

Choosing Structure Prediction Software

- There are many software tools for protein structure prediction (see https://en.wikipedia.org/wiki/List_of_protein_structure_prediction_software)

• How should you decide which to use?

of Eases of Use

- Webserver-easier for super admin use

• Dynamic and scriptable - ease of application

Accuracy

- The “Critical Assessment of protein Structure Prediction” (CASP) experiments are *blinded* tests of the ability to predict structure from sequence. (see <http://www.predictioncenter.org/index.cgi>)

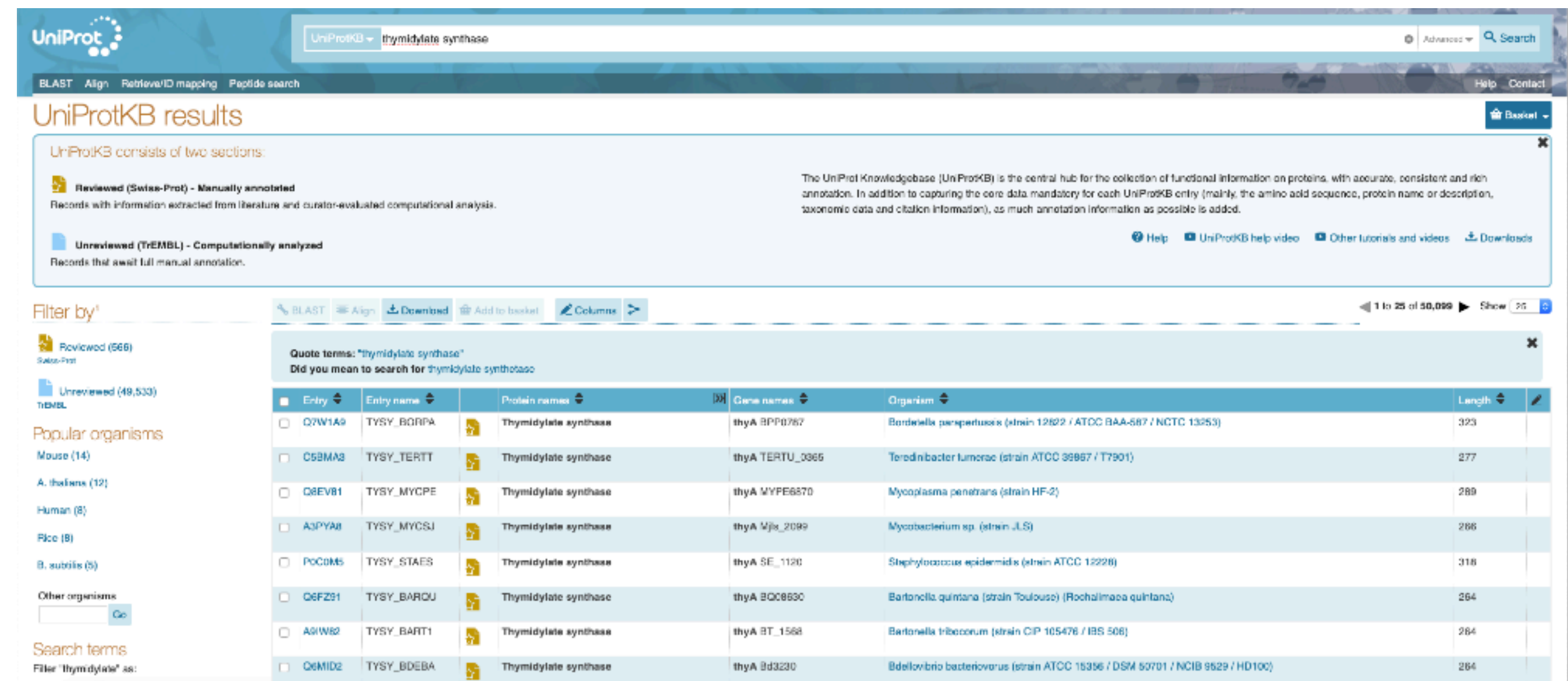
- “I-TASSER (as 'Zhang-Server') was ranked as the No 1 server for protein structure prediction in recent community-wide CASP7, CASP8, CASP9, CASP10, CASP11, CASP12, and CASP13 experiments.” So let's use it!



Choosing Structure Prediction Software

- There are many software tools for protein structure prediction (see https://en.wikipedia.org/wiki/List_of_protein_structure_prediction_software)
- How should you decide which to use?
 - Ease of use
 - Web server - easier for sporadic use
 - Downloadable and scriptable - easier for large-scale applications
 - Accuracy
- The “Critical Assessment of protein Structure Prediction” (CASP) experiments are *blinded* tests of the ability to predict structure from sequence. (see <http://www.predictioncenter.org/index.cgi>)
- “I-TASSER (as 'Zhang-Server') was ranked as the No 1 server for protein structure prediction in recent community-wide CASP7, CASP8, CASP9, CASP10, CASP11, CASP12, and CASP13 experiments.” So let’s use it!

- To reproduce the key results from Garg *et. al.*, we first need to find out what to model
- UniProt (<https://www.uniprot.org>) is a comprehensive biological sequence database
- A search for “thymidylate synthase” yields 50,099 results, including 566 that have been manually reviewed. This is much more than the 110 that were included by Garg *et. al.* in their 2015 paper!
- The two results for “thymidylate synthase wigglesworthia” is much more manageable. Select the result that has been reviewed.



UniProtKB 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.

Filter by:

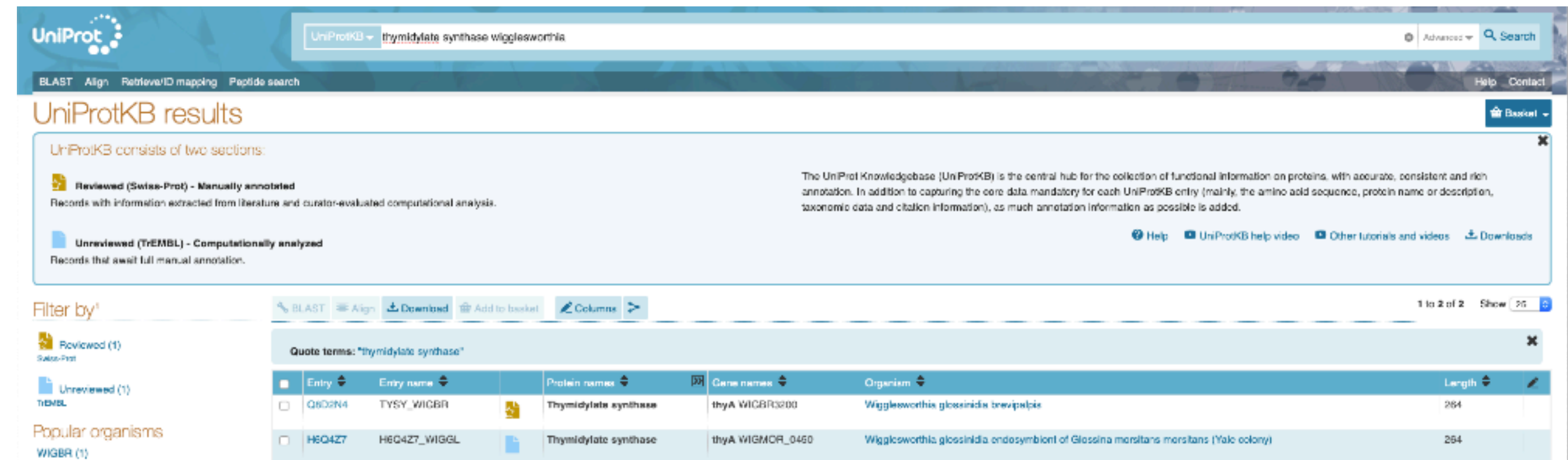
- Reviewed (566)
- Unreviewed (49,533)
- Popular organisms
- Mouse (14)
- A. thaliana (12)
- Human (8)
- Fly (8)
- B. subtilis (5)
- Other organisms

Search terms

Filter "thymidylate" as:

Quote terms: "thymidylate synthase"
Did you mean to search for thymidylate synthase?

Entry	Entry name	Protein names	Gene names	Organism	Length
<input type="checkbox"/> Q7W1A9	TYSY_BORPA	Thymidylate synthase	thyA BP0787	Bordetella pertussis (strain 12/82 / ATCC BAA-687 / NCTC 13253)	323
<input type="checkbox"/> C5BMA8	TYSY_TERTT	Thymidylate synthase	thyA TERTU_0365	Teredinibacter litoralis (strain ATCC 39867 / T7901)	277
<input type="checkbox"/> Q8EV81	TYSY_MYCPE	Thymidylate synthase	thyA MYPE6570	Mycoplasma penetrans (strain HF-2)	289
<input type="checkbox"/> A3PYA8	TYSY_MYCSJ	Thymidylate synthase	thyA Mjs_2089	Mycobacterium sp. (strain JLS)	266
<input type="checkbox"/> POC6M5	TYSY_STAES	Thymidylate synthase	thyA SE_1120	Staphylococcus epidermidis (strain ATCC 12228)	318
<input type="checkbox"/> Q6FZ31	TYSY_BAROU	Thymidylate synthase	thyA BQ08530	Bartonella quintana (strain Toulouse) (Rochalimaea quintana)	264
<input type="checkbox"/> A6IW82	TYSY_BART1	Thymidylate synthase	thyA BT_1568	Bartonella tribecorum (strain CIP 105476 / IRS 506)	264
<input type="checkbox"/> Q6MID2	TYSY_BDEBA	Thymidylate synthase	thyA Bdc320	Bdellovibrio bacteriovorus (strain ATCC 15356 / DSM 50701 / NCIB 9529 / HD100)	264



UniProtKB 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.

Filter by:

- Reviewed (1)
- Unreviewed (1)
- Popular organisms
- WIGBR (1)

Quote terms: "thymidylate synthase"

Entry	Entry name	Protein names	Gene names	Organism	Length
<input type="checkbox"/> Q6Q2N4	TYSY_WIGBR	Thymidylate synthase	thyA WIGBR0300	Wigglesworthia glossinidia brevipalpis	264
<input type="checkbox"/> H6Q4Z7	H6Q4Z7_WIGGL	Thymidylate synthase	thyA WIGMOR_0460	Wigglesworthia glossinidia endosymbiont of Glossina morsitans morsitans (Yale colony)	264