Browsing of Biological Databases and Identification of Bioinformatics Tools

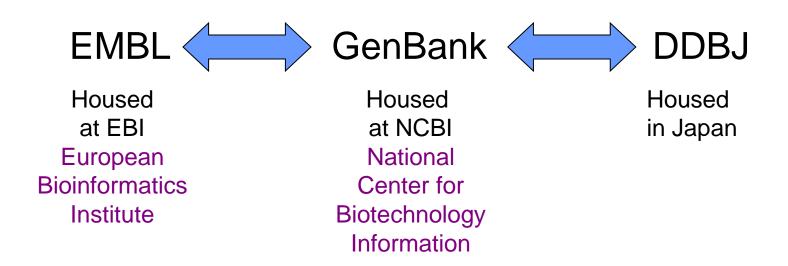
Databases

Primary (archival)

- GenBank /EMBL /DDBJ
- Uniprot
- PDB
- Medline (Pubmed)

Others are: Refseq, Taxon, OMIM etc

There are three major public DNA databases



>100,000 species are represented in GenBank

all species 128,941

viruses 6,137

bacteria 31,262

archaea 2,100

eukaryota 87,147

How can I retrieve Information Using PubMed at NCBI

PubMed

PubMed is...

- National Library of Medicine's search service
- links to participating online journals
- PubMed tutorial (via "Education" on side bar)



PubMed

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Journal List Advanced

Search



PMC

PubMed Central® (PMC) is a free full-text archive of biomedical and life sciences journal literature at the U.S. National Institutes of Health's National Library of Medicine (NIH/NLM).

PubReade

A whole new way to read scientific literature at PubMed Central

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Other Resources

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Developer Resources

PMC Citation Search

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n.gov/account/?back_url=https%3A%2F%2Fwww.ncbi.nlm....

5 MILLION Articles

are archived in PMC.

Content provided in part by:

2161 Full Participation

Journals

333 NIH Portfolio Journals

Selective Deposit Journals

4736

Public Access

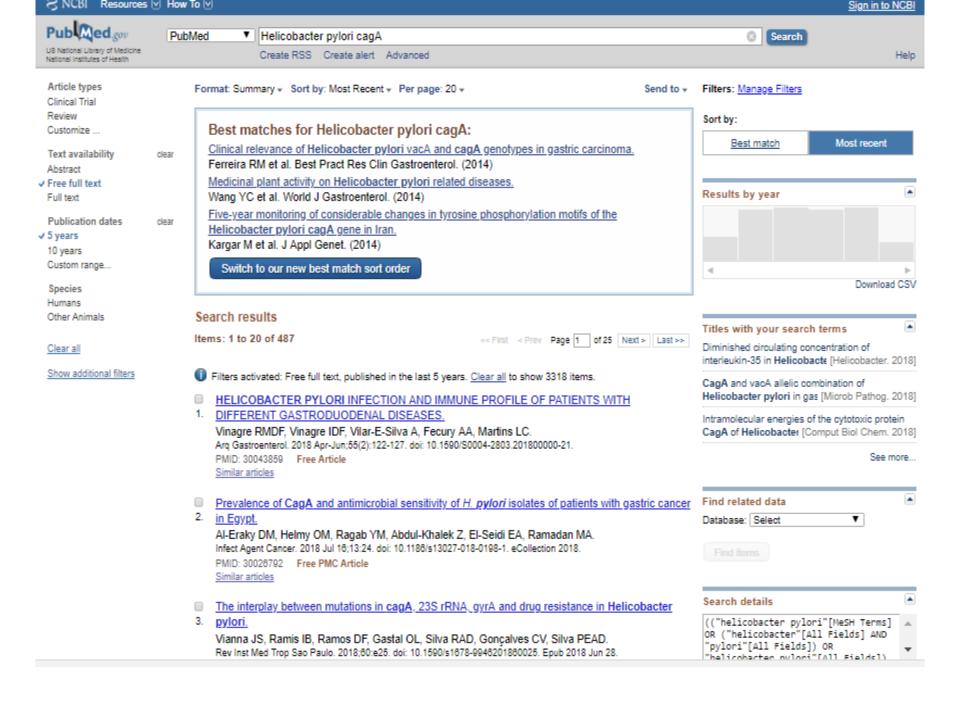
Funders and PMC

How Papers Get Into PMC

NIH Manuscript Submission System

My Bibliography

PMCID/PMID/NIHMSID Converter



OMIM

OMIM is...

- Online Mendelian Inheritance in Man
- catalog of human genes and genetic disorders
- Information about particular diseases

Books

Books is...

searchable resource of on-line books

Taxanomy

TaxBrowser is...

- browser for the major divisions of living organisms (archaea, bacteria, eukaryota, viruses)
- taxonomy information such as nucleotides and Proteins

Structure

Structure site includes...

- Molecular Modelling Database (MMDB)
- biopolymer structures obtained from the Protein Data Bank (PDB)
- 3D-structure viewer

SEQUENCE RETRIEVAL

Sequence is the nucleotides in a gene or the amino acids in a protein in their right order.

How to locate sequences:

Go to databases (I. e NCBI, iProClass, UNIPROT, etc).

Search for protein(s) or nucleotides sequence(s).

Retrieve sequences in FASTA format.

Nucleotide Sequence Retrieval

- 1 Go to the link for NCBI: http://www.ncbi.nlm.nih.gov/
- 2 In the search window, scroll and select nucleotide
- 3 Lower search window type the name of your gene or protein
- 4 Click search button

Output

- 1: Look for your query gene or protein with complete mRNA cds
- 2: Below the query gene found; look for FASTA. Click the FASTA to retrieve your nucleotide sequences in FASTA format.
- 3: Copy and save your sequence as a text file using notepad to the relevant folder.

Amino acid Sequence Retrieval

- 1 Go to the link for UNIPROT http://www.uniprot.org/
- 2 In the query window, type your gene name
- 3 Click the search button
- 4 Wait for your result to appear. Then click the gene id number.
- This takes you to the query gene/protein information page

BLAST is...

- Basic Local Alignment Search Tool
- NCBI's sequence similarity search tool
- supports analysis of DNA and protein databases

BLAST (Basic Alignment Search Tool allows rapid sequence comparison of a query sequence against a database. The BLAST algorithm is fast, accurate and Web-accessible.

BLAST searching is fundamental to understanding the relatedness of any favorite query sequence to other known proteins or DNA sequences.

Applications include

- discovering new genes or proteins
- discovering variants of genes or proteins
- exploring protein structure and function

NCBI --> Resources --> Sequence Analysis --> BLAST

- √ Select the BLAST program
- ✓ Enter query sequence in FASTA format

- ✓ Choose optional parameter i. e
 Highly similar srquences
- ✓ Click Blast

- The score of a pairwise alignment includes positive values for exact matches, and other scores for mismatches and gaps.
- Score reflects degree of similarity

Protein Sequence Analysis

- Click or Paste the web link to your browser to enter the ProtParam tool.
- The computed parameters include the molecular weight, theoretical pl, amino acid composition, atomic composition, extinction coefficient, estimated half-life, instability index, aliphatic index and grand average of hydropathicity (GRAVY) for protein sequences
- http://web.expasy.org/protparam/
- your sequence in the Protein query box in FASTA format or SwissProt accession number
- Click compute parameters.

Translation of Protein to nucleotide

Emboss Transeq ---> Sequence
 Translation

Launch back transeq (Protein sequence back translation)

Submit

Translation of nucleotides to proteins

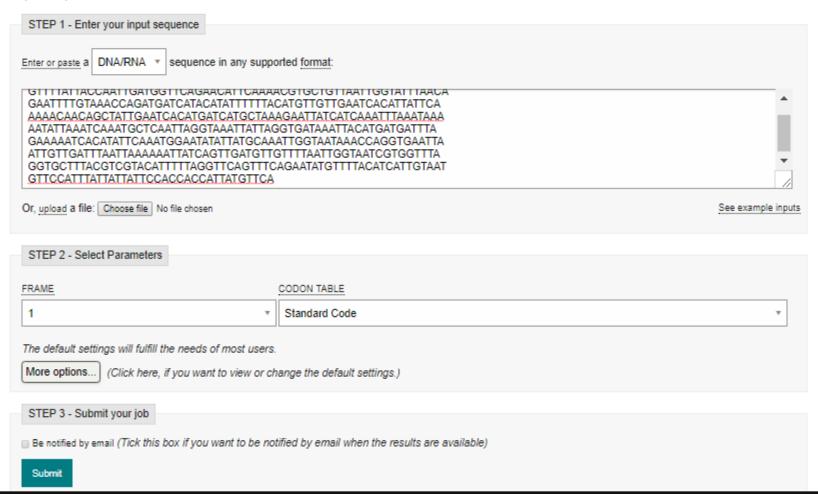
Emboss Transeq → Enter or paste DNA sequence

Submit

Tools > Sequence Translation > EMBOSS Transeq

EMBOSS Transeq

EMBOSS Transeq translates nucleic acid sequences to their corresponding peptide sequences. It can translate to the three forward and three reverse frames, and output multiple frame translations at once.



Multiple sequence alignment

- A multiple sequence alignment (MSA) is a <u>sequence alignment</u> of three or more <u>biological sequences</u>, generally <u>protein</u>, <u>DNA</u>, or <u>RNA</u>.
- In many cases, the input set of query sequences are assumed to have an <u>evolutionary</u> relationship by which they share a lineage and are descended from a common ancestor.
- From the resulting MSA, sequence <u>homology</u> can be inferred and <u>phylogenetic analysis</u> can be conducted to assess the sequences' shared evolutionary origins.
- Multiple sequence alignment is often used to assess sequence <u>conservation</u> of <u>protein domains</u>, <u>tertiary</u> and <u>secondary</u> structures, and even individual amino acids or nucleotides

MSA- Clustal Omega

- √ Go to :
 https://www.ebi.ac.uk/Tools/msa/clustalo/
- ✓ Input DNA Sequences
- ✓ Submit

Phylogenetic Analysis I

- This is a known as molecular phylogenetics, which is the analysis of hereditary molecular differences, mainly in DNA sequences, to gain information on an organism's evolutionary relationships
- It finds evolutionary ties between organisms
- It provides relationships between an ancestral sequence and its descendants
- The result of a molecular <u>phylogenetic</u> analysis is expressed or can be drawn in a hierarchical diagram called a cladogram or phylogram (<u>phylogenetic tree</u>).
- Molecular phylogenetics is one aspect of molecular <u>systematics</u>, a broader term that also includes the use of molecular data in <u>taxonomy</u> and <u>biogeography</u>.

TreeTop - Phylogenetic Tree Prediction

- Go the TreeTop web link at <u>http://www.genebee.msu.su/services/phtr</u> <u>ee reduced.html</u>
- In the alignment window, copy and paste your ClustalW save MSA.
- It is preferable to activate Bootstrap.
- Include your email to receive result or you can wait for the analysis to be completed.
- Click submit Query button

Phylogenetic Tree Prediction using Clustal Omega

- √ Go to :
 https://www.ebi.ac.uk/Tools/msa/clustalo/
- ✓ Input DNA Sequences
- ✓ Submit
- ✓ Click on Phylogenetic tree