# Web Resources

FAIR Data Practices for Omics Analysis Workshop
University of Delaware
April 18 (Day 1)





### National Center for Biotechnology Information (NCBI) Resources

- NIH National Library of Medicine
- Repository for biomedical and genomic information
- Resources include:
  - PubMed
  - PubChem
  - GenBank
  - RefSeq
  - Sequence Read Archive (SRA)
  - Many others...

All Databases **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



### NCBI News & Blog

New RefSeg Annotations!

Search

Popular Resources

PubMed

Bookshelf

BLAST

Nucleotide

Genome

SNP

Gene

Protein

PubChem

PubMed Central

13 Apr 2022

In February and March, the NCBI Eukaryotic Genome Annotation Pipeline

New feature in the MSA viewer: Search for a short sequence

12 Apr 2022

We're reading and incorporating your

MANE is published in Nature!

06 Apr 2022

We are delighted to announce that three and a half years of hard work by the

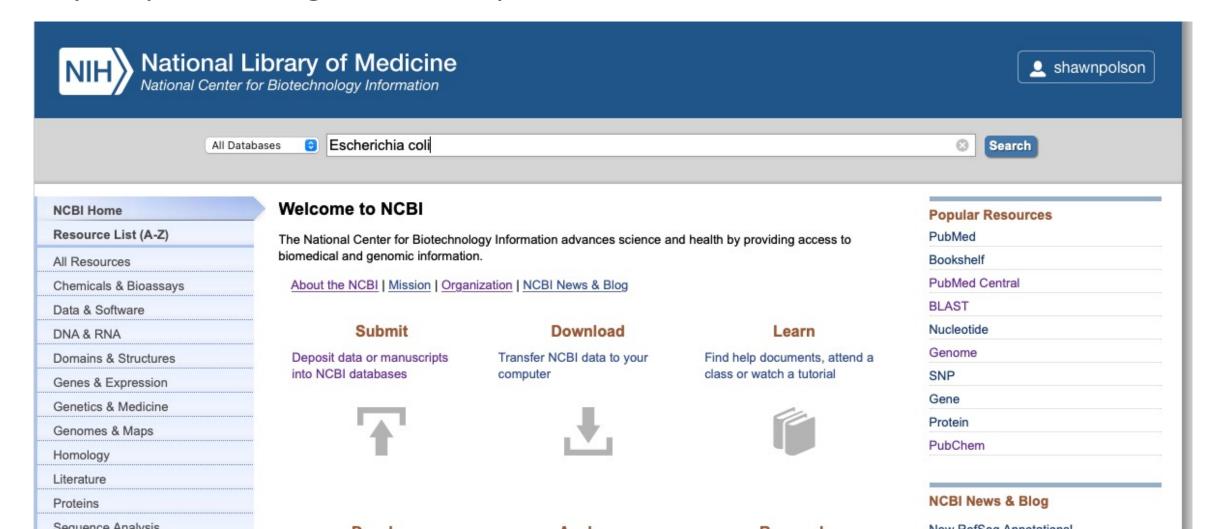
More...

#### **COVID-19 Information**

Public health information (CDC) | Research information (NIH) | SARS-CoV-2 data (NCBI) | Prevention and treatment information (HHS) | Español

### Entrez Search

In the search bar look for something in "All Databases" that interests you: protein, organism, compound, etc.



Results give a good summary of the different types of information that NCBI houses.

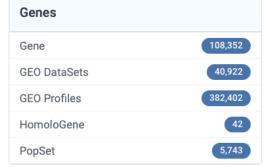
Take a few minutes and explore some of these links to see where they go...

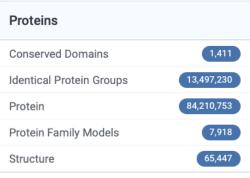


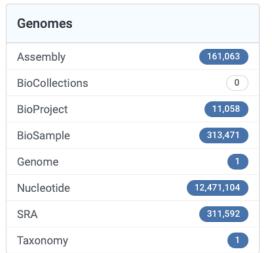
#### Results found in 32 databases

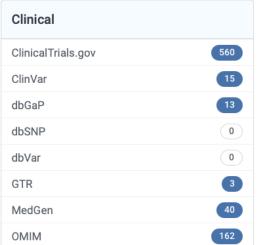






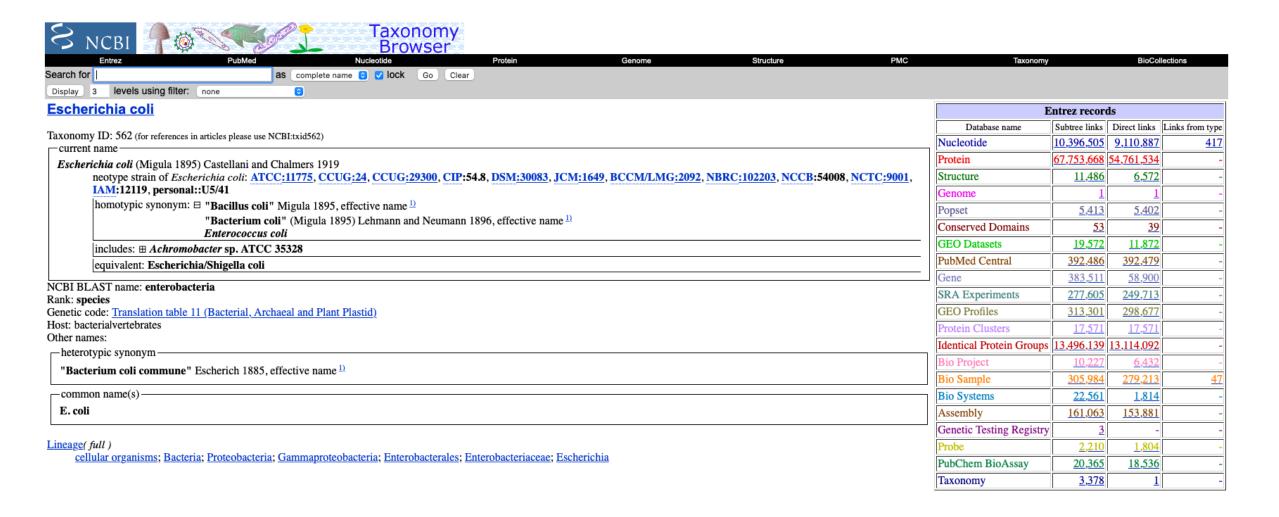






PubChem	
BioAssays	53,088
Compounds	12
Pathways	2,986
Substances	379

# The taxonomy database gives a good overview of available information for a given organism or taxonomic rank



### **BLAST Search**

Perhaps the most commonly used analysis tool at NCBI

Allows you to search by sequence

- Performs a "local alignment" allowing partial matches to be detected
  - Why would this be important?

 Several different types of BLAST are available that allow nucleotide or protein sequences against nucleotide or sequence databases





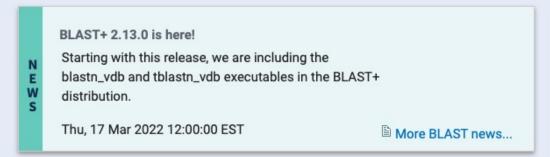
**BLAST**®

Home Recent Results Saved Strategies Help

### **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



### **Web BLAST**



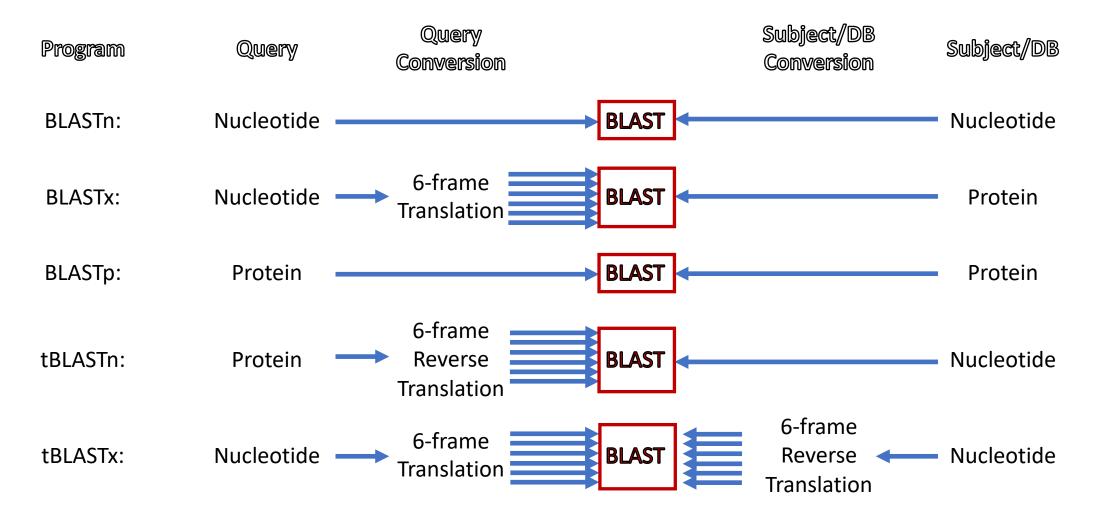
### blastx translated nucleotide ▶ protein

tblastn
protein ► translated nucleotide



https://blast.ncbi.nlm.nih.gov

### **BLAST Programs**

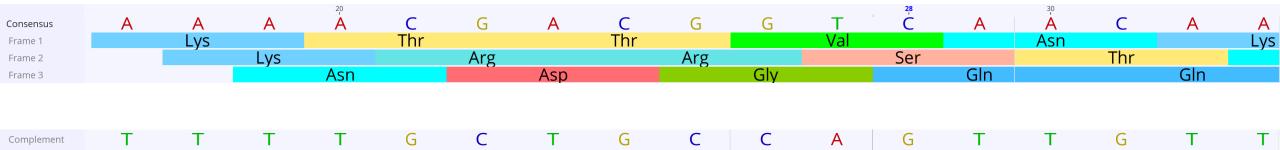


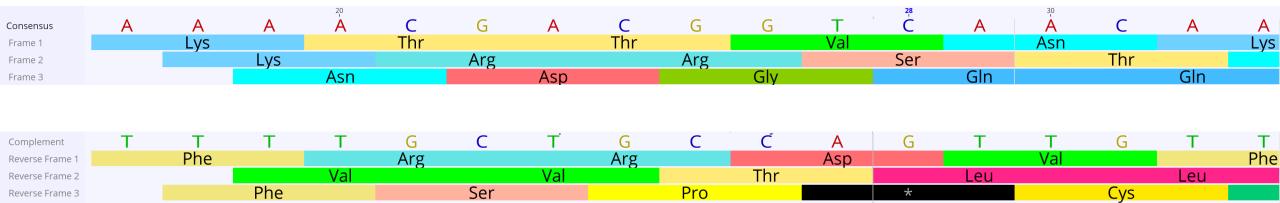
Consensus A A A Â C G A C G G T C A Â C A

UUU Phe UUC Leu UUG Leu	UCU UCC UCA UCG	UAU Tyr UAA Stop	UGU UGC UGA Stop UGG Trp
CUU	CCU	CAU His CAA GIn	CGU
CUC	CCC		CGC
CUA	CCA		CGA
CUG	CCG		CGG
AUU AUC Ble AUA Met	ACU ACC ACA ACG	AAU ASN ASN AAA AAG Lys	AGU Ser AGA AGA Arg
GUU	GCU	GAU Asp GAA GAA GAG	GGU
GUC	GCC		GGC
GUA	GCA		GGA
GUG	GCG		GGG

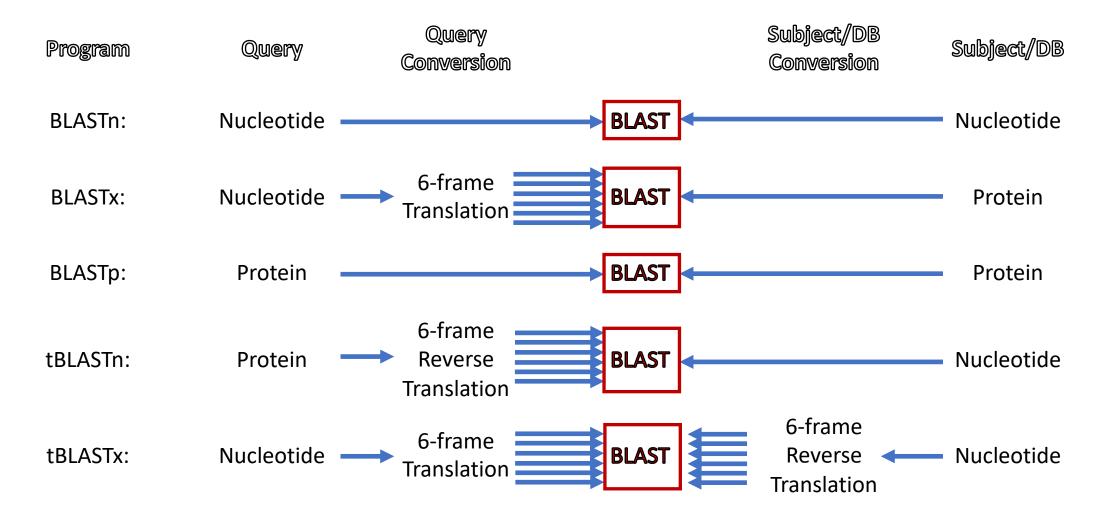


UUU Phe UUA Leu UUG	UCU UCC UCA UCG	UAU Tyr UAC Stop UAA Stop	UGU Cys UGA Stop UGG Trp
CUU	CCU	CAU His CAA GIn	CGU
CUC	CCC		CGC
CUA	CCA		CGA
CUG	CCG		CGG
AUU AUC AUA Met	ACU ACC ACA ACG	AAU ASN ASN AAA AAG Lys	AGU Ser AGA AGA Arg
GUU	GCU	GAU Asp GAA GAA GAG	GGU
GUC	GCC		GGC
GUA	GCA		GGA
GUG	GCG		GGG





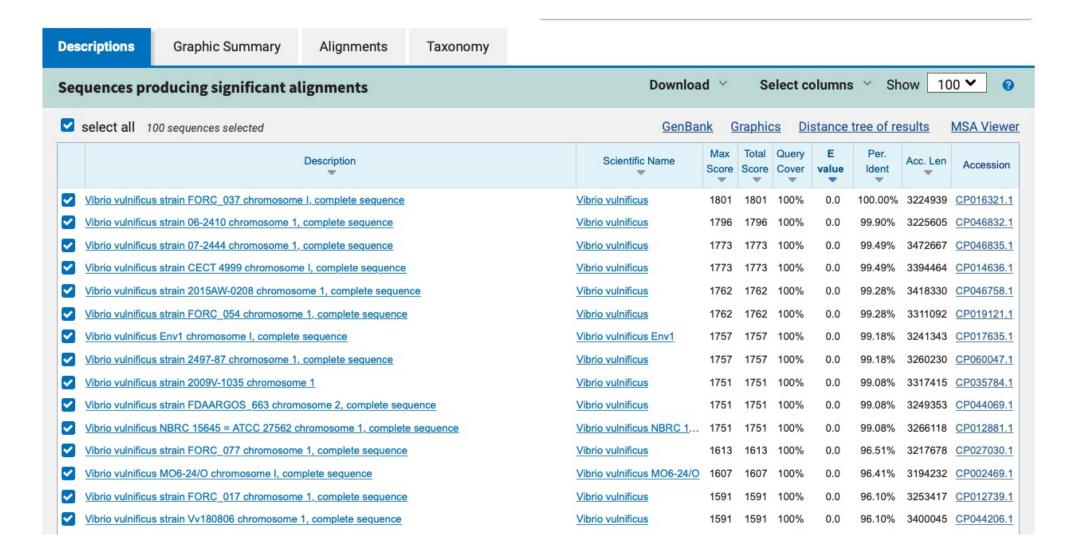
### **BLAST Programs**



# Let's try a Nucleotide BLAST (BLASTn)

#### Standard Nucleotide BLAST

blastn	blastp	blastx	tblastn	tblastx							
					BLASTN programs search nucleotide databases using a nucleotide query. more	Reset page Bookmark					
	Enter Query Sequence										
	Enter accession number(s), gi(s), or FASTA sequence(s) ? clear Query subrange ?  ATGAAACTGCAACAACTGAAGTACATTGTTGAAGTCGTTAATCACAATCT										
AAATGTCTCGGCGACCGCCG											
AAAGCTTGTATACCTCTCAGCCAGGGATCAGTAAGCAAGTCAGGCTTTT AGAAGATGAGTTAGGCATTCA  To											
	GATATTTGAACGAAGTGGTAAACACCTCACTCAAGTGACTCGAGCTGG GGAAGATATCGTGCGAATTTCG										
CAAGAAATT	TTAGCTCG	AGTTGAGAGTATT	AAAGCTGTGGC	AGGTGAGC							
	ATTTCTACC	ACCCATACACAG	CTCGTTATGCT	TTACCGGAT							
GTCATTAAA		AAA CCTTGCACATGC	ACCAAGGGACG	SCCAAGTCA							
AATGTCCGA	AAGCGATTG										
GATGCGATT	TATGTTGCC	ITGTT									
AAGGAAAA	AGTGACTAT										
Or, upload f		hoose File no file		TACCEGTC 4							
Job Title											
	Er	ter a descriptive tit	le for your BLAST	search 😯							
Align two	or more see	quences ?									
Choose	Search Se	et									
Database	0	Standard databa	ises (nr etc.):	rRNA/ITS data	pases    Genomic + transcript databases    Betacoronavirus						
		Nucleotide collect									
Organism	İ	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 ?									
Optional											
Exclude		Models (XM/XP) Uncultured/environmental sample sequences									
Optional Limit to		,									
Optional		Sequences from	т туре тпатепаг		Van Caracta australia detabase						
Entrez Quer Optional	-	ter an Entrez quen	v to limit search	<u> </u>	You Tube Create custom database						
		nor arr Entroz quor	y to mine sourch	_							
	Selection										
Optimize for	_	Highly similar se			oland)						
		Somewhat simil			nast)						
		oose a BLAST alg		,							
BLAST	r s	earch database N	lucleotide colle	ction (nr/nt) usi	ng Megablast (Optimize for highly similar sequences)						
		Show results in a	new window								



We'll briefly discuss what some of the scores and other metrics mean, but for more information check out the YouTube videos that NCBI has put together at the link below. Highly recommend the short Expect Value videos.

## **BLAST Terminology**

- Query Sequence you searched for
- **Subject** Sequence that a query aligns to (i.e. sequence from database)
- Scoring Matrix A table fo how likely different substitutions are. Allows customization in how different mismatches are penalized. (e.g. lower penalty for substitution of biochemically similar amino acids versus dissimilar)
- Raw Score Simple scoring of an alignment to reward matches/penalize mismatches for each position (uses a substitution matrix)

## **BLAST Terminology**

- **Bit Score** Score normalized for database size and use of different scoring matrices. Allow scores of the same query to be compared across searches. (High is good)
- Expect (E) value The number of alignments with scores >= to a
  given match that would occur by random chance. (Very low is good)
- Coverage Percentage of Query/Subject that were covered by the alignment
- Identity Percentage of aligned nucleotides/amino acids that were exact matches
- Similarity Percentage of aligned amino acids that were positive matches (exact matches or a substitution deemed likely (similar) by the substitution matrix

## Now try these variations

Repeat the BLASTn with only part of the query sequence

 Repeat the BLASTn with the RefSeq Representative Genome database for Organism "Bacteria (taxid:2)"

**For discussion**: Make note of how these variations change the results (both the hits themselves and the scores)

# Let's try a BLASTx with the same sequence...

 TIP: Since we know something about what type of organism has this protein we can speed up the search by limiting the "Organism"

What do these results tell you that was not apparent with BLASTn?

# Optional Exercise: Try BLASTp, tBLASTx, and tBLASTn

MKTYNVAIVGASGAVGQELIKGLENSFFPIKKFVPLASTRSAGKKIKAFNKDYEILETTH
EVFEREKIDIAFFSAGGSVSEEFATSASKTALVVDNTSFFRLNKDVPLVVPEINAKEIFN
APLNIIANPNCSTIQMTQILNPLHLHFKIKSVIVSTYQAVSGAGNKGIESLKNELKTALE
CLEKDPTIDLNQVLQAGAFAYPIAFNAIAHIDTFKENGYTKEELKMLHETHKIMGVDFPI
SATCVRVPVLRSHSESLSIAFEKEFDLKEVYEVLKNAPSVAVCDDPSHNLYPTPLKASHT
DSVFIGRLRKDLFDKKTLHGFCVADQLRVGAATNALKIALHYIKNA

### Universal Protein Resource (UniProt)

Comprehensive resource for protein sequence and annotation data

 Collaboration between the European Bioinformatics Institute (EMBL-EBI), the SIB Swiss Institute of Bioinformatics and the Protein Information Resource (PIR)

• We will not do a comprehensive overview of UniProt resources today, please check their training resources:

https://www.youtube.com/user/uniprotvideos

Help Contact

BLAST Align Retrieve/ID mapping Peptide search SPARQL

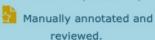
UniProt : The new UniProt website is here! Take me to UniProt BETA

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.

### **UniProtKB**

UniProt Knowledgebase

#### Swiss-Prot (566,996)



Records with information extracted from literature and curator-evaluated

#### TrEMBL (230,328,648)

computational analysis.

Automatically annotated and not reviewed.

Records that await full manual annotation.

### UniRef



The UniProt Reference Clusters (UniRef) provide clustered sets of sequences from the UniProt Knowledgebase (including isoforms) and selected UniParc records.

Literature citations

Cross-ref. databases

### UniParc



UniParc is a comprehensive and non-redundant database that contains most of the publicly available protein sequences in the world.

Supporting data

Taxonomy

4

Diseases

XXX

### Proteomes



A proteome is the set of proteins thought to be expressed by an organism. UniProt provides proteomes for species with completely sequenced genomes.

Subcellular locations

Keywords

GA

New UniProt portal for the latest SARS-CoV-2 coronavirus protein entries and receptors, updated independent of the general UniProt release cycle.

View SARS-CoV-2 Proteins and Receptors

### News









### Forthcoming changes

Planned changes for UniProt

#### UniProt release 2022 01

A phospholipase for clear vision | Cross-references to MANE-Select

#### UniProt release 2021\_04

ZTGC: bacteriophages reinvent the DNA alphabet

#### UniProt release 2021 03

The importance of being disordered | MobiDB-lite predictions for

News archive

NouTube

UniProt data

Protein spotlight

https://www.uniprot.org



BLAST Align Retrieve/ID mapping Peptide search SPARQL

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### UniProt : The new UniProt website is here! Take me to UniProt BETA 1

### UniProtKB 2022\_01 results



### UniProtKB consists of two sections:



#### Reviewed (Swiss-Prot) - Manually annotated

Records with information extracted from literature and curator-evaluated computational analysis.



#### Unreviewed (TrEMBL) - Computationally analyzed

Records that await full manual annotation.

The UniProt Knowledgebase (UniProtKB) is the central hub for the collection of functional information on proteins, with accurate, consistent and rich annotation. In addition to capturing the core data mandatory for each UniProtKB entry (mainly, the amino acid sequence, protein name or description, taxonomic data and citation information), as much annotation information as possible is added.



UniProtKB help video

Other tutorials and videos

**★** Downloads

### Filter by



### Popular organisms

VIBVL (1)

VIBVU (1)

8	BLAST = Align	n <b>≛</b> Download ⊕ Ad	d to ba	sket Columns >			1 to 2 of 2	Show 250	0
	Entry 🔷	Entry name 🗘		Protein names 🗣	<b>&gt;&gt;</b>	Gene names ♦	Organism 🗘	Length <b>♦</b>	1
	A0A087JF97	A0A087JF97_VIBVL		Cys regulon transcriptional activat		<b>cysB</b> CRN52_15695, D8T54_16205, D8T65_03355, FORC53_1863, I7730_22205 <b>№</b>	Vibrio vulnificus	324	
	A0A3Q0L6S0	A0A3Q0L6S0_VIBVU		Regulatory protein CysB		VV1_2954	Vibrio vulnificus (strain CMCP6)	324	

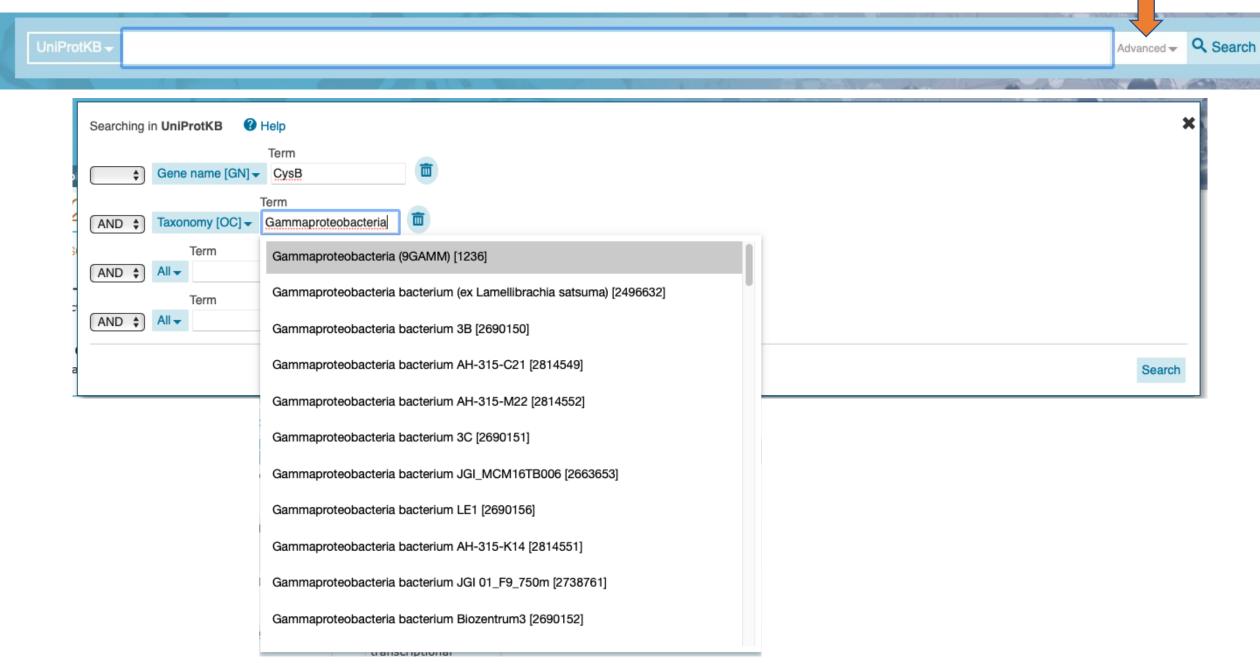
1 to 2 of 2 Show 250 3

### Reviewed vs Unreviewed Entries

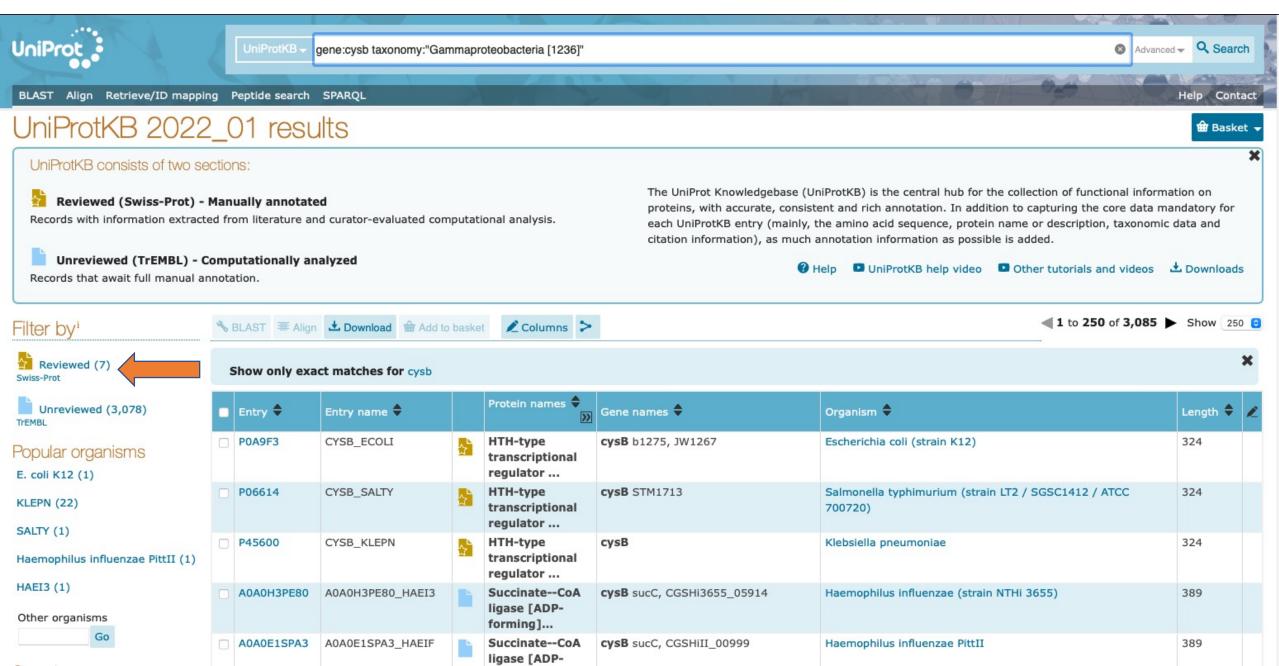
• **Unreviewed** (TrEMBL): Have been automatically annotated by a computational algorithm.

• **Reviewed** (Swiss-Prot): Have been manually annotated by a sequence curator and determined to be of high quality based on experimental evidence. In addition to the increased quality/confidence of annotation, these entries often have more types of information than TrEMBL entries.

### Broaden the Search to find Reviewed Entries



### Filter to Swiss-Prot Entries



BLAST Align Retrieve/ID mapping Peptide search SPARQL

Help Contact

### UniProtKB 2022\_01 results

**⊞** Basket **▼** 

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Help □ UniProtKB help video □ Other tutorials and videos 
 Downloads

1 to 7 of 7 Show 250 3

### Eiltor bui

Filler by:	
Reviewed (7)	
Popular organisms E. coli K12 (1)	
KLEPN (1)	
HAEIN (1)	
SALTY (1)	
ECOL6 (1)	

Go

SBLAST ≡ Align ± Download ⊕ Add to basket ∠ Columns >

	Entry 🕏	Entry name 🗣		Protein names 🗢 🔌	Gene names 🗣	Organism •	Length 🕏	1
	P0A9F3	CYSB_ECOLI	<b>☆</b>	HTH-type transcriptional regulator	<b>cysB</b> b1275, JW1267	Escherichia coli (strain K12)	324	
	P06614	CYSB_SALTY	☆	HTH-type transcriptional regulator	cysB STM1713	Salmonella typhimurium (strain LT2 / SGSC1412 / ATCC 700720)	324	
	P45600	CYSB_KLEPN	չ՝	HTH-type transcriptional regulator	cysB	Klebsiella pneumoniae	324	
	P45105	CYSB_HAEIN	<b>&amp;</b>	HTH-type transcriptional regulator	cysB HI_1200	Haemophilus influenzae (strain ATCC 51907 / DSM 11121 / KW20 / Rd)	323	
	P0A9F4	CYSB_ECOL6	☆	HTH-type transcriptional regulator	<b>cysB</b> c1742	Escherichia coli O6:H1 (strain CFT073 / ATCC 700928 / UPEC)	324	
	P0A9F5	CYSB_ECO57	☆	HTH-type transcriptional regulator	<b>cysB</b> Z2535, ECs1847	Escherichia coli O157:H7	324	
	P52675	CYSB_THIRO	⊹	HTH-type transcriptional regulator	cysB	Thiocapsa roseopersicina	136	

Coarob tormo

Other organisms

