Biological Databases

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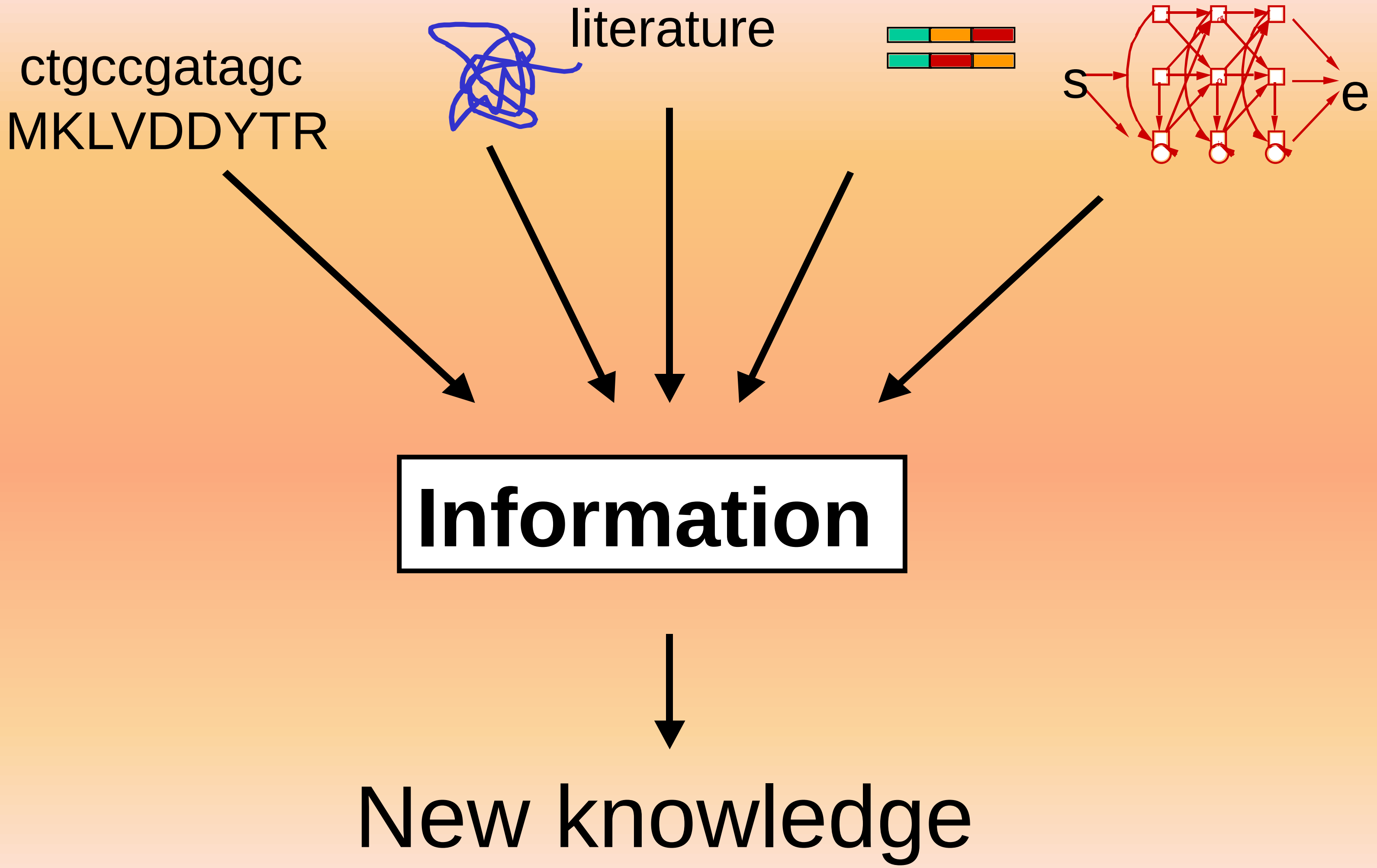
Department of Botany

Where do the data come from?
Example Databases



ctgccgatagc
MKLVDDYTR

literature

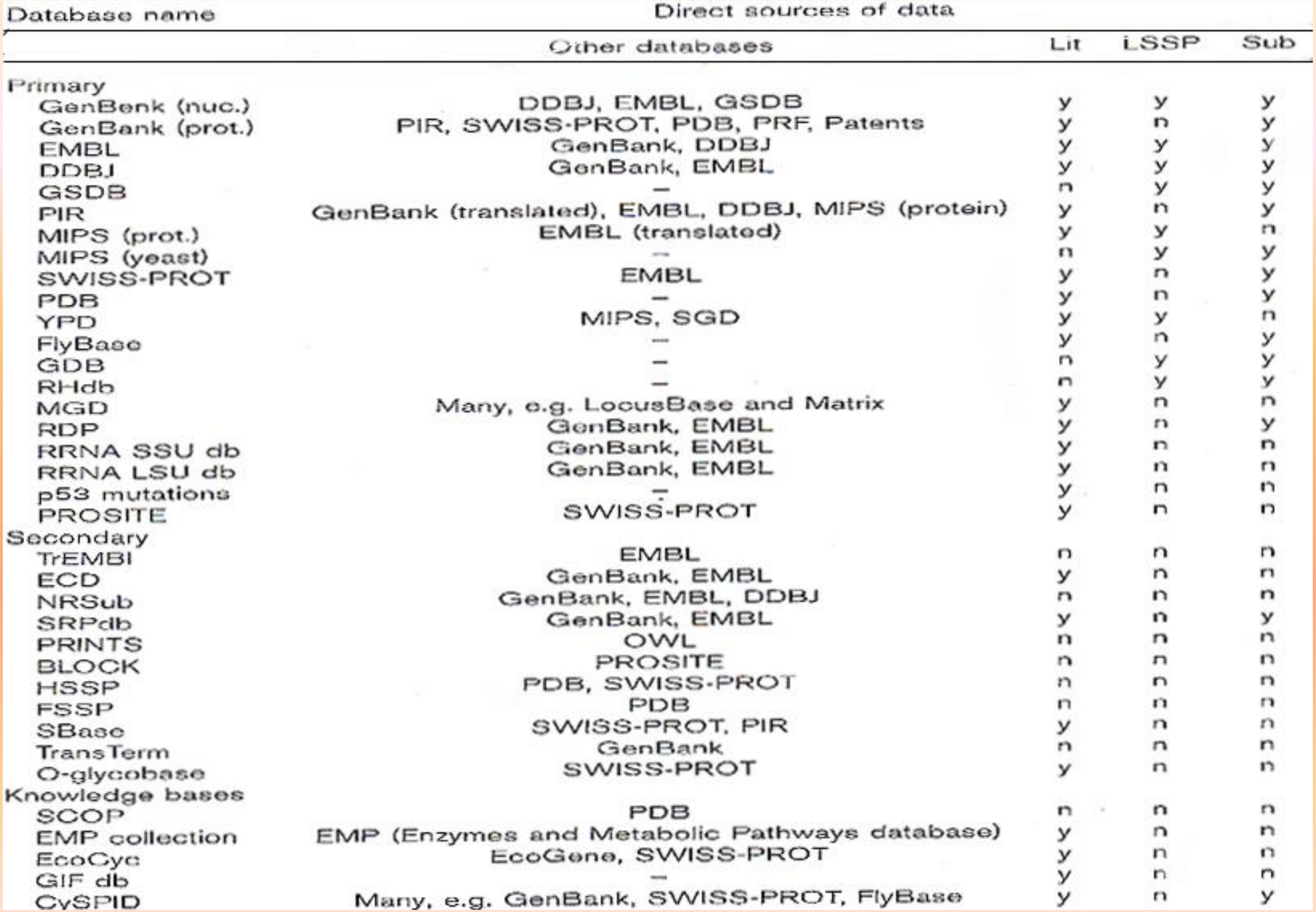
Information

New knowledge

What is a Database/Resource?

NAR Database Issue (www.nar.oupjournals.org)

- **Collection of data in the related format**
  - structured
  - searchable (index) -> table of contents
  - updated periodically (release) -> new edition
  - cross-referenced (hyperlinks) -> links with other db
- Includes also associated tools (software) necessary for db access, db updating, db information insertion, db information deletion….
- Type and Content of Data
  - Sequence or Structure
  - Nucleic acid or protein
  - Important Biological information such as about enzyme and their metabolic pathways, mutations, diseases, drugs, images etc.
- Based on source of data
  - Primary database
  - Secondary database
  - Knowledge bases
  - Integrated Database



Database name	Direct sources of data			
	Other databases	Lit	LSSP	Sub
Primary				
GenBenk (nuc.)	DDBJ, EMBL, GSDB	y	y	y
GenBank (prot.)	PIR, SWISS-PROT, PDB, PRF, Patents	y	n	y
EMBL	GenBank, DDBJ	y	y	y
DDBJ	GenBank, EMBL	y	y	y
GSDB	—	n	y	y
PIR	GenBank (translated), EMBL, DDBJ, MIPS (protein)	y	n	y
MIPS (prot.)	EMBL (translated)	y	y	n
MIPS (yeast)	—	n	y	y
SWISS-PROT	EMBL	y	n	y
PDB	—	y	n	y
YPD	MIPS, SGD	y	y	n
FlyBase	—	y	n	y
GDB	—	n	y	y
RHdb	—	n	y	y
MGD	Many, e.g. LocusBase and Matrix	y	n	n
RDP	GenBank, EMBL	y	n	y
RRNA SSU db	GenBank, EMBL	y	n	n
RRNA LSU db	GenBank, EMBL	y	n	n
p53 mutations	—	y	n	n
PROSITE	SWISS-PROT	y	n	n
Secondary				
TrEMBl	EMBL	n	n	n
ECD	GenBank, EMBL	y	n	n
NRSub	GenBank, EMBL, DDBJ	n	n	n
SRPdb	GenBank, EMBL	y	n	y
PRINTS	OWL	n	n	n
BLOCK	PROSITE	n	n	n
HSSP	PDB, SWISS-PROT	n	n	n
FSSP	PDB	n	n	n
SBase	SWISS-PROT, PIR	y	n	n
TransTerm	GenBank	n	n	n
O-glycobase	SWISS-PROT	y	n	n
Knowledge bases				
SCOP	PDB	n	n	n
EMP collection	EMP (Enzymes and Metabolic Pathways database)	y	n	n
EcoCyc	EcoGene, SWISS-PROT	y	n	n
GIF db	—	y	n	n
CySPID	Many, e.g. GenBank, SWISS-PROT, FlyBase	y	n	y

Primary biological databases

- ***Nucleic acid***

EMBL

GenBank

DDBJ (DNA Data Bank of Japan)

- ***Protein***

PIR

MIPS

SWISS-PROT

TrEMBL

NRL-3D

Nucleotide Databases

- **EMBL:**Nucleotide sequence database
- **Ensembl:** Automatics annotation of eukaryotic genomes
- **Genome Server:** Overview of completed genomes at EBI
- **Genome-MOT:** Genome monitoring table
- **EMBL-Align:** Multiple sequence alignment database
- **Parasites:** Parasite Genome databases
- **Mutations:** Sequence variation database project
- **IMGT:** Immunogenetics database, comprising-
  IMGT/LIGM- database of immunoglobulins and
  T-cell receptors, IMGT/HLA database of the human
  MHC complex and IMGT/MHC covering MHC
  complex of non-human species.

Reference site : www.ebi.ac.uk/Databases/nucleotide.html

EMBL/GenBank/DDJB

- These 3 db contain mainly the same information (few differences in the format and syntax)
- Serve as **archives** containing all sequences (single genes, ESTs, complete genomes, etc.) derived from:
  - Genome projects and sequencing centers
  - Individual scientists
  - Patent offices (i.e. USPTO, EPO)
- Non-confidential data are exchanged daily
- Currently: 2.5 x10^{7} sequences, over 3.2 x10^{10} bp;
- Sequences from > 50,000 different species;

EMBL entry: example

```
ID   HSERPG     standard; DNA; HUM; 3398 BP.
XX
AC   X02158;
XX
SV   X02158.1
XX
DT   13-JUN-1985 (Rel. 06, Created)
DT   22-JUN-1993 (Rel. 36, Last updated, Version 2)
XX
DE   Human gene for erythropoietin
XX
KW   erythropoietin; glycoprotein hormone; hormone; signal peptide.
XX
OS   Homo sapiens (human)
OC   Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi; Mammalia;
OC   Eutheria; Primates; Catarrhini; Hominidae; Homo.
XX
RN   [1]
RP   1-3398
RX   MEDLINE; 85137899.
RA   Jacobs K., Shoemaker C., Rudersdorf R., Neill S.D., Kaufman R.J.,
RA   Mufson A., Seehra J., Jones S.S., Hewick R., Fritsch E.F., Kawakita M.,
RA   Shimizu T., Miyake T.;
RT   Isolation and characterization of genomic and cDNA clones of human
RT   erythropoietin;
RL   Nature 313:806-810(1985).
XX
DR   GDB; 119110; EPO.
DR   GDB; 119615; TIMP1.
DR   SWISS-PROT; P01588; EPO_HUMAN.
XX

...
```

keyword

taxonomy

references

Cross-references

EMBL entry (cont.)

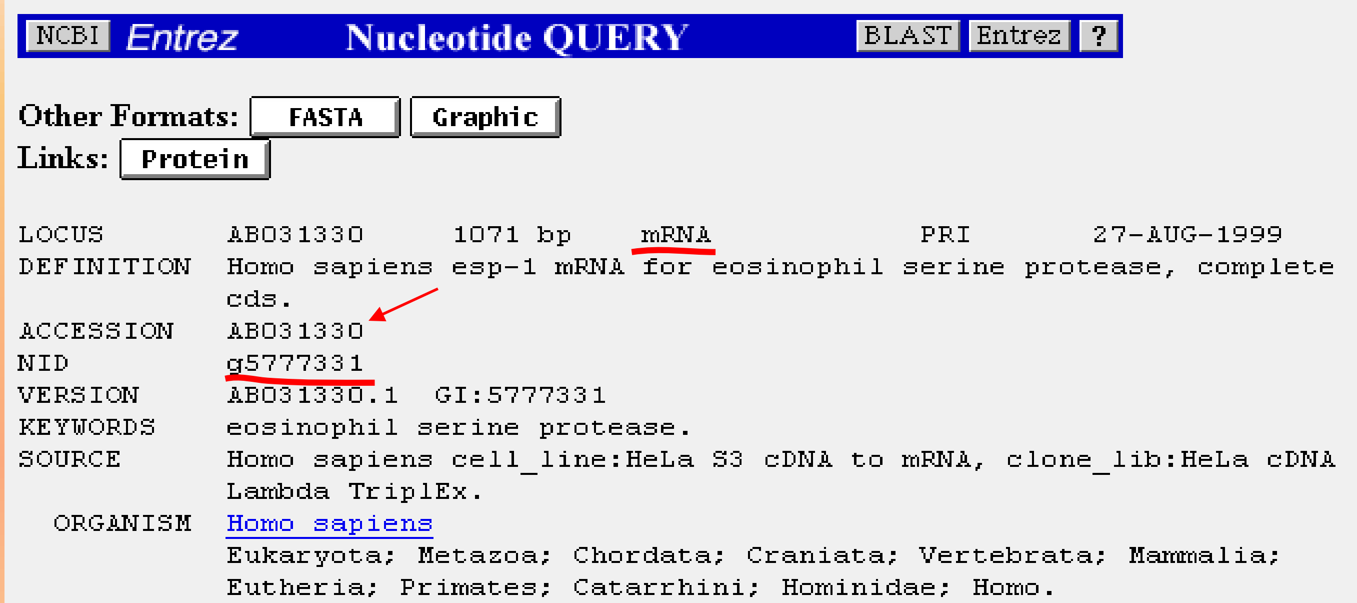
```
CC   Data kindly reviewed (24-FEB-1986) by K. Jacobs
FH   Key              Location/Qualifiers
FH
FT   source           1..3398
FT                    /db_xref=taxon:9606
FT                    /organism=Homo sapiens
FT   mRNA             join(397..627,1194..1339,1596..1682,2294..2473,2608..3327)
FT   CDS              join(615..627,1194..1339,1596..1682,2294..2473,2608..2763)
FT                    /db_xref=SWISS-PROT:P01588
FT                    /product=erythropoietin
FT                    /protein_id=CAA26095.1
FT                    /translation=MGVHECPAWLWLLLSLLSLPLGLPVLGAPPRLICDSRVLQRYLLE
FT                    AKEAENITTGCAEHCSLNENITVPDTKVNFYAWKRMEVGQQAVEVWQGLALLSEAVLRG
FT                    QALLVNSSQPWEPLQLHVDKAVSGLRSLTTLLRALGAQKEAISPPDAASAAPLRTITAD
FT                    TFRKLFRVYSNFLRGKLKLYTGEACRTGDR
FT   mat_peptide      join(1262..1339,1596..1682,2294..2473,2608..2763)
FT                    /product=erythropoietin
FT   sig_peptide      join(615..627,1194..1261)
FT   exon             397..627
FT                    /number=1
FT   intron           628..1193
FT                    /number=1
FT   exon             1194..1339
FT                    /number=2
FT   intron           1340..1595
FT                    /number=2
FT   exon             1596..1682
FT                    /number=3
FT   intron           1683..2293
FT                    /number=3
FT   exon             2294..2473
FT                    /number=4
FT   intron           2474..2607
FT                    /number=4
FT   exon             2608..3327
FT                    /note=3' untranslated region
FT                    /number=5
XX
```

annotation

sequence

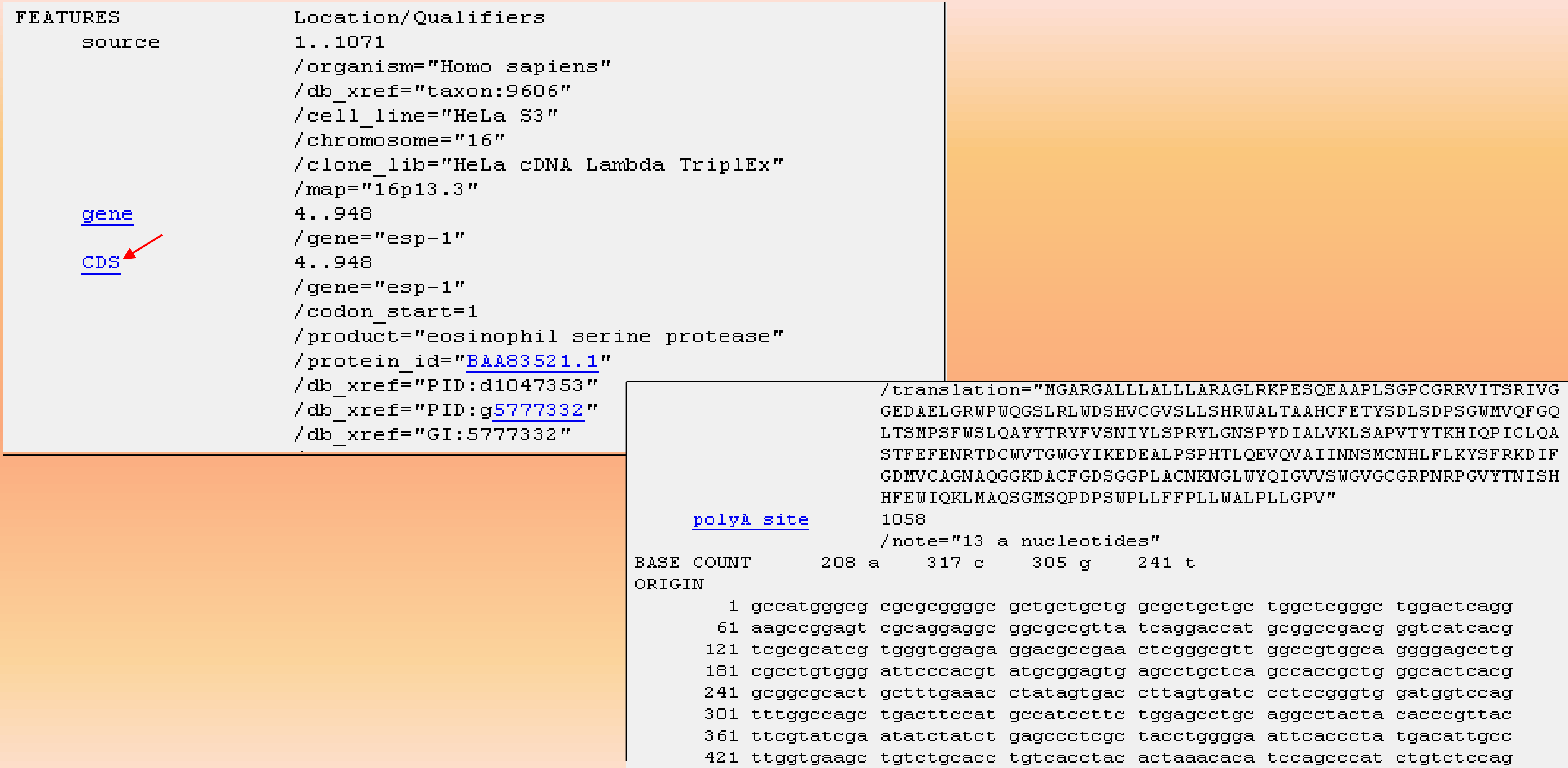
```
SQ   Sequence 3398 BP; 698 A; 1034 C; 991 G; 675 T; 0 other;
     agcttctggg cttccagacc cagctacttt gcggaactca gcaacccagg catctctgag        60
     tctccgccca agaccgggat gccccccagg aggtgtccgg gagcccagcc tttcccagat       120
```

GenBank file format



```
LOCUS       AB031330     1071 bp    mRNA            PRI       27-AUG-1999
DEFINITION  Homo sapiens esp-1 mRNA for eosinophil serine protease, complete
            cds.
ACCESSION   AB031330
NID         g5777331
VERSION     AB031330.1  GI:5777331
KEYWORDS    eosinophil serine protease.
SOURCE      Homo sapiens cell_line:HeLa S3 cDNA to mRNA, clone_lib:HeLa cDNA
            Lambda TriplEx.
  ORGANISM  Homo sapiens
            Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Mammalia;
            Eutheria; Primates; Catarrhini; Hominidae; Homo.
```

GenBank file format

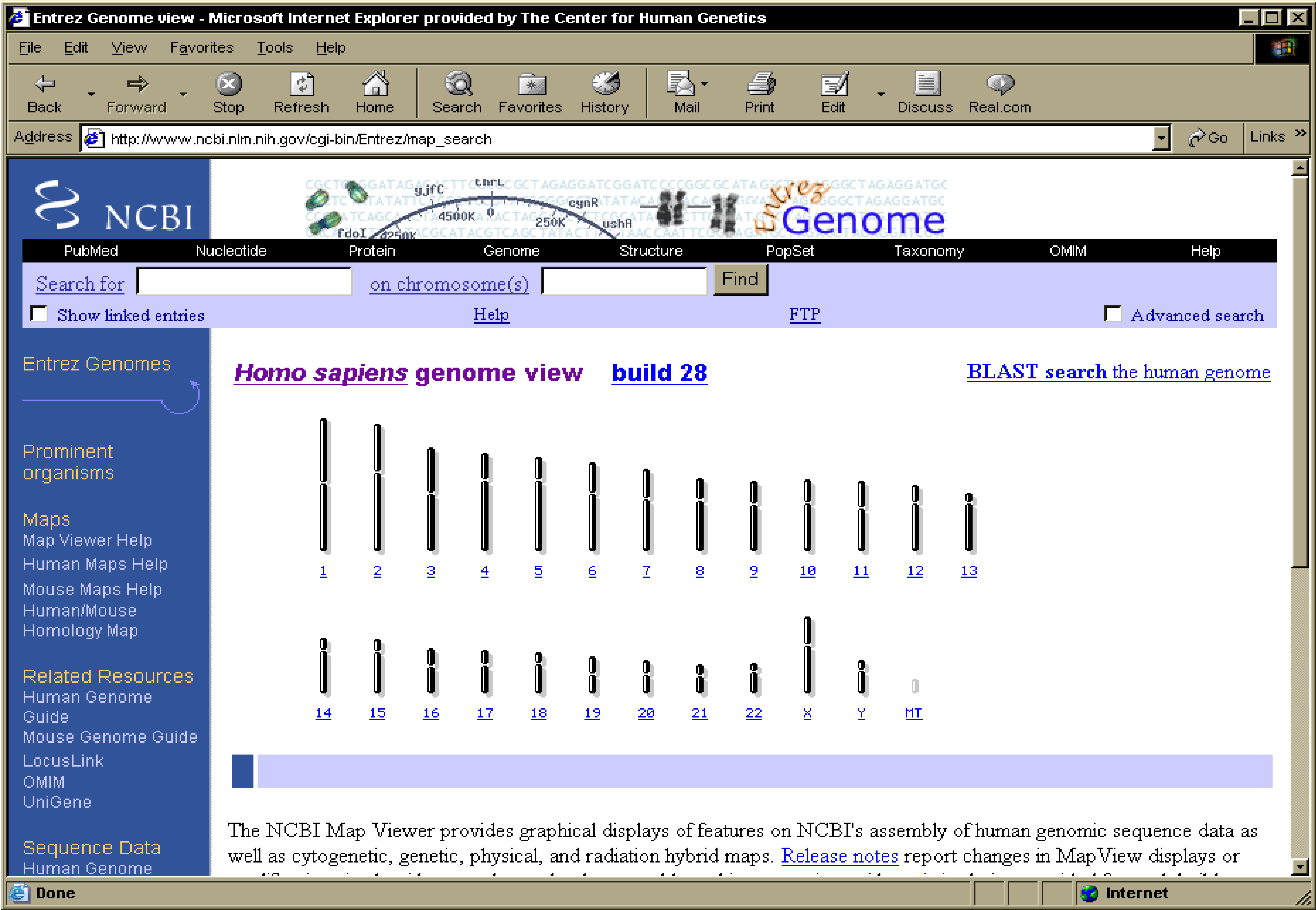


```
FEATURES             Location/Qualifiers
     source          1..1071
                     /organism="Homo sapiens"
                     /db_xref="taxon:9606"
                     /cell_line="HeLa S3"
                     /chromosome="16"
                     /clone_lib="HeLa cDNA Lambda TriplEx"
                     /map="16p13.3"
     gene            4..948
                     /gene="esp-1"
     CDS             4..948
                     /gene="esp-1"
                     /codon_start=1
                     /product="eosinophil serine protease"
                     /protein_id="BAA83521.1"
                     /db_xref="PID:d1047353"
                     /db_xref="PID:g5777332"
                     /db_xref="GI:5777332"
```

```
                     /translation="MGARGALLLALLLARAGLRKPESQEAAPLSGPCGRRVITSRIVG
                     GEDAELGRWPWQGSLRLWDSHVCGVSLLSHRWALTAAHCFETYSDLSDPSGWMVQFGQ
                     LTSMPSFWSLQAYYTRYFVSNIYLSPRYLGNSPYDIALVKLSAPVTYTKHIQPICLQA
                     STFEFENRTDCWVTGWGYIKEDEALPSPHTLQEVQVAIINNSMCNHLFLKYSFRKDIF
                     GDMVCAGNAQGGKDACFGDSGGPLACNKNGLWYQIGVVSWGVGCGRPNRPGVYTNISH
                     HFEWIQKLMAQSGMSQPDPSWPLLFFPLLWALPLLGPV"
     polyA site      1058
                     /note="13 a nucleotides"
BASE COUNT      208 a    317 c    305 g    241 t
ORIGIN
        1 gccatgggcg cgcgcggggc gctgctgctg gcgctgctgc tggctcgggc tggactcagg
       61 aagccggagt cgcaggaggc ggcgccgtta tcaggaccat gcggccgacg ggtcatcacg
      121 tcgcgcatcg tgggtggaga ggacgccgaa ctcgggcgtt ggccgtggca ggggagcctg
      181 cgcctgtggg attcccacgt atgcggagtg agcctgctca gccaccgctg ggcactcacg
      241 gcggcgcact gctttgaaac ctatagtgac cttagtgatc cctccgggtg gatggtccag
      301 tttggccagc tgacttccat gccatccttc tggagcctgc aggcctacta cacccgttac
      361 ttcgtatcga atatctatct gagccctcgc tacctgggga attcacccta tgacattgcc
      421 ttggtgaagc tgtctgcacc tgtcacctac actaaacaca tccagcccat ctgtctccag
```

Databases related to Genomics

- Contain information on genes, gene location (mapping), gene nomenclature and links to sequence databases;
- Exist for most organisms important for life science research;
- Examples: MIM, GDB (human), MGD (mouse), FlyBase (Drosophila), SGD (yeast), MaizeDB (maize), SubtiList (B.subtilis), etc.
- Format: generally relational (Oracle, SyBase or AceDb).



Address: http://www.ncbi.nlm.nih.gov/cgi-bin/Entrez/map_search

Search for □ on chromosome(s) □ Find

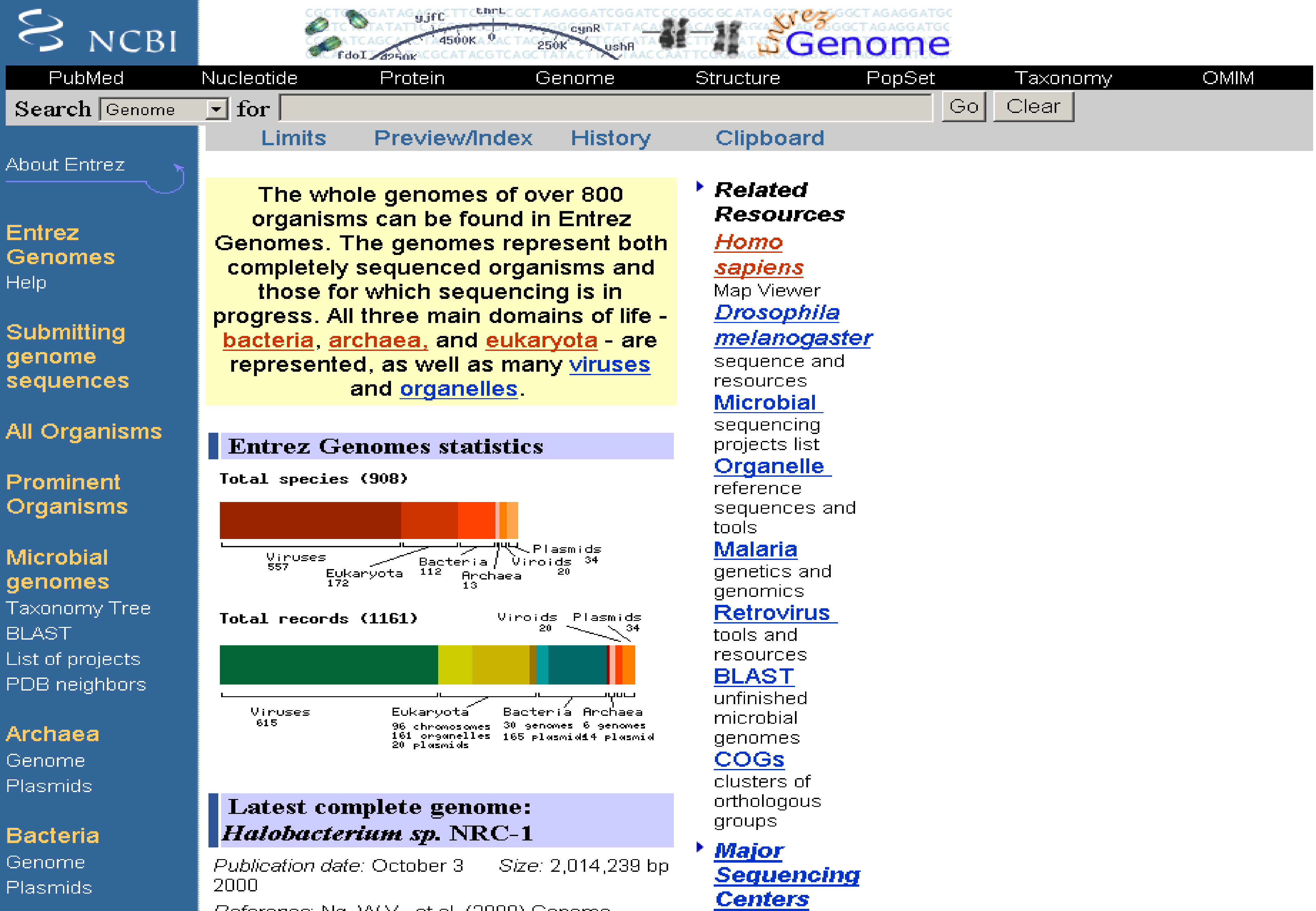
□ Show linked entries

□ Advanced search

Homo sapiens genome view **build 28**

BLAST search the human genome

The NCBI Map Viewer provides graphical displays of features on NCBI's assembly of human genomic sequence data as well as cytogenetic, genetic, physical, and radiation hybrid maps. Release notes report changes in MapView displays or



About Entrez

Entrez Genomes
Help

Submitting genome sequences

All Organisms

Prominent Organisms

Microbial genomes
Taxonomy Tree
BLAST
List of projects
PDB neighbors

Archaea
Genome
Plasmids

Bacteria
Genome
Plasmids

The whole genomes of over 800 organisms can be found in Entrez Genomes. The genomes represent both completely sequenced organisms and those for which sequencing is in progress. All three main domains of life - bacteria, archaea, and eukaryota - are represented, as well as many viruses and organelles.

Entrez Genomes statistics

Total species (908)

Total records (1161)

Latest complete genome: *Halobacterium sp.* NRC-1

Publication date: October 3 2000 *Size:* 2,014,239 bp

Reference: Ng, W.V., et al. (2000) Genome

Related Resources

Homo sapiens
Map Viewer

Drosophila melanogaster
sequence and resources

Microbial
sequencing projects list

Organelle
reference sequences and tools

Malaria
genetics and genomics

Retrovirus
tools and resources

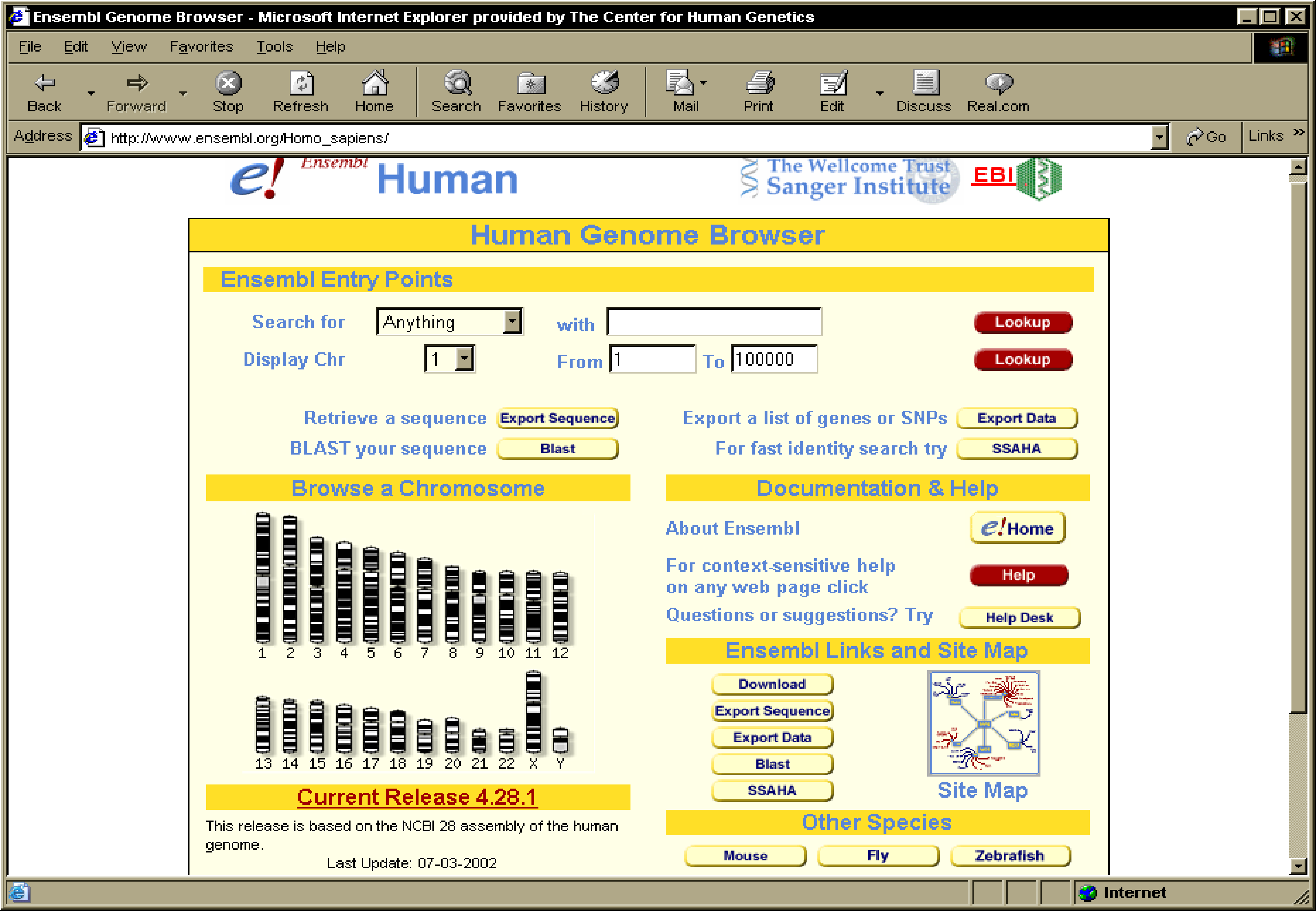
BLAST
unfinished microbial genomes

COGs
clusters of orthologous groups

Major Sequencing Centers

Ensembl

- Contains all the human genome DNA sequences currently available in the public domain.
- Automated annotation: by using different software tools, features are identified in the DNA sequences:
  - Genes (known or predicted)
  - Single nucleotide polymorphisms (SNPs)
  - Repeats
  - Homologies
- Created and maintained by the EBI and the Sanger Center (UK)
- www.ensembl.org



Ensembl Genome Browser - Microsoft Internet Explorer provided by The Center for Human Genetics

Address http://www.ensembl.org/Homo_sapiens/

Ensembl Human

The Wellcome Trust Sanger Institute

EBI

Human Genome Browser

Ensembl Entry Points

Search for: Anything with

Display Chr: 1 From 1 To 100000

Retrieve a sequence Export Sequence

BLAST your sequence Blast

Export a list of genes or SNPs Export Data

For fast identity search try SSAHA

Browse a Chromosome

Current Release 4.28.1

This release is based on the NCBI 28 assembly of the human genome.

Last Update: 07-03-2002

Documentation & Help

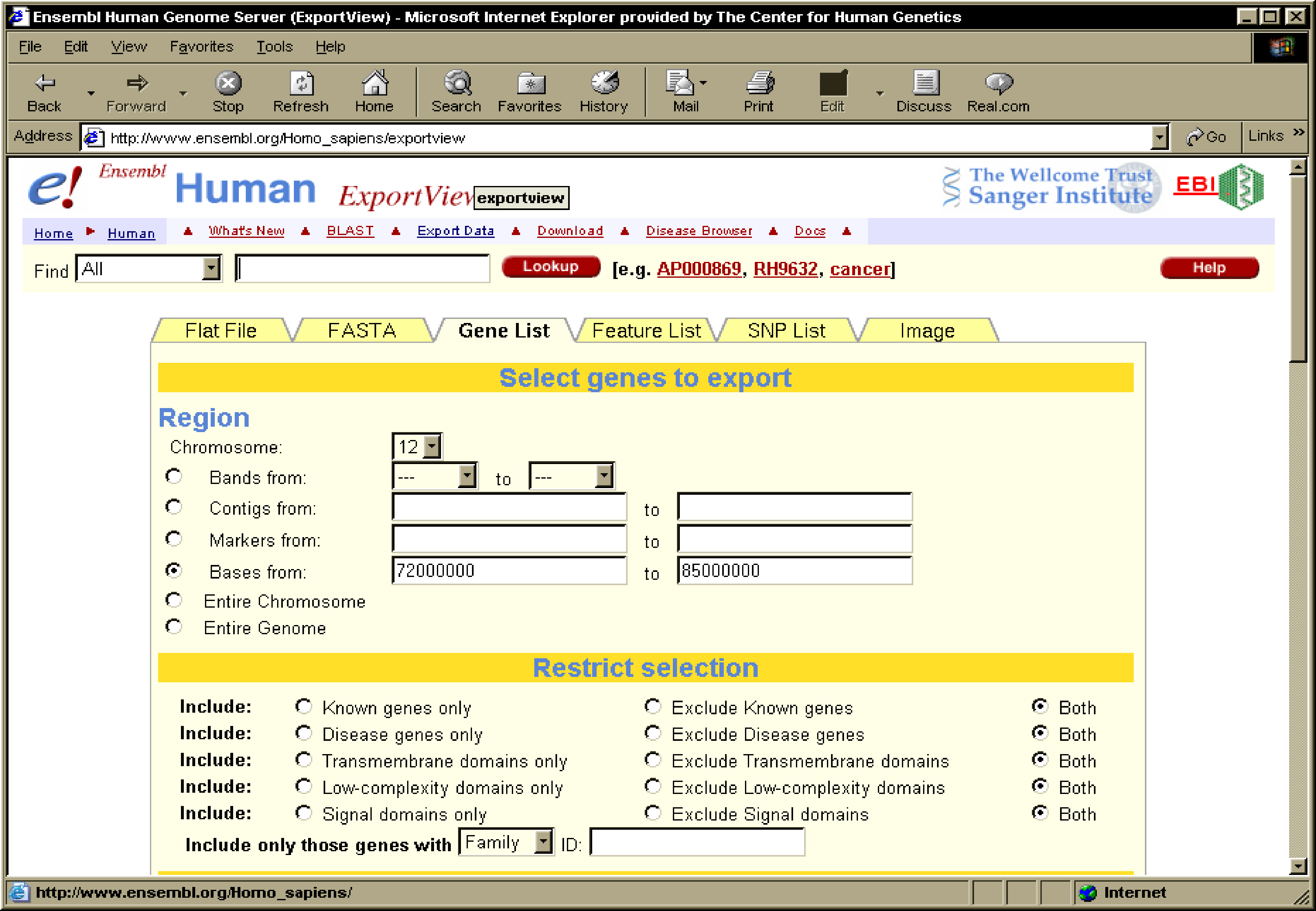
About Ensembl e! Home

For context-sensitive help on any web page click Help

Questions or suggestions? Try Help Desk

Ensembl Links and Site Map

Other Species


File Edit View Favorites Tools Help
Back Forward Stop Refresh Home Search Favorites History Mail Print Edit Discuss Real.com
Address
Go
Links
Home ▸ Human ▲ What's New ▲ BLAST ▲ Export Data ▲ Download ▲ Disease Browser ▲ Docs ▲
Lookup
Help
Internet

Ensembl Human Genome Server (ExportView) - Microsoft Internet Explorer provided by The Center for Human Genetics

Address: http://www.ensembl.org/Homo_sapiens/exportview

e! Ensembl Human ExportView exportview

The Wellcome Trust Sanger Institute EBI

Find All [e.g. AP000869, RH9632, cancer]

Flat File | FASTA | Gene List | Feature List | SNP List | Image

Select genes to export

Region

Chromosome: 12

○ Bands from: --- to ---

○ Contigs from: to

○ Markers from: to

● Bases from: 72000000 to 85000000

○ Entire Chromosome

○ Entire Genome

Restrict selection

Include:	○ Known genes only	○ Exclude Known genes	● Both
Include:	○ Disease genes only	○ Exclude Disease genes	● Both
Include:	○ Transmembrane domains only	○ Exclude Transmembrane domains	● Both
Include:	○ Low-complexity domains only	○ Exclude Low-complexity domains	● Both
Include:	○ Signal domains only	○ Exclude Signal domains	● Both

Include only those genes with Family ID:

http://www.ensembl.org/Homo_sapiens/

Protein Databases

- **SWISS-PROT:** Annotated Sequence Database
- **TrEMBL:** Database of EMBL nucleotide translated sequences
- **InterPro:**Integrated resource for protein families, domains and functional sites.
- **CluSTr:**Offers an automatic classification of SWISS-PROT and TrEMBL.
- **IPI:** A non-redundant human proteome set constructed from SWISS-PROT, TrEMBL, Ensembl and RefSeq.
- **GOA:** Provides assignments of gene products to the Gene Ontology (GO) resource.
- **Proteome Analysis:** Statistical and comparative analysis of the predicted proteomes of fully sequenced organisms
- **Protein Profiles:** Tables of SWISS-PROT and TrEMBL entries and alignments for the protein families of the Protein Profile.
- **IntEnz:** The Integrated relational Enzyme database (IntEnz) will contain enzyme data approved by the Nomenclature Committee.

Reference site : www.ebi.ac.uk/Databases/protein.html

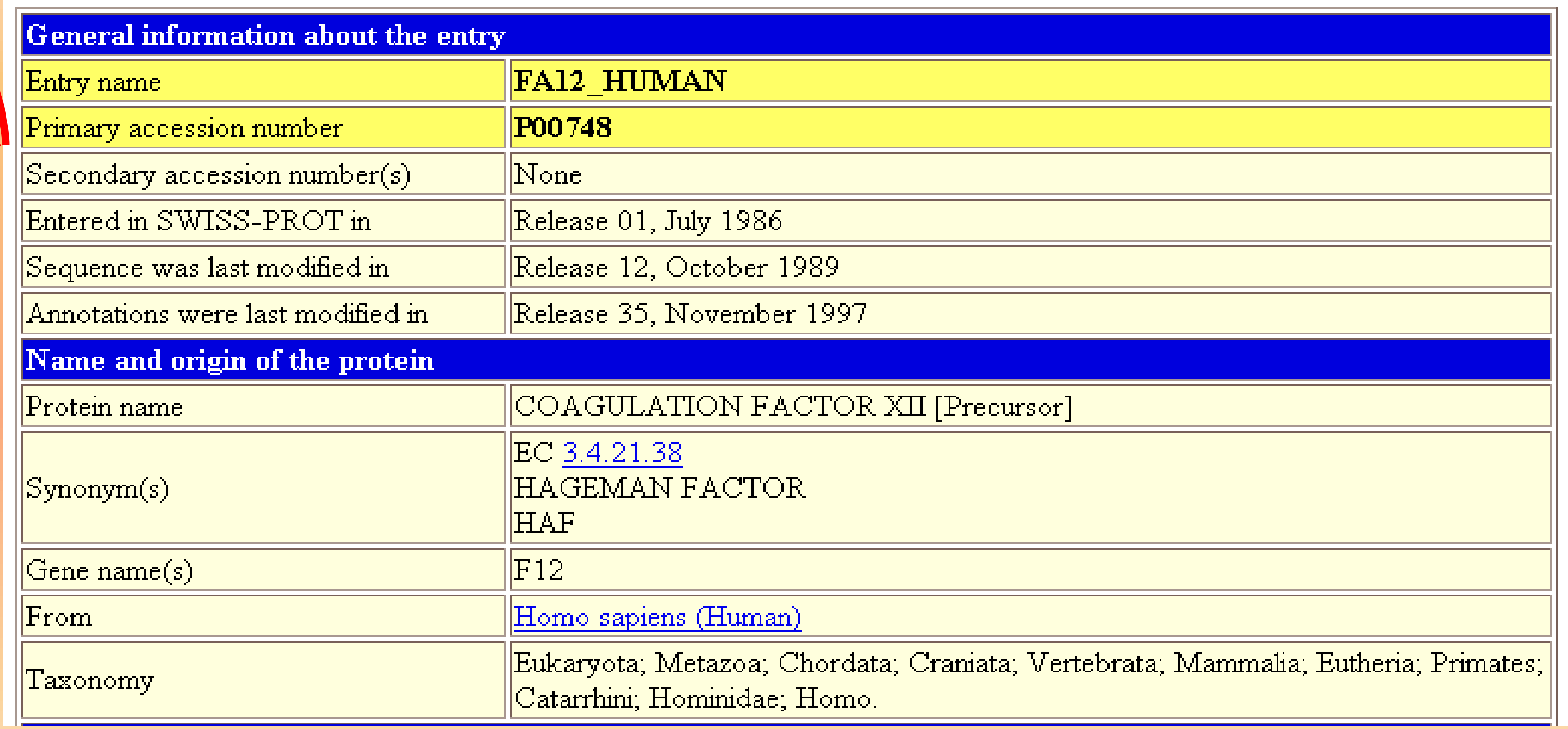
Swiss-Prot

- Annotated protein sequence database established in 1986 and maintained collaboratively since 1987, by the Department of Medical Biochemistry of the University of Geneva and EBI
- Complete, Curated, Non-redundant and cross-referenced with 34 other databases
- Highly cross-referenced
- Available from a variety of servers and through sequence analysis software tools
- More than 8,000 different species
- First 20 species represent about 42% of all sequences in the database
- More than 1,29,000 entries with 4.7 X 10^{10} amino acids
- More than 6,22,000 entries in TrEMBL

TrEMBL (Translation of EMBL)

- Computer-annotated supplement to SWISS-PROT, as it is impossible to cope with the flow of data…
- Well-structure SWISS-PROT-like resource
- Derived from automated EMBL CDS translation maintained at the EBI, UK.
- TrEMBL is automatically generated and annotated using software tools (incompatible with the SWISS-PROT in terms of quality)
- TrEMBL contains all what is **not yet** in SWISS-PROT

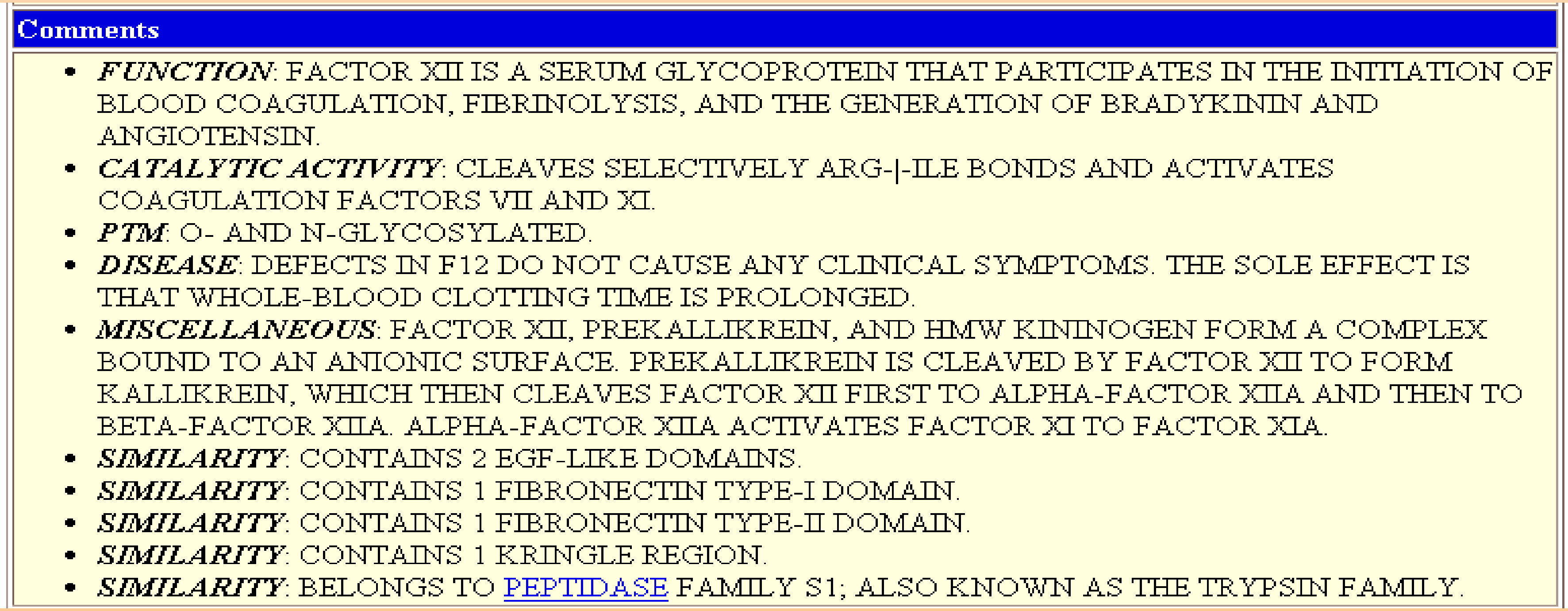
SWISS-PROT file format



General information about the entry	
Entry name	**FA12_HUMAN**
Primary accession number	**P00748**
Secondary accession number(s)	None
Entered in SWISS-PROT in	Release 01, July 1986
Sequence was last modified in	Release 12, October 1989
Annotations were last modified in	Release 35, November 1997
Name and origin of the protein	
Protein name	COAGULATION FACTOR XII [Precursor]
Synonym(s)	EC 3.4.21.38 HAGEMAN FACTOR HAF
Gene name(s)	F12
From	Homo sapiens (Human)
Taxonomy	Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Mammalia; Eutheria; Primates; Catarrhini; Hominidae; Homo.

SWISS-PROT file format

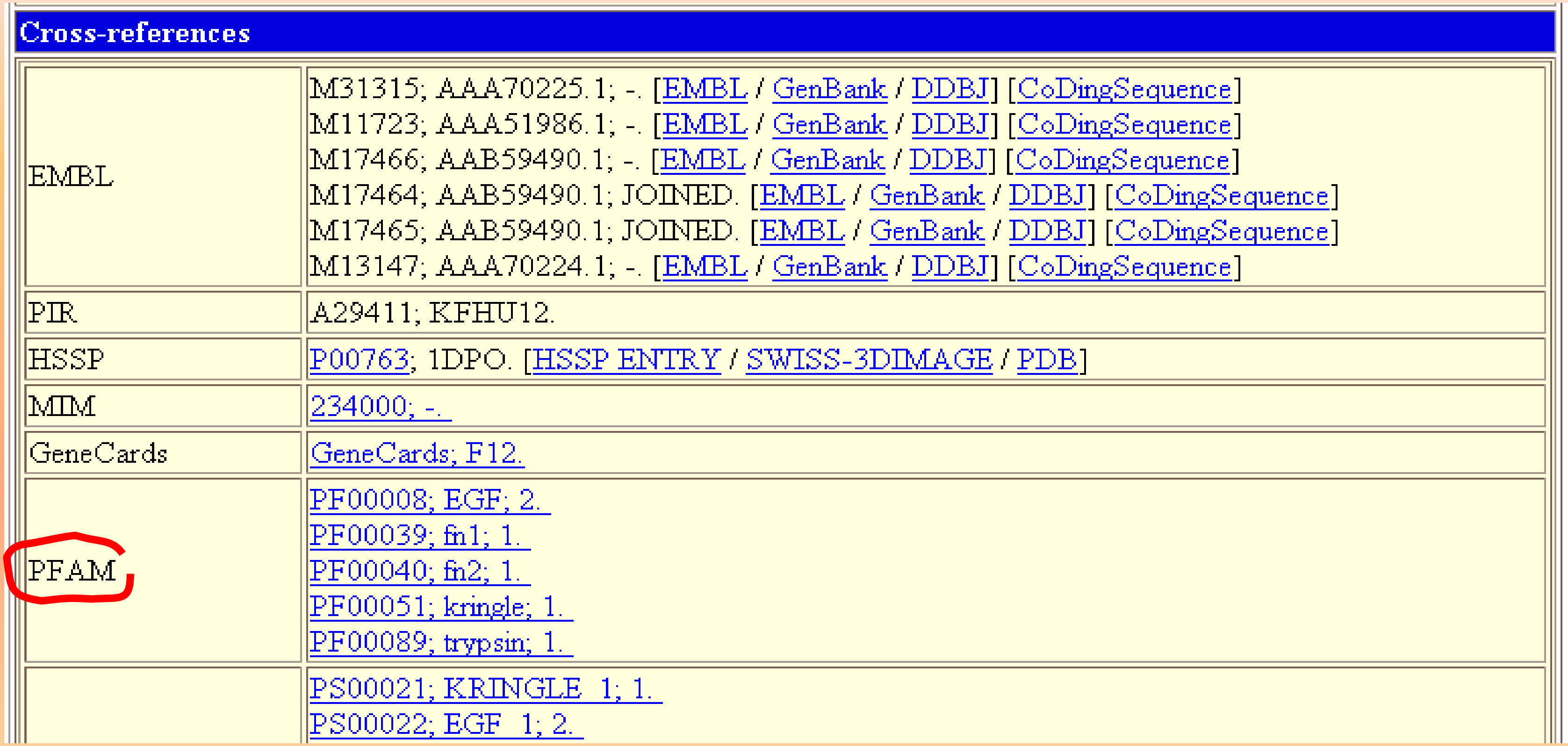
!



Comments

- ***FUNCTION***: FACTOR XII IS A SERUM GLYCOPROTEIN THAT PARTICIPATES IN THE INITIATION OF BLOOD COAGULATION, FIBRINOLYSIS, AND THE GENERATION OF BRADYKININ AND ANGIOTENSIN.
- ***CATALYTIC ACTIVITY***: CLEAVES SELECTIVELY ARG-|-ILE BONDS AND ACTIVATES COAGULATION FACTORS VII AND XI.
- ***PTM***: O- AND N-GLYCOSYLATED.
- ***DISEASE***: DEFECTS IN F12 DO NOT CAUSE ANY CLINICAL SYMPTOMS. THE SOLE EFFECT IS THAT WHOLE-BLOOD CLOTTING TIME IS PROLONGED.
- ***MISCELLANEOUS***: FACTOR XII, PREKALLIKREIN, AND HMW KININOGEN FORM A COMPLEX BOUND TO AN ANIONIC SURFACE. PREKALLIKREIN IS CLEAVED BY FACTOR XII TO FORM KALLIKREIN, WHICH THEN CLEAVES FACTOR XII FIRST TO ALPHA-FACTOR XIIA AND THEN TO BETA-FACTOR XIIA. ALPHA-FACTOR XIIA ACTIVATES FACTOR XI TO FACTOR XIA.
- ***SIMILARITY***: CONTAINS 2 EGF-LIKE DOMAINS.
- ***SIMILARITY***: CONTAINS 1 FIBRONECTIN TYPE-I DOMAIN.
- ***SIMILARITY***: CONTAINS 1 FIBRONECTIN TYPE-II DOMAIN.
- ***SIMILARITY***: CONTAINS 1 KRINGLE REGION.
- ***SIMILARITY***: BELONGS TO PEPTIDASE FAMILY S1; ALSO KNOWN AS THE TRYPSIN FAMILY.

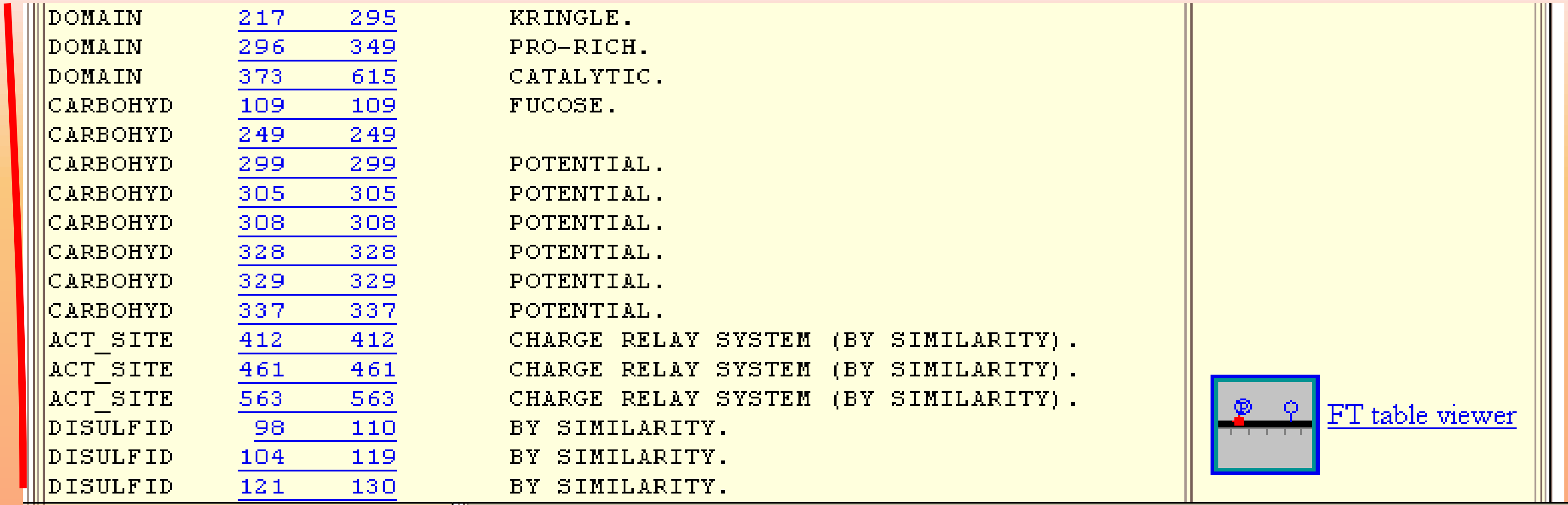
SWISS-PROT file format



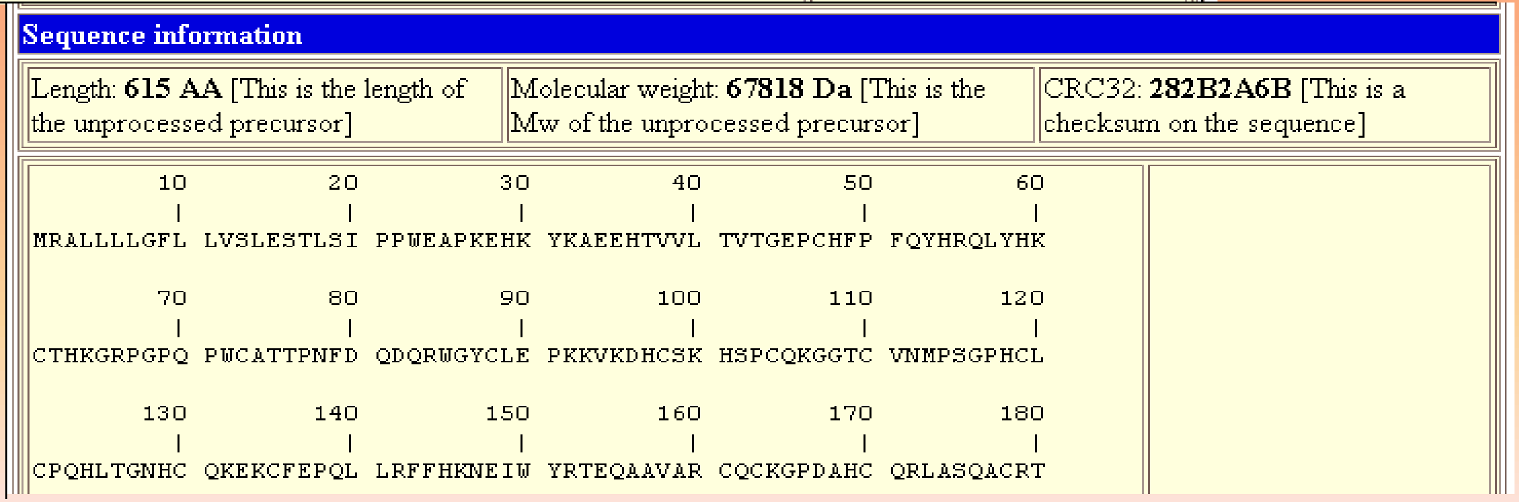
Cross-references

EMBL	M31315; AAA70225.1; -. [EMBL / GenBank / DDBJ] [CoDingSequence] M11723; AAA51986.1; -. [EMBL / GenBank / DDBJ] [CoDingSequence] M17466; AAB59490.1; -. [EMBL / GenBank / DDBJ] [CoDingSequence] M17464; AAB59490.1; JOINED. [EMBL / GenBank / DDBJ] [CoDingSequence] M17465; AAB59490.1; JOINED. [EMBL / GenBank / DDBJ] [CoDingSequence] M13147; AAA70224.1; -. [EMBL / GenBank / DDBJ] [CoDingSequence]
PIR	A29411; KFHU12.
HSSP	P00763; 1DPO. [HSSP ENTRY / SWISS-3DIMAGE / PDB]
MIM	234000; -.
GeneCards	GeneCards; F12.
PFAM	PF00008; EGF; 2. PF00039; fn1; 1. PF00040; fn2; 1. PF00051; kringle; 1. PF00089; trypsin; 1.
	PS00021; KRINGLE_1; 1. PS00022; EGF_1; 2.

SWISS-PROT file format



```
DOMAIN        217      295        KRINGLE.
DOMAIN        296      349        PRO-RICH.
DOMAIN        373      615        CATALYTIC.
CARBOHYD      109      109        FUCOSE.
CARBOHYD      249      249
CARBOHYD      299      299        POTENTIAL.
CARBOHYD      305      305        POTENTIAL.
CARBOHYD      308      308        POTENTIAL.
CARBOHYD      328      328        POTENTIAL.
CARBOHYD      329      329        POTENTIAL.
CARBOHYD      337      337        POTENTIAL.
ACT_SITE      412      412        CHARGE RELAY SYSTEM (BY SIMILARITY).
ACT_SITE      461      461        CHARGE RELAY SYSTEM (BY SIMILARITY).
ACT_SITE      563      563        CHARGE RELAY SYSTEM (BY SIMILARITY).
DISULFID       98      110        BY SIMILARITY.
DISULFID      104      119        BY SIMILARITY.
DISULFID      121      130        BY SIMILARITY.
```



Sequence information

Length: **615 AA** [This is the length of the unprocessed precursor]	Molecular weight: **67818 Da** [This is the Mw of the unprocessed precursor]	CRC32: **282B2A6B** [This is a checksum on the sequence]

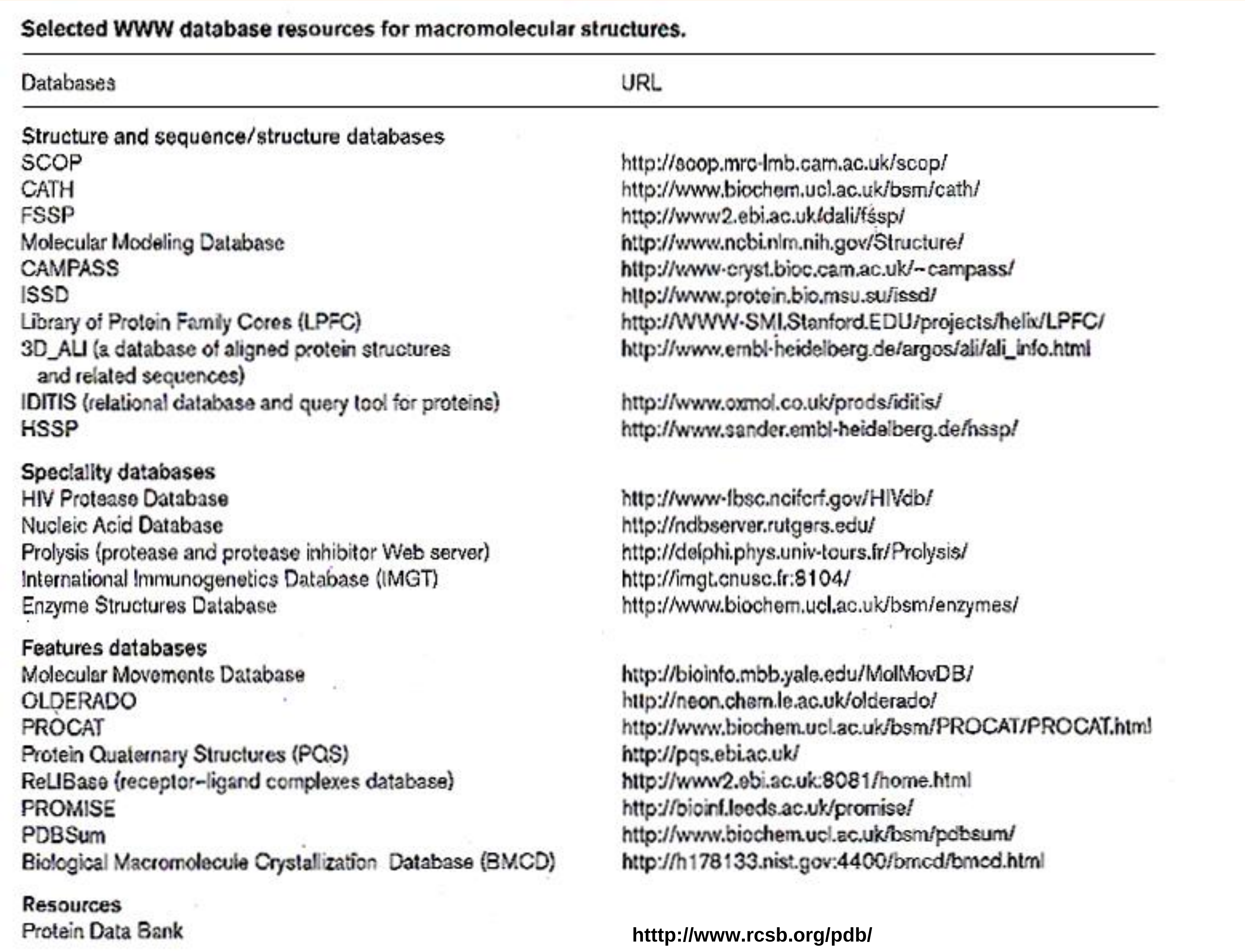
```
        10         20         30         40         50         60
         |          |          |          |          |          |
MRALLLLGFL LVSLESTLSI PPWEAPKEHK YKAEEHTVVL TVTGEPCHFP FQYHRQLYHK

        70         80         90        100        110        120
         |          |          |          |          |          |
CTHKGRPGPQ PWCATTPNFD QDQRWGYCLE PKKVKDHCSK HSPCQKGGTC VNMPSGPHCL

       130        140        150        160        170        180
         |          |          |          |          |          |
CPQHLTGNHC QKEKCFEPQL LRFFHKNEIW YRTEQAAVAR CQCKGPDAHC QRLASQACRT
```

Structure Databases

- **MSD:**The Macromolecular Structure Database – A relational database representation of clean Protein Data Bank (PDB)
- **3DSeq:** 3D sequence alignment server- Annotation of the alignments between sequence database and the PDB
- **FSSP:** Based on exhaustive all-against-all 3D structure comparison of protein structures currently in the Protein Data Bank (PDB)
- **DALI:** Fold Classification based on Structure-Structure Assignments
- **3Dee:** Database of protein domain definitions wherein the domains have been clustered on sequence and structural similarity
- **NDB:** Nucleic Acid Structure Database



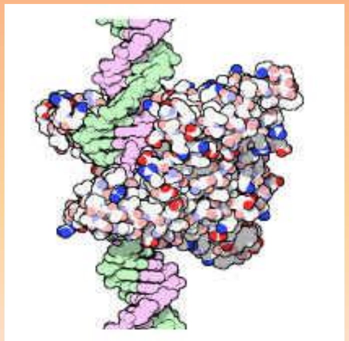
Selected WWW database resources for macromolecular structures.

Databases	URL
Structure and sequence/structure databases	
SCOP	http://scop.mrc-lmb.cam.ac.uk/scop/
CATH	http://www.biochem.ucl.ac.uk/bsm/cath/
FSSP	http://www2.ebi.ac.uk/dali/fssp/
Molecular Modeling Database	http://www.ncbi.nlm.nih.gov/Structure/
CAMPASS	http://www-cryst.bioc.cam.ac.uk/~campass/
ISSD	http://www.protein.bio.msu.su/issd/
Library of Protein Family Cores (LPFC)	http://WWW-SMI.Stanford.EDU/projects/helix/LPFC/
3D_ALI (a database of aligned protein structures and related sequences)	http://www.embl-heidelberg.de/argos/ali/ali_info.html
IDITIS (relational database and query tool for proteins)	http://www.oxmol.co.uk/prods/iditis/
HSSP	http://www.sander.embl-heidelberg.de/hssp/
Speciality databases	
HIV Protease Database	http://www-fbsc.ncifcrf.gov/HIVdb/
Nucleic Acid Database	http://ndbserver.rutgers.edu/
Prolysis (protease and protease inhibitor Web server)	http://delphi.phys.univ-tours.fr/Prolysis/
International Immunogenetics Database (IMGT)	http://imgt.cnusc.fr:8104/
Enzyme Structures Database	http://www.biochem.ucl.ac.uk/bsm/enzymes/
Features databases	
Molecular Movements Database	http://bioinfo.mbb.yale.edu/MolMovDB/
OLDERADO	http://neon.chem.le.ac.uk/olderado/
PROCAT	http://www.biochem.ucl.ac.uk/bsm/PROCAT/PROCAT.html
Protein Quaternary Structures (PQS)	http://pqs.ebi.ac.uk/
ReLIBase (receptor–ligand complexes database)	http://www2.ebi.ac.uk:8081/home.html
PROMISE	http://bioinf.leeds.ac.uk/promise/
PDBSum	http://www.biochem.ucl.ac.uk/bsm/pdbsum/
Biological Macromolecule Crystallization Database (BMCD)	http://h178133.nist.gov:4400/bmcd/bmcd.html
Resources	
Protein Data Bank	**http://www.rcsb.org/pdb/**

Protein DataBank (PDB)

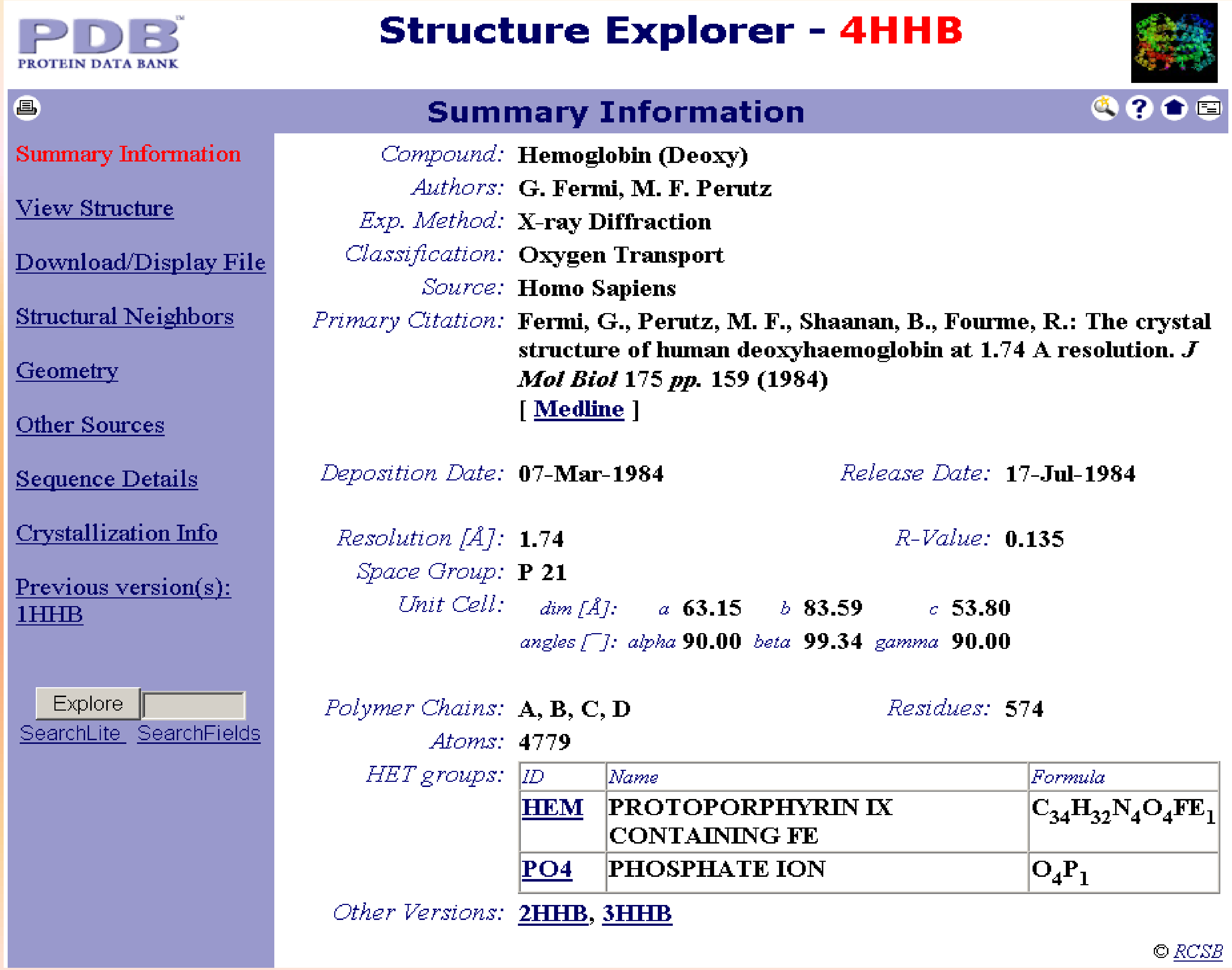
- Important in solving real problems in molecular biology
- Protein Databank
  - PDB Established in 1972 at Brookhaven National Laboratory (BNL)
  - Sole international repository of macromolecular structure data
  - Moved to Research Collaboratory
    for Structural Bioinformatics

http://www.rcsb.org/



Effective use of PDB

- Queries are of three types
  - PDBid - As quoted in paper
  - Search Lite - one or more keywords
  - Search Fields - A detailed query form
- Query results
  - Structure Explorer - details of the structure
  - Query Result Browser - for multiple structures
- PDB Viewer



Structure Explorer - 4HHB

Summary Information

- Summary Information
- View Structure
- Download/Display File
- Structural Neighbors
- Geometry
- Other Sources
- Sequence Details
- Crystallization Info
- Previous version(s): 1HHB

Compound: Hemoglobin (Deoxy)

Authors: G. Fermi, M. F. Perutz

Exp. Method: X-ray Diffraction

Classification: Oxygen Transport

Source: Homo Sapiens

Primary Citation: Fermi, G., Perutz, M. F., Shaanan, B., Fourme, R.: The crystal structure of human deoxyhaemoglobin at 1.74 A resolution. ***J Mol Biol*** 175 ***pp.*** 159 (1984)
[Medline]

Deposition Date: 07-Mar-1984 *Release Date:* 17-Jul-1984

Resolution [Å]: 1.74 *R-Value:* 0.135

Space Group: P 21

Unit Cell:

dim [Å]:	*a*	63.15	*b*	83.59	*c*	53.80
angles [ ]:	*alpha*	90.00	*beta*	99.34	*gamma*	90.00

Polymer Chains: A, B, C, D *Residues:* 574

Atoms: 4779

HET groups:

ID	*Name*	*Formula*
HEM	PROTOPORPHYRIN IX CONTAINING FE	$C_{34}H_{32}N_4O_4FE_1$
PO4	PHOSPHATE ION	O_4P_1

Other Versions: 2HHB, 3HHB

© *RCSB*

PDB: example

```
HEADER    LYASE(OXO-ACID)                         01-OCT-91   12CA      12CA   2
COMPND    CARBONIC ANHYDRASE /II (CARBONATE DEHYDRATASE) (/HCA II)    12CA   3
COMPND   2 (E.C.4.2.1.1) MUTANT WITH VAL 121 REPLACED BY ALA (/V121A)  12CA   4
SOURCE    HUMAN (HOMO SAPIENS) RECOMBINANT PROTEIN                    12CA   5
AUTHOR    S.K.NAIR,D.W.CHRISTIANSON                                   12CA   6
REVDAT   1   15-OCT-92 12CA    0                                      12CA   7
JRNL        AUTH   S.K.NAIR,T.L.CALDERONE,D.W.CHRISTIANSON,C.A.FIERKE    12CA   8
JRNL        TITL   ALTERING THE MOUTH OF A HYDROPHOBIC POCKET.          12CA   9
JRNL        TITL 2 STRUCTURE AND KINETICS OF HUMAN CARBONIC ANHYDRASE   12CA  10
JRNL        TITL 3 /II$ MUTANTS AT RESIDUE VAL-121                      12CA  11
JRNL        REF    J.BIOL.CHEM.                  V. 266 17320 1991      12CA  12
JRNL        REFN   ASTM JBCHA3  US ISSN 0021-9258                 071  12CA  13
REMARK   1                                                          12CA  14
REMARK   2                                                          12CA  15
REMARK   2 RESOLUTION. 2.4  ANGSTROMS.                              12CA  16
REMARK   3                                                          12CA  17
REMARK   3 REFINEMENT.                                              12CA  18
REMARK   3   PROGRAM                    PROLSQ                      12CA  19
REMARK   3   AUTHORS                    HENDRICKSON,KONNERT         12CA  20
REMARK   3   R VALUE                    0.170                       12CA  21
REMARK   3   RMSD BOND DISTANCES        0.011  ANGSTROMS            12CA  22
REMARK   3   RMSD BOND ANGLES           1.3    DEGREES              12CA  23
REMARK   4                                                          12CA  24
REMARK   4 N-TERMINAL RESIDUES SER 2, HIS 3, HIS 4 AND C-TERMINAL      12CA  25
REMARK   4 RESIDUE LYS 260 WERE NOT LOCATED IN THE DENSITY MAPS AND,    12CA  26
REMARK   4 THEREFORE, NO COORDINATES ARE INCLUDED FOR THESE RESIDUES.   12CA  27
………
```

PDB (cont.)

```
SHEET    3   S10 PHE    66  PHE    70 -1  O  ASN    67   N  LEU    60   12CA  68
SHEET    4   S10 TYR    88  TRP    97 -1  O  PHE    93   N  VAL    68   12CA  69
SHEET    5   S10 ALA   116  ASN   124 -1  O  HIS   119   N  HIS    94   12CA  70
SHEET    6   S10 LEU   141  VAL   150 -1  O  LEU   144   N  LEU   120   12CA  71
SHEET    7   S10 VAL   207  LEU   212  1  O  ILE   210   N  GLY   145   12CA  72
SHEET    8   S10 TYR   191  GLY   196 -1  O  TRP   192   N  VAL   211   12CA  73
SHEET    9   S10 LYS   257  ALA   258 -1  O  LYS   257   N  THR   193   12CA  74
SHEET   10   S10 LYS    39  TYR    40  1  O  LYS    39   N  ALA   258   12CA  75
TURN     1  T1 GLN    28  VAL    31     TYPE VIB (CIS-PRO 30)          12CA  76
TURN     2  T2 GLY    81  LEU    84     TYPE II(PRIME) (GLY 82)        12CA  77
TURN     3  T3 ALA   134  GLN   137     TYPE I (GLN 136)               12CA  78
TURN     4  T4 GLN   137  GLY   140     TYPE I (ASP 139)               12CA  79
TURN     5  T5 THR   200  LEU   203     TYPE VIA (CIS-PRO 202)         12CA  80
TURN     6  T6 GLY   233  GLU   236     TYPE II (GLY 235)              12CA  81
CRYST1   42.700   41.700   73.000  90.00 104.60  90.00 P 21          2  12CA  82
ORIGX1      1.000000  0.000000  0.000000        0.00000                12CA  83
ORIGX2      0.000000  1.000000  0.000000        0.00000                12CA  84
ORIGX3      0.000000  0.000000  1.000000        0.00000                12CA  85
SCALE1      0.023419  0.000000  0.006100        0.00000                12CA  86
SCALE2      0.000000  0.023981  0.000000        0.00000                12CA  87
SCALE3      0.000000  0.000000  0.014156        0.00000                12CA  88
ATOM      1  N   TRP     5       8.519  -0.751  10.738  1.00 13.37      12CA  89
ATOM      2  CA  TRP     5       7.743  -1.668  11.585  1.00 13.42      12CA  90
ATOM      3  C   TRP     5       6.786  -2.502  10.667  1.00 13.47      12CA  91
ATOM      4  O   TRP     5       6.422  -2.085   9.607  1.00 13.57      12CA  92
ATOM      5  CB  TRP     5       6.997  -0.917  12.645  1.00 13.34      12CA  93
ATOM      6  CG  TRP     5       5.784  -0.209  12.221  1.00 13.40      12CA  94
ATOM      7  CD1 TRP     5       5.681   1.084  11.797  1.00 13.29      12CA  95
ATOM      8  CD2 TRP     5       4.417  -0.667  12.221  1.00 13.34      12CA  96
ATOM      9  NE1 TRP     5       4.388   1.418  11.515  1.00 13.30      12CA  97
ATOM     10  CE2 TRP     5       3.588   0.375  11.797  1.00 13.35      12CA  98
ATOM     11  CE3 TRP     5       3.837  -1.877  12.645  1.00 13.39      12CA  99
ATOM     12  CZ2 TRP     5       2.216   0.208  11.656  1.00 13.39      12CA 100
ATOM     13  CZ3 TRP     5       2.465  -2.043  12.504  1.00 13.33      12CA 101
ATOM     14  CH2 TRP     5       1.654  -1.001  12.009  1.00 13.34      12CA 102
…….
```

A comprehensive help document

Cn3D FAQ

Frequently Asked Questions

Cn3D Install

Installation and Configuration

MMDB

NCBI's structure database

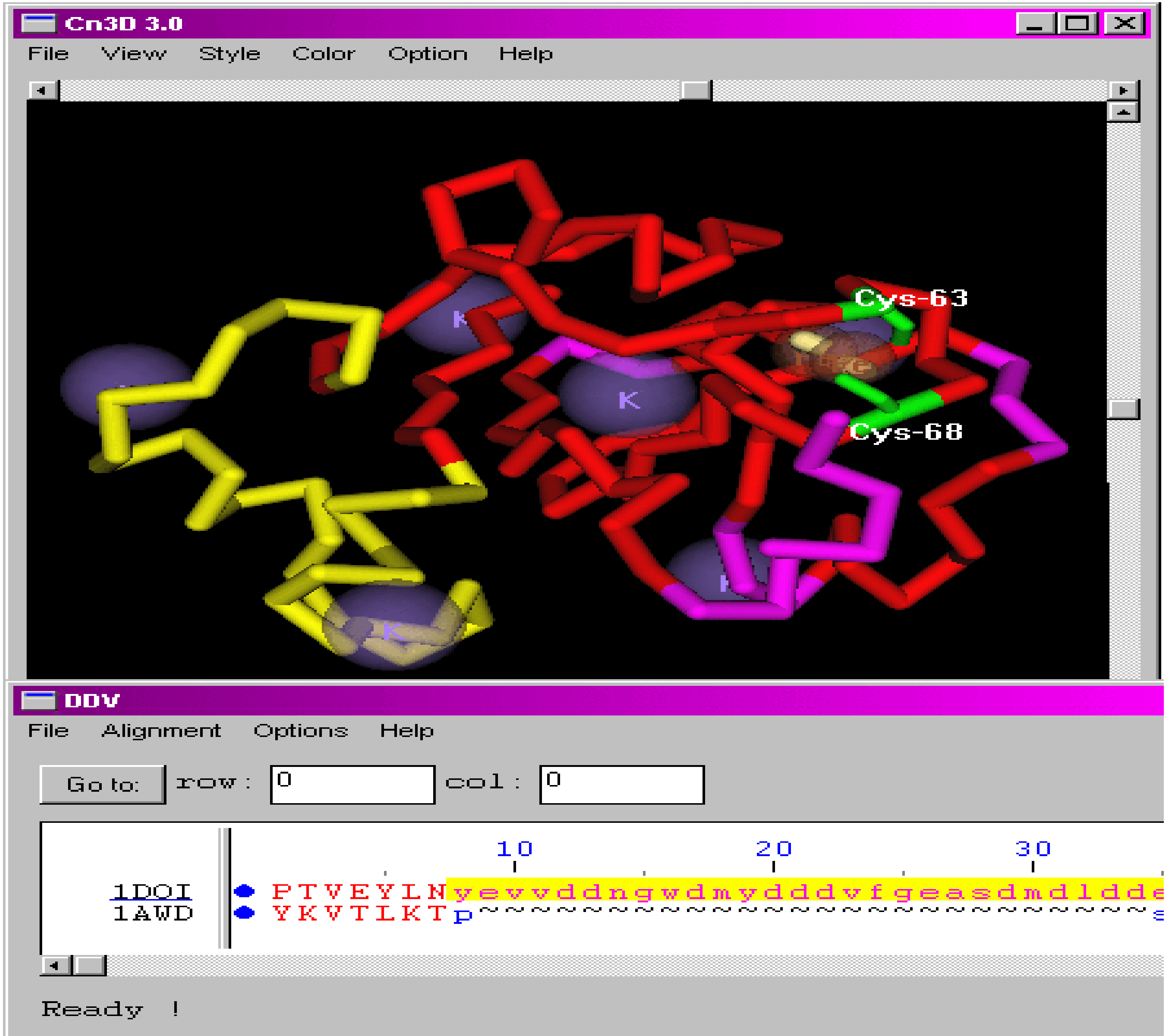
PDBeast

Taxonomy in MMDB

VAST

Structure comparisons

VAST Search



```
1DOI ● PTVEYLNyevvddngwdmydddvfgeasdmdlddе
1AWD ● YKVTLKTp~~~~~~~~~~~~~~~~~~~~~~~~~~s
```

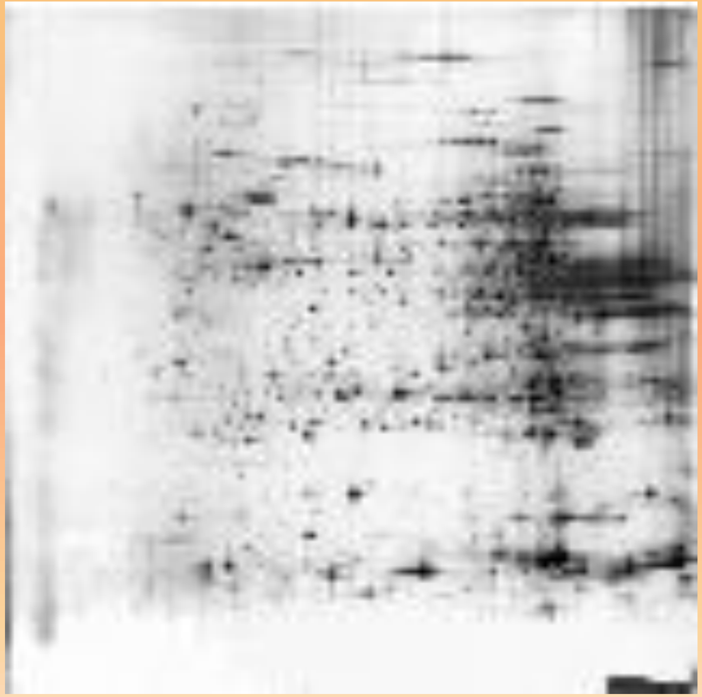
Ready !

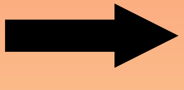
Databases related to Proteomics

- Contain information obtained by 2D-PAGE: master images of the gels and description of identified proteins
- Examples: SWISS-2DPAGE, ECO2DBASE, Maize-2DPAGE, Sub2D, Cyano2DBase, etc.
- Format: composed of image and text files
- Most 2D-PAGE databases are “federated” and use SWISS-PROT as a master index
- Mass Spectrometry (MS) database

Proteomics

1978-1998





MALDI-TOF?

ESI-MS?

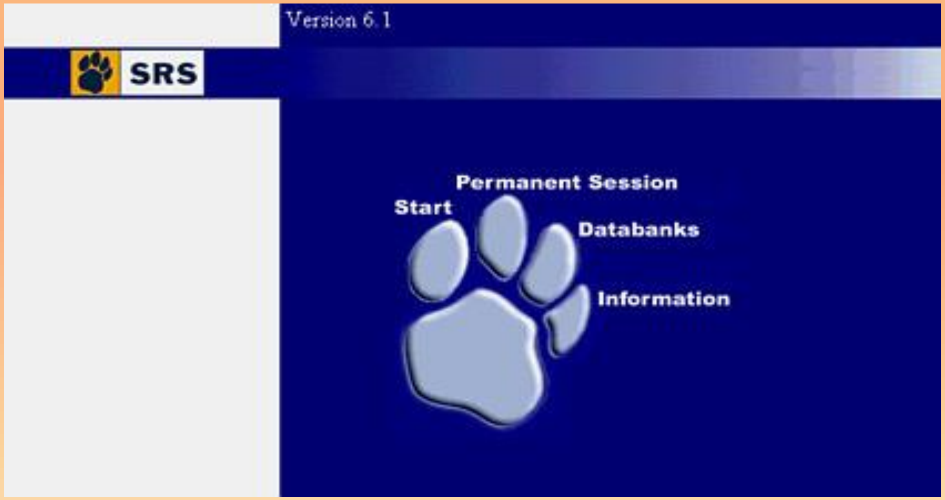
Database Mining Tools

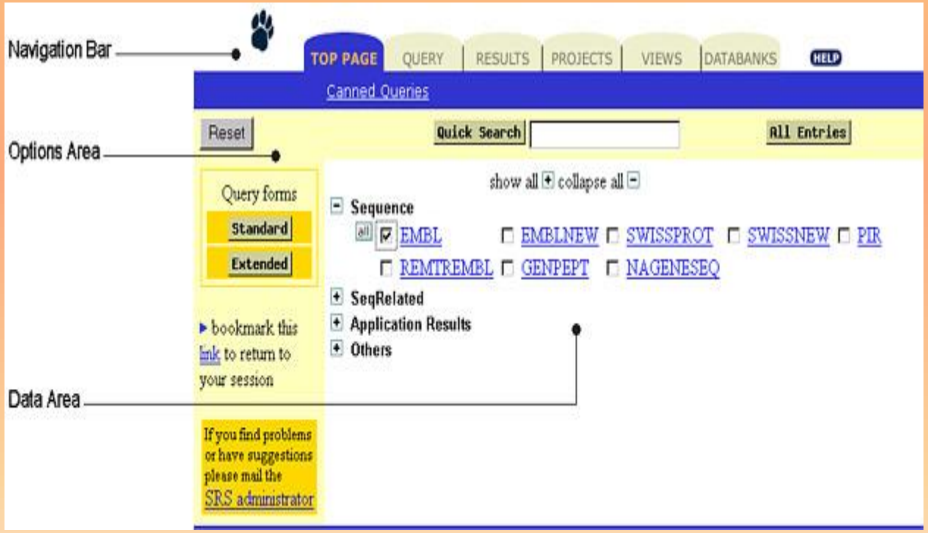
- **SRS:** Sequence Retrieval System
- **Entrez:** Search Engine at NCBI, US
- **Bankit:** World Wide Web sequence submission server
- Sequence Similarity Search Tools-**BLAST & FASTA**
  - Finding sequence homologs to deduce the identity of query sequence
  - Identify potential sequence homologs with known three dimensional structure

Sequence Retrieval System

SRS is a powerful data integration platform

- •Provides rapid, easy and user friendly access
- •Large volumes of heterogeneous Life Science data
- •Stored in more than 400 internal and public domain databases
- •Available at http://srs.ebi.ac.uk/




Navigation Bar
TOP PAGE
QUERY
RESULTS
PROJECTS
VIEWS
DATABANKS
HELP
Canned Queries
Options Area
Reset
Quick Search
All Entries
show all ⊞ collapse all ⊟
Query forms
Standard
Extended
⊟ Sequence
all ☑ EMBL
□ EMBLNEW □ SWISSPROT □ SWISSNEW □ PIR
□ REMTREMBL □ GENPEPT □ NAGENESEQ
⊞ SeqRelated
⊞ Application Results
⊞ Others
▸ bookmark this link to return to your session
Data Area
If you find problems or have suggestions please mail the SRS administrator

….SRS

SRS performs searches on the following categories:

References
Sequence libraries - subsections
SeqRelated
User Owned Databanks
Protein3DStruct
Mapping
Locus Specific Mutations
Others
EMBOSS DOCS

Sequence libraries - complete
InterPro&Related
TransFac
Application Results
Genome
Mutations
Metabolic Pathways
SNP
System

Searches can be carried out using

- •Quick search on all entries
- •Standard form with Boolean operators
- •Extended form with field names

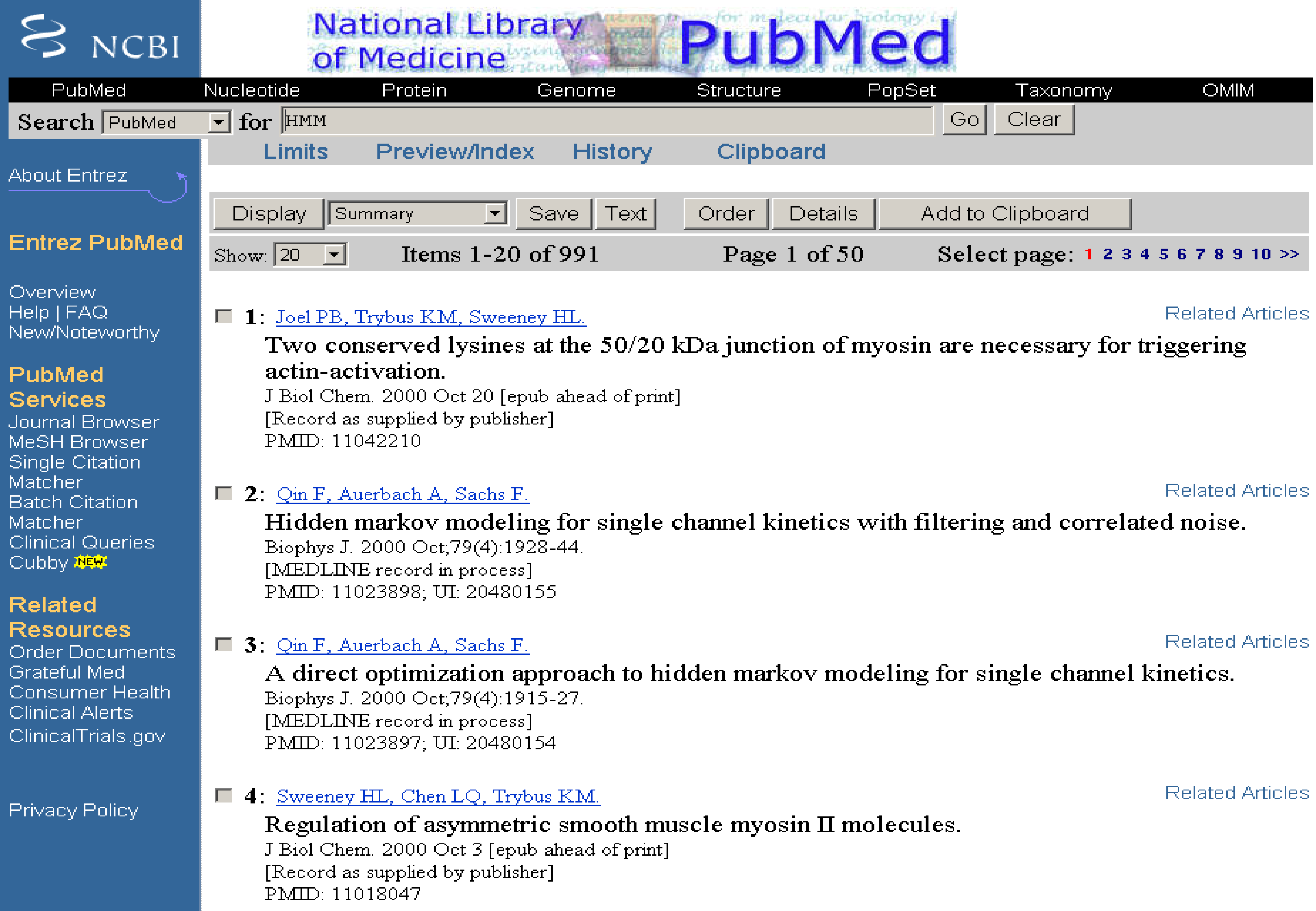
Entrez at NCBI

It is a retrieval system for searching several linked databases such as

- PubMed: The biomedical literature (PubMed)
- Nucleotide sequence database (Genbank)
- Protein sequence database
- Structure: Three-dimensional macromolecular structures
- Genome: Complete genome assemblies
- PopSet: Population study data sets
- OMIM: Online Mendelian Inheritance in Man
- Taxonomy: Organisms in GenBank
- Books: Online books
- ProbeSet: Gene expression and microarray datasets
- 3D Domains: Domains from Entrez Structure
- UniSTS: Markers and mapping data
- SNP: Single nucleotide polymorphisms
- CDD: Conserved domains

Entrez: Search fields

- Keyword allows to search a set of indexed terms
- Accession allows to search accession numbers
- Author Name
- Affiliations of authors
- Journal Title
- E.C. Numbers
- Feature Key searches for particular DNA feature
- SeqId is string identifier
- Title Words
- Text Words
- Organism
- Pubmed ID
- Publication and modification date
- Protein Name



Items 1-20 of 991 Page 1 of 50

□ 1: Joel PB, Trybus KM, Sweeney HL.

Two conserved lysines at the 50/20 kDa junction of myosin are necessary for triggering actin-activation.
J Biol Chem. 2000 Oct 20 [epub ahead of print]
[Record as supplied by publisher]
PMID: 11042210

□ 2: Qin F, Auerbach A, Sachs F.

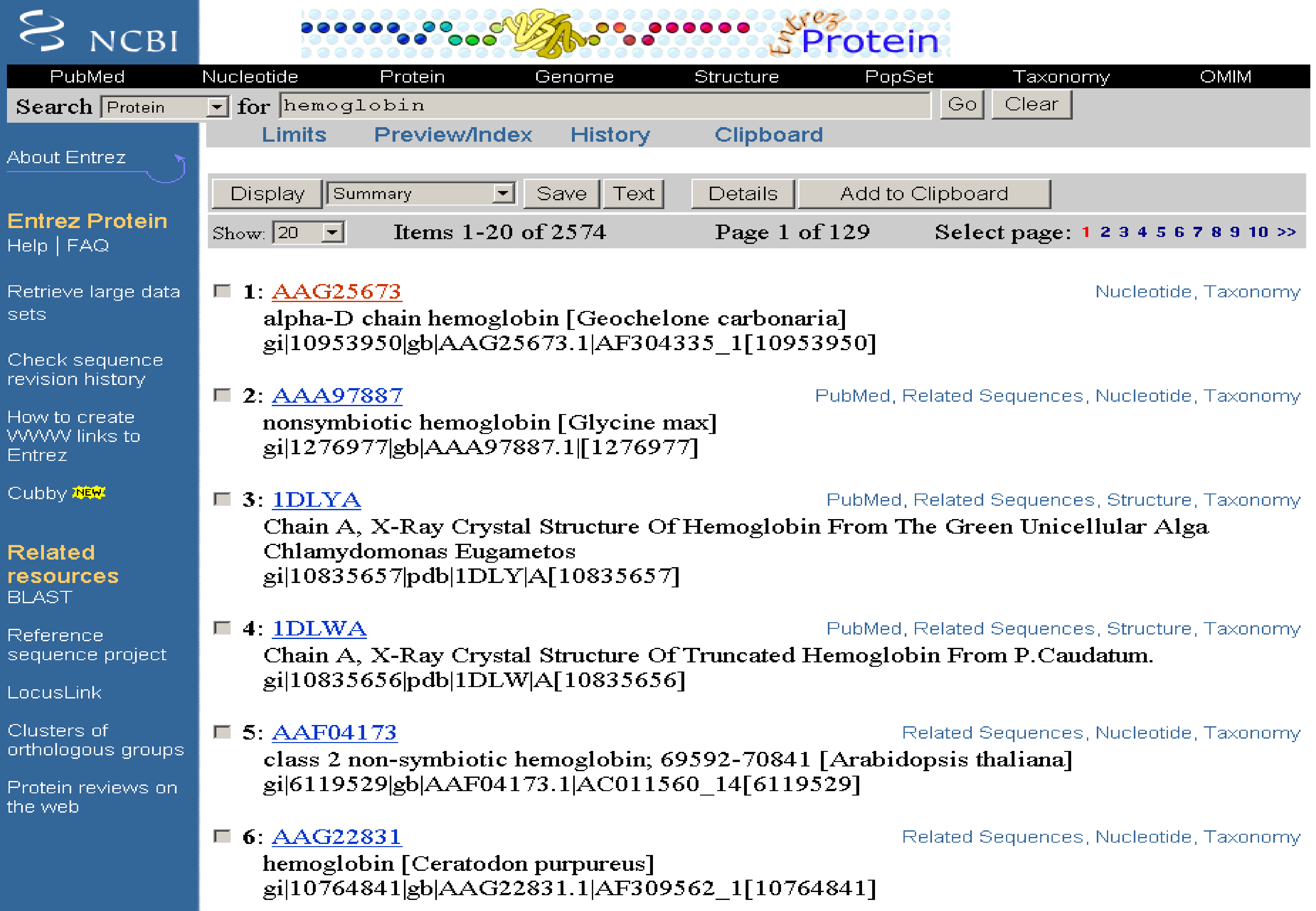
Hidden markov modeling for single channel kinetics with filtering and correlated noise.
Biophys J. 2000 Oct;79(4):1928-44.
[MEDLINE record in process]
PMID: 11023898; UI: 20480155

□ 3: Qin F, Auerbach A, Sachs F.

A direct optimization approach to hidden markov modeling for single channel kinetics.
Biophys J. 2000 Oct;79(4):1915-27.
[MEDLINE record in process]
PMID: 11023897; UI: 20480154

□ 4: Sweeney HL, Chen LQ, Trybus KM.

Regulation of asymmetric smooth muscle myosin II molecules.
J Biol Chem. 2000 Oct 3 [epub ahead of print]
[Record as supplied by publisher]
PMID: 11018047



Search Protein for hemoglobin

Items 1-20 of 2574 Page 1 of 129

□ 1: AAG25673 Nucleotide, Taxonomy
alpha-D chain hemoglobin [Geochelone carbonaria]
gi|10953950|gb|AAG25673.1|AF304335_1[10953950]

□ 2: AAA97887 PubMed, Related Sequences, Nucleotide, Taxonomy
nonsymbiotic hemoglobin [Glycine max]
gi|1276977|gb|AAA97887.1|[1276977]

□ 3: 1DLYA PubMed, Related Sequences, Structure, Taxonomy
Chain A, X-Ray Crystal Structure Of Hemoglobin From The Green Unicellular Alga Chlamydomonas Eugametos
gi|10835657|pdb|1DLY|A[10835657]

□ 4: 1DLWA PubMed, Related Sequences, Structure, Taxonomy
Chain A, X-Ray Crystal Structure Of Truncated Hemoglobin From P.Caudatum.
gi|10835656|pdb|1DLW|A[10835656]

□ 5: AAF04173 Related Sequences, Nucleotide, Taxonomy
class 2 non-symbiotic hemoglobin; 69592-70841 [Arabidopsis thaliana]
gi|6119529|gb|AAF04173.1|AC011560_14[6119529]

□ 6: AAG22831 Related Sequences, Nucleotide, Taxonomy
hemoglobin [Ceratodon purpureus]
gi|10764841|gb|AAG22831.1|AF309562_1[10764841]

File Formats of the sequences

Readseq (http://bimas.dcrt.nih.gov/molbio/readseq/)

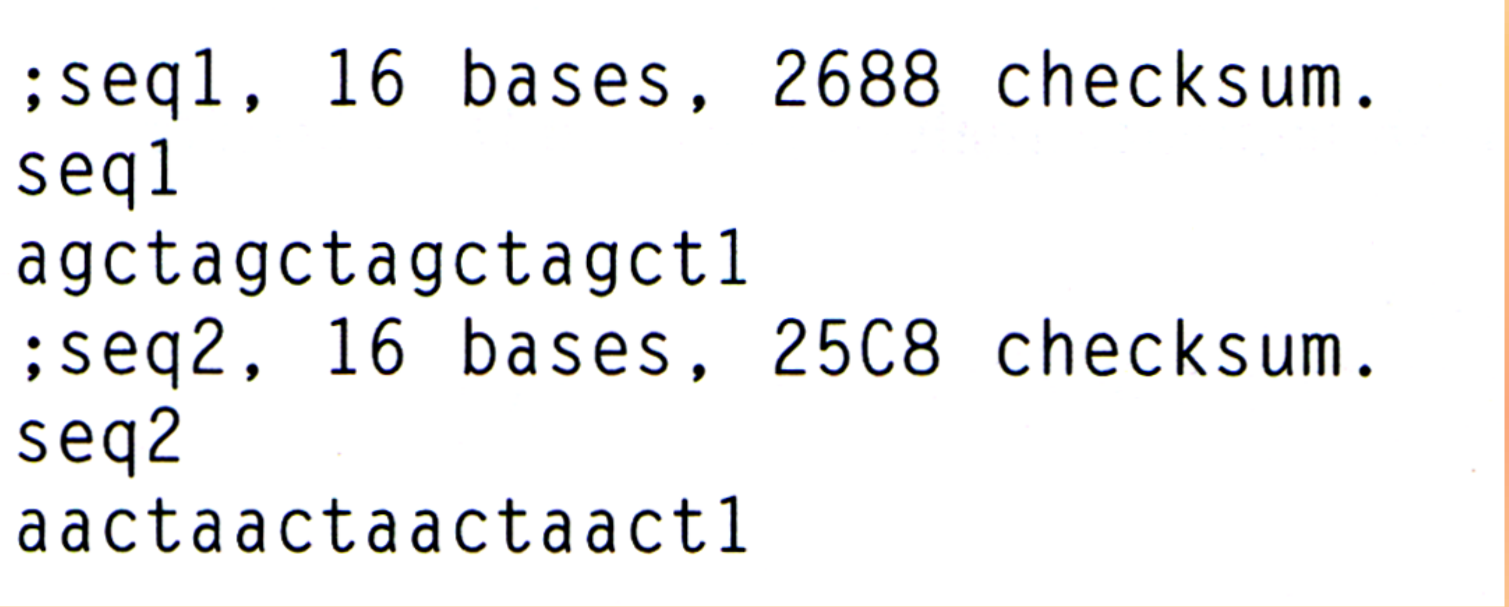
1. IG/Stanford
2. GenBank/GB
3. NBRF
4. EMBL
5. GCG
6. DNAStrider
7. Fitch
8. Pearson/Fasta
9. Zuker (in-only)
10. Olsen (in-only)
11. Phylip3.2
12. Phylip
13. Plain/Raw
14. PIR/CODATA
15. MSF
16. ASN.1
17. PAUP
18. Pretty (out-only)

FAST Format

- Popular Format and commonly used

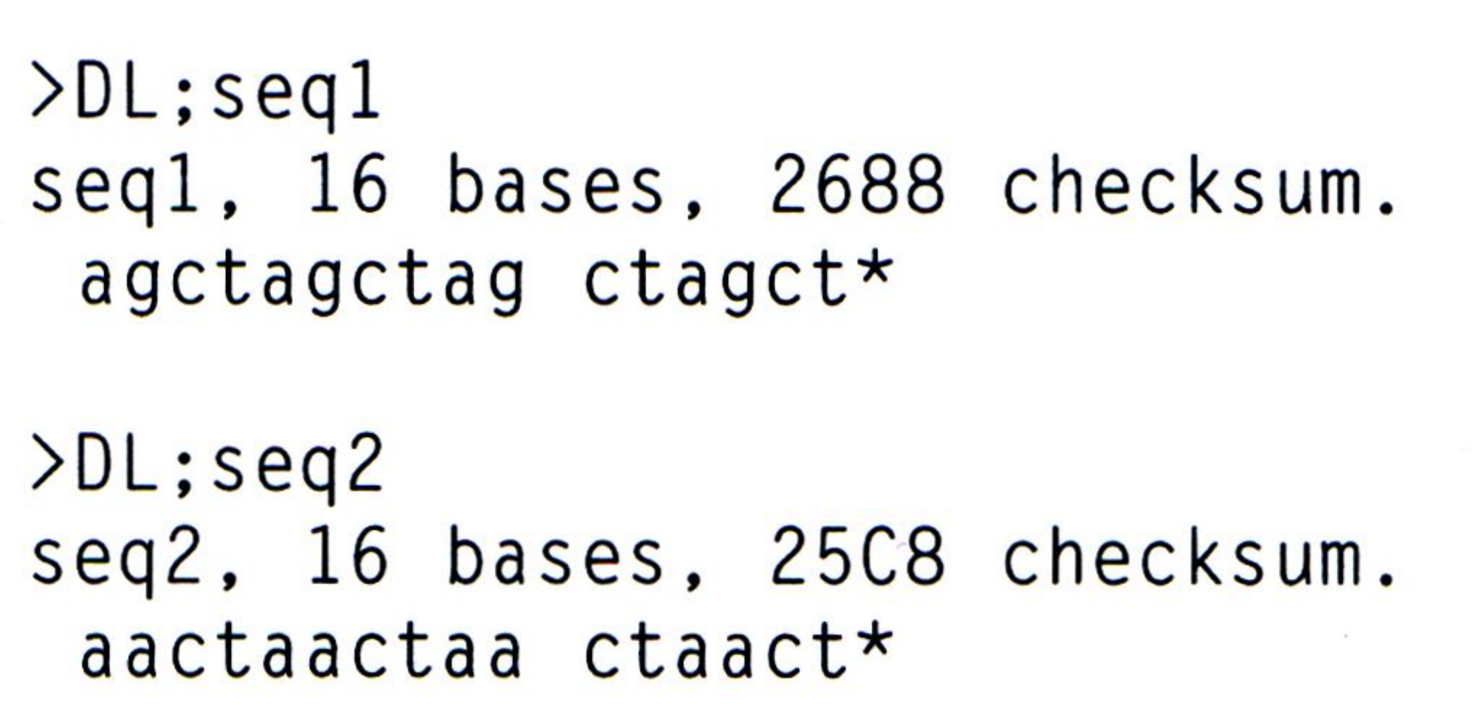
```
> Seq1
ALVLRARLATGPATGCTRTARARLATGALVLRARLATGPARARLATGPATGCTRTARA
RLATGALVLRARRLATGPATGCTRRLATGPATGCTRRARLATGPATGCTRTARARLAT
GALVLRAR
>Seq2
TGCTRTARARLATGALVLRARLATGPARARALVLRARLATGPATGCTRTARATGALVL
RARLATGPARARALVLRARLATG
>Seq 3
……..
```

Intelligenetics format



```
;seq1, 16 bases, 2688 checksum.
seq1
agctagctagctagct1
;seq2, 16 bases, 25C8 checksum.
seq2
aactaactaactaact1
```

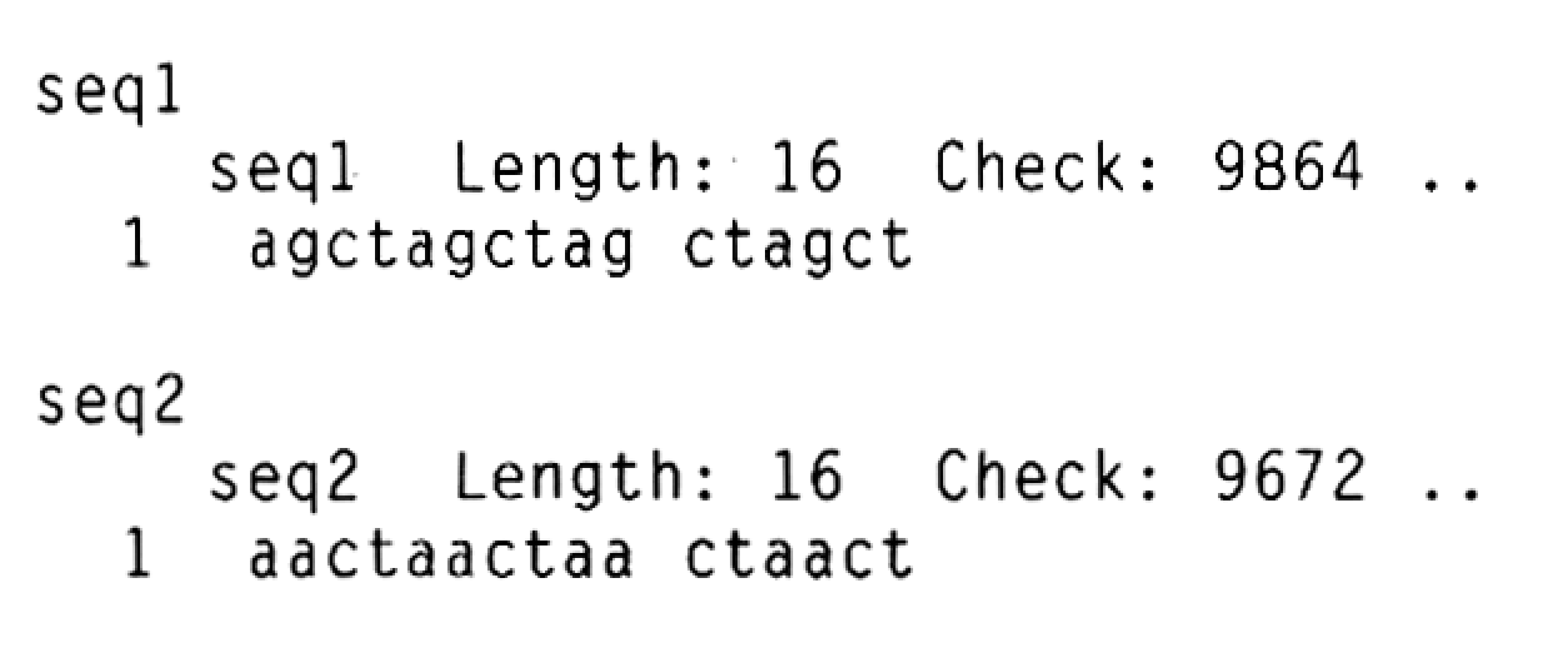
NBRF format



```
>DL;seq1
seq1, 16 bases, 2688 checksum.
 agctagctag ctagct*

>DL;seq2
seq2, 16 bases, 25C8 checksum.
 aactaactaa ctaact*
```

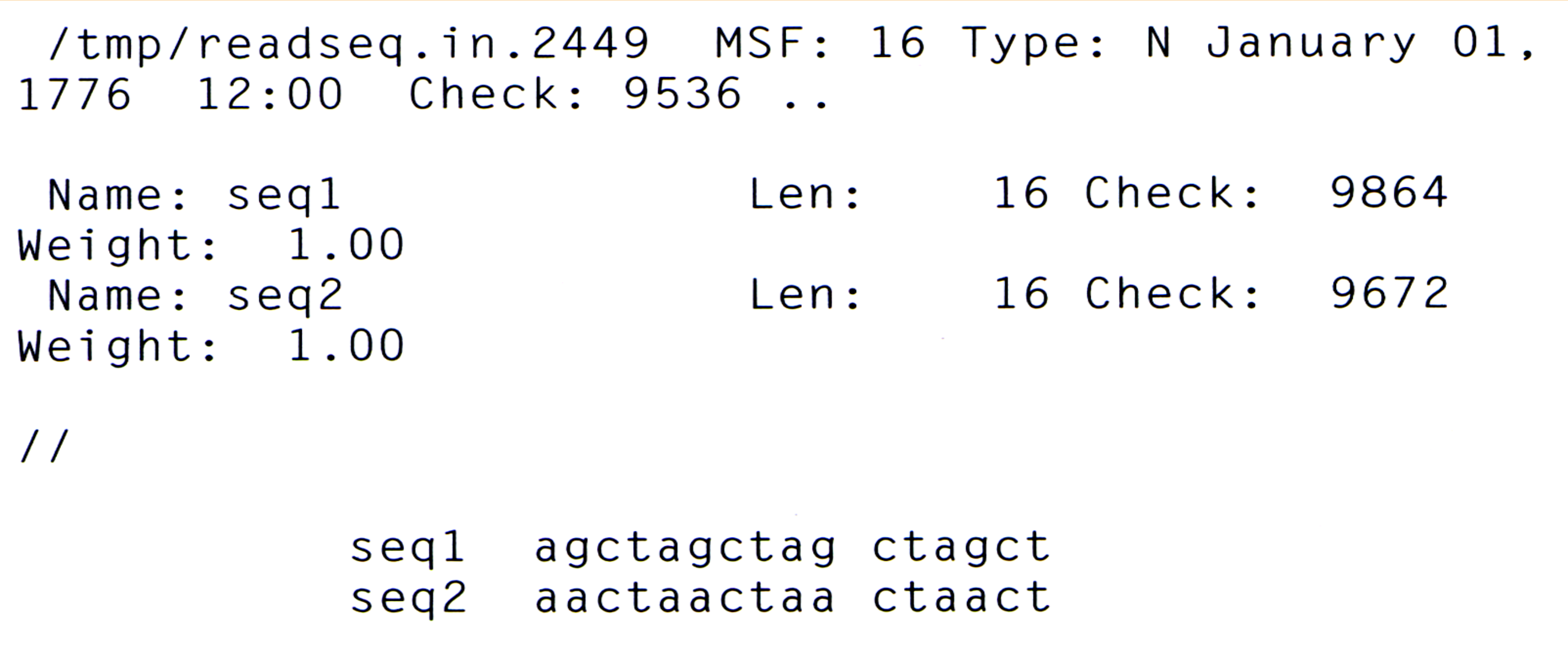
GCG format



```
seq1
    seq1  Length: 16  Check: 9864 ..
  1  agctagctag ctagct

seq2
    seq2  Length: 16  Check: 9672 ..
  1  aactaactaa ctaact
```

GCG multiple sequence format (MSF)



```
 /tmp/readseq.in.2449  MSF: 16 Type: N January 01,
1776  12:00  Check: 9536 ..

 Name: seq1             Len:    16 Check:  9864
Weight:  1.00
 Name: seq2             Len:    16 Check:  9672
Weight:  1.00

//

           seq1  agctagctag ctagct
           seq2  aactaactaa ctaact
```