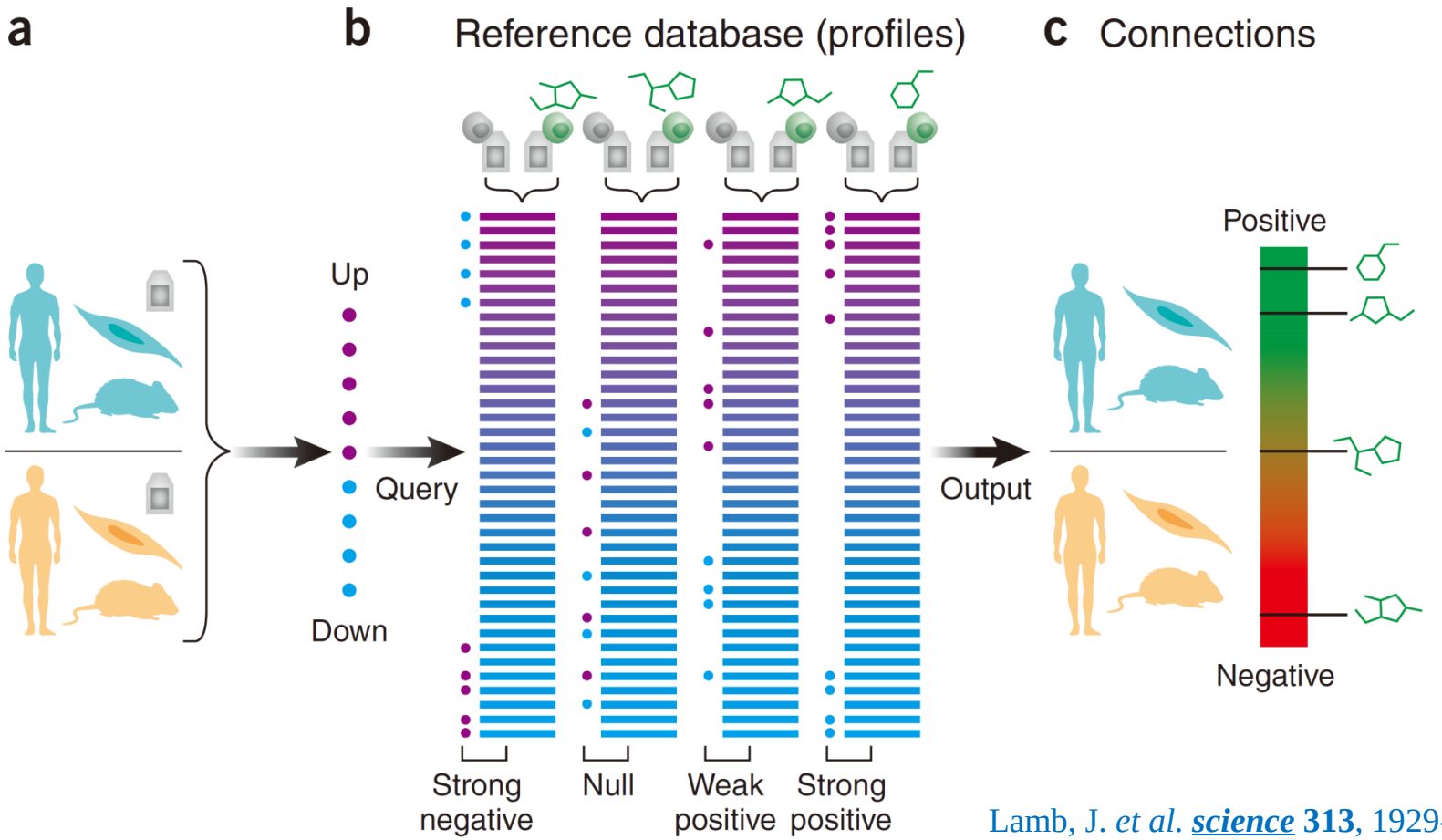
InvivoGen



Traditional de novo *drug discovery process versus drug repurposing process*

CMap: a new tool for drug discovery

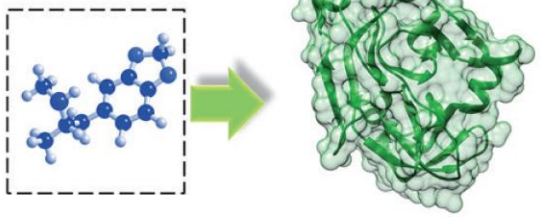
Connectivity Map: *using gene-expression signatures to connect small molecules, genes, and disease*



Lamb, J. *et al.* ***science*** **313**, 1929-1935 (2006).

Lamb, J. The. ***Nature reviews cancer*** **7**, 54 (2007).

Subramanian, A. *et al.* ***Cell*** **171**, 1437-1452. e17 (2017).



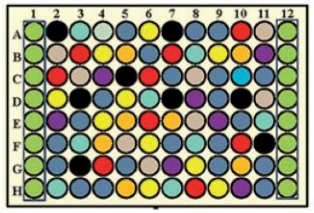
Drug

Target Protein

Drug-Disease Pathway analysis

Genome sequence analysis

Phenotype-Based Drug Repurposing



High throughput screening

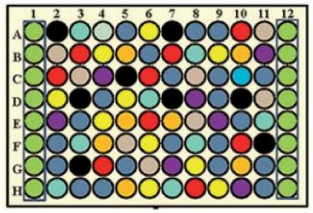
Lead identification

Poly-Pharmacology Analysis

Drug repurposed for New Indication and Treatment

Lead identification

Structure and Phenotype-Based Drug Repurposing



High throughput screening

Identified leads

Pharmacophore Modeling Based on previous Dataset

1861 FDA approved drugs Experimental Knowledge-Based Drug Repositioning Database (EK-DRD) http://www.idruglab.com/drd/index.php.

Microbial Protein Target(s)

Virtual High throughput screening

Drug repurposed for new indication and treatment

Strategies for drug repurposing

【实例8】从NCBI数据库大批量获取数据（借助FTP）

Help for Programmers

NCBI Toolbox: In-house source code useful for incorporating NCBI-like functionality into their programs.
Three main parts: Data Model, Data Encoding and Programming Libraries.

- Examples: BLAST, Cn3D, Sequin, Data format conversion scripts

http://www.ncbi.nlm.nih.gov/IEB/ToolBox/index.cgi

E-Utilities: Guidelines for Entrez "URL calls" used to access data.
Designed for use in scripts.

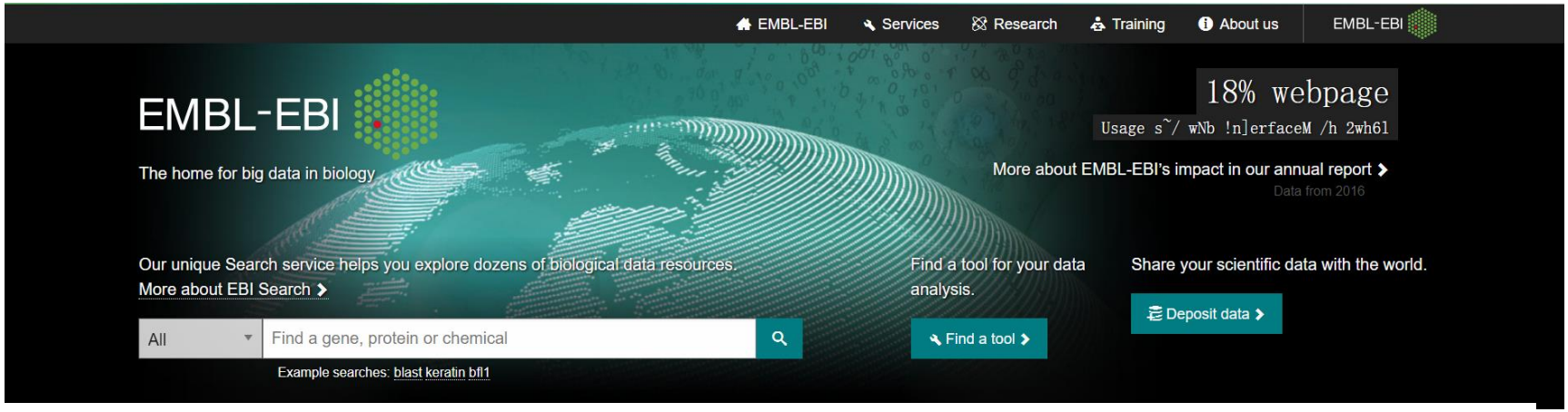
- Examples: ESearch, EPost, ESummary, EFetch and ELink

http://www.ncbi.nih.gov/entrez/query/static/eutils_help.html

Caution: *Overuse may result in blocked IPs!*

Software	Description
rentrez	An R package for the NCBI eUtils API
biodbNcbi	a library for connecting to NCBI Databases
ExpressionAtlas	Download datasets from EMBL-EBI Expression Atlas
gwascat	representing and modeling data in the EMBL-EBI GWAS catalog
prideR	obtain data from the EMBL-EBI PRIDE Archive and PRIDE Cluster)
BiomaRt	quick, easy and powerful way to access BioMart right from your R software terminal
biofiles	An Interface for GenBank/GenPept Flat Files
GEOquery	
SRAdb	A compilation of metadata from NCBI SRA and tools
ensembldb	Utilities to create and use Ensembl-based annotation databases
proActiv	Estimate Promoter Activity from RNA-Seq data
TSRchitect	Promoter identification from large-scale TSS profiling data
CAGEr	Analysis of CAGE (Cap Analysis of Gene Expression) sequencing data for precise mapping of transcription start sites and promoterome mining
UniprotR	Retrieving and visualizing protein sequence and functional information from Universal Protein Resource
AssessORF	Assess Gene Predictions Using Proteomics and Evolutionary Conservation
LedPred	Learning from DNA to Predict Enhancers
ORFhunteR	Predict open reading frames in nucleotide sequences
ORFik	analysis of transcript and translation features through manipulation of sequence data and NGS data like Ribo-Seq, RNA-Seq, TCP-Seq and CAGE

第3节：EMBL数据库与数据资源



We are EMBL-EBI

The European Bioinformatics Institute (EMBL-EBI) is part of EMBL, Europe's flagship laboratory for the life sciences. More about EMBL-EBI and our impact.

Data resources

Explore our open data resources to enrich your research. Browse data, perform analyses or share your own results.

Research

Find out about our research groups, postdoctoral schemes and PhD Programme

Training

Access a wealth of world-leading training in bioinformatics and scientific service provision, regardless of your career stage or sector

Industry

Explore our knowledge-exchange Industry Programme and take part in translational partnerships and projects

ELIXIR

We support, as an ELIXIR node, the coordination of biological data provision throughout Europe

Latest news

Research highlights, service updates and more

Our events

Thurs 27th Sep | Seminar

Deep Learning Double Bill - Dr Antony Rix & Dr Tom Whitehead

In this double bill, they will talk about the potential use of AI in a range of life science applications and when using sparse data.

Tues 2nd Oct - Fri 5th | Course

Introduction to Next Generation Sequencing

This course will provide an introduction to the technology, data analysis, tools and resources for next generation sequencing (NGS) data.

Wed 3rd Oct | Course

Ensembl Browser Workshop, Rabat, 3 October 2018

The Ensembl project at www.ensembl.org provides a comprehensive and integrated source of annotation of mainly

EBI

- 欧洲生物信息学研究所(European Bioinformatics Institute)
- 1994年建于英国剑桥,前身是德国海德堡的欧洲分子生物学实验室的信息服务部门
- EBI接收了原来*EMBL*数据库的管理和维护
- 是欧洲分子生物学网(EMBnet)的一个特别节点
- http://www.ebi.ac.uk/ (主页)
- http://www2.ebi.ac.uk/ (工具)
- http://www3.ebi.ac.uk/ (服务)

EMBL European Molecular Biology Laboratory

Heidelberg

OTHER LOCATIONS

Research | Services | Training | Jobs | About Us

Donate | Staff services | Intranet

Research

RESEARCH UNITS

- Cell Biology and Biophysics
- Developmental Biology
- Directors' Research
- Genome Biology
- Structural and Computational Biology
- Research at other EMBL Sites

SEMINARS

EMBL AND THE TARA OCEAN FOUNDATION

VENTURE CAPITAL

INTERDISCIPLINARY RESEARCH

- Bioinformatics at EMBL
- Chemistry at EMBL
- Physics and Engineering at EMBL
- Mathematics and Statistics at EMBL
- EMBL Centres

FACULTY

PARTNERSHIPS

LIFE SCIENCE ALLIANCE

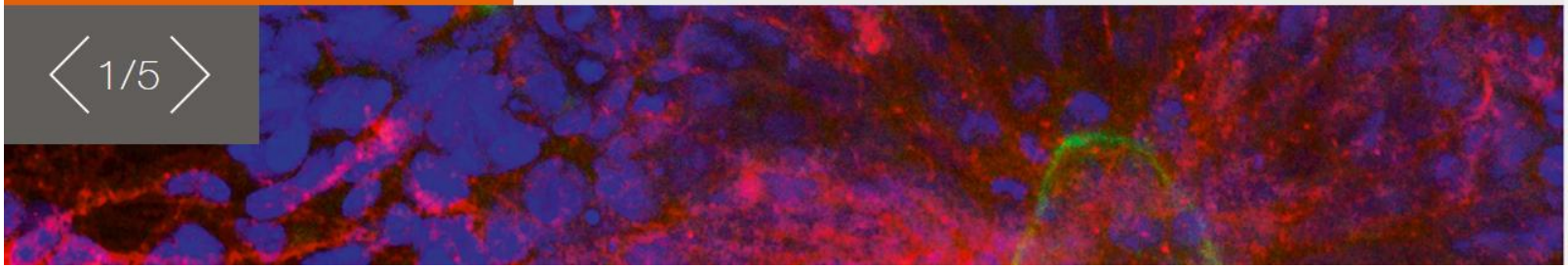
TECHNOLOGY TRANSFER

EMBL International PhD Programme: Winter recruitment 2020

TRAINING

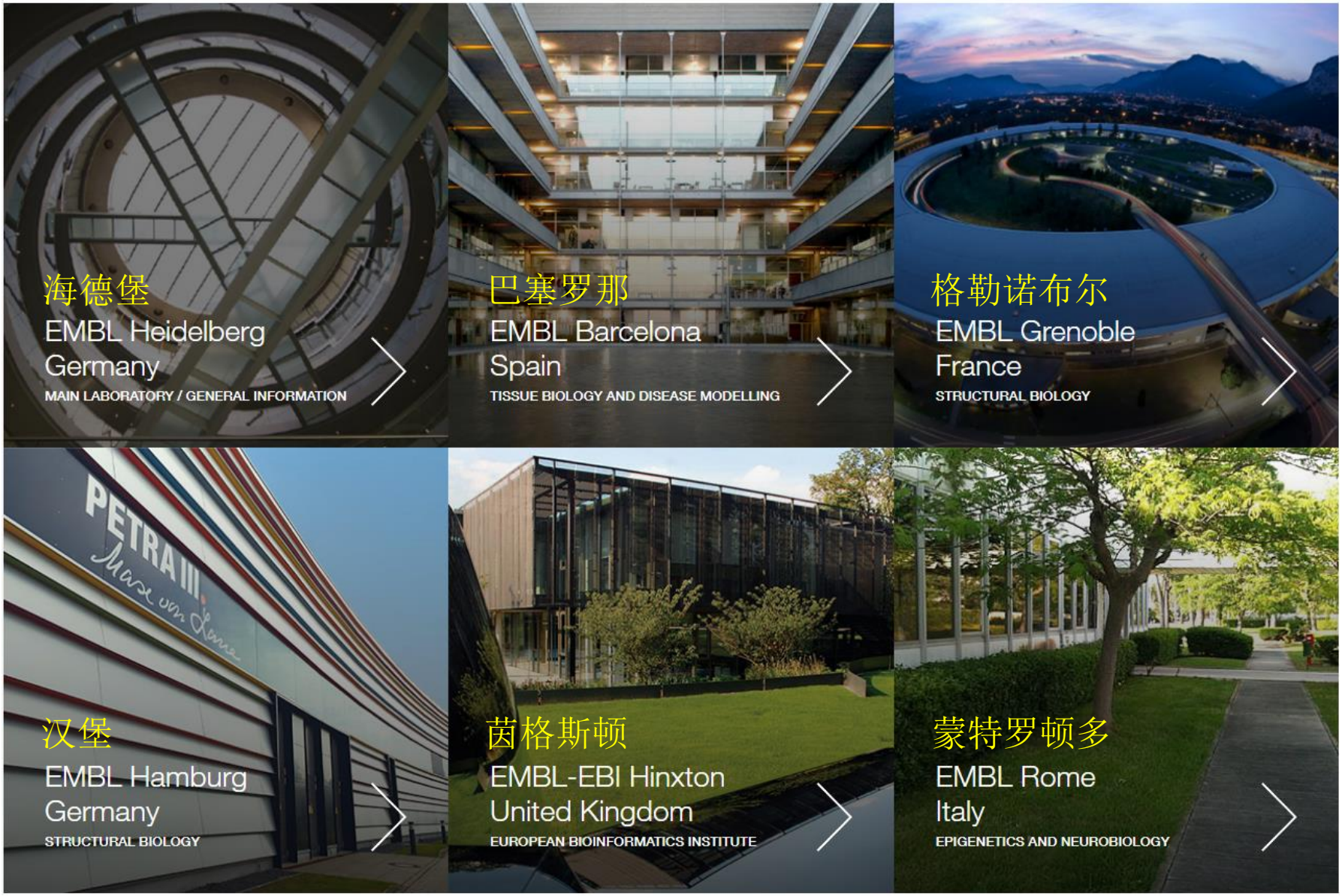
READ MORE

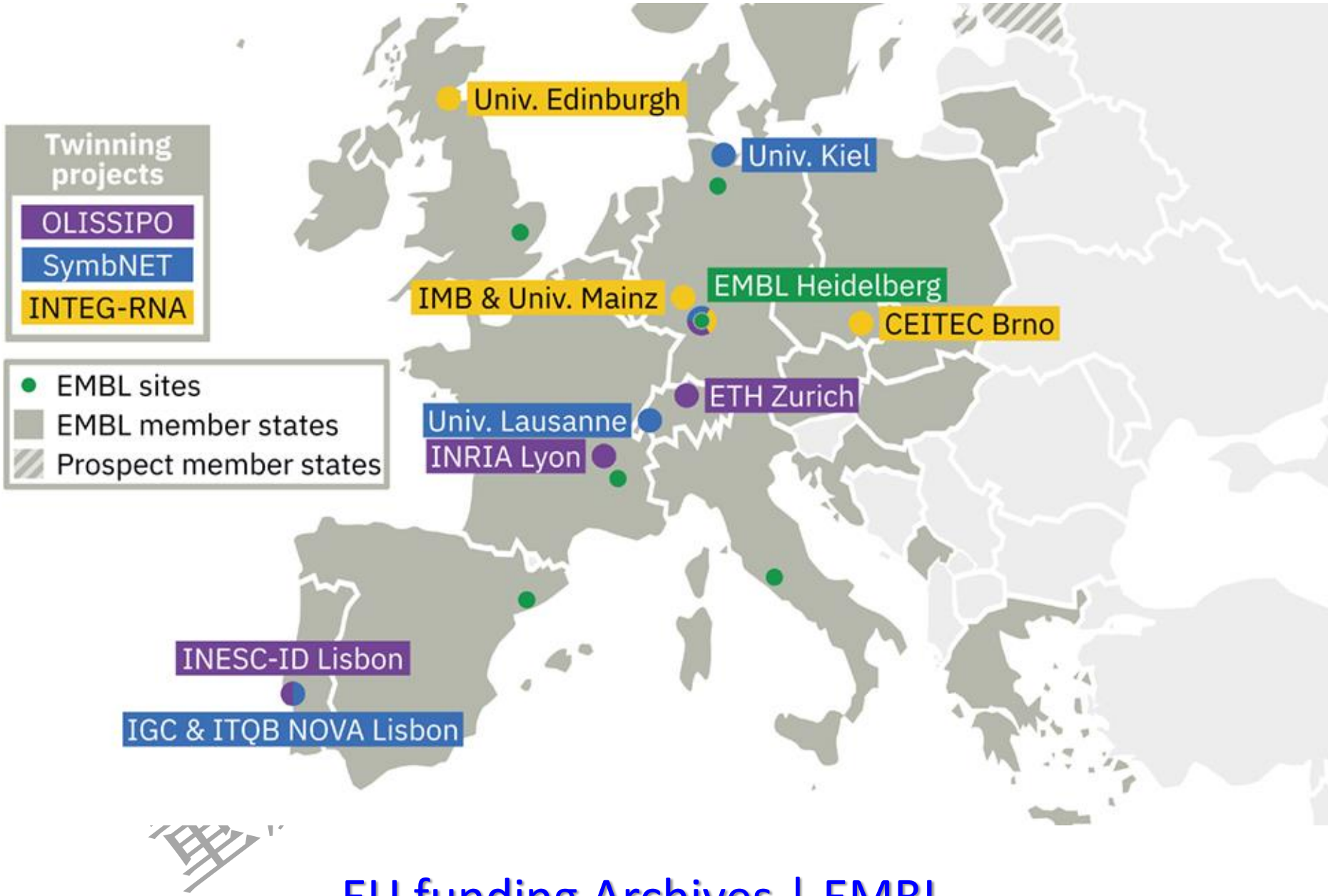
1/5



EMBL的六处的节点

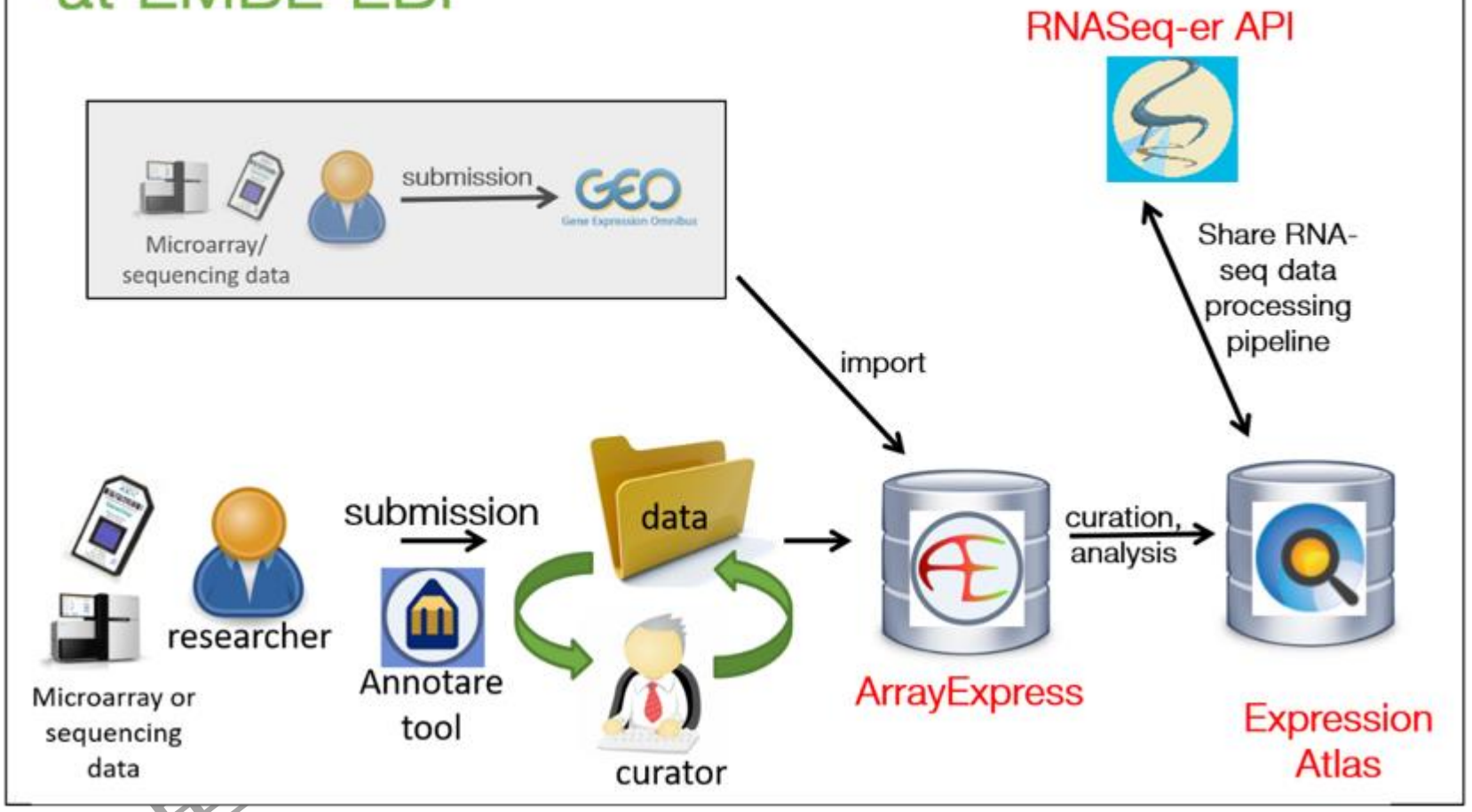
Locations





[EU funding Archives | EMBL]

Summary of functional genomics resources at EMBL-EBI



EBI旗下的数据库资源

Ensembl

Genome browser, API and database, providing access to reference genome annotation

Expression Atlas

An added-value database that shows which genes/proteins are expressed under which conditions, and how expression differs between conditions.

UniProt

A comprehensive resource for protein sequence and functional annotation.

ChEMBL

An open data resource of binding, functional and ADMET bioactivity data.

PDBe

The European resource for the collection, organisation and dissemination of 3D structural data (from PDB and EMDB) on biological macromolecules and their complexes.

See all data resources ›

Europe PMC

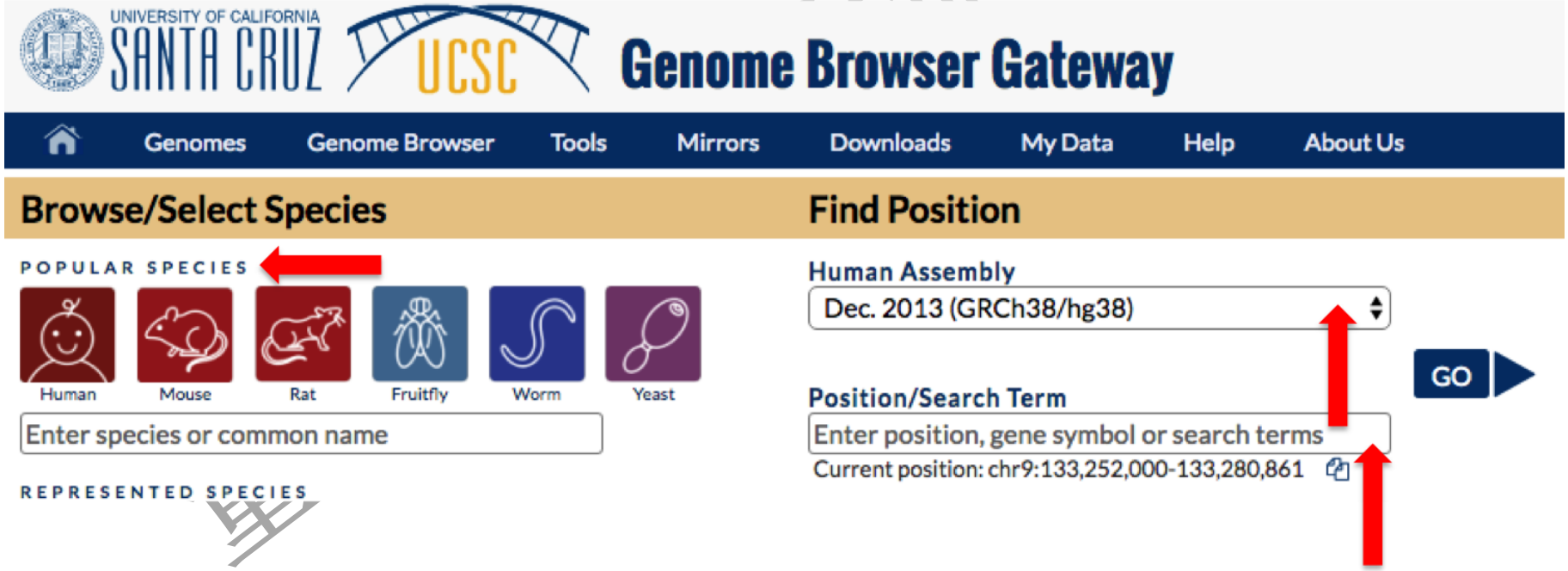
A database to search the worldwide life sciences literature

https://www.ebi.ac.uk/services/all

第4节：UCSC基因组浏览器与数据资源

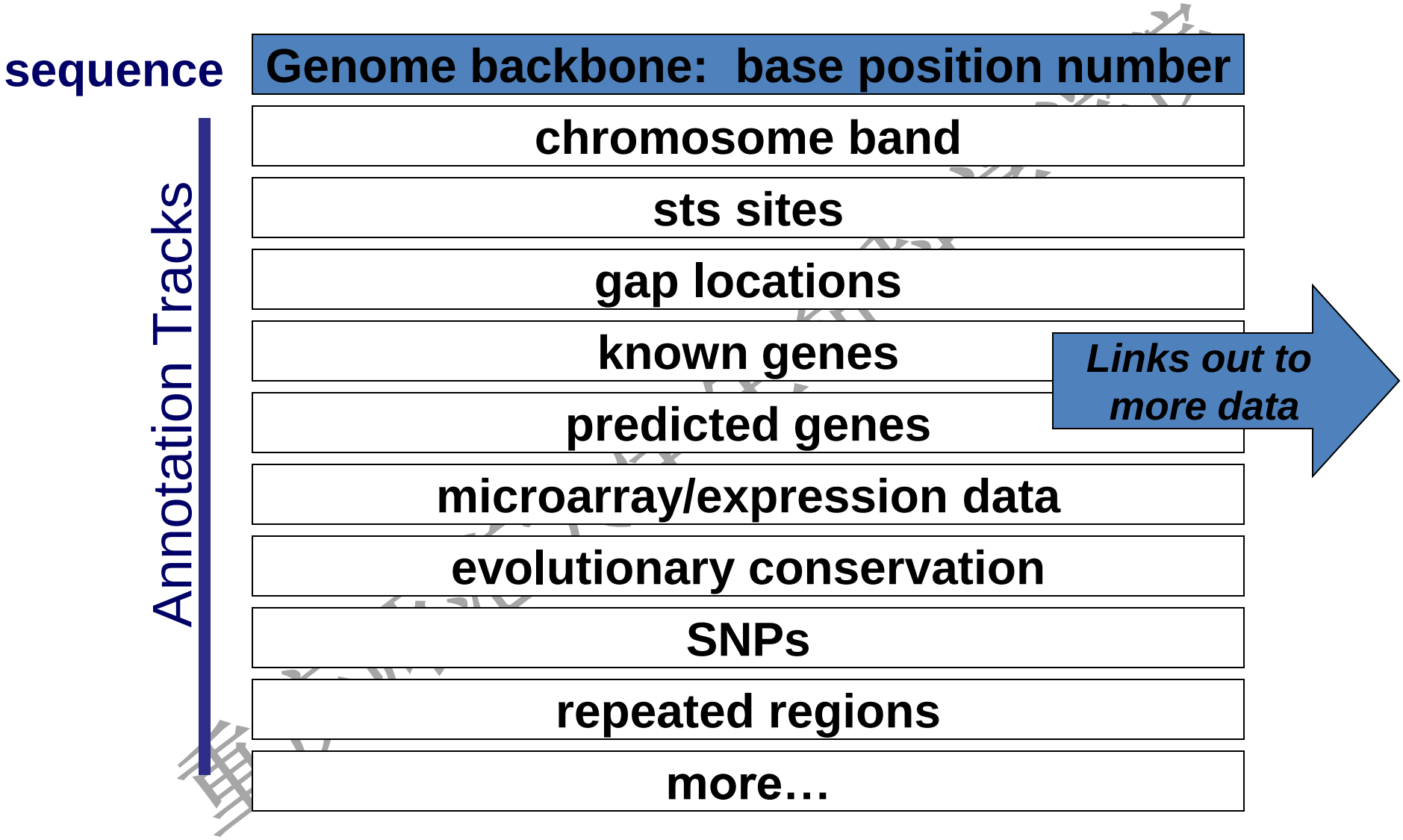
UCSC Genome Browser

UCSC Genome Browser是由University of California Santa Cruz （UCSC)）创立和维护的，该站点包含有人类、小鼠和大鼠等多个物种的基因组草图，并提供一系列的网页分析工具。(可以在任何尺度上快速查询和显示基因组内容。)

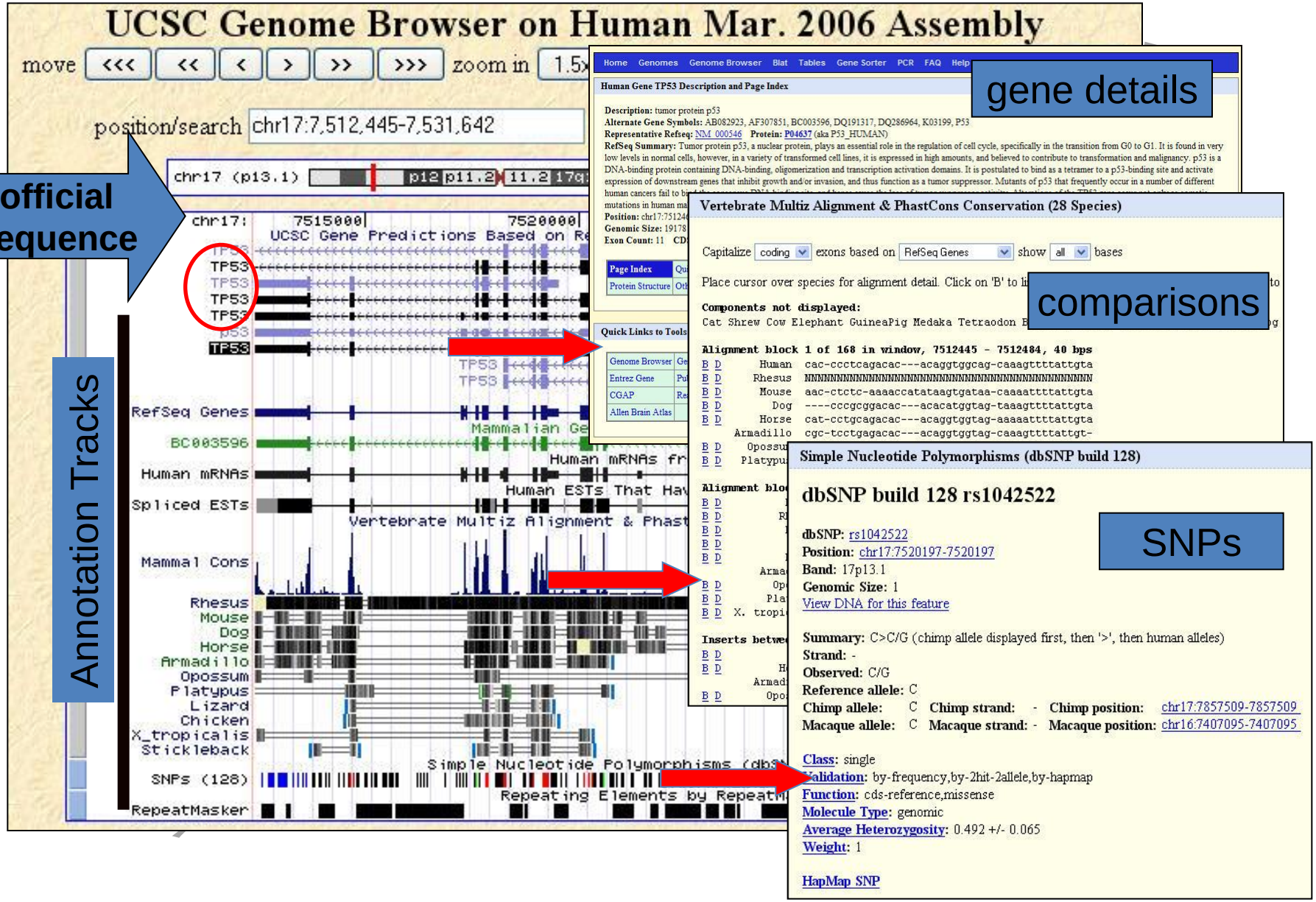


如果想将测序的reads对于到染色体上，可以用UCSc Genome Browser或IGV.

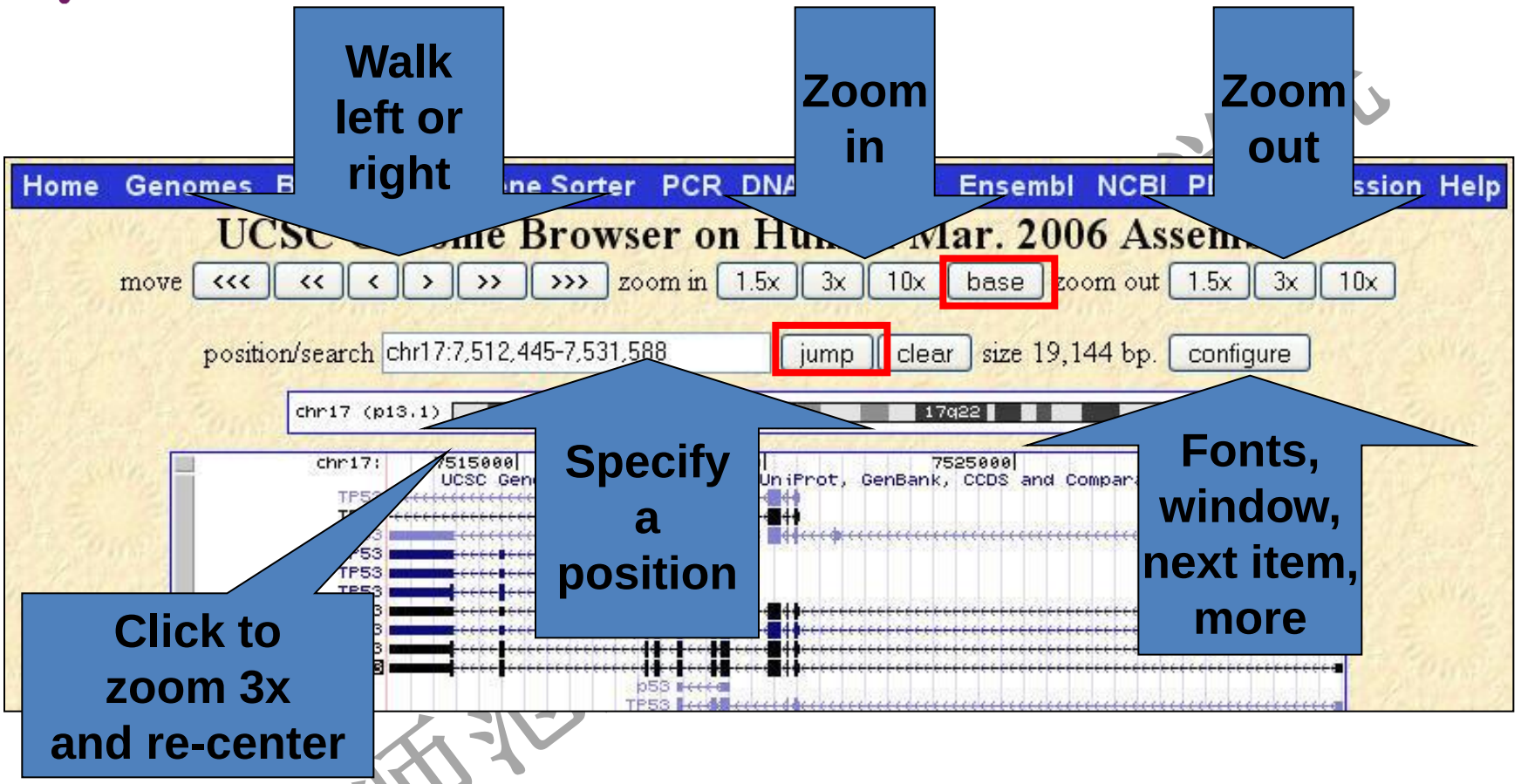
Organization of Genomic Data



A Sample of the UCSC Genome Browser

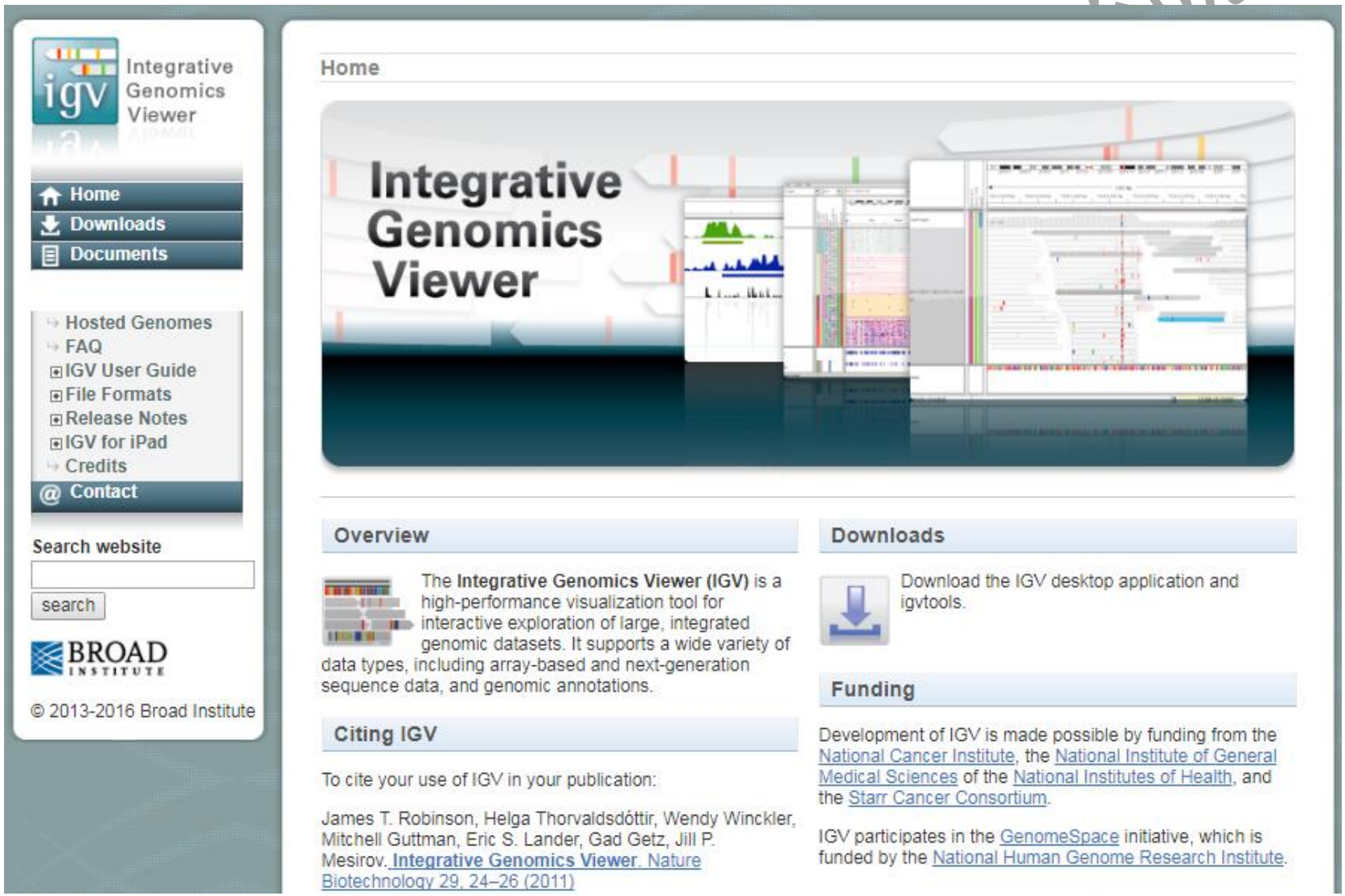


Options for Changing Images: Upper Section



- Next iteChange your view or location with controls at the top
- Use "base" to get right down to the nucleotides
- Configure: to change font, window size, more…
  - m, next exon navigation assistance can be turned on

IGV is a high-performance visualization tool for interactive exploration of large, integrated genomic datasets. It supports a wide variety of data types, including array-based and next-generation sequence data, and genomic annotations.



重庆师范大学
CHONG QING NORMAL UNIVERSIYT

Thanks for your attention!

Acknowledgement

College of Life Sciences, Chongqing Normal University

2022, Chongqing of P. R. C