

生物信息学：导论与方法

Bioinformatics: Introduction and Methods



<https://www.coursera.org/course/pkubioinfo>



生物信息学：导论与方法

Bioinformatics: Introduction and Methods

北京大学生物信息学中心 高歌、魏丽萍

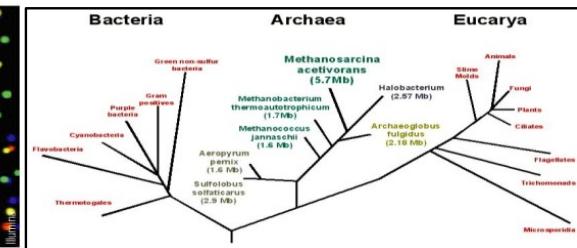
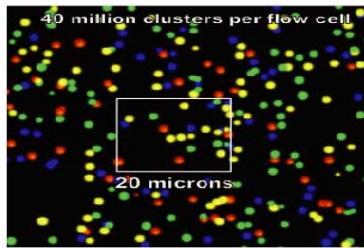
Ge Gao & Liping Wei

Center for Bioinformatics, Peking University





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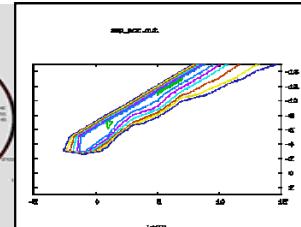
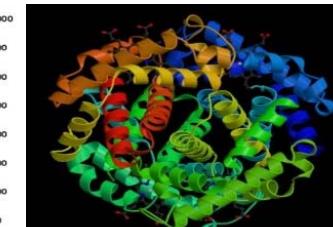
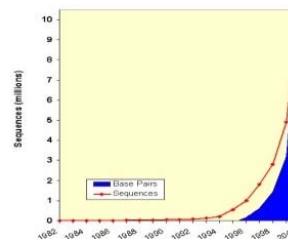
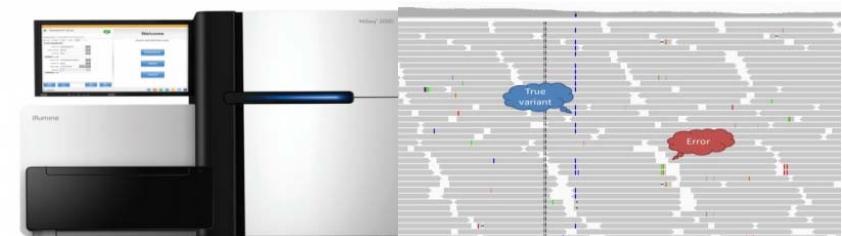


Sequence Database Search

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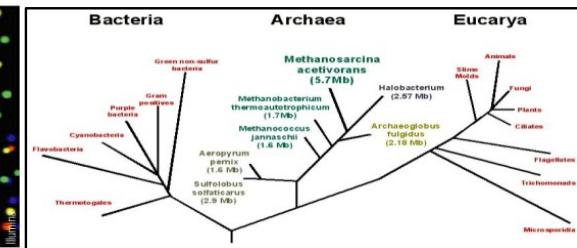
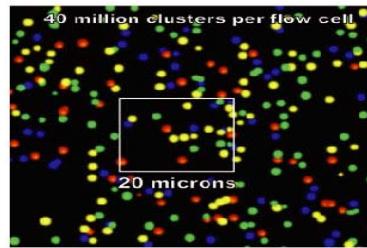
Ge Gao, Ph.D.

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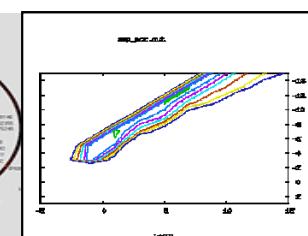
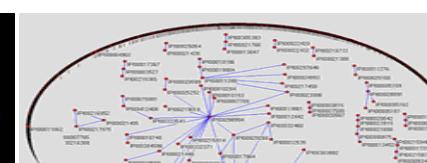
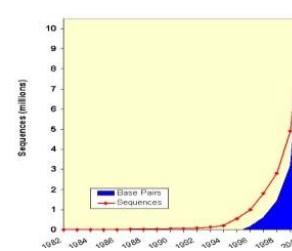
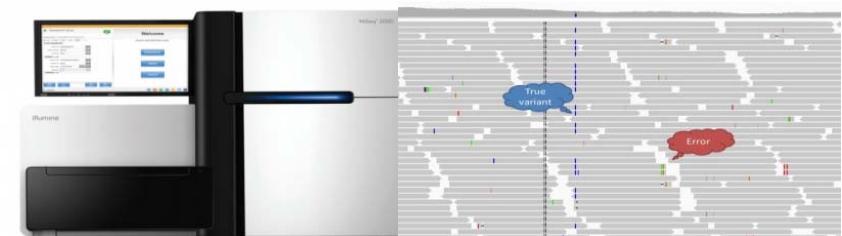


Unit 1: Sequence Databases

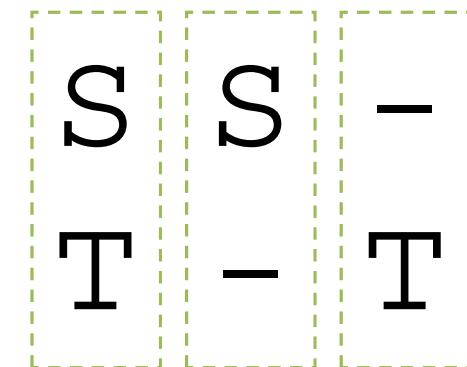
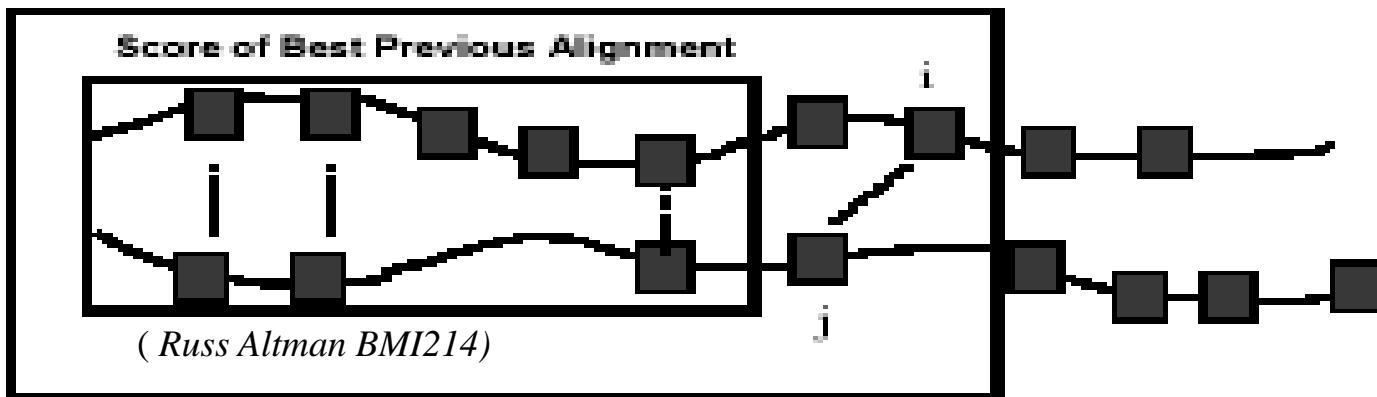
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New Best Alignment = Previous Best + Local Best



Global alignment (Needleman-Wunsch)

$$F(0,0) = 0$$

$$F(i, j) = \max \begin{cases} F(i - 1, j - 1) + s(x_i, y_j) \\ F(i - 1, j) + d \\ F(i, j - 1) + d \end{cases}$$

Local alignment (Smith-Waterman)

$$F(0,0) = 0$$

$$F(i, j) = \max \begin{cases} F(i - 1, j - 1) + s(x_i, y_j) \\ F(i - 1, j) + d \\ F(i, j - 1) + d \\ 0 \end{cases}$$

Sequence Alignment

“How can we determine the similarity
between two sequences?”

Why is it important?

- Similar sequence → Similar structure → Similar function (The “*Sequence-to-Structure-to-Function Paradigm*”)
- Similar sequence → Common ancestor (“*Homology*”)

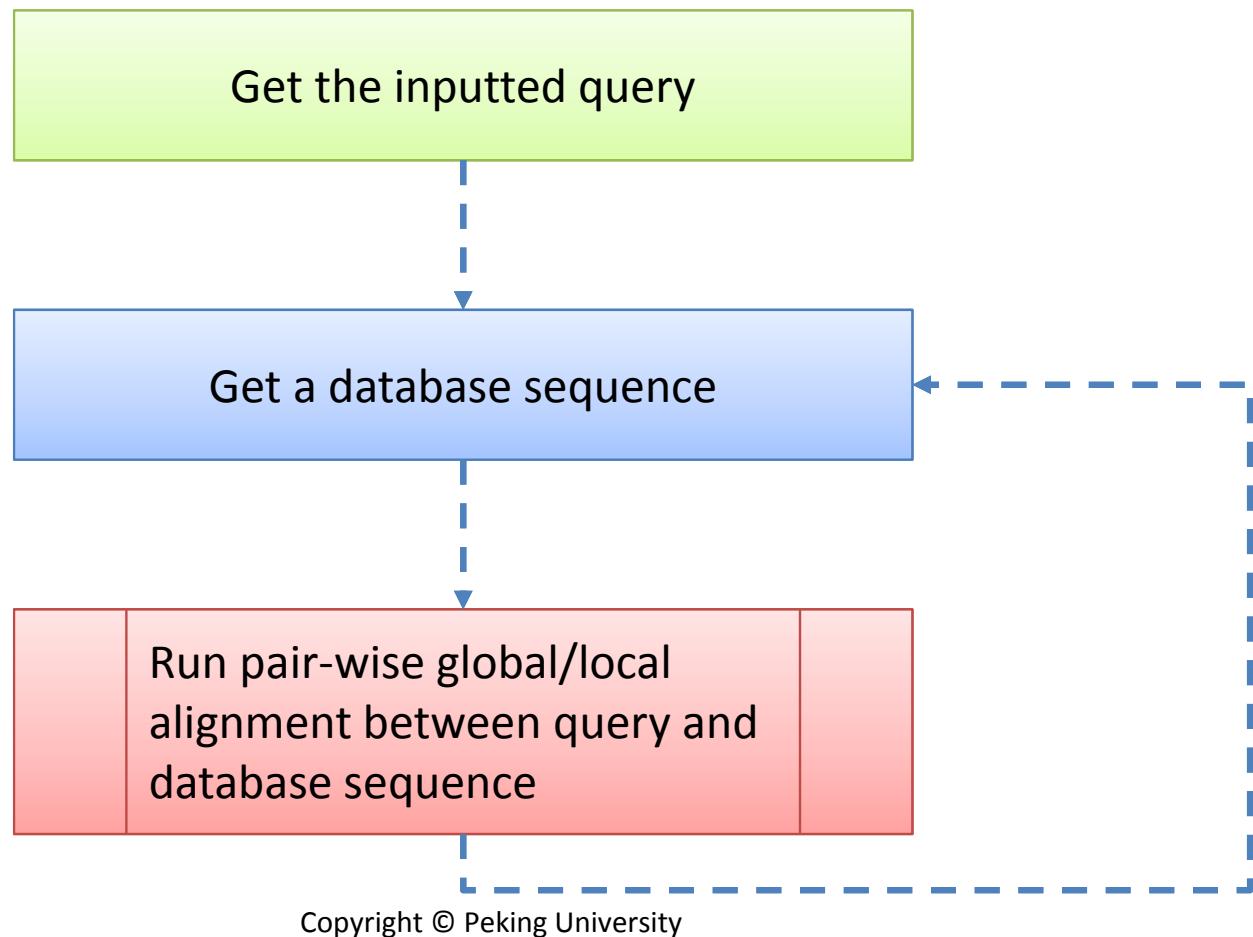
Sequence Database Searching

- Rather than do the alignment pair-wise, it's more often to search **sequence database** in a **high-throughput** style.
- Or, identify similarities between
 - **novel query sequence**
whose structures and functions are usually unknown and/or uncharacterized
 - **sequences in (public) databases**
whose structures and functions have been elucidated and annotated.

Sequence Database Searching

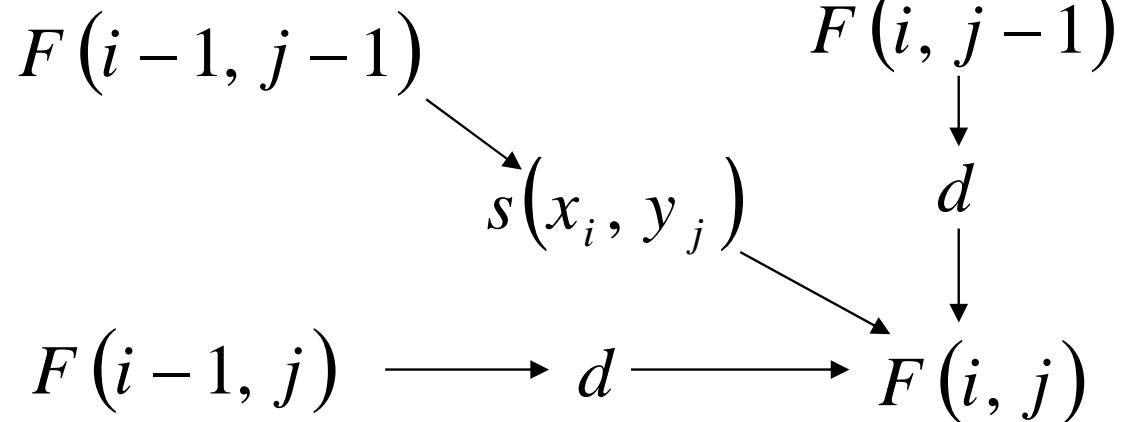
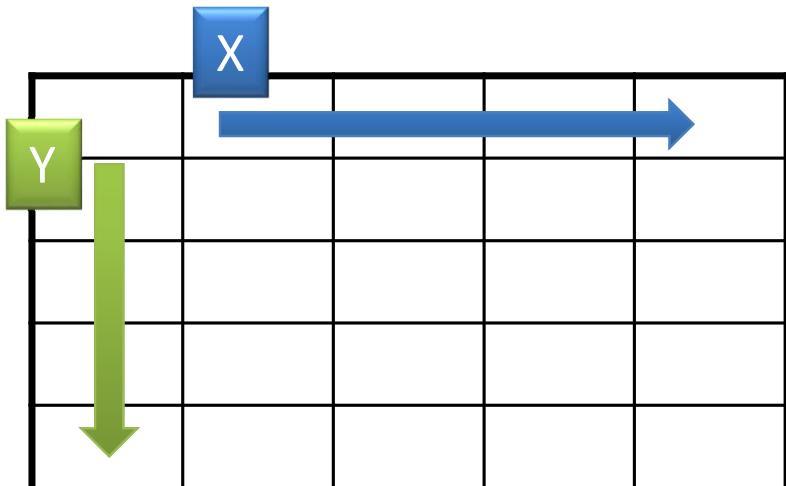
- The **query sequence** is compared/aligned with every sequence in the database
- **Statistically significant hits** are assumed to be related to the query sequence
 - Similar **function/structure**
 - Common **evolutionary ancestor**

A (naïve) algorithm for database searching



$$F(0,0) = 0$$

$$F(i, j) = \max \begin{cases} F(i - 1, j - 1) + s(x_i, y_j) & x_i \text{ aligned to } y_j \\ F(i - 1, j) + d & x_i \text{ aligned to a gap} \\ F(i, j - 1) + d & y_j \text{ aligned to a gap} \end{cases}$$



There are nm entries in the matrix.

Sequence X of length m

Sequence Y of length n

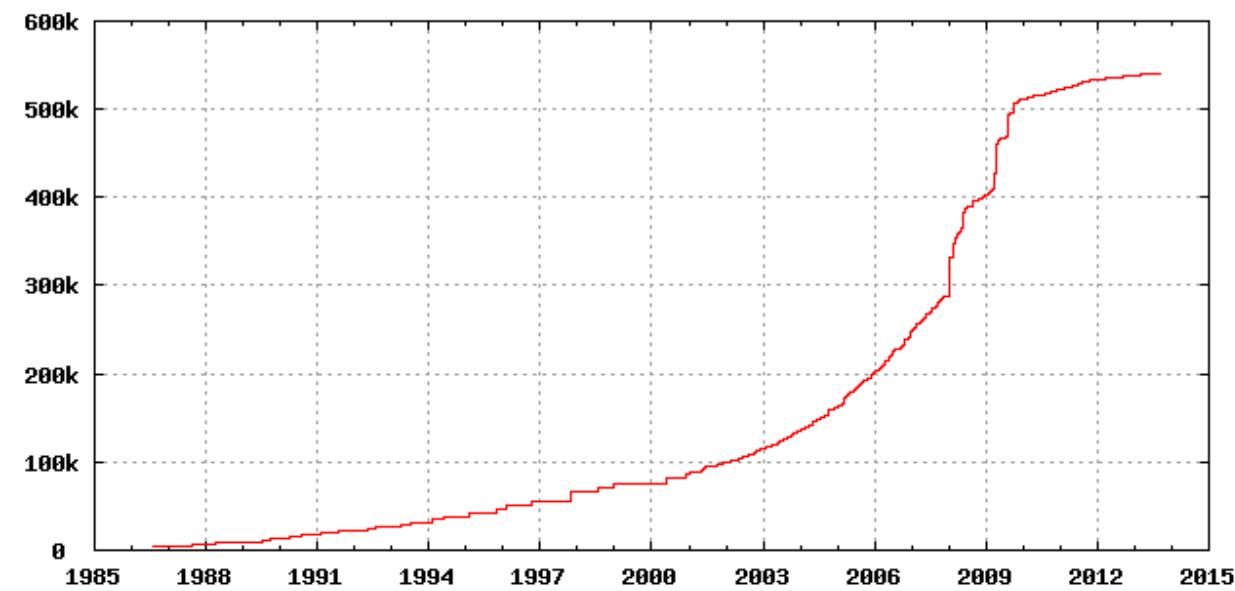
Dynamic programming matrix

Each entry requires a constant number c of operation(s).

$c * m * n$ operations needed in total, for one pair-wise alignment.

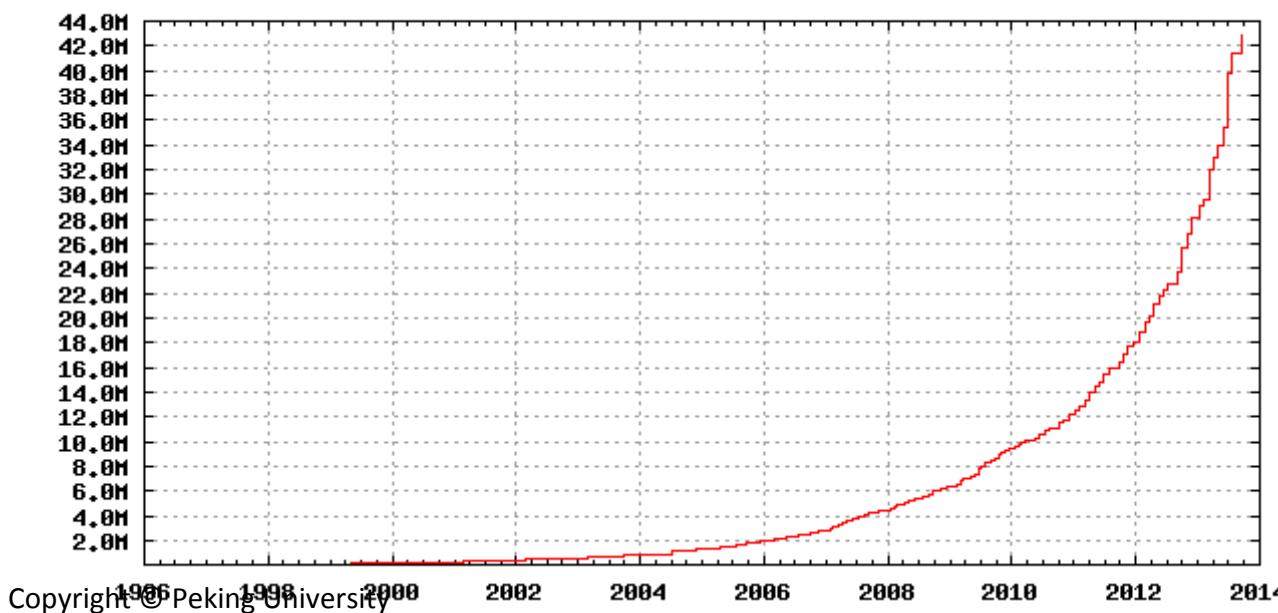
- Say your query sequence (HBA_HUMAN) has 142 amino acids
- Most recent release of human-curated Swiss-Prot protein databases contains 540,958 sequences with 192,206,270 amino acids (Sept 18th, 2013);
 - On average, the sequence length is $192,206,270 / 540,958 = 355.30$ aa
- And assume your super-fast computer can run one operation in $1\mu\text{s} = (0.000001\text{s})$
- Then, you will need **7.8 hr** for **ONE** comparison!

Number of entries in UniProtKB/Swiss-Prot



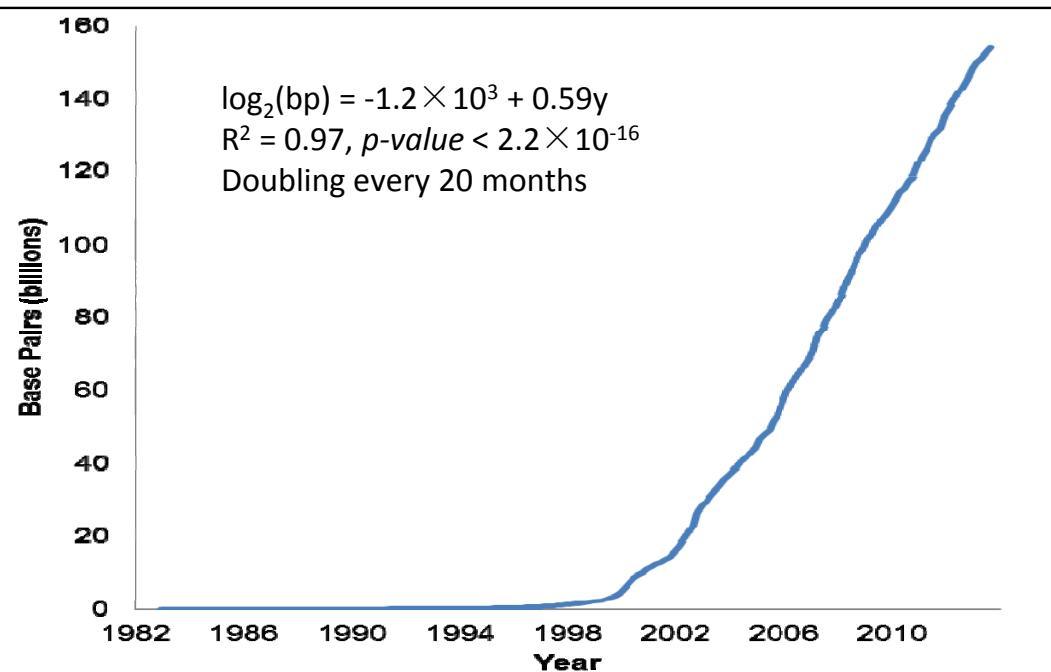
Source: <http://web.expasy.org/docs/relnotes/relstat.html>

Number of entries in UniProtKB/TrEMBL

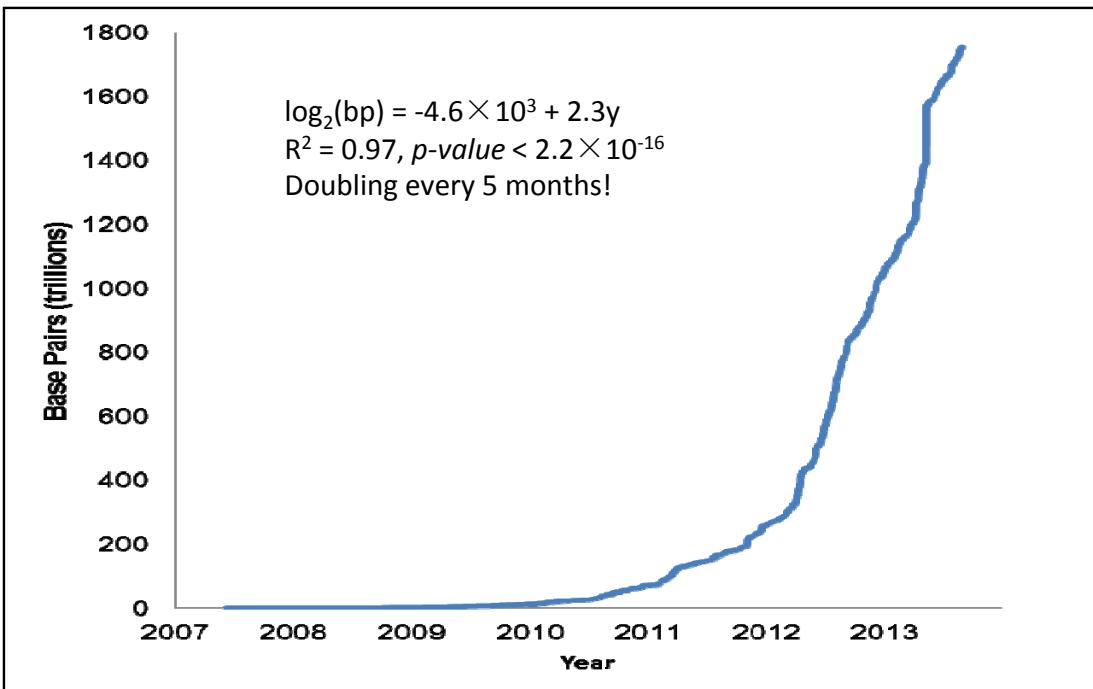


Source: <http://www.ebi.ac.uk/uniprot/TrEMBLstats>

Genbank

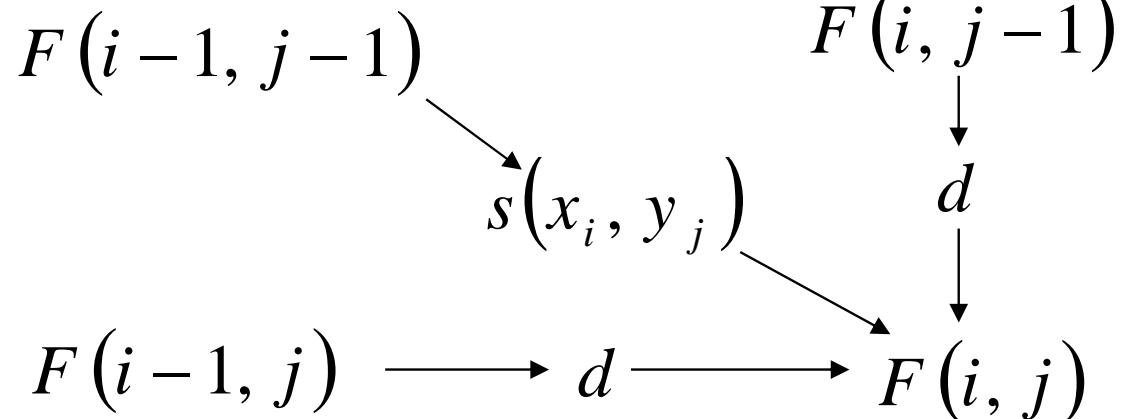
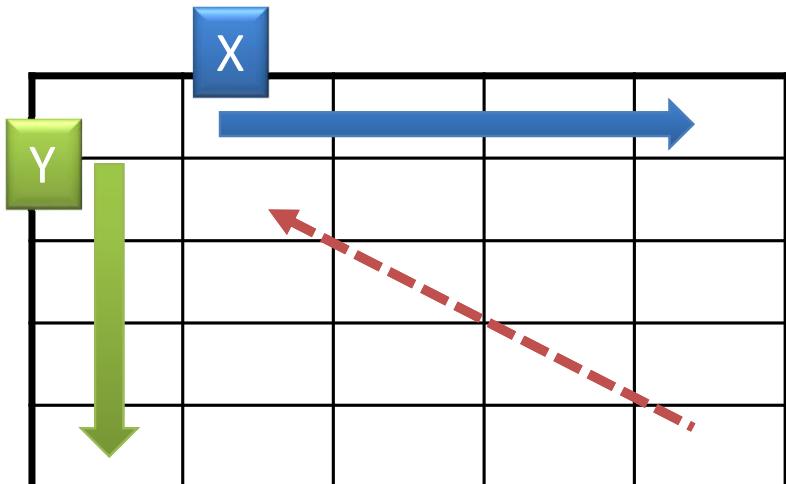


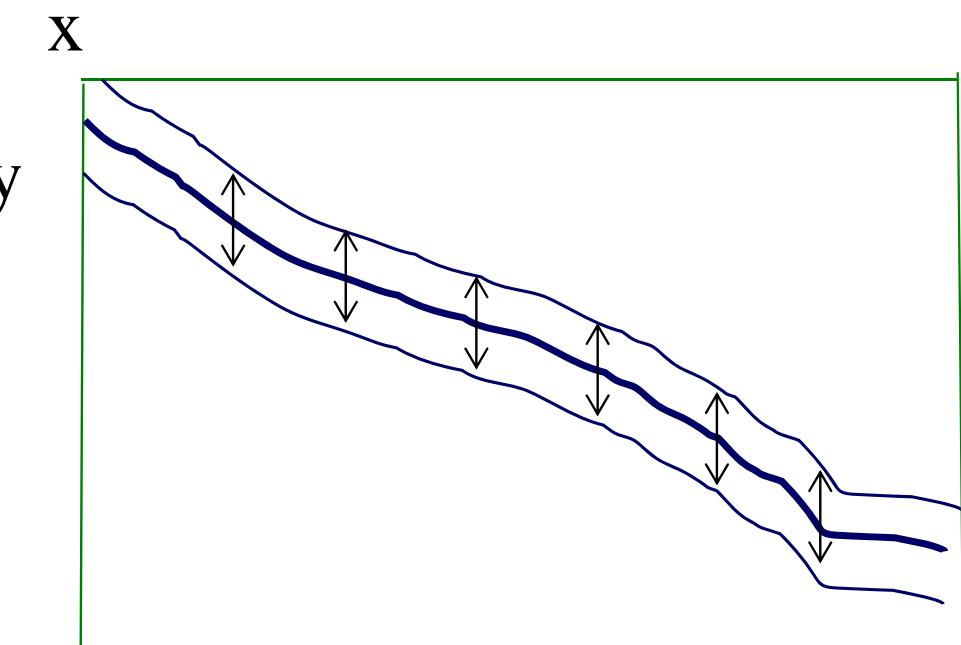
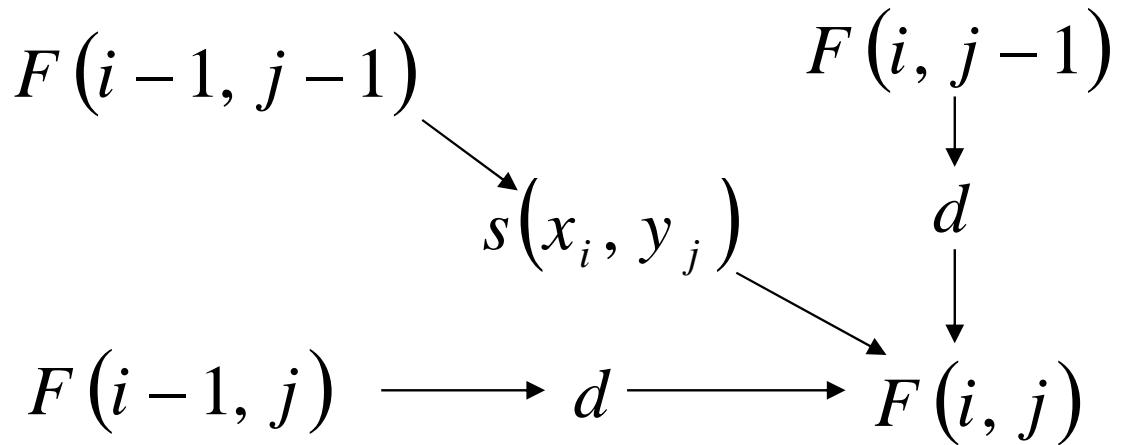
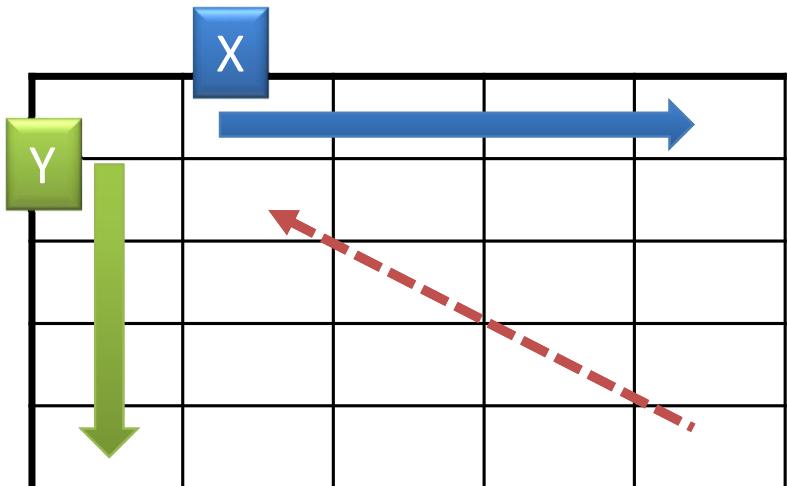
SRA



$$F(0,0) = 0$$

$$F(i, j) = \max \begin{cases} F(i - 1, j - 1) + s(x_i, y_j) & x_i \text{ aligned to } y_j \\ F(i - 1, j) + d & x_i \text{ aligned to a gap} \\ F(i, j - 1) + d & y_j \text{ aligned to a gap} \end{cases}$$

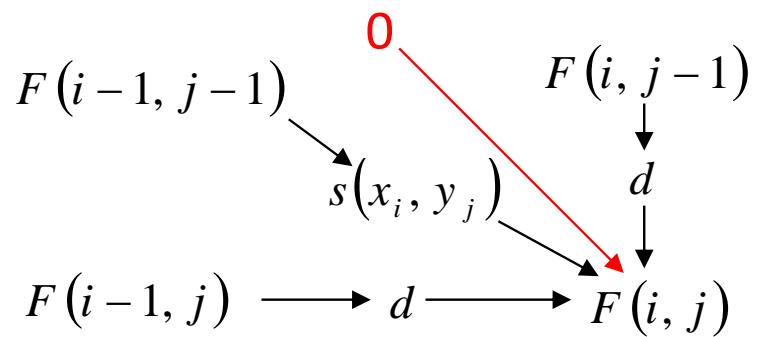




HBA_HUMAN	1 MV-LSPADKTNVKAAWGKVGAHAGEYGAEALERMFLSPTTTKTYFPHF-D	48
HBB_HUMAN	1 MVHLTPEEKSAAVTALWGRV--NVDEVGGGEALGRLLIVVYPWTQRFESFGD	48
HBA_HUMAN	49 LS-----HGSAQVKGHGKKVADALTNAVAHVDDMPNALSALSDLHAHKLR	93
HBB_HUMAN	49 LSTPDAVMGNPKVKAHGKKVLGAFSDGLAHLDNLKGTFATLSELHCDKLH	98
HBA_HUMAN	94 VDPVNFKILLSHCLLVTAAHLPAEFTPASVHASLDKFLASVSTVLTSKYR	142
HBB_HUMAN	94 VDPENFRILLGNVLVCVLAHHFGKEFTPPVQAAYQKVVAGVANALAHKYH	147

A G
A G

		A	A	G
	0	0	0	0
A	0	2	2	0
G	0	0	0	4
C	0	0	0	0



BLAST: Intro

- To make the alignment effectively, a *Heuristic algorithm* BLAST (Basic Local Alignment Search Tool) is proposed by Altschul *et al* in 1990.
- BLAST finds the highest scoring **locally optimal alignments** between a query sequence and a database.
 - Very **fast** algorithm
 - Can be used to search **extremely large** databases
 - Sufficiently **sensitive** and **selective** for most purposes
 - **Robust** – the default parameters just work for most cases



Basic Local Alignment Search Tool

Stephen F. Altschul¹, Warren Gish¹, Webb Miller²
Eugene W. Myers³ and David J. Lipman¹

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National Library of Medicine, National Institutes of Health
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²Department of Computer Science
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³Department of Computer Science
University of Arizona, Tucson, AZ 85721, U.S.A.

(Received 26 February 1990; accepted 15 May 1990)

Basic local alignment search tool

SF Altschul, W Gish, W Miller, EW Myers... - Journal of molecular ..., 1990 - Elsevier

A new approach to rapid sequence comparison, **basic local alignment search tool** (BLAST), directly approximates alignments that optimize a measure of **local** similarity, the maximal segment pair (MSP) score. Recent mathematical results on the stochastic properties of ...

Cited by 47577 Related articles All 98 versions Cite

blast.ncbi.nlm.nih.gov/Blast.cgi

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NCBI/ BLAST Home

BLAST finds regions of similarity between biological sequences. [more...](#)

New DELTA-BLAST, a more sensitive protein-protein search [Go](#)

BLAST Assembled RefSeq Genomes

Choose a species genome to search, or [list all genomic BLAST databases](#).

<input type="checkbox"/> Human	<input type="checkbox"/> Oryza sativa	<input type="checkbox"/> Gallus gallus
<input type="checkbox"/> Mouse	<input type="checkbox"/> Bos taurus	<input type="checkbox"/> Pan troglodytes
<input type="checkbox"/> Rat	<input type="checkbox"/> Danio rerio	<input type="checkbox"/> Microbes
<input type="checkbox"/> Arabidopsis thaliana	<input type="checkbox"/> Drosophila melanogaster	<input type="checkbox"/> Apis mellifera

Basic BLAST

Choose a BLAST program to run.

nucleotide blast	Search a nucleotide database using a nucleotide query <i>Algorithms:</i> blastn, megablast, discontiguous megablast
protein blast	Search protein database using a protein query <i>Algorithms:</i> blastp, psi-blast, phi-blast, delta-blast
blastx	Search protein database using a translated nucleotide query
tblastn	Search translated nucleotide database using a protein query
tblastx	Search translated nucleotide database using a translated nucleotide query

Specialized BLAST

Choose a type of specialized search (or database name in parentheses.)

- Make specific primers with [Primer-BLAST](#)
- Search [trace archives](#)
- Find [conserved domains](#) in your sequence (cds)
- Find sequences with similar [conserved domain architecture](#) (cdart)
- Search sequences that have [gene expression profiles](#) (GEO)
- Search [immunoglobulins and T cell receptor sequences](#) (IgBLAST)
- Screen sequence for [vector contamination](#) (vecscren)
- Align two (or more) sequences using BLAST (bl2seq)
- Search [protein](#) or [nucleotide](#) targets in PubChem BioAssay
- Search [SRA by experiment](#)
- Constraint Based Protein [Multiple Alignment Tool](#)
- Needleman-Wunsh [Global Sequence Alignment Tool](#)
- Search [RefSeqGene](#)

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Protein BLAST: seal x

blast.ncbi.nlm.nih.gov/Blast.cgi?PROGRAM=blastp&BLAST_PROGRAMS=blastp&PAGE_TYPE=Bla:☆

BLAST® Basic Local Alignment Search Tool

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NCBI/ BLAST/ blastp suite Standard Protein BLAST

blast blastp blastx tblastn tblastx

Enter Query Sequence

BLASTP programs search protein databases using a protein query. [more...](#)

Reset page Bookmark

Enter accession number(s), gi(s), or FASTA sequence(s) [?](#)

?"/>

From
To

Or, upload file No file chosen [?](#)

Job Title
Enter a descriptive title for your BLAST search [?](#)

Align two or more sequences [?](#)

Choose Search Set

Database Non-redundant protein sequences (nr) [?](#)

Organism Optional Enter organism name or id—completions will be suggested Exclude [+](#)
Enter organism common name, binomial, or taxid. Only 20 top taxa will be shown. [?](#)

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

Entrez Query Optional Enter an Entrez query to limit search [?](#)

Program Selection

Algorithm blastp (protein-protein BLAST)
 PSI-BLAST (Position-Specific Iterated BLAST)
 PHI-BLAST (Pattern Hit Initiated BLAST)
 DELTA-BLAST (Domain Enhanced Lookup Time Accelerated BLAST)
Choose a BLAST algorithm [?](#)

BLAST Search database Non-redundant protein sequences (nr) using Blastp (protein-protein BLAST)

Show results in a new window

[Algorithm parameters](#)

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Protein BLAST: sea x

blast.ncbi.nlm.nih.gov/Blast.cgi?PROGRAM=blastp&BLAST_PROGRAMS=blastp&PAGE_TYPE=Bla:☆ a

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NCBI/ BLAST/ blastp suite Standard Protein BLAST

blastn blastp blastx tbblastn tbblastx

Enter Query Sequence

BLASTP programs search protein databases using a protein query. [more...](#)

Enter accession number(s), gi(s), or FASTA sequence(s) [?](#)

>sp|P69905|HBA_HUMAN
MVLSPADKINIKAAANGKVGAHAGEYGAELERMFLSFPITIKIVFPHEDLSHGSAQVK
GHGKXUADALTNAAVHVDIMPNALSLSDIHAKHLRVDPNFKLILSHCLIVTIAAHL
PAEFTPAVHASLQKFLASVSTVLISKYR

Clear Query subrange [?](#)

From _____ To _____

Or, upload file Choose File No file chosen [?](#)

Job Title sp|P69905|HBA_HUMAN

Enter a descriptive title for your BLAST search [?](#)

Align two or more sequences [?](#)

Choose Search Set

Database Non-redundant protein sequences (nr)

Organism Reference proteins (refseq_protein)

Optional UniProtKB/Swiss-Prot(swissprot)

Exclude Patented protein sequences(pat)

Optional Protein Data Bank proteins(pdb)

Entrez Query Metagenomic proteins(env_nr)

Optional Transcriptome Shotgun Assembly proteins (tsa_nr)

Enter an Entrez query to limit search [?](#)

Program Selection

Algorithm blastp (protein-protein BLAST)
 PSI-BLAST (Position-Specific Iterated BLAST)
 PHI-BLAST (Pattern Hit Initiated BLAST)
 DELTA-BLAST (Domain Enhanced Lookup Time Accelerated BLAST)

Choose a BLAST algorithm [?](#)

BLAST

Search database Non-redundant protein sequences (nr) using Blastp (protein-protein BLAST)

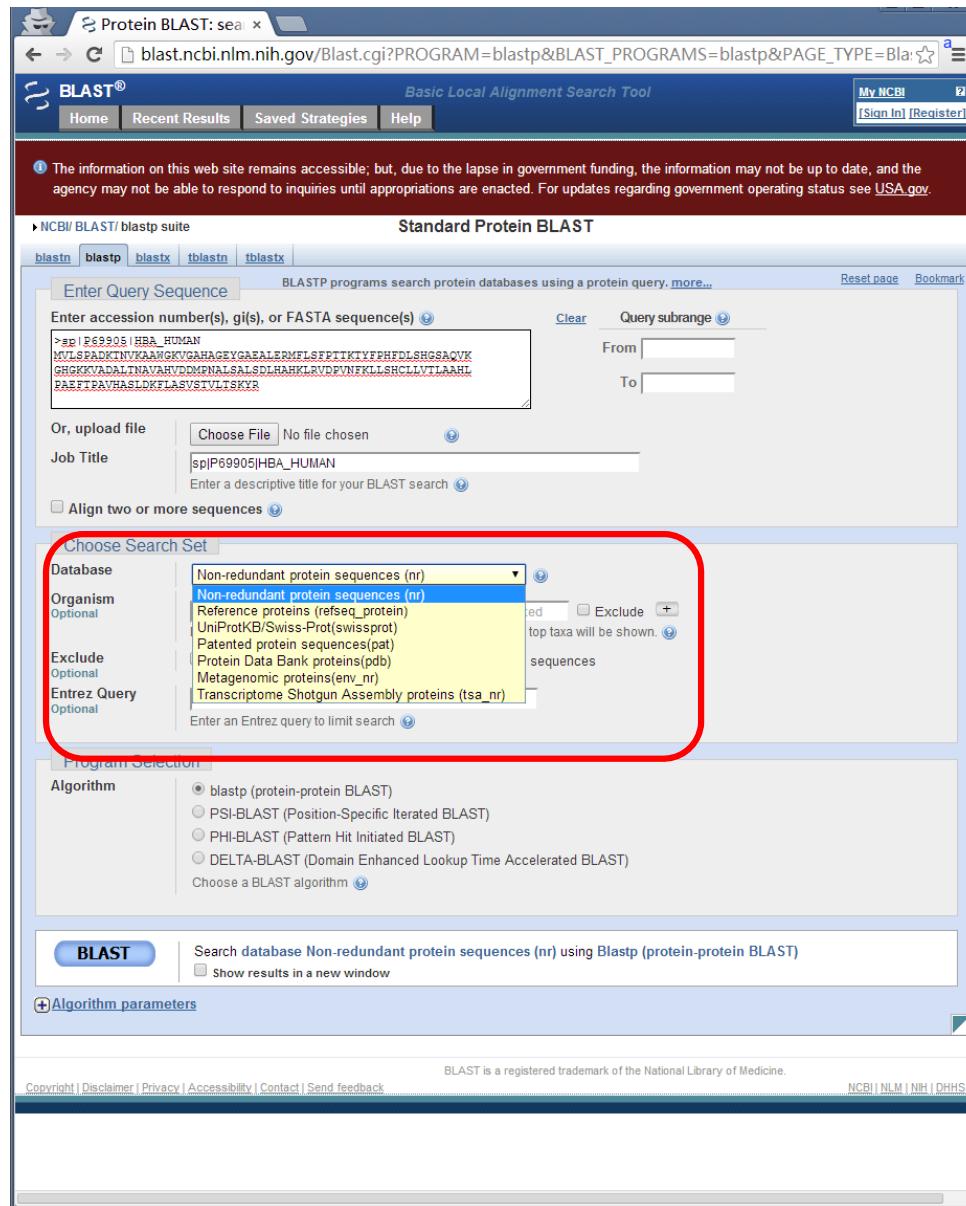
Show results in a new window

+ Algorithm parameters

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WELCOME

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

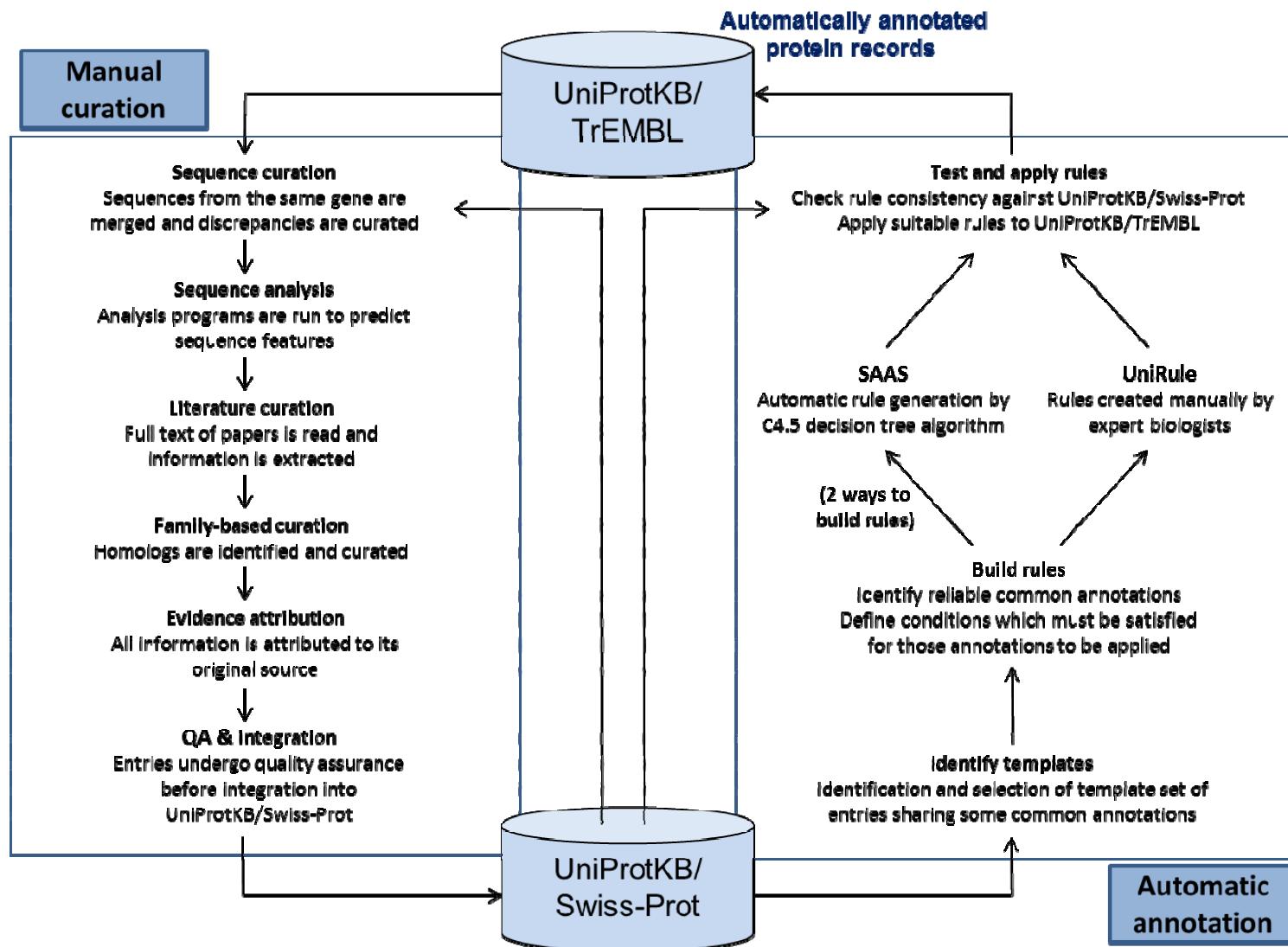
data
protein sequence



knowledge
functional information

(Modified from http://education.expasy.org/cours/Turin/UniProtKB_Turin.ppt)

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The diagram illustrates the UniProtKB/Swiss-Prot annotation interface and its features, with several highlighted sections and arrows pointing to specific annotations.

Annotations:

- Names and origin:** Shows protein names (Elongation factor Tu 1), gene names (POCE47), organism (Escherichia coli), and taxonomic lineage (Bacteria > Proteobacteria > Gammaproteobacteria > Enterobacteriales > Enteracteriaceae > Escherichia).
- References:** Lists three references, with one highlighted: "The nucleotide sequence of the cloned tufA gene of Escherichia coli." by Yokota T, Sugisaki H, Takamori M, Kaziro Y. (1980) [PubMed: 7011903] [Abstract].
- Cross-references:** Links to various databases including EMBL, GenBank, DDBJ, PIR, RefSeq, and 3D structures.
- Protein and gene names Taxonomic information:** A central box containing the protein name, gene name, and taxonomic information.
- General annotation (Comments):** Describes the protein's function as promoting GTP-dependent binding of aminoacyl-tRNA to the ribosomal subunit.
- Manual annotation:** A large blue box covering Function, Subcellular location, Catalytic activity, Disease, Tissue specificity, and Pathway.
- Sequence annotation (Features):** Shows initiator methionine removed at position 4.
- Manual annotation:** Post-translational modifications, variants, transmembrane domains, signal peptide.
- Ontologies:** Lists biological processes, cellular components, ligands, molecular functions, and technical terms.
- Gene Ontology (GO):** Lists biological processes, cellular components, and molecular functions.
- Keywords:** Lists antibiotic resistance, protein biosynthesis, cell membrane, cytoplasm, membrane, GTP-binding, nucleotide-binding, elongation factor, acetylation, methylation, phosphoprotein, 3D-structure, complete proteome, and direct protein sequencing.

Annotations in focus:

 - One protein sequence, One gene, One species:** A central statement supported by the UniProtKB entry for POCE47.
 - Alternative products:** Protein sequences produced by alternative splicing, alternative promoter usage, and alternative initiation.
 - Post-translational modifications:** N-acetylysine at position 2 and N6,N5-dimethyllysine at position 57.
 - Gene Ontology:** Response to antibiotic, cytoplasm, plasma membrane, GTP-binding, GTPase activity, protein binding, and translation elongation factor activity.

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Organism-specific

AGD
ArachnoServer
CGD
ConoServer
CTD
CYGD
dictyBase
EchoBASE
EcoGene
euHCVdb
EuPathDB
FlyBase
GeneCards
GeneDB_Spombe
GeneFarm
GenoList
Gramene
H-InvDB
HGNC
HPA
LegioList
Leproma
MaizeGDB
MGI
MIM
neXtProt
Orphanet
PharmGKB
PseudoCAP
RGD
SGD
TAIR
TuberCuList
WormBase
Xenbase
ZFIN

Phylogenomic dbs

eggNOG
GeneTree
HOGENOM
HOVERGEN
InParanoid
OMA
OrthoDB
PhylomeDB
ProtClustDB

Sequence

EMBL
IPI
PIR
RefSeq
UniGene

Gene expression

ArrayExpress
Bgee
CleanEx
Genevestigator
GermOnline

Ontologies

GO

Proteomic

PeptideAtlas
PRIDE
ProMEX

Genome annotation

Ensembl
EnsemblBacteria
EnsemblFungi
EnsemblMetazoa
EnsemblPlants
EnsemblProtists
GenID
GenomeReviews
KEGG
NMPDR
TIGR
UCSC
VectorBase

Polymorphism

dbSNP

Family and domain

Gene3D
HAMAP
InterPro
PANTHER
Pfam
PIRSF
PRINTS
ProDom
PROSITE
SMART
SUPFAM
TIGRFAMs

Protein family/group

Allergome
CAZy
MEROPS
PeroxiBase
PptaseDB
REBASE
TCDB

2D gel

2DBase-Ecoli
ANU-2DPAGE
Aarhus/Ghent-2DPAGE (no server)
COMPLUYEAST-2DPAGE
Cornea-2DPAGE
DOSAC-COBS-2DPAGE
ECO2DBASE (no server)
OGP
PHCI-2DPAGE
PMMA-2DPAGE
Rat-heart-2DPAGE
REPRODUCTION-2DPAGE
Siena-2DPAGE
SWISS-2DPAGE
UCD-2DPAGE
World-2DPAGE

Enzyme and pathway

BioCyc
BRENDA
Pathway_Interaction_DB
Reactome

UniProtKB/Swiss-Prot:
129 explicit links

and 14 implicit links!

PTM

GlycoSuiteDB
PhosphoSite
PhosSite

Other

BindingDB
DrugBank
NextBio
PMAP-CutDB

PPI

DIP
IntAct
MINT
STRING

3D structure

DisProt
HSSP
PDB
PDBsum
ProteinModelPortal
SMR

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Protein BLAST: sea x

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NCBI/ BLAST/ blastp suite Standard Protein BLAST

blastn blastp blastx tblastn tblastx

Enter Query Sequence

Enter accession number(s), gi(s), or FASTA sequence(s) [more...](#)

>sp|P69905|HBA_HUMAN
MVLSPADTKNVKAAGKVGAAHGEYGAELERMFLSFTTITKTYFPHFDLSHGSAQVK
GHGKKVADALTNNAVHDDNPNALSDLHAKLRLVDPVNFKLLSHCLVTLA AHL
PAEFTPAVHALDKFLASVSTVLTSKYR

Clear Query subrange [From](#) [To](#) [Reset page](#) [Bookmark](#)

Or, upload file Choose File No file chosen

Job Title sp|P69905|HBA_HUMAN

Enter a descriptive title for your BLAST search [more...](#)

Align two or more sequences [more...](#)

Choose Search Set

Database UniProtKB/Swiss-Prot(swissprot)

Title: Non-redundant UniProtKB/SwissProt sequences.
Molecule Type: Protein
Update date: 2013/10/10
Number of sequences: 456016

Organism Enter organism name or id—completions will be suggested Exclude [+ Add](#)
Enter organism common name, binomial, or tax id. Only 20 top taxa will be shown. [more...](#)

Exclude Models (XML/XP) Uncultured/environmental sample sequences

Entrez Query Enter an Entrez query to limit search [more...](#)

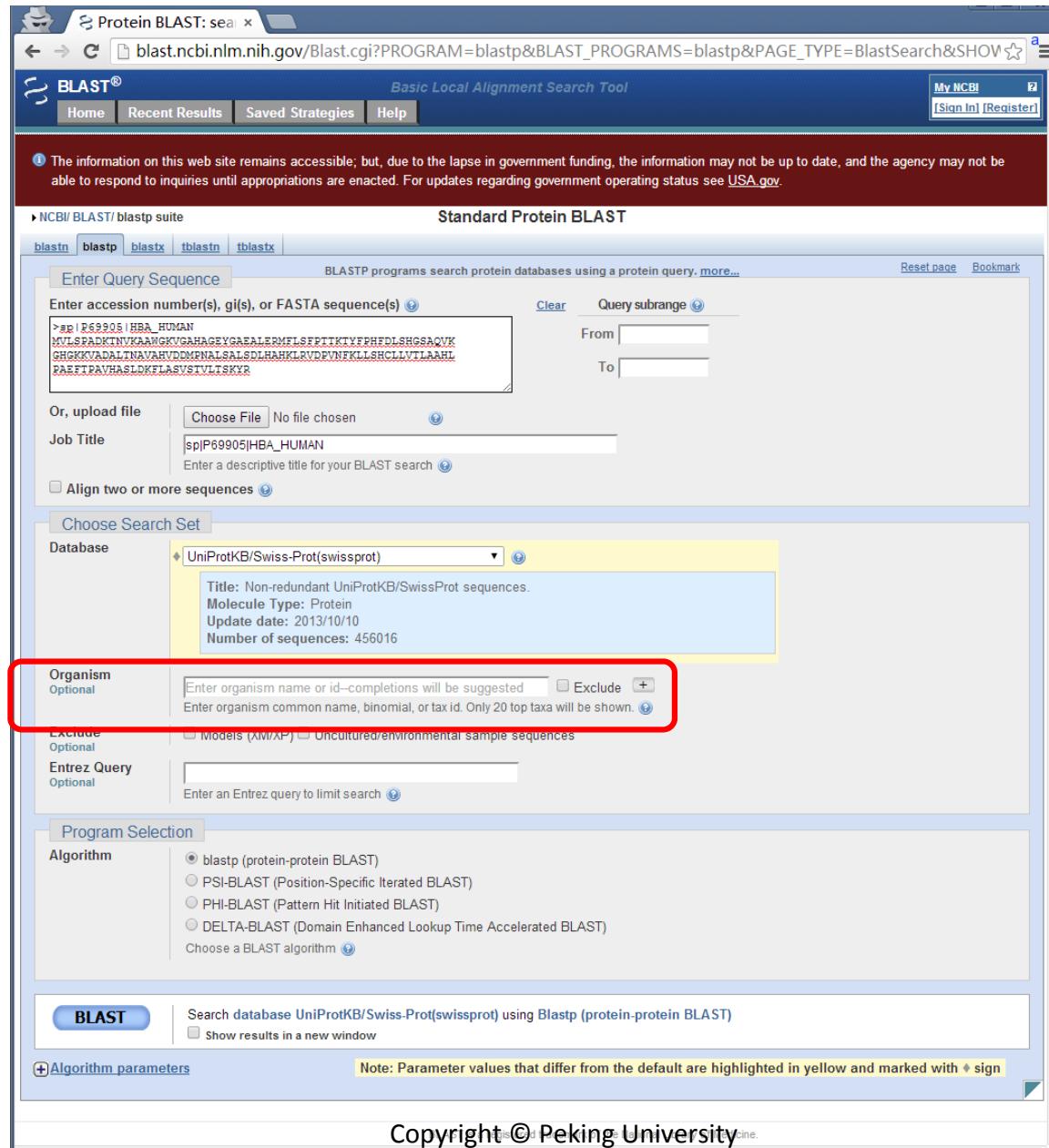
Program Selection

Algorithm blastp (protein-protein BLAST)
 PSI-BLAST (Position-Specific Iterated BLAST)
 PHI-BLAST (Pattern Hit Initiated BLAST)
 DELTA-BLAST (Domain Enhanced Lookup Time Accelerated BLAST)
Choose a BLAST algorithm [more...](#)

BLAST Search database UniProtKB/Swiss-Prot(swissprot) using Blastp (protein-protein BLAST)
 Show results in a new window

[Algorithm parameters](#) Note: Parameter values that differ from the default are highlighted in yellow and marked with * sign

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Protein BLAST: sea x

blast.ncbi.nlm.nih.gov/Blast.cgi

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NCBI/ BLAST/ blastp suite Standard Protein BLAST

blast blastp blastx tblastn tblastx

Enter Query Sequence

BLASTP programs search protein databases using a protein query. more... Reset page Bookmark

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

From To

Or, upload file No file chosen

Job Title Enter a descriptive title for your BLAST search

Align two or more sequences

Choose Search Set

Database

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

Exclude Models (XMP/XP) Uncultured/environmental sample sequences

Entrez Query Enter an Entrez query to limit search

Program Selection

Algorithm blastp (protein-protein BLAST) PSI-BLAST (Position-Specific Iterated BLAST) PHI-BLAST (Pattern Hit Initiated BLAST) DELTA-BLAST (Domain Enhanced Lookup Time Accelerated BLAST)

BLAST Search database UniProtKB/Swiss-Prot(swissprot) using Blastp (protein-protein BLAST) Show results in a new window

Note: Parameter values that differ from the default are highlighted in yellow and marked with * sign

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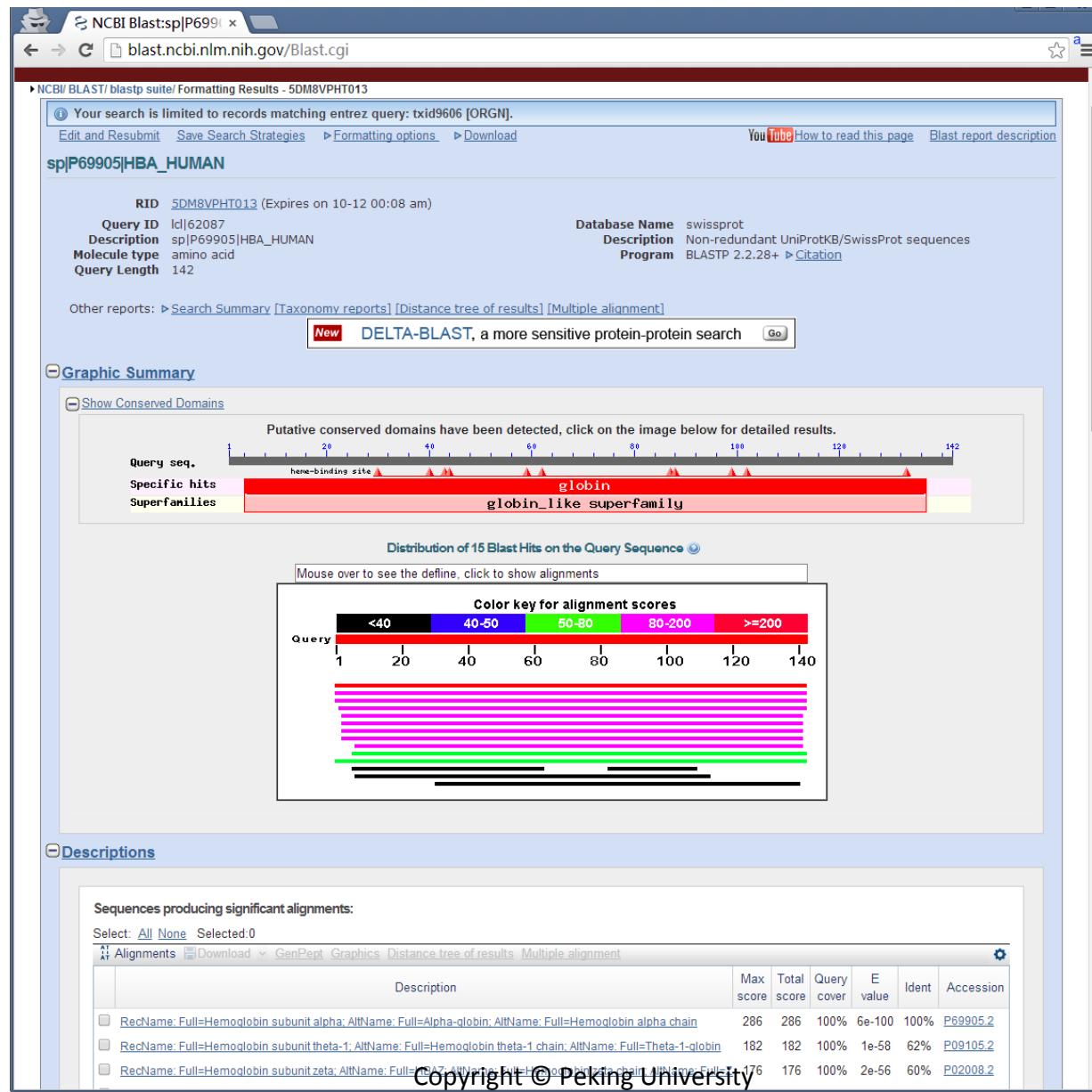
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NCBI | NLM | NIH | DHHS

Summary

Domain(s)

Hits summary



Sequences producing significant alignments:

Select: All None Selected:0

	Description	Max score	Total score	Query cover	E value	Ident	Accession
<input type="checkbox"/>	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	286	286	100%	6e-100	100%	P69905.2
<input type="checkbox"/>	RecName: Full=Hemoglobin subunit theta-1; AltName: Full=Hemoglobin theta-1 chain; AltName: Full=Theta-1-globin	182	182	100%	1e-58	62%	P09105.2
<input type="checkbox"/>	RecName: Full=Hemoglobin subunit zeta; AltName: Full=HBAZ; AltName: Full=Hemoglobin zeta chain; AltName: Full=Z	176	176	100%	2e-56	60%	P02008.2
<input type="checkbox"/>	RecName: Full=Hemoglobin subunit mu; AltName: Full=Hemoglobin mu chain; AltName: Full=Mu-globin	135	135	99%	2e-40	45%	Q6B0K9.1
<input type="checkbox"/>	RecName: Full=Hemoglobin subunit delta; AltName: Full=Delta-globin; AltName: Full=Hemoglobin delta chain	114	114	97%	2e-32	43%	P02042.2
<input type="checkbox"/>	RecName: Full=Hemoglobin subunit beta; AltName: Full=Beta-globin; AltName: Full=Hemoglobin beta chain; Contains:	114	114	97%	2e-32	43%	P68871.2
<input type="checkbox"/>	RecName: Full=Hemoglobin subunit gamma-1; AltName: Full=Gamma-1-globin; AltName: Full=Hb F Agamma; AltNam	113	113	97%	6e-32	41%	P69891.2
<input type="checkbox"/>	RecName: Full=Hemoglobin subunit gamma-2; AltName: Full=Gamma-2-globin; AltName: Full=Hb F Ggamma; AltNam	113	113	97%	6e-32	41%	P69892.2
<input type="checkbox"/>	RecName: Full=Hemoglobin subunit epsilon; AltName: Full=Epsilon-globin; AltName: Full=Hemoglobin epsilon chain	101	101	95%	2e-27	39%	P02100.2
<input type="checkbox"/>	RecName: Full=Cytochrome c; AltName: Full=Histoglobin; Short=HGb; AltName: Full=Stellate cell activation-associated pr	68.9	68.9	96%	5e-15	28%	Q8WWM9.1
<input type="checkbox"/>	RecName: Full=Myoglobin	51.2	51.2	100%	5e-09	28%	P02144.2
<input type="checkbox"/>	RecName: Full=Neurobeachin-like protein 1; AltName: Full=Amyotrophic lateral sclerosis 2 chromosomal region candi	27.7	27.7	19%	2.7	37%	Q6ZS30.3
<input type="checkbox"/>	RecName: Full=StAR-related lipid transfer protein 9; AltName: Full=START domain-containing protein 9; Short=StARD9	26.6	26.6	40%	6.5	30%	Q9P2P6.3
<input type="checkbox"/>	RecName: Full=Intraflagellar transport protein 140 homolog; AltName: Full=WD and tetratricopeptide repeats protein 2	26.6	26.6	75%	7.0	27%	Q96RY7.1
<input type="checkbox"/>	RecName: Full=Ubiquitin carboxyl-terminal hydrolase 34; AltName: Full=Deubiquitinating enzyme 34; AltName: Full=Ub	26.2	26.2	77%	8.6	24%	Q70CQ2.2

HBA_HUMAN

Download ▾ GenPept Graphics ▾ Next ▲ Previous ▲ Descriptions

RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain
Sequence ID: [sp|P69905.2|HBA_HUMAN](#) Length: 142 Number of Matches: 1

Range 1: 1 to 142 GenPept Graphics ▾ Next Match ▲ Previous Match

Score	Expect	Method	Identities	Positives	Gaps
286 bits(733)	6e-100	Compositional matrix adjust.	142/142(100%)	142/142(100%)	0/142(0%)

Query 1 MVLSPADKTNVKGAAGKVGAHAGEYGAELERMFLSFPTITKTYFPHFDSLHSQAVKGHG 60
Sbjct 1 MVLSPADKTNVKGAAGKVGAHAGEYGAELERMFLSFPTITKTYFPHFDSLHSQAVKGHG 60

Query 61 KKVA DALINAVAHVDDMPNALSALSDLAHKLRLVDVNFKL LSHCLLVTLAAHLPAEFTP 120
Sbjct 61 KKVA DALINAVAHVDDMPNALSALSDLAHKLRLVDVNFKL LSHCLLVTLAAHLPAEFTP 120

Query 121 AVHASLDKFLASVSTVLISKIR 142
Sbjct 121 AVHASLDKFLASVSTVLISKIR 142

Related Information

- [Gene](#) - associated gene details
- [Map Viewer](#) - aligned genomic context
- [Identical Proteins](#) - Proteins identical to the subject

HBB_HUMAN

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RecName: Full=Hemoglobin subunit beta; AltName: Full=Beta-globin; AltName: Full=Hemoglobin beta chain; Contains: RecName: Full=LVV-hemorphin-7
Sequence ID: [sp|P68871.2|HBB_HUMAN](#) Length: 147 Number of Matches: 1

Range 1: 4 to 146 GenPept Graphics ▾ Next Match ▲ Previous Match

Score	Expect	Method	Identities	Positives	Gaps
114 bits(286)	2e-32	Compositional matrix adjust.	63/145(43%)	88/145(60%)	8/145(5%)

Query 3 ISPADKTNVKGAAGKVGAHAGEYGAELERMFLSFPTITKTYFPHF-DLS-----HGSQV 56
Sbjct 4 L+P K+ V A WGKV + E G E AL R+ + *P I+ +F F DLS G+ +V 61

Query 57 KGGGKKVADALINAVAHVDDMPNALSALSDLHAHKLRLVDVNFKL LSHCLLVTLAAHLPA 116
Sbjct 62 KAHGKVKVLGAFSDGLAHLNDLKGTATLSELHCDKLHVDPENFRLLGNVLVCVLAHHFGK 121

Query 117 EFTPAVHASLDKFLASVSTVLISKY 141
Sbjct 122 EFTPPVQAAYQKVVAAGVANALAHKY 146

Related Information

- [Gene](#) - associated gene details
- [PubChem BioAssay](#) - bioactivity screening
- [Map Viewer](#) - aligned genomic context
- [Identical Proteins](#) - Proteins identical to the subject

Needleman-Wunsch Global alignment

HBA_HUMAN	1 MV-LS PADKTNVKAAWGKVGAHAGEYGAEALERMFLSFPTTKTYFPHF-D : .: : . . .:. . . . :..: . : ..	48
HBB_HUMAN	1 MVHLT PEEKSAVTALWGKV--NVDEVGGEALGRLLVVYPWTQRFFESFGD	48
HBA_HUMAN	49 LS----HGSAQVKGHGKKVADALTNAVAHVDDMPNALSALSDLHAHKLR . : . . .:: : :.... : ..	93
HBB_HUMAN	49 LSTPDAVMGNPKVKAHGKKVLGAFSDGLAHLDNLKGTFATLSELHCDKLH	98
HBA_HUMAN	94 VDPVN FKLLSHCLLVTLA AHLPAEFTP AVHASLDKFLASVSTVLT SKYR . : : 	142
HBB_HUMAN	99 VDPEN FRLLGNVLVCVLAHHFGKEFTP PVQAAYQKV VAGVANALAHKYH	147
HBA_HUMAN	3 LSPADKTNVKAAWGKVGAHAGEYGAEALERMFLSFPTTKTYFPHF-DLS- : .: : . . .:. . . . :..: . : ..	50
HBB_HUMAN	4 LTPEEKSAVTALWGKV--NVDEVGGEALGRLLVVYPWTQRFFESFGDLST	51
HBA_HUMAN	51 ----HGSAQVKGHGKKVADALTNAVAHVDDMPNALSALSDLHAHKLRVDP . : . . .:: : :.... : ..	96
HBB_HUMAN	52 PDAVMGNPKVKAHGKKVLGAFSDGLAHLDNLKGTFATLSELHCDKLHVDP	101
HBA_HUMAN	97 VNFKLLSHCLLVTLA AHLPAEFTP AVHASLDKFLASVSTVLT SKY . : 	141
HBB_HUMAN	102 ENFRLLGNVLVCVLAHHFGKEFTP PVQAAYQKV VAGVANALAHKY	146

Smith-Waterman Local alignment

Query 3	LSPADKTNVKAAWGKVGAHAGEYGAEALERMFLSFPTTKTYFPHF-DLS-----HGSAQV	56
Sbjct 4	L+P +K+ V A WGKV + E G EAL R+ +P T+ +F F DLS G+ +V LTPEEKSAVTALWGKV--NVDEVGGEALGRLLVVYPWTQRFFESFGDLSTPDAVMGNPKV	61
Query 57	KGHGKKVADALTNAVAHVDDMPNALSALSDLHAHKLRVDPVNFKLLSHCLLVTLA AHLPA	116
Sbjct 62	K HGKKV A ++ +A+D++ + LS+LH KL VDP NF+LL + L+ LA H KAHGKKVLGAFSDGLAHLDNLKGTFATLSELHCDKLHVDPENFRLLGNVLVCVLAHHFGK	121
Query 117	EFTP AVHASLDKFLASVSTVLT SKY 141	
Sbjct 122	EFTP V A+ K +A V+ L KY EFTPVQAAYQKV VAGVANALAHKY 146	

BLAST Local alignment

Protein BLAST: sea x

blast.ncbi.nlm.nih.gov/Blast.cgi?PROGRAM=blastp&BLAST_PROGRAMS=blastp&PAGE_TYPE=BlastSearch&SHOW

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NCBI/ BLAST/ blastp suite Standard Protein BLAST

blastn blastp blastx tblastn tblastx

Enter Query Sequence

Enter accession number(s), gi(s), or FASTA sequence(s) [more...](#)

>sp|P69905|HBA_HUMAN
MVLSPADKTVKAAGKVGAHAGEYGAELERMFLSFTTITKTYFPHFDLSHGSAQVK
GHGKKVADALTNAVAHVDDNPNALSDLHAKLRLVDPVNFKLSSHCLVLA AHL
PAEFTPAVHALDKFLASVSTVLTSKYR

Clear Query subrange [From](#) [To](#)

Reset page Bookmark

Or, upload file Choose File No file chosen

Job Title sp|P69905|HBA_HUMAN

Enter a descriptive title for your BLAST search

Align two or more sequences

Choose Search Set

Database UniProtKB/Swiss-Prot(swissprot)

Title: Non-redundant UniProtKB/SwissProt sequences.
Molecule Type: Protein
Update date: 2013/10/10
Number of sequences: 456016

Organism Optional Enter organism name or id—completions will be suggested Exclude +
Enter organism common name, binomial, or tax id. Only 20 top taxa will be shown.

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

Entrez Query Optional Enter an Entrez query to limit search

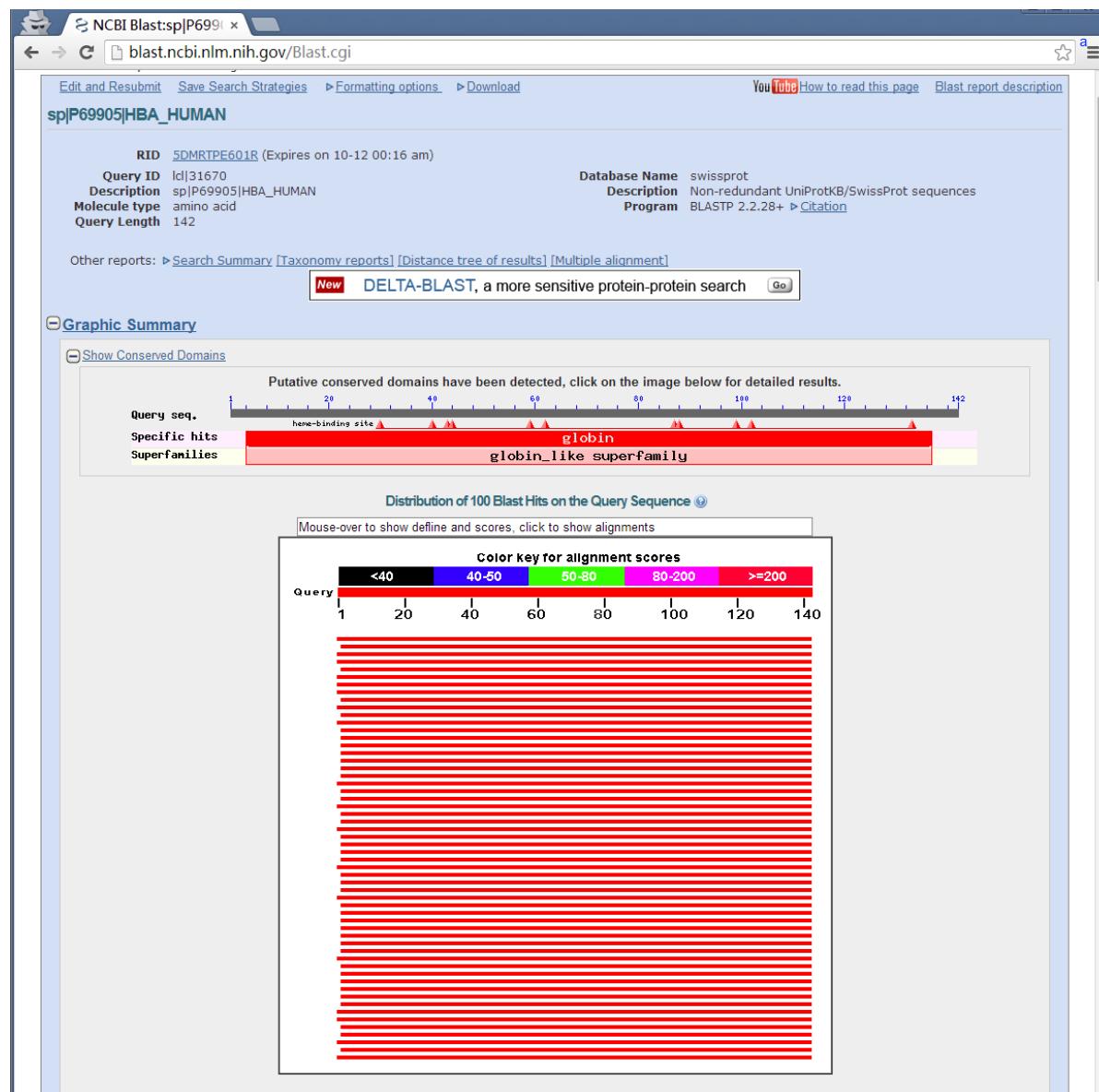
Program Selection

Algorithm blastp (protein-protein BLAST)
 PSI-BLAST (Position-Specific Iterated BLAST)
 PHI-BLAST (Pattern Hit Initiated BLAST)
 DELTA-BLAST (Domain Enhanced Lookup Time Accelerated BLAST)
Choose a BLAST algorithm

BLAST Search database UniProtKB/Swiss-Prot(swissprot) using Blastp (protein-protein BLAST)
 Show results in a new window

[Algorithm parameters](#) Note: Parameter values that differ from the default are highlighted in yellow and marked with * sign

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NCBI Blast:sp|P6991

blast.ncbi.nlm.nih.gov/Blast.cgi

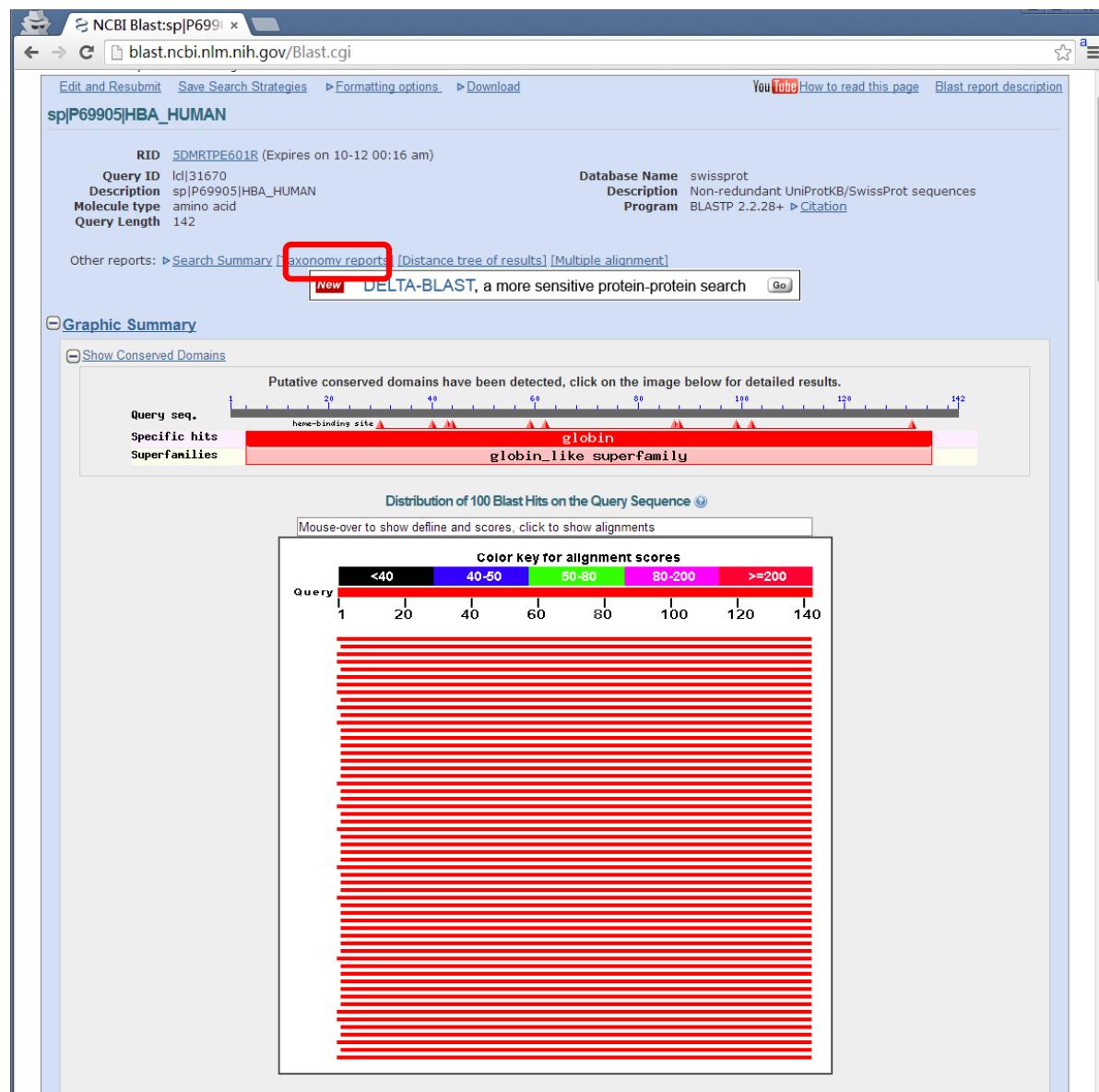
Descriptions

Sequences producing significant alignments:

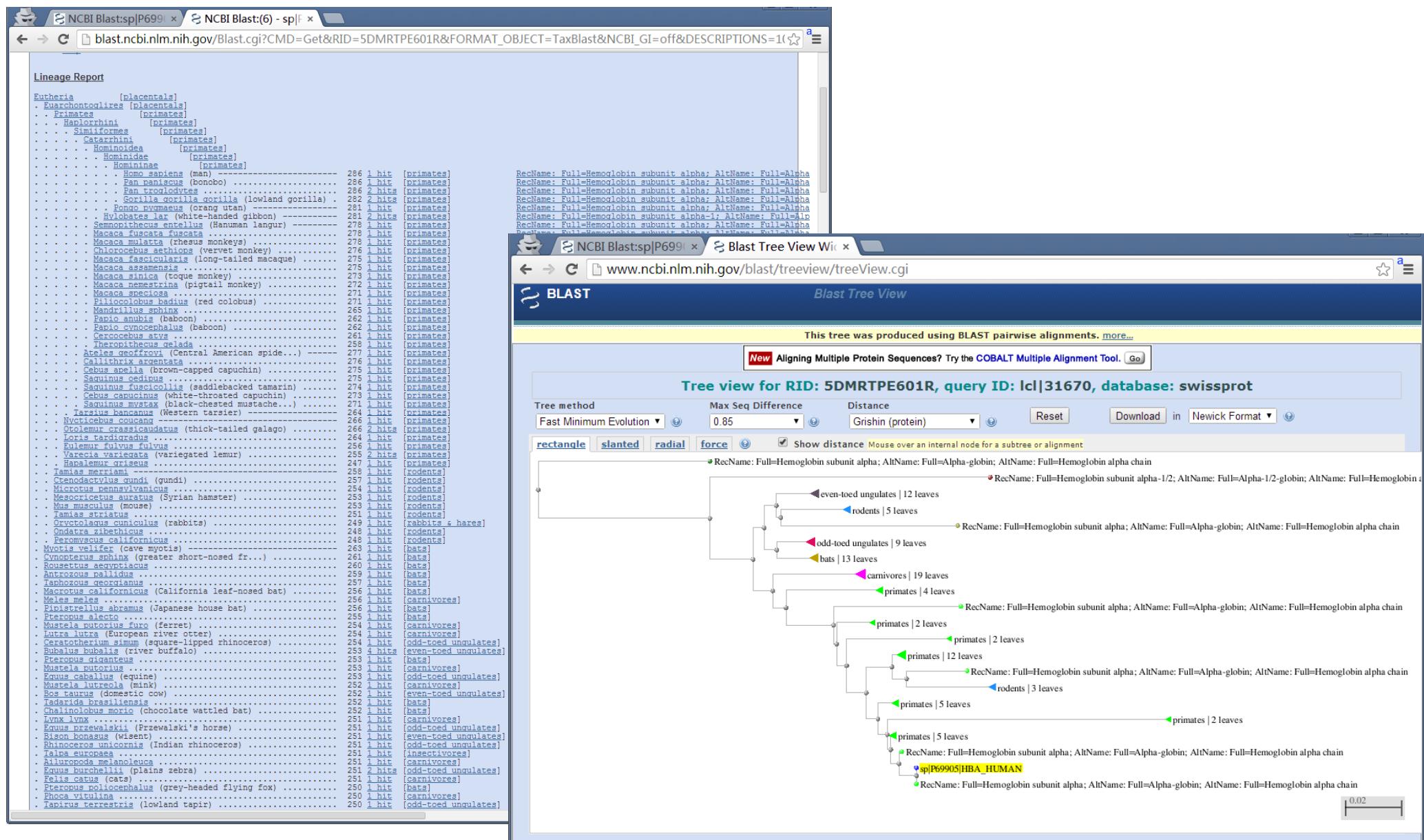
Select: All None Selected 0

Alignments Download GenPept Graphics Distance tree of results Multiple alignment

	Description	Max score	Total score	Query cover	E value	Ident	Accession
1	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain >sp P6991	286	286	100%	9e-99	100%	P69905_2
2	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	282	282	99%	5e-97	99%	P01923_1
3	RecName: Full=Hemoglobin subunit alpha-1; AltName: Full=Alpha-1-globin; AltName: Full=Hemoglobin alpha-1 chain	281	281	100%	1e-96	99%	Q9TS35_2
4	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	281	281	100%	2e-96	98%	P06353_2
5	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	278	278	99%	1e-95	98%	P01924_1
6	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain >sp P63	278	278	100%	1e-95	97%	P63107_2
7	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	277	277	100%	5e-95	96%	P67817_2
8	RecName: Full=Hemoglobin subunit alpha-2; AltName: Full=Alpha-2-globin; AltName: Full=Hemoglobin alpha-2 chain	277	277	100%	6e-95	96%	Q9TS34_2
9	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	276	276	99%	6e-95	97%	P18972_1
10	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	276	276	100%	2e-94	96%	P01926_2
11	RecName: Full=Hemoglobin subunit alpha-A/O/R/T; AltName: Full=Alpha-A/O/R/T-globin; AltName: Full=Hemoglobin alph	275	275	99%	2e-94	97%	P21767_1
12	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	275	275	100%	2e-94	96%	P01928_2
13	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	275	275	99%	4e-94	96%	P67818_1
14	RecName: Full=Hemoglobin subunit alpha-1/2/3; AltName: Full=Alpha-1/2/3-globin; AltName: Full=Hemoglobin alpha-1/2	275	275	99%	5e-94	97%	P21766_1
15	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	274	274	99%	5e-94	96%	P01929_1
16	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	273	273	99%	2e-93	96%	P07421_1
17	RecName: Full=Hemoglobin subunit alpha-1/2; AltName: Full=Alpha-1/2-globin; AltName: Full=Hemoglobin alpha-1/2 ch	273	273	99%	2e-93	96%	P21768_1
18	RecName: Full=Hemoglobin subunit alpha-1/2/3; AltName: Full=Alpha-1/2/3-globin; AltName: Full=Hemoglobin alpha-1/2	272	272	99%	3e-93	96%	P19002_1
19	RecName: Full=Hemoglobin subunit alpha-1/2; AltName: Full=Alpha-1/2-globin; AltName: Full=Hemoglobin alpha-1/2 ch	271	271	99%	7e-93	96%	P07402_1
20	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	271	271	100%	1e-92	95%	P01930_2
21	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	271	271	99%	1e-92	96%	Q7IM386_1
22	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	266	266	99%	6e-91	94%	P01937_1
23	RecName: Full=Hemoglobin subunit alpha-B; AltName: Full=Alpha-B-globin; AltName: Full=Alpha-II; AltName: Full=Hemo	266	266	100%	8e-91	92%	P01939_3
24	RecName: Full=Hemoglobin subunit alpha-3; AltName: Full=Alpha-3-globin; AltName: Full=Hemoglobin alpha-2 chain	266	266	99%	1e-90	89%	P01935_1
25	RecName: Full=Hemoglobin subunit alpha-3; AltName: Full=Alpha-3-globin; AltName: Full=Hemoglobin alpha-2 chain	265	265	99%	2e-90	89%	P01934_1
26	RecName: Full=Hemoglobin subunit alpha-A; AltName: Full=Alpha-A-globin; Short=Alpha-I; AltName: Full=Hemoglobin al	265	265	100%	3e-90	92%	P14259_2
27	RecName: Full=Hemoglobin subunit alpha-1/2; AltName: Full=Alpha-1/2-globin; AltName: Full=Hemoglobin alpha-1/2 ch	265	265	99%	4e-90	94%	P08258_1
28	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	264	264	99%	6e-90	93%	P01938_2
29	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	264	264	99%	6e-90	91%	P01940_1
30	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	263	263	99%	1e-89	91%	P11757_1
31	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain >sp P63	262	262	100%	5e-89	92%	P63111_2
32	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	261	261	99%	6e-89	93%	P01933_1
33	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	261	261	99%	9e-89	90%	P11753_1
34	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	260	260	99%	2e-88	90%	P01956_1
35	RecName: Full=Hemoglobin subunit alpha; AltName: Full=Alpha-globin; AltName: Full=Hemoglobin alpha chain	259	259	100%	3e-88	90%	P14387_2



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Summary Questions

- Why do we need to perform a database searching?
- What's the major challenge/obstacle when searching sequence database?

生物信息学：导论与方法

Bioinformatics: Introduction and Methods



<https://www.coursera.org/course/pkubioinfo>