

Introduction to applied bioinformatics

„Protein bioinformatics II“

Retrieving protein sequences from databases (Uniprot: FASTA formate)

Computing amino-acids compositions, molecular weight, isoelectric point, and other parameters (SMS)

Prediction of proteases cutting (PeptideCutter)

Predicting elements of protein secondary structure, signal peptide, transmembrane helix

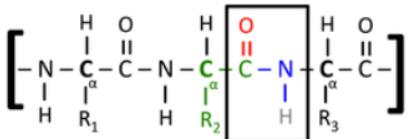
Finding 3-D structure and the domain organization of proteins

Finding all proteins that share a similar sequence and Classifying proteins into families

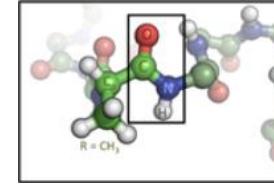
Finding evolutionary relationships between proteins, drawing proteins' family trees

Computing the optimal alignment between two or more protein sequences

...



Proteins



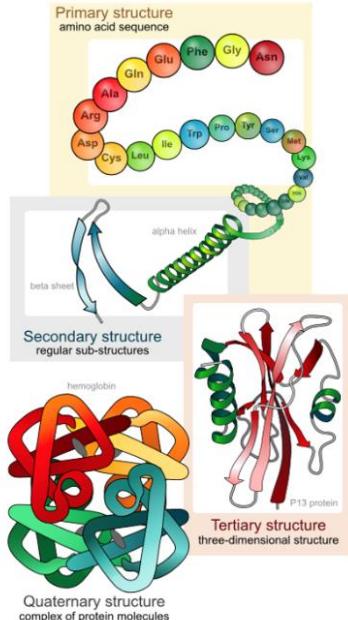
20 Aminoacids – primary structure:

(Frederick Sanger-1958 Nobel prize for insulin sequencing)

Secondary structure

Tertiary structure

Quaternary structure

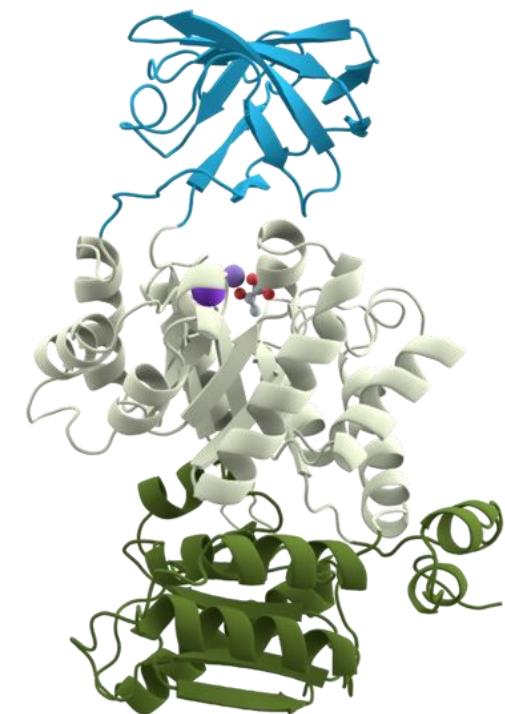
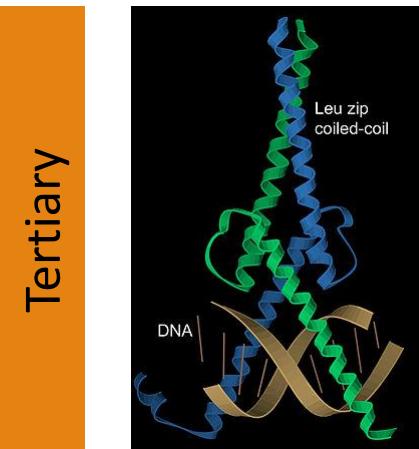
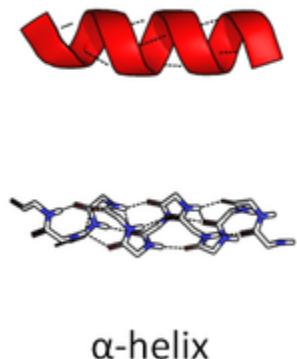
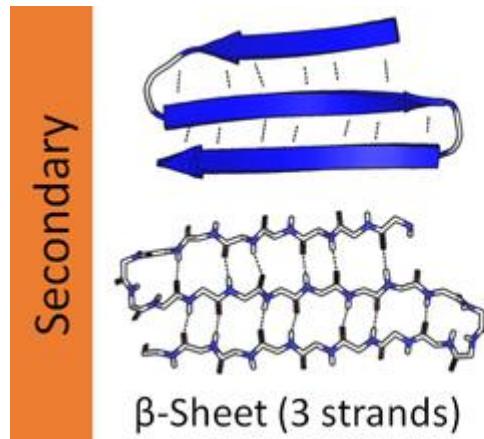


1-letter code	3-letter code	Amino acid	Possible codons
A	Ala	Alanine	GCA, GCC, GCG, GCT
B	Asx	Asparagine or Aspartic acid	AAC, AAT, GAC, GAT
C	Cys	Cysteine	TGC, TGT
D	Asp	Aspartic acid	GAC, GAT
E	Glu	Glutamic acid	GAA, GAG
F	Phe	Phenylalanine	TTC, TTT
G	Gly	Glycine	GGA, GGC, GGG, GGT
H	His	Histidine	CAC, CAT
I	Ile	Isoleucine	ATA, ATC, ATT
K	Lys	Lysine	AAA, AAG
L	Leu	Leucine	CTA, CTC, CTG, CTT, TTA, TTG
M	Met	Methionine	ATG
N	Asn	Asparagine	AAC, AAT
P	Pro	Proline	CCA, CCC, CCG, CCT
Q	Gln	Glutamine	CAA, CAG
R	Arg	Arginine	AGA, AGG, CGA, CGC, CGG, CGT
S	Ser	Serine	AGC, AGT, TCA, TCC, TCG, TCT
T	Thr	Threonine	ACA, ACC, ACG, ACT
V	Val	Valine	GTA, GTC, GTG, GTT
W	Trp	Tryptophan	TGG
X	X	Stop codon	TAA, TAG, TGA
Y	Tyr	Tyrosine	TAC, TAT
Z	Glx	Glutamine or Glutamic acid	CAA, CAG, GAA, GAG

SEQUENCE \Rightarrow STRUCTURE \Rightarrow FUNCTION

Protein domain

- region of a protein's polypeptide chain that folds independently from the rest
- forms a compact folded three-dimensional structure
- many proteins consist of several domains



Conserved domain search

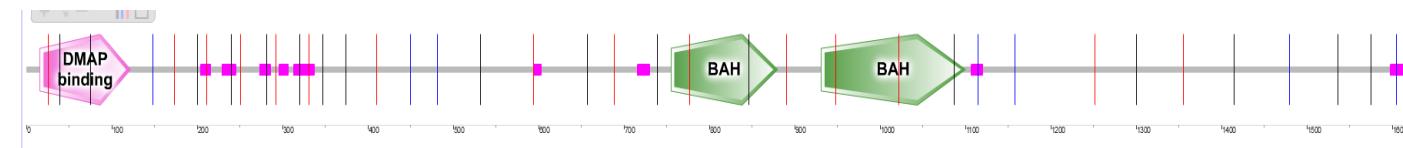
SEQUENCE ⇔ STRUCTURE ⇔ FUNCTION

- Conserved domain databases:

NCBI/CDD



SMART



EMBL/InterPro



Pfam



Conserved domain search - CD (NCBI)

NCBI Resources How To

Conserved Domains

Conserved Domains p15559 Search

Advanced Help

Conserved Domains and Protein Classification

How to use CDD: examples

This page provides **quick start guides** for some common types of searches. The **CDD Help document** provides detailed descriptions of the database content, search system, and display formats. Once records of interest are retrieved, follow Entrez's "Links" to **discover associations among previously disparate data**.

• Identify the putative **function of a protein** sequence.

• Identify a **protein's classification** based on domain architecture.

• Identify the specific **amino acids** in a protein sequence that are putatively **involved in functions such as binding or catalysis**, as mapped from conserved domain annotations to the query sequence.

• View a **protein query sequence embedded within the multiple sequence alignment of a domain model**.

• **Interactively view the 3D structure** of a conserved domain.

• Find other **proteins with similar domain architecture**.

• Interactively view the **phylogenetic sequence tree** for a conserved domain model of interest, with or without a query sequence embedded.

Conserved domain search - CD (NCBI)

CD-Search Results: Concise Display
shows only the best scoring domain model for each region on the query sequence

Identifikátor sekvence Délka sekvence Menu pro omezení úrovně zobrazených detailů

Conserved domains on [gi|157830769|pdb|1CYG|A]
Chain A, Cyclodextrin Glucanotransferase (E.C.2.4.1.19) (Cgtase)

View Concise Results

Graphical summary Zoom to residue level Hide extra options << Show site features Horizontal zoom: x 1 Update graph

Query seq. 1 100 200 300 400 500 600 680

active site starch-binding site 1 starch-binding site 2

Co binding site catalytic site

Specific hits AmyAc_betaMalt_CGTase_1like

Superfamilies AmyAc_family superfamily

Multi-domains Alpha amylase

IPT_CGTD IPT superfamily

CBM20_CGTree CBM20 superFamily

Search for similar domain architectures Refine search

Hit types vary based on confidence level and specificity.

Follow the text links below this illustration for more information about each hit type.

Small triangles indicate the amino acids involved in conserved features/sites, such as catalytic and binding sites

Click on the colored bar representing any domain model to view the detailed information for that domain, including a multiple sequence alignment of the proteins used to generate the domain, with your query sequence embedded.

Specific hits are shown in bright colors as the top hit type. They represent a high confidence association between the query sequence and a domain model, and therefore a high confidence level in the inferred function of the query protein.

The **superfamily** to which a specific hit belongs is shown beneath it in a similar, **pastel color**.

If CD-Search finds only **non-specific hits** for a region of the query sequence, only the **superfamily** to which the hits belong will be shown in the concise display. The non-specific hits can be viewed in the full display.

Multi-domains are domain models that were computationally detected and are likely to contain multiple single domains. They are typically shown as **grey bars**.

Conserved domain search / NQO1

NCBI Resources ▾ How To ▾

jostovap My NCBI Sign Out

Help

NCBI

HOME SEARCH GUIDE Structure

Search for

Enter protein or nucleotide query as

Submit

References:

Conserved Domains

Conserved domains on [gi|118607|sp|P1559.1|NQO1_HUMAN]

RecName: Full=NAD(P)H dehydrogenase [quinone] 1; AltName: Full=Azoreductase; AltName: Full=DT-diaphorase; Short=DTD; AltName: Full=Menadione reductase; AltName: Full=NAD(P)H:quinone oxidoreductase 1; AltName: Full=Phylloquinone reductase; AltName: Full=Quinone reductase 1; Short=QR1

Protein Classification

flavodoxin family protein (domain architecture ID 10495002)
flavodoxin family protein containing a flavodoxin-like fold domain, similar to *Bradyrhizobium diazoefficiens* FMN-dependent NADH-azoreductase 1, which catalyzes the reductive cleavage of the azo bond in aromatic azo compounds to the corresponding amine

Graphical summary Zoom to residue level show extra options »

Query seq. 50 100 150 200 250 274

Specific hits Flavodoxin_2

Superfamilies FMN_red superfamily

Search for similar domain architectures Refine search

List of domain hits

Name	Accession	Description	Interval	E-value
Flavodoxin_2	pfam02525	Flavodoxin-like fold; This family consists of a domain with a flavodoxin-like fold. The family ...	5-212	4.06e-46

References:

- Marchler-Bauer A et al. (2017), "CDD/SPARCLE: functional classification of proteins via subfamily domain architectures.", *Nucleic Acids Res.* 45(D)200-3.
- Marchler-Bauer A et al. (2015), "CDD: NCBI's conserved domain database.", *Nucleic Acids Res.* 43(D)222-6.
- Marchler-Bauer A et al. (2011), "CDD: a Conserved Domain Database for the functional annotation of proteins.", *Nucleic Acids Res.* 39(D)225-9.
- Marchler-Bauer A, Bryant SH (2004). "CD-Search: protein domain annotations on the fly." *Nucleic Acids Res.* 32(W)227-231.

Conserved domain search - SMART

SMART 

Letunic et al. (2017) Nucleic Acids Res doi: 10.1093/nar/gkx922
Letunic et al. (2020) Nucleic Acids Res doi: 10.1093/nar/gkaa837

SMART MODE: **NORMAL GENOMIC**

Simple Modular Architecture Research Tool

keywords...
Search SMART

[HOME](#) [SETUP](#) [FAQ](#) [ABOUT](#) [GLOSSARY](#) [WHAT'S NEW](#) [FEEDBACK](#)

Select your default SMART mode

You can use SMART in two different modes: **normal** or **genomic**. The main difference is in the underlying protein database used. In **Normal SMART**, the database contains Swiss-Prot, SP-TrEMBL and stable Ensembl proteomes. In **Genomic SMART**, only the proteomes of completely sequenced genomes are used; Ensembl for metazoans and Swiss-Prot for the rest. The complete list of genomes in Genomic SMART is [available here](#).

The protein database in Normal SMART has significant redundancy, even though identical proteins are removed. If you use SMART to explore domain architectures, or want to find exact domain counts in various genomes, consider switching to **Genomic** mode. The numbers in the domain annotation pages will be more accurate, and there will not be many protein fragments corresponding to the same gene in the architecture query results. Remember you are exploring a limited set of genomes, though.

Different color schemes are used to easily identify the mode you're in.

Normal mode	Genomic mode
SMART MODE: NORMAL GENOMIC	SMART MODE: NORMAL GENOMIC
Simple Modular Architecture Research Tool	Simple Modular Architecture Research Tool

Click on the images above to select your default mode.

Information about your selected mode is stored in a browser cookie. If you for whatever reason don't want/can't use cookies, access SMART [through this page](#).

You can easily change modes later, by clicking on the links in the 'SMART MODE' header box, or in your personal preference settings ('SETUP' link in the menu):

SMART 

Schultz et al. (1998) Proc. Natl. Acad. Sci. USA 95, 5857-5864
Letunic et al. (2004) Nucleic Acids Res 32, D142-D144

[HOME](#) [SETUP](#) [FAQ](#) [ABOUT](#) [GLOSSARY](#) [WHAT'S NEW](#) [FEEDBACK](#)

Conserved domain search - SMART

The screenshot shows the SMART web interface. At the top, there's a banner with the SMART logo and a background of green and blue grid patterns. Below the banner, the header includes links for "HOME", "SETUP", "FAQ", "ABOUT", "GLOSSARY", "WHAT'S NEW", and "FEEDBACK". A "SMART MODE:" dropdown is set to "NORMAL GENOMIC". To its right is the "Simple Modular Architecture Research Tool" (SMART) logo. Further right is a search bar with "keywords" and a "Search SMART" button.

Sequence analysis

You may use either a [Uniprot/Ensembl](#) sequence identifier (ID) / accession number (ACC) or the protein sequence itself to perform the SMART analysis service.

Sequence ID or ACC

Examples: #1, #2 [?](#)

Protein sequence

Examples: #1, #2 [?](#)

Sequence SMART **Reset**

HMMER searches of the SMART database occur by default. You may also find:

Outlier homologues and homologues of known structure
 PFAM domains
 signal peptides
 internal repeats

Architecture analysis

You can search for proteins with combinations of [specific domains](#) in different species or taxonomic ranges. You can input the domains directly into "Domain selection" box, or use "GO terms query" to get a list of domains.

Domain selection

Examples: #1, #2 [?](#)

GO terms query

Examples: #1, #2 [?](#)

Taxonomic selection

If you wish to restrict your domain architecture query to a particular species or taxonomic class, start typing its name in the box, and select a match from the popup list.

Architecture query **Resetovat**

You can try an [Advanced Query](#) if you're familiar with SQL.

Conserved domain search - SMART

SMART - SMART domains

SMART MODE: Simple

keywords... keywords... Search SMART

SETUP FAQ ABOUT GLOSSARY WHAT'S NEW FEEDBACK

Domains within *Homo sapiens* protein NQO1_HUMAN (P15559)

NAD(P)H dehydrogenase [quinone] 1; The enzyme apparently serves as a quinone reductase in connection with conjugation reactions of hydroquinones involved in detoxification pathways as well as in biosynthetic processes such as the vitamin K-dependent gamma-carboxylation of glutamate residues in prothrombin synthesis; Belongs to the NAD(P)H dehydrogenase (quinone) family.

+ = - Introns SAVE Alternative representations: 1 / 2 << >>

0 100 200

Information Architecture Interactions Pathways PTMs Orthology

Length 274 aa
Source UniProt
Identifiers NQO1_HUMAN, 9606.ENSPO0000319788, P15559, ENSP00000319788.5, ENSP00000319788, B2R5Y9, B4DNM7, B7ZAD1, Q86UK1, H3BNV2_HUMAN, H3BNV2, K7BKZ6_PANTR, K7BKZ6, A0A2I2YI80_GORGO, A0A2I2YI80, A0A2J8Q3V7_PANTR, A0A2J8Q3V7, H2QBF4_PANTR, H2QBF4, G3QL89_GORGO, G3QL89
Source ENSG00000181019 gene

The SMART diagram above represents a summary of the results shown below. Domains with scores less significant than established cutoffs are not shown in the diagram. Features are also not shown when two or more occupy the same piece of sequence; the priority for display is given by SMART > PFAM > PROSPERO repeats > Signal peptide > Transmembrane > Coiled coil > Unstructured regions > Low complexity. In either case, features not shown in the above diagram are marked as 'overlap' in the right side table below.

Conserved domain search - SMART

SMART | [SETUP](#) [FAQ](#) [ABOUT](#) [GLOSSARY](#) [WHAT'S NEW](#) [FEEDBACK](#)

Domains within *Homo sapiens* protein [NQO1_HUMAN](#) (P15559)

NAD(P)H dehydrogenase [quinone] 1; The enzyme apparently serves as a quinone reductase in connection with conjugation reactions of hydroquinones involved in detoxification pathways as well as in biosynthetic processes such as the vitamin K-dependent gamma-carboxylation of glutamate residues in prothrombin synthesis; Belongs to the NAD(P)H dehydrogenase (quinone) family.

+ = - Introns SAVE Alternative representations: 1 / 2 << >>



Information Architecture Interactions Pathways PTMs Orthology

Posttranslational modifications

PTM annotation is taken from [PTMcode](#), a resource of known and predicted functional associations between protein posttranslational modifications (PTMs).

There are 19 PTMs annotated in this protein:

PTM	Count
Ub	Ubiquitination 14
Ac	Acetylation 3
Ph	Phosphorylation 2

To see the full details, including possible functional associations between the PTMs, please visit the PTMcode [annotation page for protein NQO1](#).



Conserved domain search - InterPro

InterPro Classification of protein families

Home ▶ Search ▶ Browse ▶ Results Release notes Download ▶ Help ▶ About

Job ID: iprscan5-R20230301-115158-0009-77866479-p1m

Length: 274 amino acids

Actions: Delete Edit

Status: ✓ finished

Expires: Wed Mar 08 2023

Protein family membership

None predicted

Entry matches to this protein

1 20 40 60 80 100 120 140 160 180 200 220 240 260 274

Options Export

Domain: IPR003680, PF02525

Homologous Superfamily: IPR029039, G3DSA:3.40.50.360, SSF52218
Flavodoxin_fold: 5 - 211

Unintegrated: G3DSA:3.40.50.360:FF:000029, PTHR10204

The screenshot shows the InterPro search results for a protein sequence. At the top, there's a navigation bar with links for Home, Search, Browse, Results, Release notes, Download, Help, and About. Below the navigation is a summary section with details like Job ID, Length (274 amino acids), Status (finished), and Expiry date. The main content area is titled 'Protein family membership' and indicates 'None predicted'. Below this, a section titled 'Entry matches to this protein' displays a sequence alignment from position 1 to 274. A green bar highlights a domain from position 5 to 211, which is identified as 'Flavodoxin_fold'. This domain is associated with InterPro entry IPR003680 and Pfam entry PF02525. Other homologous superfamily entries shown include IPR029039, G3DSA:3.40.50.360, and SSF52218. The bottom part of the page lists 'Unintegrated' entries: G3DSA:3.40.50.360:FF:000029 and PTHR10204.

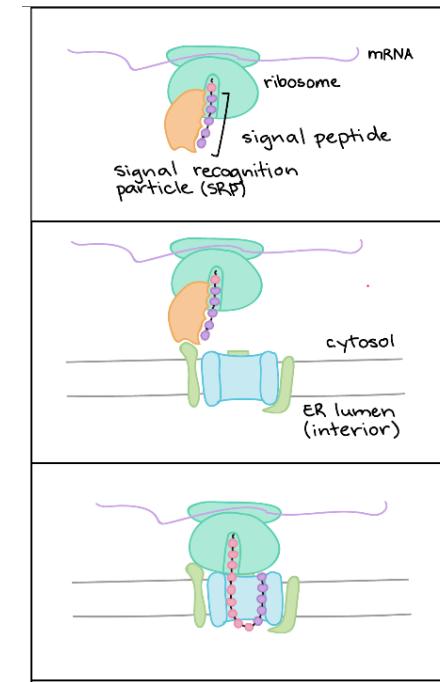
Practical part

Try
CD / SMART/ InterPro
search

Find domains in your sequence

ER signal peptide prediction

Endoplasmic reticulum signal peptide: 15-60 amino acids on protein N-terminus



Signal recognition particle (SRP) binds to the signal peptide as it emerges from the ribosome.

SRP brings the ribosome to the ER by binding to a receptor on the ER surface. The receptor is associated with other proteins that make a pore.

The ribosome resumes translating, feeding the polypeptide through the pore and into the ER lumen (interior).

Signal peptides

SignalP

DTU Health Tech

Research Publications Education Collaboration Services and Products News About

SignalP 6.0 is based on a [matrix-based protein language model](#) with a convolutional random field for structured prediction.

Behind the Paper: Check out the [blog post about the SignalP 6.0 publication](#) in the Nature Portfolio Bioengineering Community.

History paper: Click here to read "[A Brief History of Protein Sorting Prediction](#)", The Protein Journal, 2019

Eukaryotic proteins: Remember, the presence or absence of a signal peptide is not the whole story about the localization of a protein! If you want to find out more about the sorting of your eukaryotic proteins, try the protein subcellular localization predictor [DeepLoc](#). You may also want to check whether proteins with signal peptides have GPI anchors that keep them attached to the outer face of the plasma membrane using the predictor [NetGPI](#).

Submission Instructions Data Article abstract FAQ Version history Portable Downloads

Submit data

Sequence submission: paste the sequence(s) and/or upload a local file

Protein sequences should be not less than 10 amino acids. The maximum number of proteins is 5000.

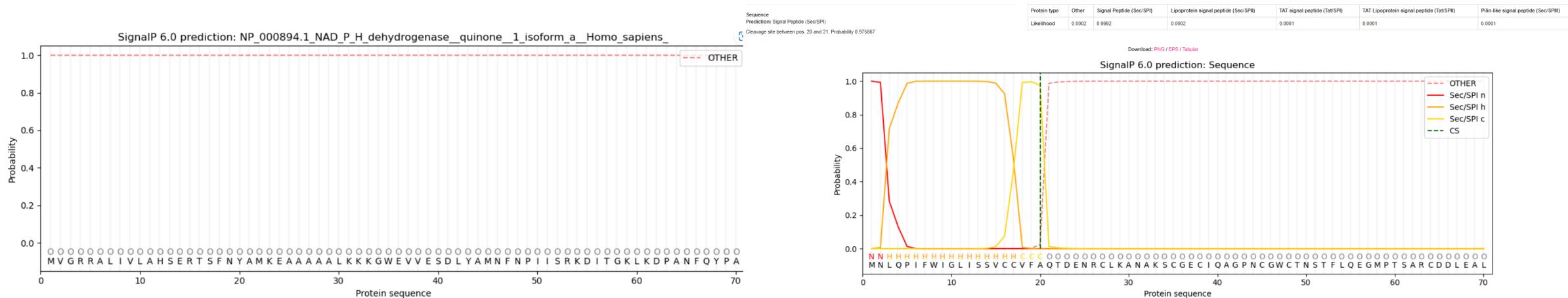
The long output format might timeout for more than 100 entries.

[Mirror](#) Use SignalP 6.0 on BioLib if this server is heavily loaded.

```
>NP_000894.1 NAD(P)H dehydrogenase [quinone] 1 isoform a [Homo sapiens]
MVGRRALIVLAHSERTSFNYAMKEAAAAALKKGWEVVESDLYAMNFNPIISRKDITGKLK
DPANFQYPA
ESVLAYKEGHLSPLDIVAEQKKLEAADLVIQFPLQWFGVPAILKGWFERVFIGEFAYTAAMY
DKGPFRS
KKAVLSITTGGSGSMYSLQGIHGDMNVILWPIQSGILHFCGFQVLEPQLTYSIGHTPADARIQI
LEGWKK
RLENIWDETPLYFAPSSLFDLNFQAGFLMKKEVQDEEKKKFGLSVGHHLGKSIPTDNQIK
ARK|
```

Signal peptides

SignalP



protein does not have signal peptide

Protein has signal peptide
(with certain probability)

Signal peptides

SMART  **Simple Modular Architecture Research Tool**

Schultz et al. (1998) Proc. Natl. Acad. Sci. USA 95, 5857-5864
Letunic et al. (2014) Nucleic Acids Res. doi: 10.1093/nar/gku949

SMART MODE: NORMAL GENOMIC

Sequence analysis

You may use either a [Uniprot/Ensembl](#) sequence identifier (ID) / accession number (ACC) or the protein sequence itself to perform the SMART analysis.

Sequence ID or ACC
 Examples: #1, #2

Protein sequence

MVAATVAAAWLLWAAACAQQEQDFYDFKAVNIRGKLVSLEKYRGSVSLVVNVASECGFTDOHYRALQQQLQRDLGPHHFNVLAFPCNCQFGQQEPDSNKEIESFARRTYSVSFPMFSKIAVTGTGAHPFKYLAQTSGKEPTWNFWKYLVAPDGKVVGAWDPTVSVVEVRPQITAIVRKLIILKREDL
Examples: #1, #2

Sequence SMART **Reset**

HMMER searches of the SMART database occur by default. You may also find:

Outlier homologues and homologues of known structure
 PFAM domains
 signal peptides
 internal repeats

Architecture

Domain architecture analysis

Display all proteins with similar:

- **Domain organisation:** Proteins having all the domains as the query in the same order. Additional domains are allowed.
- **Domain composition:** Proteins with the same domain composition have at least one copy of each of domains of the query

The SMART diagram above represents a summary of the results shown below. Domains with scores less significant than establish the priority for display is given by SMART > PFAM > PROSPERO repeats > Signal peptide > Transmembrane > Coiled coil > I the right side table below.

Confidently predicted domains, repeats, motifs and features:

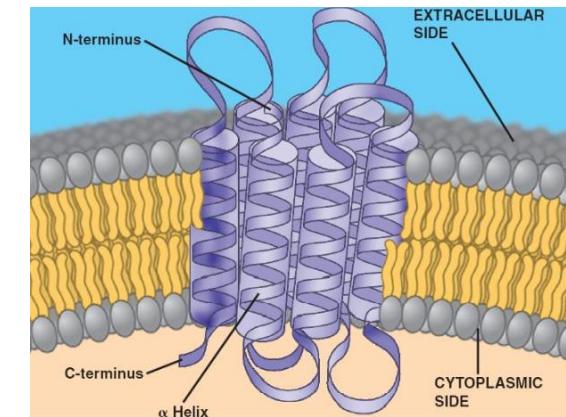
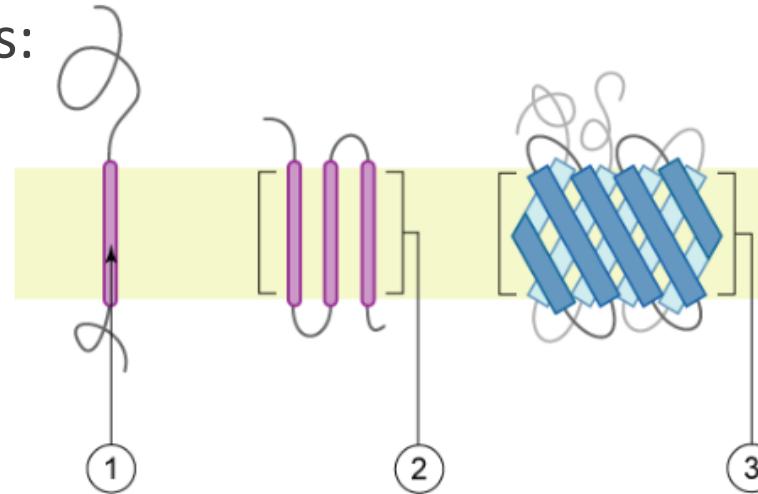
Name	Start ▲	End	E-value
signal peptide	1	18	N/A
Pfam:UDPGT	19	523	8e-64

Practical part

search for signal peptide in
your sequence

Prediction of transmembrane helices

Transmembrane proteins:

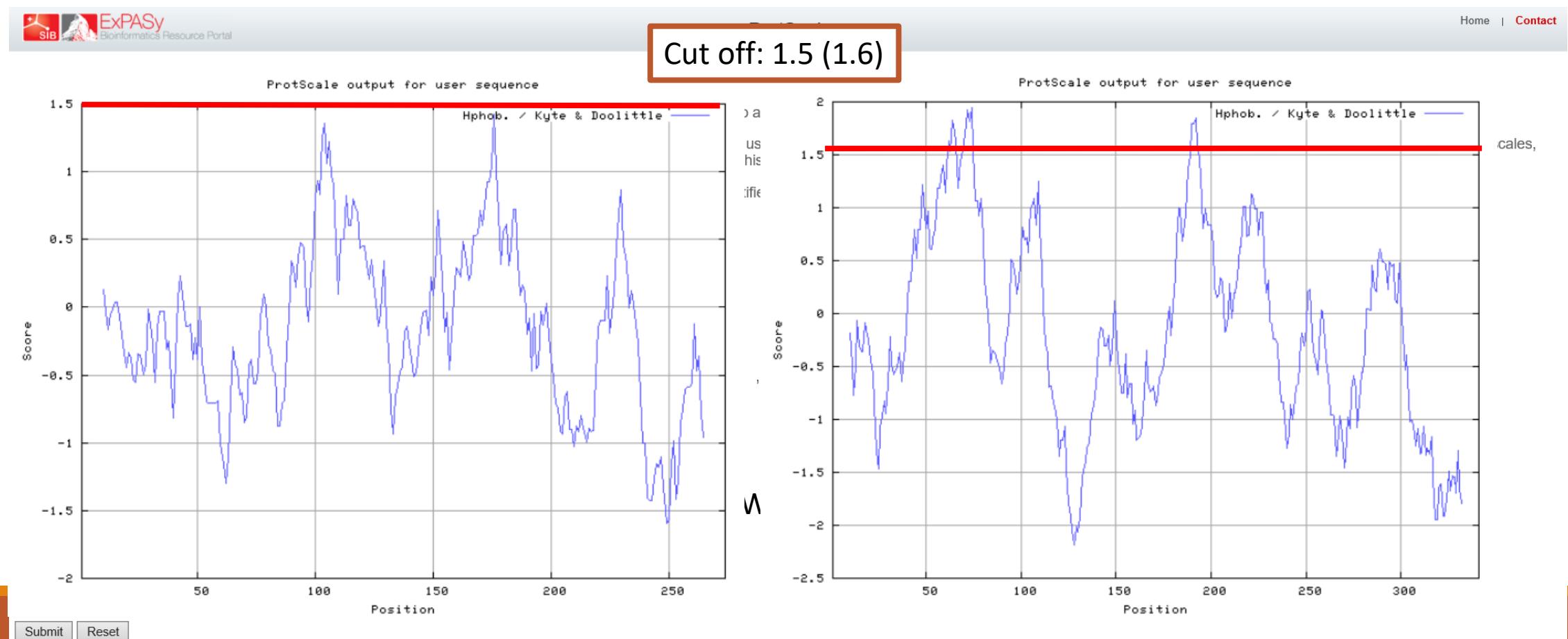


Amino acid Hydrofobicity

- various programs – different algorithms – different results
- Topological predictions (estimation of in and out topology)

Prediction of transmembrane helices

Profile of amino acids hydrofobicity



TMHMM

CENTER FOR BIOLOGICAL SIGNALING CBS

EVENTS NEWS RESEARCH GROUPS CBS PREDICTION SERVERS CBS DATA SETS PUBLICATIONS EDUCATION CENTER FOR BIOLOGICAL SIGNALING CBS >> CBS Prediction Servers >> TMHMM

STAFF CONTACT ABOUT CBS INTERNAL CBS BIOINFORMATICS TOOLS CBS COURSES OTHER BIOINFORMATICS LINKS

TMHMM Server v. 2.0

Prediction of transmembrane helices in proteins

TMHMM result

[HELP](#) with output formats

no TM helix

SUBMISSION

Submission of a local file in [FASTA](#) form Procházel...

OR by pasting sequence(s) in [FASTA](#) for

Output format:

- Extensive, with graphics
- Extensive, no graphics
- One line per protein

Other options:

Use old model (version 1)

Restrictions:
At most 10,000 sequences and 4,000,000 amino acids.

Confidentiality:
The sequences are kept confidential and will not be stored or analyzed.

[Submit](#) [Clear](#)

TMHMM posterior probabilities for WEBSEQUENCE

probability

transmembrane — inside — outside —

WEBSEQUENCE Length: 274
WEBSEQUENCE Number of predicted TMHs: 0
WEBSEQUENCE Exp number of AAs in TMHs: 0.20324
WEBSEQUENCE Exp number, first 60 AAs: 0
WEBSEQUENCE Total prob of N-in: 0.04315
WEBSEQUENCE TMHMM2.0 outside 1 274

TMHMM result

[HELP](#) with output formats

five predicted TM helices

TMHMM posterior probabilities for WEBSEQUENCE

probability

transmembrane — inside — outside —

WEBSEQUENCE Length: 321
WEBSEQUENCE Number of predicted TMHs: 5
WEBSEQUENCE Exp number of AAs in TMHs: 108.47546
WEBSEQUENCE Exp number, first 60 AAs: 21.62676
WEBSEQUENCE Total prob of N-in: 0.05151
WEBSEQUENCE POSSIBLE N-term signal sequence
WEBSEQUENCE TMHMM2.0 outside 1 34
WEBSEQUENCE TMHMM2.0 TMhelix 35 57
WEBSEQUENCE TMHMM2.0 inside 58 63
WEBSEQUENCE TMHMM2.0 TMhelix 64 86
WEBSEQUENCE TMHMM2.0 outside 87 95
WEBSEQUENCE TMHMM2.0 TMhelix 96 118
WEBSEQUENCE TMHMM2.0 inside 119 179
WEBSEQUENCE TMHMM2.0 TMhelix 180 202
WEBSEQUENCE TMHMM2.0 outside 203 216
WEBSEQUENCE TMHMM2.0 TMhelix 217 236
WEBSEQUENCE TMHMM2.0 inside 237 321

TOPCONS

TOPCONS



Consensus prediction of membrane peptides

Please paste your amino acid sequences in **FASTA** format:
Allowed characters: "ABCDEFGHIJKLMNPQRSTVWYZX*",
(Sequences should be no shorter than 10 amino acids)

Alternatively, upload a text file in FASTA format upto 100 KB
[Procházel...](#)

Job name (optional):

Email (recommended for batch submissions):

Force run (do not use cached results):

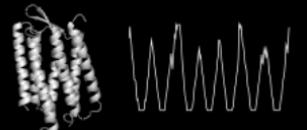
[Submit](#) [Clear](#) [Generate example input](#)

New query
Batch WSDL API
Download
References
News
Server status
Example results
Old TOPCONS
Help

Your recent jobs:
Queued 0
Running 0
Finished 5
Failed 0

© Arne Elofsson

TOPCONS



Results

- Submitted: 2018-03-05 15:59:14
- Status: **Finished**
- Waiting time: 0 sec
- Running Time: 0 sec

Results of your prediction with jobid: **rst_BKOIKK**

Zipped folder of your result can be found in [rst_BKOIKK.zip](#)

Dumped prediction in one text file can be found in [query.result.txt](#)

The sequence(s) you submitted can be found in [query.raw.fa](#)

Predicted topologies and predicted ΔG values:

Legend: Inside (red), Outside (blue), TM-helix (IN->OUT) (grey), TM-helix (OUT->IN) (white), Signal peptide (black)

Method	Topology	Value
TOPCONS	Inside	Highly Consistent
	Outside	Highly Consistent
	TM-helix (IN->OUT)	Low Consistency
	TM-helix (OUT->IN)	Low Consistency
	Signal peptide	Highly Consistent
OCTOPUS	Inside	Highly Consistent
	Outside	Highly Consistent
	TM-helix (IN->OUT)	Low Consistency
	TM-helix (OUT->IN)	Low Consistency
	Signal peptide	Highly Consistent
Philius	Inside	Highly Consistent
	Outside	Highly Consistent
	TM-helix (IN->OUT)	Low Consistency
	TM-helix (OUT->IN)	Low Consistency
	Signal peptide	Highly Consistent
PolyPhobius	Inside	Highly Consistent
	Outside	Highly Consistent
	TM-helix (IN->OUT)	Low Consistency
	TM-helix (OUT->IN)	Low Consistency
	Signal peptide	Highly Consistent
SCAMPI	Inside	Highly Consistent
	Outside	Highly Consistent
	TM-helix (IN->OUT)	Low Consistency
	TM-helix (OUT->IN)	Low Consistency
	Signal peptide	Highly Consistent
SPOCTOPUS	Inside	Highly Consistent
	Outside	Highly Consistent
	TM-helix (IN->OUT)	Low Consistency
	TM-helix (OUT->IN)	Low Consistency
	Signal peptide	Highly Consistent
PDB-homology	Inside	Highly Consistent
	Outside	Highly Consistent
	TM-helix (IN->OUT)	Low Consistency
	TM-helix (OUT->IN)	Low Consistency
	Signal peptide	***No homologous TM proteins detected***

© Arne Elofsson

Predicted topologies and predicted ΔG values:

Legend: Inside (red), Outside (blue), TM-helix (IN->OUT) (grey), TM-helix (OUT->IN) (white), Signal peptide (black)

Method	Topology	Value
TOPCONS	Inside	Highly Consistent
	Outside	Highly Consistent
	TM-helix (IN->OUT)	Low Consistency
	TM-helix (OUT->IN)	Low Consistency
	Signal peptide	Highly Consistent
OCTOPUS	Inside	Highly Consistent
	Outside	Highly Consistent
	TM-helix (IN->OUT)	Low Consistency
	TM-helix (OUT->IN)	Low Consistency
	Signal peptide	Highly Consistent
Philius	Inside	Highly Consistent
	Outside	Highly Consistent
	TM-helix (IN->OUT)	Low Consistency
	TM-helix (OUT->IN)	Low Consistency
	Signal peptide	Highly Consistent
PolyPhobius	Inside	Highly Consistent
	Outside	Highly Consistent
	TM-helix (IN->OUT)	Low Consistency
	TM-helix (OUT->IN)	Low Consistency
	Signal peptide	Highly Consistent
SCAMPI	Inside	Highly Consistent
	Outside	Highly Consistent
	TM-helix (IN->OUT)	Low Consistency
	TM-helix (OUT->IN)	Low Consistency
	Signal peptide	Highly Consistent
SPOCTOPUS	Inside	Highly Consistent
	Outside	Highly Consistent
	TM-helix (IN->OUT)	Low Consistency
	TM-helix (OUT->IN)	Low Consistency
	Signal peptide	Highly Consistent

Phobius



Normal prediction

Paste your protein sequence here in Fasta format:



Or: Select the sequence file you wish to use Nevybrán žádný soubor

Select output format:

- Short
- Long without Graphics
- Long with Graphics

Phobius

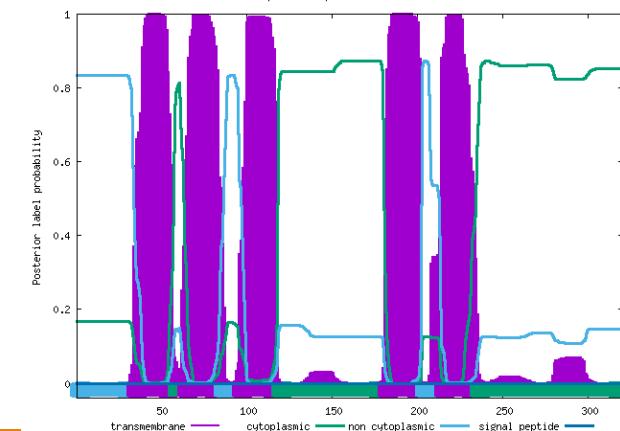
A combined transmembrane topology and signal peptide predictor

Phobius prediction

Prediction of UNNAMED

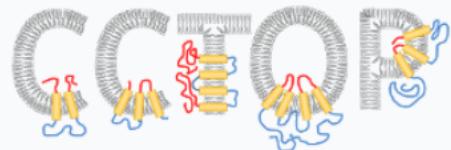
ID	UNNAMED	1	33	NON CYTOPLASMIC.
FT	TOPO_DOM	34	57	CYTOPLASMIC.
FT	TRANSMEM	58	63	CYTOPLASMIC.
FT	TOPO_DOM	64	84	CYTOPLASMIC.
FT	TRANSMEM	85	95	NON CYTOPLASMIC.
FT	TOPO_DOM	96	118	CYTOPLASMIC.
FT	TOPO_DOM	119	180	CYTOPLASMIC.
FT	TRANSMEM	181	202	CYTOPLASMIC.
FT	TOPO_DOM	203	213	NON CYTOPLASMIC.
FT	TRANSMEM	214	234	CYTOPLASMIC.
FT	TOPO_DOM	235	320	CYTOPLASMIC.
//				

Phobius posterior probabilities for UNNAMED

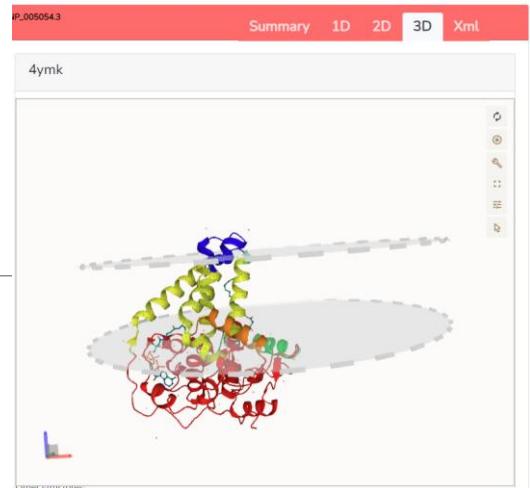


The probability data used in the plot is found [here](#), and the gnuplot script is [here](#).

CCTOP

[Submit](#)[Manual](#)[About](#)[Standalone](#)[MyJobs](#)

Job ID



Results for job 92e87f663074d81d642456ea6e9d63a6

Proteins:

sequences: 1/1

> NP_005054.3

Control panel

NP_005054.3

Summary

1D

2D

Download results

XML file

>sequence
MPAHLQLDDISSSYTTTTITAPPSRVLQNGGDKLETMPLYLEDDIRPDIKDDIYDPTYKDKEGSPKVVEVWR
LYGITLTPTCKFYTWLWGVFYYEVSALEGITAGAHLWHSRSYKARLPLRLFLIIANTMAFQNDVYEWARDHRAH
SRRGFFFSHVGWLVRKHPAVKEKGSTLDSLDEAEKLMFQRRYYKPGGLMMCFILPTLVPAHYFWGETFQN5V
NAWTWLVSAAHLFGYRPYDKNISPENILVSLGAVGEGFHNYHHSFPYDYSASEYRWHINFTEFFIDCMAALGL
LARIKRTGDGNYKSG
>topology
II
MMMMMMM00000MMNN
II
MII
II

NP_005054.3

Summary 1D 2D 3D Xml

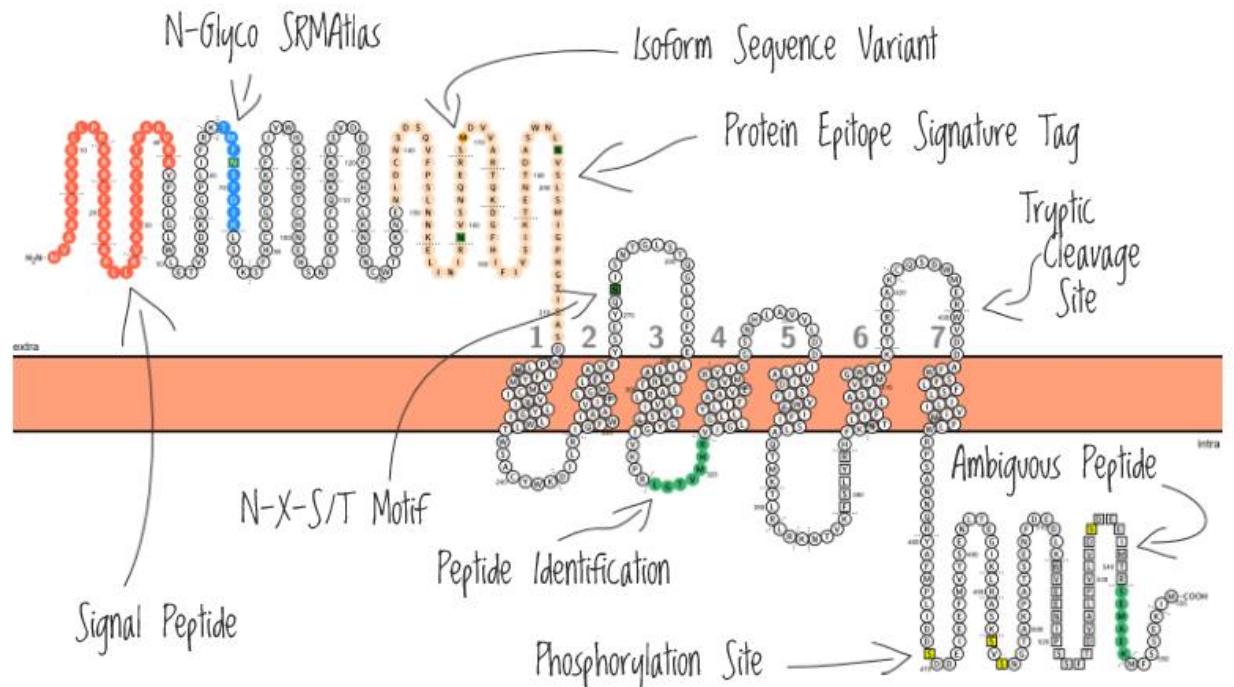


PROTTER-figure!

-creates figure from the UniProt data

PROTTER

Welcome to Protter — the open-source tool for visualization of proteoforms and interactive integration of annotated and predicted sequence features together with experimental proteomic evidence!



start PROTTER

PROTTER-figure!

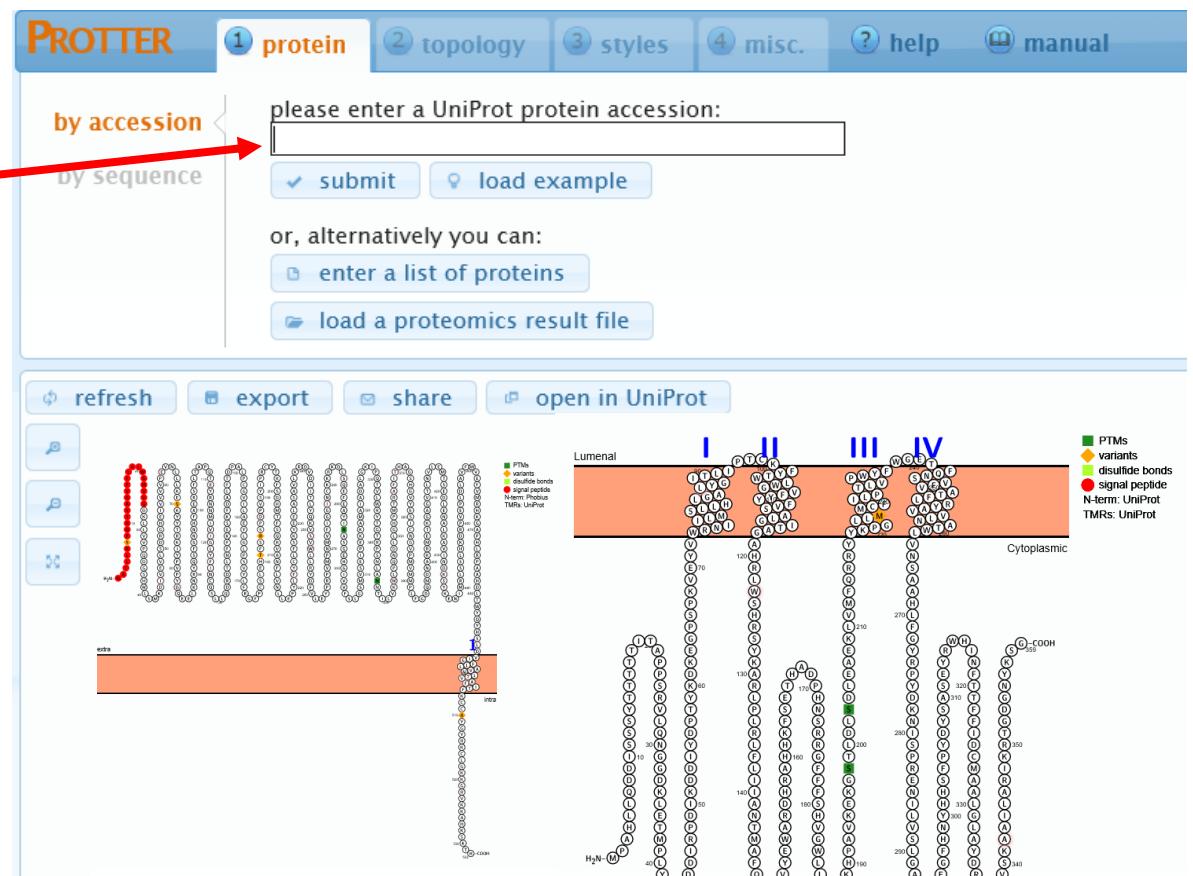
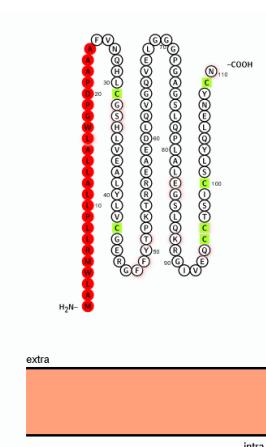
-creates figure from the UniProt data

-uses UniProt ID:

UGT1A6 (P19224)

Desaturase (O00767)

(prepro) insulin (P01308)



PROTTER-figure!

PROTTER

① protein ② topology ③ styles ④ misc. ⑤ help ⑥ manual

by accession

please enter a UniProt protein accession:
O00767

or, alternatively you can:

PROTTER

① protein ② topology ③ styles ④ misc. ⑤ help ⑥ manual

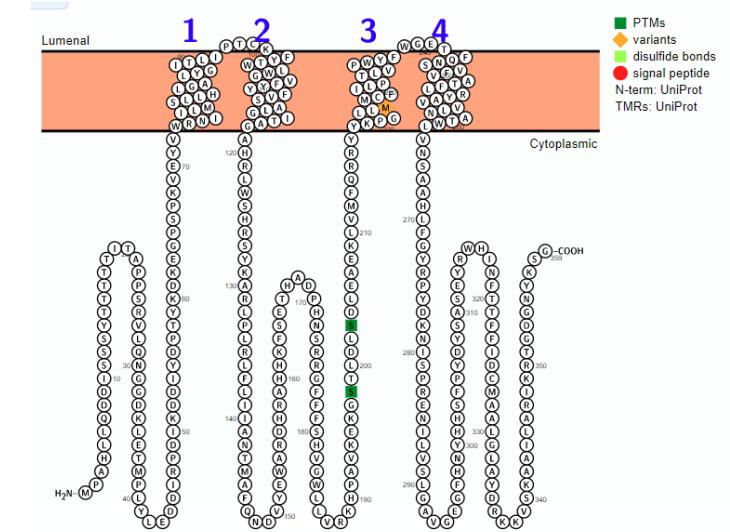
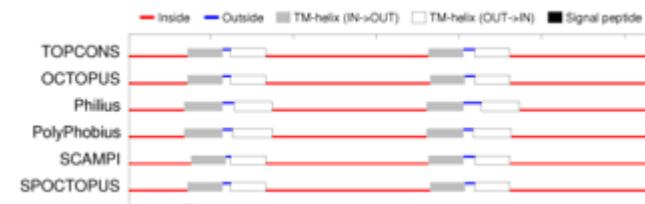
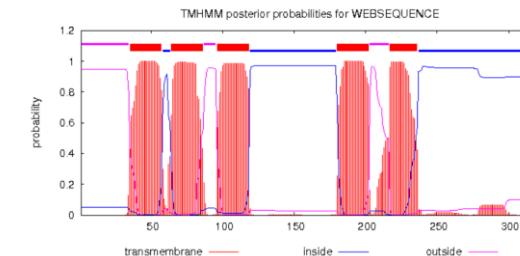
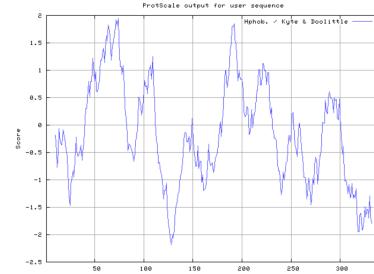
by accession

enter a custom protein sequence or multiple sequences in FASTA format:

```
MPAHLLQDDISSLSSYTTTTITAPPSRVLQNGGDKLETMPYLEDDIRPDIKDDIYDPTYK
DKEGPSPKVEVWWRNIILMSLLHLGALYGITLIPTCKFYTLWGVFYYFVSALGITAGAH
RLWSHRSYKARLPLRLFLIANTMAFQNNDVYEWARDHRAHHKFSETHADPHNSRRGFFS
HVGWLLVRKHPAVKEKGSTLDSLDEAEKLVMFQRYYKPGLLMMMCFLPTLVPWYFWGE
TFQNSFEVATFLRYAVVNLNATWLVNSAAHLFCGYRPYDKNISPRENILVSLGAVGEGFHNY
HHSFPYDYSASEYRWHINFTFFFIDCMAALGLAYDRKKVSKAAILARIKRTGDNYKSG
```

Prediction of transmembrane helices

ProtScale
TMHMM
TOPCONS



➤ Always try more programs!

Practical part

Try more programs.

Does your sequence have any TMHs?
and/or signal peptide?

„Protein bioinformatics I“

Retrieving protein sequences from databases (Uniprot: FASTA formate)

Computing amino-acids compositions, molecular weight, isoelectric point, and other parameters (SMS)

Prediction of proteases cutting (PeptideCutter)

Predicting elements of protein secondary structure, signal peptide, transmembrane helix

Finding 3-D structure and the domain organization of proteins

Finding all proteins that share a similar sequence and Classifying proteins into families

Finding evolutionary relationships between proteins, drawing proteins' family trees

Computing the optimal alignment between two or more protein sequences

...

Searching for similar sequences

Similarity x Homology

BLAST: Basic Local Alignment and Search Tool

Finds regions of similarity between biological sequences. The program compares nucleotide or protein sequences to sequence databases and calculates the statistical significance.

Similarity matrix:

„Leucine is more similar to Isoleucine than Histidine“

The BLOSUM62 similarity matrix

A	B	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	X	Y	Z
A	4	-2	0	-2	-1	-2	0	-2	-1	-1	-1	-2	-1	-1	-1	1	0	0	-3	-1	-2	-1
B	-2	6	-3	6	2	-3	-1	-1	-3	-1	-4	-3	1	-1	0	-2	0	-1	-3	-4	-1	-3
C	0	-3	9	-3	-4	-2	-3	-3	-1	-3	-1	-3	-3	-3	-1	-1	-1	-2	-1	-2	-4	
D	-2	6	-3	6	2	-3	-1	-1	-3	-1	-4	-3	1	-1	0	-2	0	-1	-3	-4	-1	-3
E	-1	2	-4	2	5	-3	-2	0	-3	1	-3	-2	0	-1	2	0	0	-1	-2	-3	-1	-2
F	-2	-3	-2	-3	-3	6	-3	-1	0	-3	0	0	-3	-4	-3	-3	-2	-2	-1	1	-1	3
G	0	-1	-3	-1	-2	3	6	-2	-4	-2	-4	-3	0	-2	-2	-2	0	-2	-3	-2	-1	-3
H	-2	-1	-3	-1	0	-1	-2	8	-3	-1	-3	-2	1	-2	0	0	-1	-2	-3	-2	-1	2
I	-1	-3	-1	-3	-3	0	-4	-3	4	-3	2	1	-3	-3	-3	-3	-2	-1	3	-3	-1	-3
K	-1	-1	-3	-1	1	-3	-2	-1	-3	5	-2	-1	0	-1	1	2	0	-1	-2	-3	-1	-2
L	-1	-4	-1	-4	-3	0	-4	-3	2	-2	4	2	-3	-3	-2	-2	-2	-1	1	-2	-1	-1
M	-1	-3	-1	-3	-2	0	-3	-2	1	-1	2	5	-2	-2	0	-1	-1	1	-1	-1	-1	-2
N	-2	1	-3	1	0	-3	0	1	-3	0	-3	-2	6	-2	0	0	1	0	-3	-4	-1	2
P	-1	-1	-3	-1	-1	-4	-2	-2	-3	-1	-3	-2	-2	7	-1	-2	-1	-1	-2	-4	-1	-3
Q	-1	0	-3	0	2	-3	-2	0	-3	1	-2	0	0	-1	5	1	0	-1	-2	-2	-1	2
R	-1	-2	-3	-2	0	-3	2	-2	-1	0	-2	1	5	-1	-1	-3	-3	-1	-2	0		
S	1	0	-1	0	0	-2	0	-1	-2	0	-2	-1	1	-1	0	-1	4	1	-2	-3	-1	2
T	0	-1	-1	-1	-1	-2	-2	-2	-1	-1	-1	0	-1	-1	1	5	0	-2	-1	-2	-1	
V	0	-3	-1	-3	-2	-1	-3	-3	3	-2	1	1	-3	-2	-2	-3	-2	0	4	-3	-1	-1
W	-3	-4	-2	-4	-3	1	-2	-2	-3	-3	-2	-1	-4	-4	-2	-3	-3	-2	-3	11	-1	2
X	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	
Y	-2	-3	-2	-3	-2	3	-3	2	-1	-2	-1	-1	-2	-3	-1	-2	-2	-2	-1	2	-1	7
Z	-1	2	-4	2	5	-3	-2	0	-3	1	-3	-2	0	-1	2	0	0	-1	-2	-3	-1	-2

NCBI/BLAST

<http://blast.ncbi.nlm.nih.gov/Blast.cgi>

The screenshot shows the NCBI BLAST homepage. At the top left is the NIH National Library of Medicine logo. On the right is a user profile for "jostovap". The main navigation bar includes links for Home, Recent Results, Saved Strategies, and Help. Below the navigation is a section titled "Basic Local Alignment Search Tool" with a sub-section for "Web BLAST". The "Nucleotide BLAST" and "tblastn" options are shown as blue arrows pointing left. The "blastx" and "Protein BLAST" options are shown as blue arrows pointing right. The "Protein BLAST" option is highlighted with a red box. To the right of the "blastx" arrow is a "NEWS" box containing a message about ElasticBLAST 1.0.0. At the bottom is a search bar for "BLAST Genomes" with a dropdown menu showing "Human", "Mouse", "Rat", and "Microbes".

NIH National Library of Medicine
National Center for Biotechnology Information

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](#)

NEWS

ElasticBLAST 1.0.0 is Now available!
ElasticBLAST version 1.0.0 has support for faster cheaper disks at AWS and better supports Kubernetes on GCP!

Mon, 09 Jan 2023 [More BLAST news...](#)

Web BLAST

Nucleotide BLAST
nucleotide ► nucleotide

blastx
translated nucleotide ► protein

tblastn
protein ► translated nucleotide

Protein BLAST
protein ► protein

Enter organism common name, scientific name, or tax id

Search

Human Mouse Rat Microbes

NCBI/BLAST

<http://blast.ncbi.nlm.nih.gov/Blast.cgi>

NCBI Resources How To

jostovap My NCBI Sign Out

NCBI National Center for Biotechnology Information

All Databases Search

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

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 | Research | NCBI News

Get Started

- Tools: Analyze data using NCBI software
- Downloads: Get NCBI data or software
- How-To's: Learn how to accomplish specific tasks at NCBI
- Submissions: Submit data to GenBank or other NCBI databases

NCBI YouTube channel

Learn how to get the most out of NCBI tools and databases with video tutorials on the NCBI YouTube Channel.

Popular Resources

PubMed

Bookshelf

PubMed Central

PubMed Health

BLAST

Nucleotide

Genome

SNP

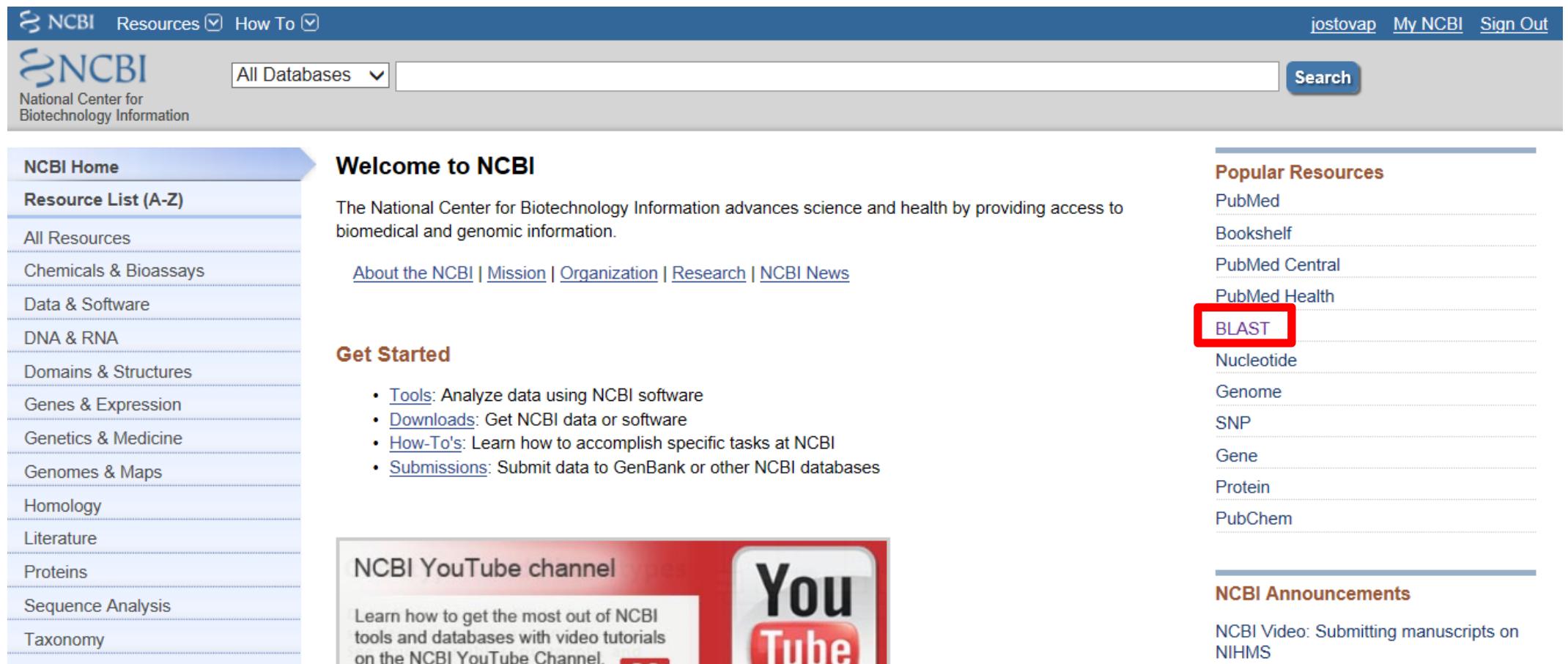
Gene

Protein

PubChem

NCBI Announcements

NCBI Video: Submitting manuscripts on NIHMS



NCBI/BLAST

NCBI BLAST® Basic Local Alignment Search Tool My NCBI
Home Recent Results Saved Strategies Help Welcome jostovap. [Sign Out]

NCBI/ BLAST/ blastp suite Standard Protein BLAST

blastn blastp blastx tblastn tblastx

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

MAARRALIVLAHSEKTSFNYAMKEAAVEALKKRGWEVLESMDLYAMMNFPPIISRNDITGELKDSKNFQ
YPS
ESSLAHKERGLSPDIVAEHKLEAADLVIFQFPLQWFGVPAILKGWFERVLVAGFAYTYAAMYDNGP
FQN
KKTLLSITGGSGSMYSLQGVHDMNVILWPIQSGILRFGFQVLEPQLVYSIGHTPPDARMQILEG

From _____ To _____

Or, upload file Procházen...
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 common name, binomial, or tax id. Only 20 top taxa will be shown.
 Exclude +
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 using Blastp (protein-protein BLAST)
 Show results in a new window

Algorithm parameters

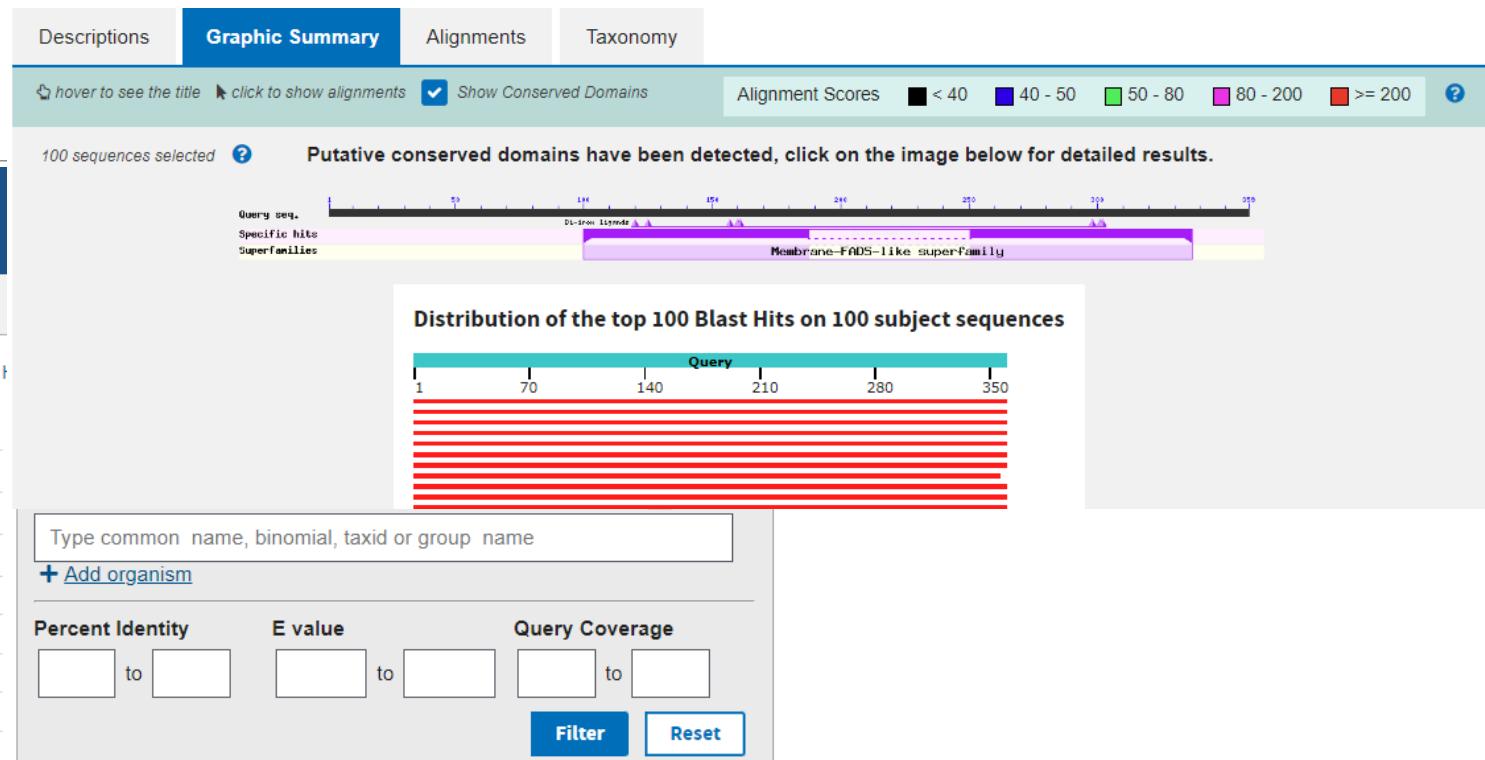
NCBI/BLAST

National Library of Medicine
National Center for Biotechnology Information

BLAST® » blastp suite » results for RID-ZYHJKTA1013

< Edit Search Save Search Search Summary

Job Title NP_005054.3 stearoyl-CoA desaturase [Homo...
RID ZYHJKTA1013 Search expires on 03-02 19:34 pm Download All
Program BLASTP Citation
Database nr See details
Query ID lcl|Query_51026
Description NP_005054.3 stearoyl-CoA desaturase [Homo sapiens]
Molecule type amino acid
Query Length 359
Other reports Distance tree of results Multiple alignment MSA viewer



Compare these results against the new Clustered nr database ? BLAST

Descriptions Graphic Summary Alignments Taxonomy

Links

E-value (expectancy)

Sequences producing significant alignments

Download Select columns Show 100 ?

select all 100 sequences selected

GenPept Graphics Distance tree of results Multiple alignment MSA Viewer

	Description	Scientific Name	Max Score	Total Score	Query Cover	E value	Per. Ident	Acc. Len	Accession
<input checked="" type="checkbox"/>	stearoyl-CoA desaturase [Homo sapiens]	Homo sapiens	748	748	100%	0.0	100.00%	3.9	NP_005054.3
<input checked="" type="checkbox"/>	stearoyl-CoA desaturase [Homo sapiens]	Homo sapiens	747	747	100%	0.0	99.72%	3.9	AAD29870.1
<input checked="" type="checkbox"/>	stearoyl-CoA desaturase variant [Homo sapiens]	Homo sapiens	746	746	100%	0.0	99.72%	3.6	BAD92219.1
<input checked="" type="checkbox"/>	stearoyl-CoA desaturase variant [Homo sapiens]	Homo sapiens	744	744	100%	0.0	99.72%	3.9	BAD96582.1

NCBI/BLAST

Descriptions Graphic Summary **Alignments** Taxonomy

Alignment view Pairwise [Restore defaults](#) [Download](#)

100 sequences selected [?](#)

[Download](#) [GenPept](#) [Graphics](#) [▼ Next](#) [▲ Previous](#) [◀ Descriptions](#)

stearoyl-CoA desaturase [Homo sapiens]
Sequence ID: [NP_005054.3](#) Length: 359 Number of Matches: 1
[See 2 more title\(s\)](#) [▼](#) [See all Identical Proteins\(IPG\)](#)

Range 1: 1 to 359 [GenPept](#) [Graphics](#) [▼ Next Match](#) [▲ Previous Match](#)

Score	Expect	Method	Identities	Positives	Gaps
748 bits(1931)	0.0	Compositional matrix adjust.	359/359(100%)	359/359(100%)	0/359(0%)

Query 1 MPAHLLQDDISSLSSYTTTTITAPPSRVLQNGGDKLETMPLYLEDDIRPDIKDDIYDPTYK 60
MPAHLHQDDISSLSSYTTTTITAPPSRVLQNGGDKLETMPLYLEDDIRPDIKDDIYDPTYK
Sbjct 1 MPAHLLQDDISSLSSYTTTTITAPPSRVLQNGGDKLETMPLYLEDDIRPDIKDDIYDPTYK 60

Query 61 DKEGPSPKVEYWRNIILMSLLHLGALYGITLIPTCKFYTWLWGVFYYFVSALGITAGAH 120
DKEGPSPKVEYWRNIILMSLLHLGALYGITLIPTCKFYTWLWGVFYYFVSALGITAGAH
Sbjct 61 DKEGPSPKVEYWRNIILMSLLHLGALYGITLIPTCKFYTWLWGVFYYFVSALGITAGAH 120

Query 121 RLWSHRSYKARLPLRLFLIIANTMAFQNDVYEWARDHRAHHKFSETHADPHNSRRGFFFS 180
RLWSHRSYKARLPLRLFLIIANTMAFQNDVYEWARDHRAHHKFSETHADPHNSRRGFFFS
Sbjct 121 RLWSHRSYKARLPLRLFLIIANTMAFQNDVYEWARDHRAHHKFSETHADPHNSRRGFFFS 180

Query 181 HVGWLLVRKHPAVKEKGSTLDLSDEAEKLVMFQRRYYKPGLLMMCFILPTLVPWYFWGE 240
HVGWLLVRKHPAVKEKGSTLDLSDEAEKLVMFQRRYYKPGLLMMCFILPTLVPWYFWGE

Related Information

[Gene](#) - associated gene details
[Genome Data Viewer](#) - aligned genomic context
[Identical Proteins](#) - Identical proteins to NP_005054.3

NCBI/BLAST

→change sequences (FASTA) names into organism only

Descriptions Graphic Summary Alignments Taxonomy

Sequences producing significant alignments

select all 5 sequences selected

	Description
<input checked="" type="checkbox"/>	stearoyl-CoA desaturase [Homo sapiens]
<input type="checkbox"/>	stearoyl-CoA desaturase [Homo sapiens]
<input type="checkbox"/>	stearoyl-CoA desaturase variant [Homo sapiens]
<input type="checkbox"/>	stearoyl-CoA desaturase variant [Homo sapiens]
<input checked="" type="checkbox"/>	acyl-CoA desaturase [Gorilla gorilla gorilla]
<input type="checkbox"/>	SCD isoform 1 [Pongo abelii]
<input type="checkbox"/>	stearoyl-CoA desaturase [Pongo abelii]
<input type="checkbox"/>	SCD protein [Homo sapiens]
<input checked="" type="checkbox"/>	acyl-CoA desaturase [Pan troglodytes]
<input type="checkbox"/>	acyl-CoA desaturase [Hylobates moloch]
<input type="checkbox"/>	stearoyl CoA desaturase [Homo sapiens]
<input type="checkbox"/>	acyl-CoA desaturase [Nomascus leucogenys]

Download

- GenPe
- FASTA (complete s)
- FASTA (aligned sec)
- GenBank (complet
- Hit Table (text)

```
*seqdump (1).txt - Poznámkový blok
Soubor Úpravy Formát Zobrazení Nápověda
>Homo sapiens
MPAHLQLDDISSSYTTTTITAPPSRVLQNGGDKLETMPLYLEDDIRPDIKDDIYDPTYKDKEGPSPKVEVWRNIILMS
LLHLGALYGITLIPTCKFYTWLWGVFYYFVSALGITAGAHLRLWSHRSYKARLPLRLFLIIANTMAFQNDVYEWARDHRAH
HKFSETHADPHNSRRGGFFFSHVGLLVRKHPAVKEKGSTLDLSDLEAEKLVMFQRRYYKPGLLMCFILPTLVPWYWFGE
TFQNSVFVATFLRYAVVNLATWLVNSAAHLFGYRPyDKNISPRENILVSLGAVGEGFHNYHHSFPYDYSASEYRHINFT
TFFIDCMAALGLAYDRKKVSKAAILARIKRTGDNYSKG
>Gorilla gorilla gorilla
MPAHLQLDDISSSYTTTTITAPPSRVLQNGGDKLETMPLYLEDDIRPDIKDDIYDPTYKDKEGPSPKVEVWRNIILMS
LLHLGALYGITLIPTCKFYTWLWGVFYYFVSALGITAGAHLRLWSHRSYKARLPLRLFLIIANTMAFQNDVYEWARDHRAH
HKFSETHADPHNSRRGGFFFSHVGLLVRKHPAVKEKGSTLDLSDLEAEKLVMFQRRYYKPGLLMCFILPTLVPWYWFGE
TFQNSVFVATFLRYAVVNLATWLVNSAAHLFGYRPyDKNISPRENILVSLGAVGEGFHNYHHSFPYDYSASEYRHINFT
TFFIDCMAALGLAYDRKKVSKAAILARIKRTGDNYSKG
>Pan troglodytes
MPAHLQLDDITAPPSRVLQNGGDKLETMPLYLEDDIRPDIKDDIYDPTYKDKEGPSPKVEVWRNIILMS
LLHLGALYGITLIPTCKFYTWLWGVFYYFVSALGITAGAHLRLWSHRSYKARLPLRLFLIIANTMAFQNDVYEWARDHRAH
HKFSETHADPHNSRRGGFFFSHVGLLVRKHPAVKEKGSTLDLSDLEAEKLVMFQRRYYKPGLLMCFILPTLVPWYWFGE
TFQNSVFVATFLRYAVVNLATWLVNSAAHLFGYRPyDKNISPRENILVSLGAVGEGFHNYHHSFPYDYSASEYRHINFT
TFFIDCMAALGLAYDRKKVSKAAILARIKRTGDNYSKG
>Camelus ferus
MPAHLQEEISSSYTTTTITAPPSRVLQNGGDKLEKTPLYLEEDIRPEMKDDIYDPSYQDKEGPKPKVYVWRNIILMG
LLHLGALYGITLIPTCKFYTWCWLFYYIISALGITAGAHLRLWSHRSYKARLPLRLFLIIANTMAFQNDVYEWARDHRAH
HKFSETHADPHNSRRGGFFFSHVGLLVRKHPAVKEKGLLDLSLKAEKLVMFQRRYYKPGILLMCFIMPTLVPWYWFGE
TFQHSLYLATFLRYAVVNLTVLVSAAHLFGYRPyDKTINPRENILVSLGAVGEGFHNYHHSFPYDYSASEYRHINFT
TFFIDCMAALGLAYDRKKVSKAAILAKVKTGDSYKG
>Ovis aries
MPAHLQEEISSSYTTTTITAPPSRVLQNGGDKLEKTPLYLEEDIRPEMKDDIYDPSYQDKEGPKPKEYVWRNIILMG
LLHLGALYGITLIPTCKFYTFLWLFYYVISALGITAGVHRLWSHRTYKARLPLRVFLIIANTMAFQNDVFEWSRDHRAH
HKFSETHADPHNSRRGGFFFSHVGLLVRKHPAVREKGATLDLSDLRAEKLVMFQRRYYKPGVLLCFILPTLVPWYLWGE
TFQNSLFFFATFLRYAVVNLATWLVNSAAHMYGYRPyDKTINPRENILVSLGAVGEGFHNYHHTFPYDYSASEYRHINFT
TFFIDCMAAIGLAYDRKKVSKAAVLARMKRTGEESYKG
seqdump.txt - Poznámkový blok
Soubor Úpravy Formát Zobrazení Nápověda
>gi|13435426|gb|AAH04579.1| Nqo1 pr
MAARRALIVLAHSEKTSFNYAMKEAAVEALKRGW
LSPDIVAEHKKLEAADLVIQFPLQWFVGPAIKG
VHGMNVILWPIQSGILHFCGFQVLEPQLVSYIGH
>gi|524939198|ref|XP_005071892.1| P
MAVRALILLAHSEKTSFNYAMKEAAVEALKKKG
LSPDIVAEQKKLEAADLVIQFPLWVGVPAIKG
VHGMNVILWPIQSGILHFCGFQVLEPQLVSYIGH
>gi|227430403|ref|NP_001153085.1| NAD(P)H dehydrogenase [quinone] 1 [sus scrofa]
MAVRKALIILAHSER TSFNYAMKEAAVEALKRGGWEAVS5DLYAMMNFPVISRKDITGKLKDPGNFQYPAETALAYKEGR
LSPDIVAEQKKLEAADLVIQFPLQWFVGPAIKGWEVRLVIGEFAYTYAMYDKGPFRNNKKAVLSTITGGSGSMYSLQG
IHGMNILLWPIQSGTLHFCGFQVLEPQLTYSIGHTPEDIARQIILEEWKKRLENIDETPLFAPSSLFDLNFQAGFLMKKEVQDEEKNKKFLSVGHHLGKSIPTDNQIKARK
>gi|386781783|ref|NP_001247927.1| NAD(P)H dehydrogenase [quinone] 1 [Macaca mulatta]
MVGRKALIILAHSER TSFNYAMKEAAVAALKKKGWEVAESDLYAMMNFPVISRKDITGKLKDPGNFQYPAETALAYKEGR
LSPDIVAEQKKLEAADLVIQFPLQWFVGPAIKGWEVRLVIGEFAYTLAAMYDKGPFRQSKKAVLSTITGGSGSMYSLQG
IHGMNILLWPIQSGILHFCGFQVLEPQLTYSIGHTPADIARQIILEGWKKRLENIDETPLFAPSSLFDLNFQAGFLMKKEVQDEEKNKKFLSVGHHLGKSIPTDNQIKARK
>gi|426242583|ref|XP_004015151.1| PREDICTED: NAD(P)H dehydrogenase [quinone] 1 [ovis aries]
MAVRKALIILAHSER TSFNYAMKEAAIAEALKRGKWEVTLVSDLYAMMNFPVISRKDITGKLKDPGNFQYPAETALAYKEGR
LSPDIVAEQKKLEAADLVIQFPLQWFVGPAIKGWEVRLVIGEFAYTYAMYDKGPFRNNKKAVLSTITGGSGSMYSLQG
IHGMNILLWPIQSGTLHFCGFQVLEPQLTYSIGHTPEDIARQIILEGWKKRLENIDETPLFAPSSLFDLNFQAGFLMKKEVQDEEKNKKFLSVGHHLGKSIPTDNQIKARK
>gi|30230685|gb|AAP20940.1| NAD(P)H dehydrogenase, quinone 1 [Homo sapiens]
RRAILVLAHSEKTSFNYAMKEAAAALKKKGWEVESDLYAMMNFPVISRKDITGKLKDPGNFQYPAESVLAYKEGHLP
DIVAEQKKLEAADLVIQFPLQWFVGPAIKGWEVRLVIGEFAYTYAMYDKGPFRSKAVLSTITGGSGSMYSLQG
DMNVILWPIQSGILHFCGFQVLEPQLTYSIGHTPADIARQIILEGWKKRLENIDETPLFAPSSLFDLNFQAGFLMKKEVQDEEKNKKFLSVGHHLGKSIPMDNQIKARK
```

NCBI/BLAST (reference proteins)

BLAST® Basic Local Alignment Search Tool My NCBI
Home Recent Results Saved Strategies Help Welcome jostovap. [Sign Out]

NCBI/ BLAST/ blastp suite Standard Protein BLAST

blastn blastp blastx tblastn tblastx

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

is using a protein query. more... Reset page Bookmark

From _____ To _____

MAARRALIVLAHSEKTSFNYAMKEAAVEALKRGWEVLESMDLYAMMNFPPIISRNDITGELKDSKNFQ
YPS
ESSLAHKERGLSPDIVAEHKLEADLVIFQFPLQWFGVPAILKGWFERVLVAGFAYTYAAMYDNGP
FQN
KKTLLSITGGSGSMYSLQGVHGMNVILWPIQSGILRFGFQVLEPQLVYSIGHTPPDARMQILEG

Or, upload file Procházen...
Job Title Enter a descriptive title for your BLAST search
 Align two or more sequences

Standard

Database Reference proteins (refseq_protein)
Non-redundant protein sequences (nr)
RefSeq Select proteins (refseq_select)
Reference proteins (refseq_protein) taxa will be shown
Model Organisms (landmark)
UniProtKB/Swiss-Prot(swissprot)
Patented protein sequences(patent)
Protein Data Bank proteins(pdb)
Metagenomic proteins(env_nr)
Transcriptome Shotgun Assembly proteins (tsa_nr)

Organism exclude Add organism
(WP) Uncultured/environmental sample sequences

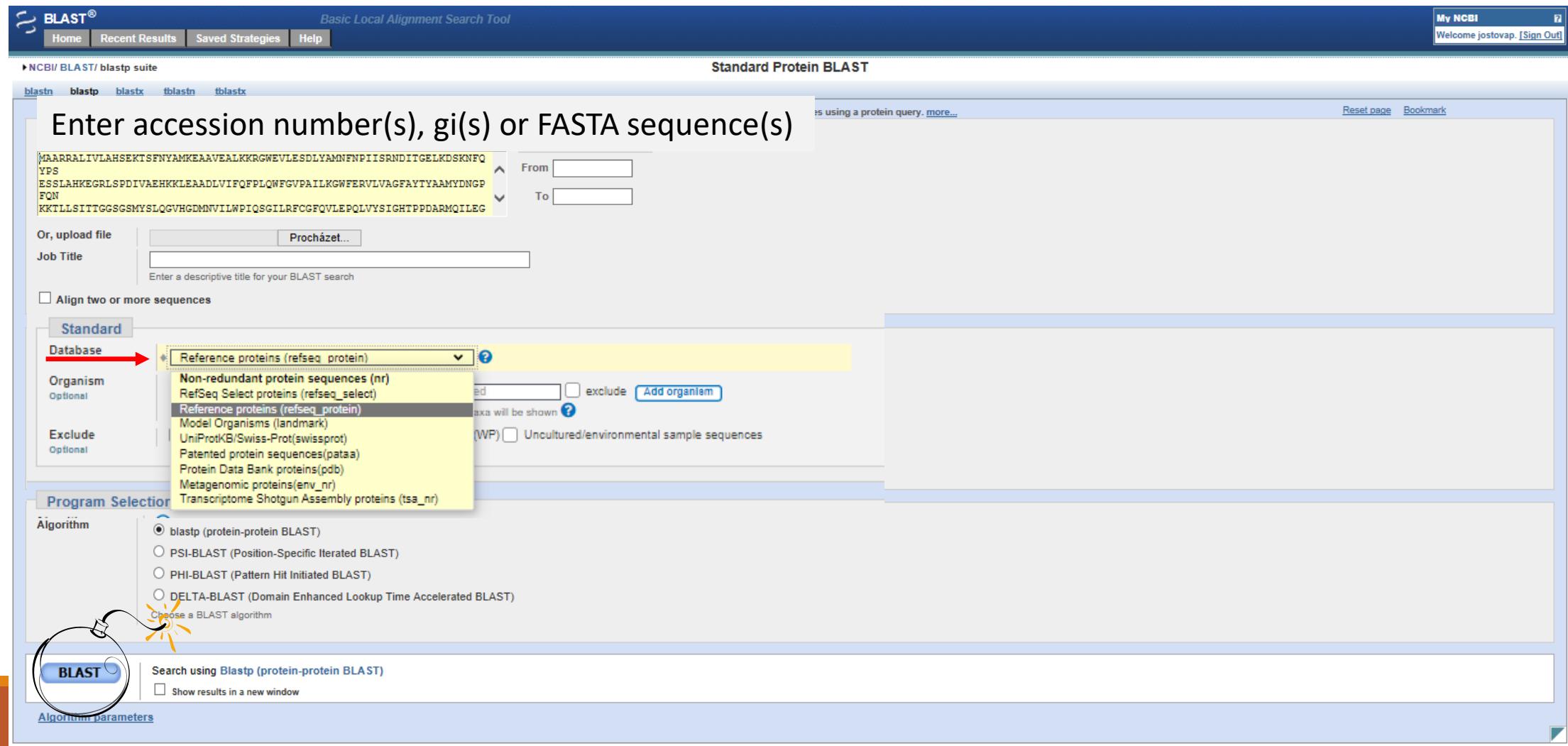
Exclude Optional

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 using Blastp (protein-protein BLAST)
 Show results in a new window

Algorithm parameters



Practical part

Try BLAST.

Download five similar sequences from different organisms.

Homework 3

- 1) How many times will be the whole sequence cut by trypsin?
- 2) Does your sequence have a typical domain?
- 3) Does your sequence have transmembrane helix?
- 4) Does your sequence have ER retention signal?
- 5) Find and download five similar sequences.

E.g use „výstřížky“



„snipping tool“

- Compile in „one note“ (or word, or pdf)
- Submit via Moodle

Homework 3 - example

1) Trypsin

33



2)

TMIMOD

# Annotation	NON-TM PROTEIN
# Length	274
# Number of predicted TMHs	0
# Exp number of AAs in TMHs	0.000000
# Exp number, first 60 AAs	0.000000
# Total prob of N-in	0.493699
outside	1 274

3)

>Macaca mulatta
MVGGRALIVLAHSERTSFNYAMKEAAEALRKKGWNEVAESDLYAMKGNFNPVIIISRKDITGKLKDPMNFQYAAESTLAYKGR
LSPDITVAEQRKLEADLVIPIQFFPLQWFGVPAILKGWPERFVYGEPEPAYTIAAMTDKGPFQSGGGAVLSITTTGGGSMYSLGQ
IHGGMONVILWPIQSGILIPCGFQVLEPQLTTSIGHTPADARIQILEGWGGGLENIWEDETFPLYTAFSSLFLDNFQAGFLMK
KEVQDEERKNGKFGLSVGHMLGKSIPTDNQVKANK

>Sus scrofa
MVGGRALIVLAHSERTSFNYAMKEAAEALRKKGWNEVTISDLYAMMNFNPVIIISRKDITGKLKDPMNFQYPAETLAYKGR
LSPDITVAEQRKLEADLVIPIQFFPLQWFGVPAILKGWPERFVYGEPEPAYTIAAMTDKGPFQSGGGAVLSITTTGGGSMYSLGQ
IHGGMONVILWPIQSGILIPCGFQVLEPQLTTSIGHTPEDARQILEGWGGGLENIWEDETFPLYTAFSSLFLDNFQAGFLMK
KEVQDEERKNGKFGLSVGHMLGKSIPTDNQVKANK

5)

>Bos taurus
MAVRKALIVLAHSERTSFNYAMKEAAEALRKKGWNEVTVSDLYAMMNFNPVIIISRKDITGKLKDPMNFQYPAETLAYKGR
LSPDITVAEQRKLEADLVIPIQFFPLQWFGVPAILKGWPERFVYGEPEPAYTIAAMTDKGPFQSGGGAVLSITTTGGGSMYSLGQ
IHGGMONVILWPIQSGILIPCGFQVLEPQLTTSIGHTPEDARQILEGWGGGLENIWEDETFPLYTAFSSLFLDNFQAGFLMK
KEVQDEERKNGKFGLSVGHMLGKSIPTDNQVKANK

>Mus musculus
MAARRKALIVLAHSERTSFNYAMKEAAEALRKKGWNEVLESDLYAMMNFNPVIIISRKDITGKLKDPMNFQYPSSESSLAYKGR
LSPDITVAEQRKLEADLVIPIQFFPLQWFGVPAILKGWPERFVYGEPEPAYTIAAMTDKGPFQSGGGAVLSITTTGGGSMYSLGQ
IHGGMONVILWPIQSGILIPCGFQVLEPQLTTSIGHTPPDARQILEGWGGGLENIWEETFLPLYTAFSSLFLDNFQAGFLMK
KEVQDEERKNGKFGLSVGHMLGKSIPTDNQVKANK

>Alligator mississippiensis
MAJJKKALIVLAHAKTSTNHAMPDAAVDALQKGKGNWSVAUSDLYAMKGNFNPVQSREDITGKLKDPMNFNYAEMGLAMKGR
LSSDITVAEQRKLEADLVIPIQFFPLQWFGVPAILKGWPERFVYGEPEAYTIAAMTDKGPFQSGGGAVLSITTTGGGSMYSLGQ
IHGGMONVILWPIQNGTLYFCGFQVLEPQLTTSIGHTPEDVRSQILMGWGRERLGSIMEEKPLSFVFSSEFMSFGGGFLMK
AEIQEQQQKDQKYGSLVQMLGKAIIPPDNQVKAQRK

4)

