Introduction to applied bioinformatics

PETRA MATOUŠKOVÁ

2024/2025

2/10

„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, domains

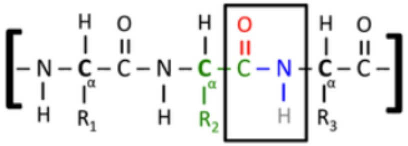
Predicting 3-D structure and the domain organization of proteins

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

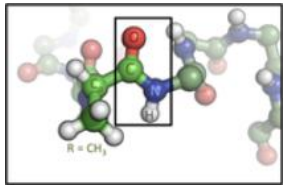
Finding evolutionary relationships between proteins, drawing proteins’ family trees

Computing the optimal alignment between two or more protein sequences

…



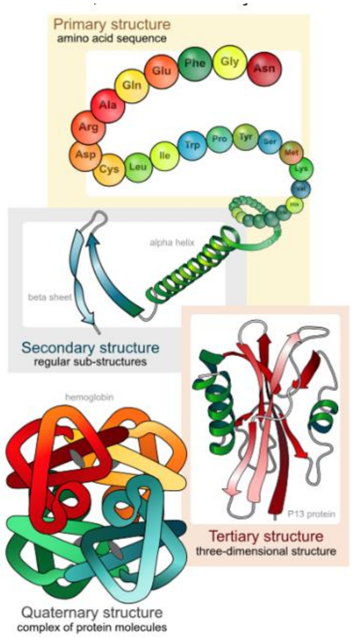
Proteins

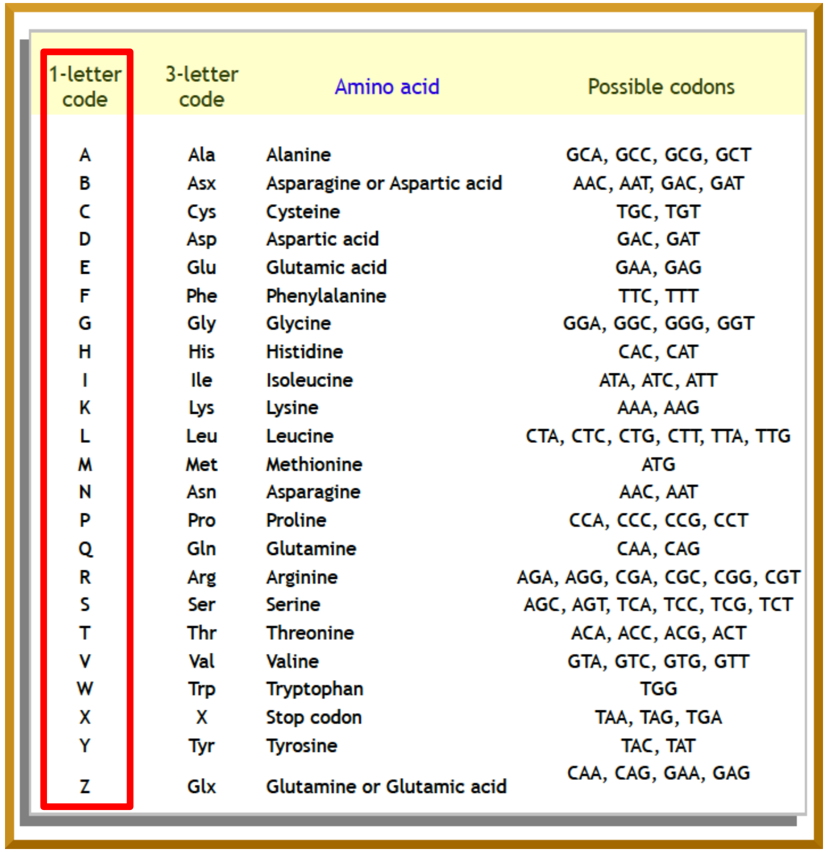


20 Aminoacids – primary structure:

(Frederick Sanger-1958 Nobel prize for insulin sequencing)

Secondary structure
Tertiary structure
Quaternary structure

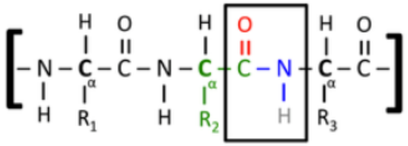




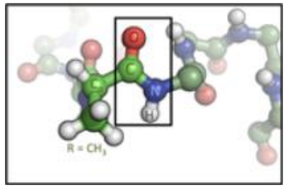
1-letter code	3-letter code	Amino acid	Possible codons
A	Ala	Alanine	GCA, GCC, GCG, GCT
B	Asx	Asparagine or Aspartic acid	AAC, AAT, GAC, GAT
C	Cys	Cysteine	TGC, TGT
D	Asp	Aspartic acid	GAC, GAT
E	Glu	Glutamic acid	GAA, GAG
F	Phe	Phenylalanine	TTC, TTT
G	Gly	Glycine	GGA, GGC, GGG, GGT
H	His	Histidine	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 ⇨ STRUCTURE ⇨ FUNCTION

Protein sequences are the fundamental determinants of biological structure and function.

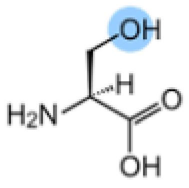


Proteins

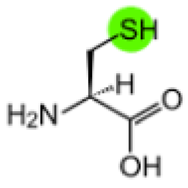


20 Aminoacids – primary structure:

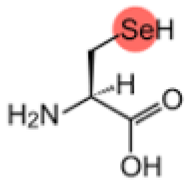
J	Xle	Isoleucine/Leucine
O	Pyl	Pyrrolysine
U	Sec	Selenocysteine
X	Xaa	Any residue



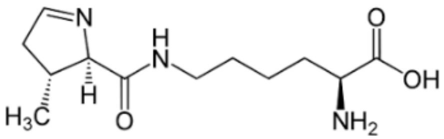
Serine (Ser)



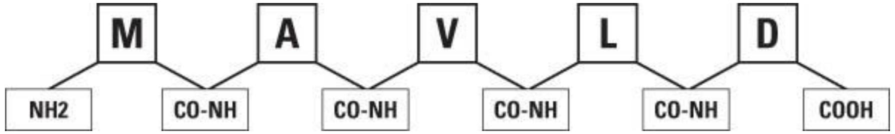
Cysteine (Cys)

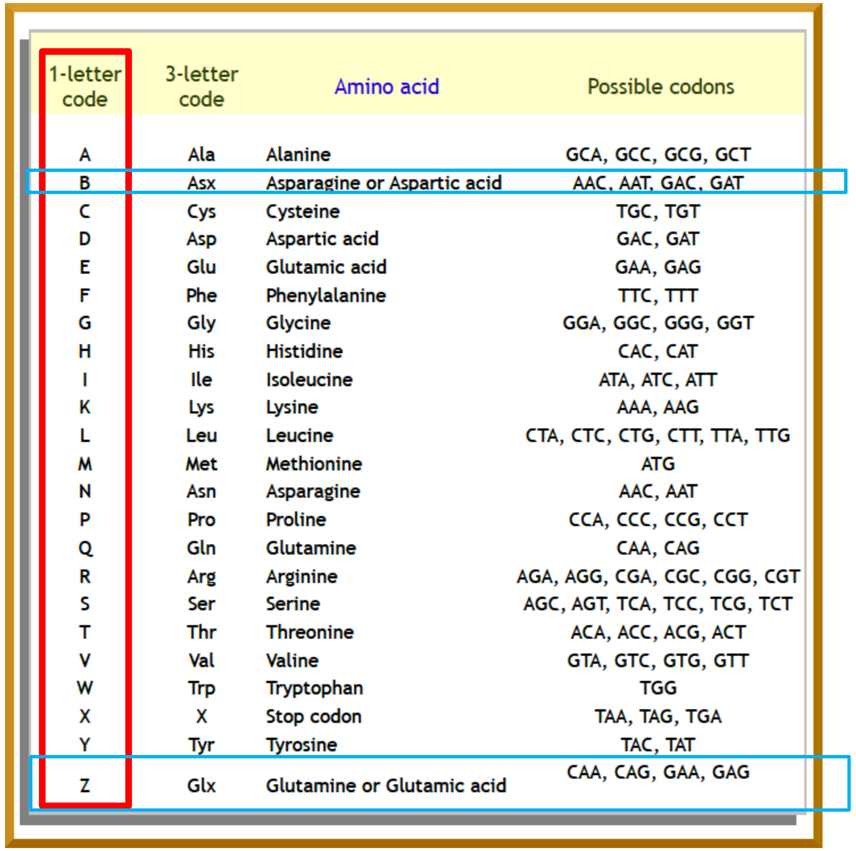


Selenocysteine (Sec)



N-terminus → C-terminus





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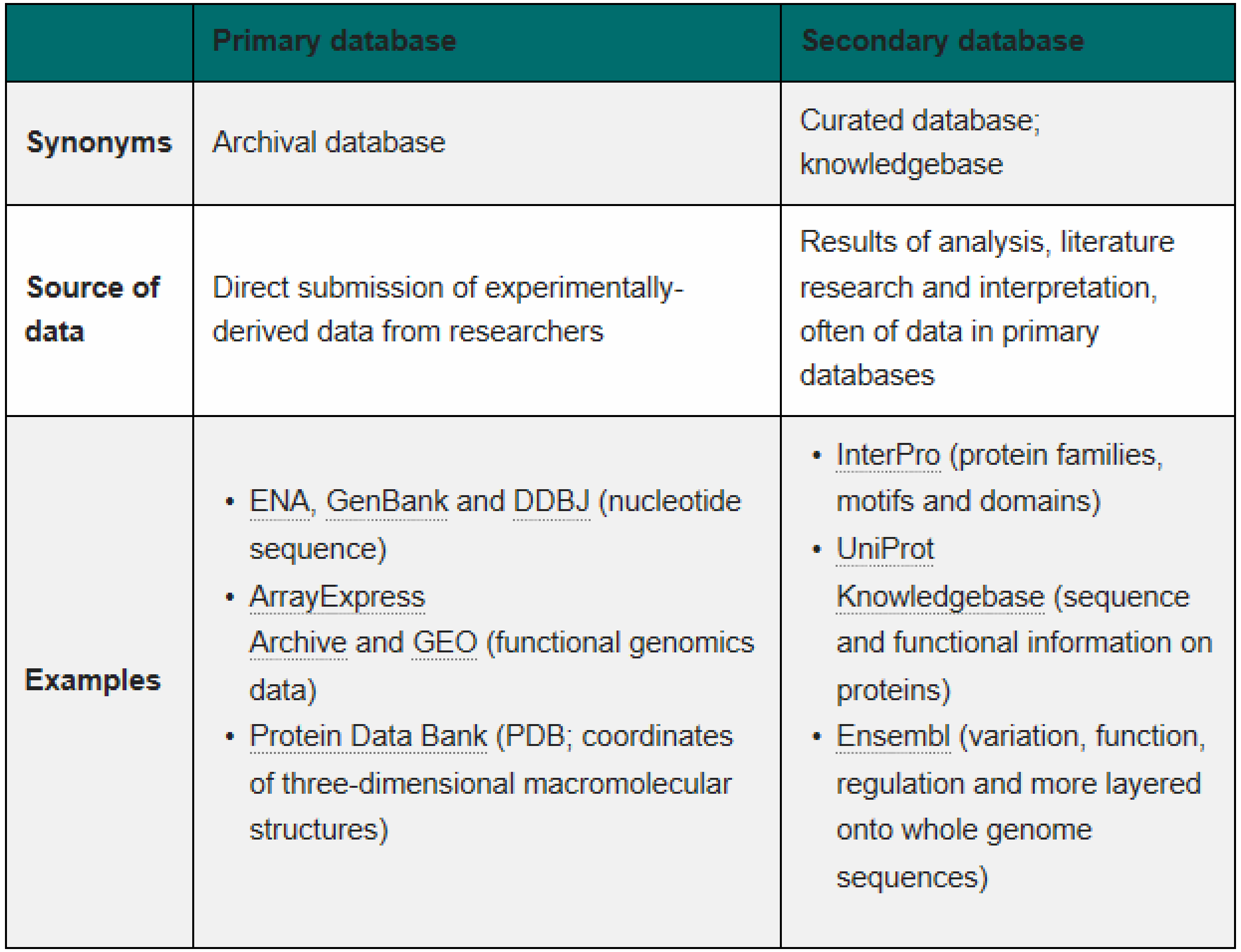
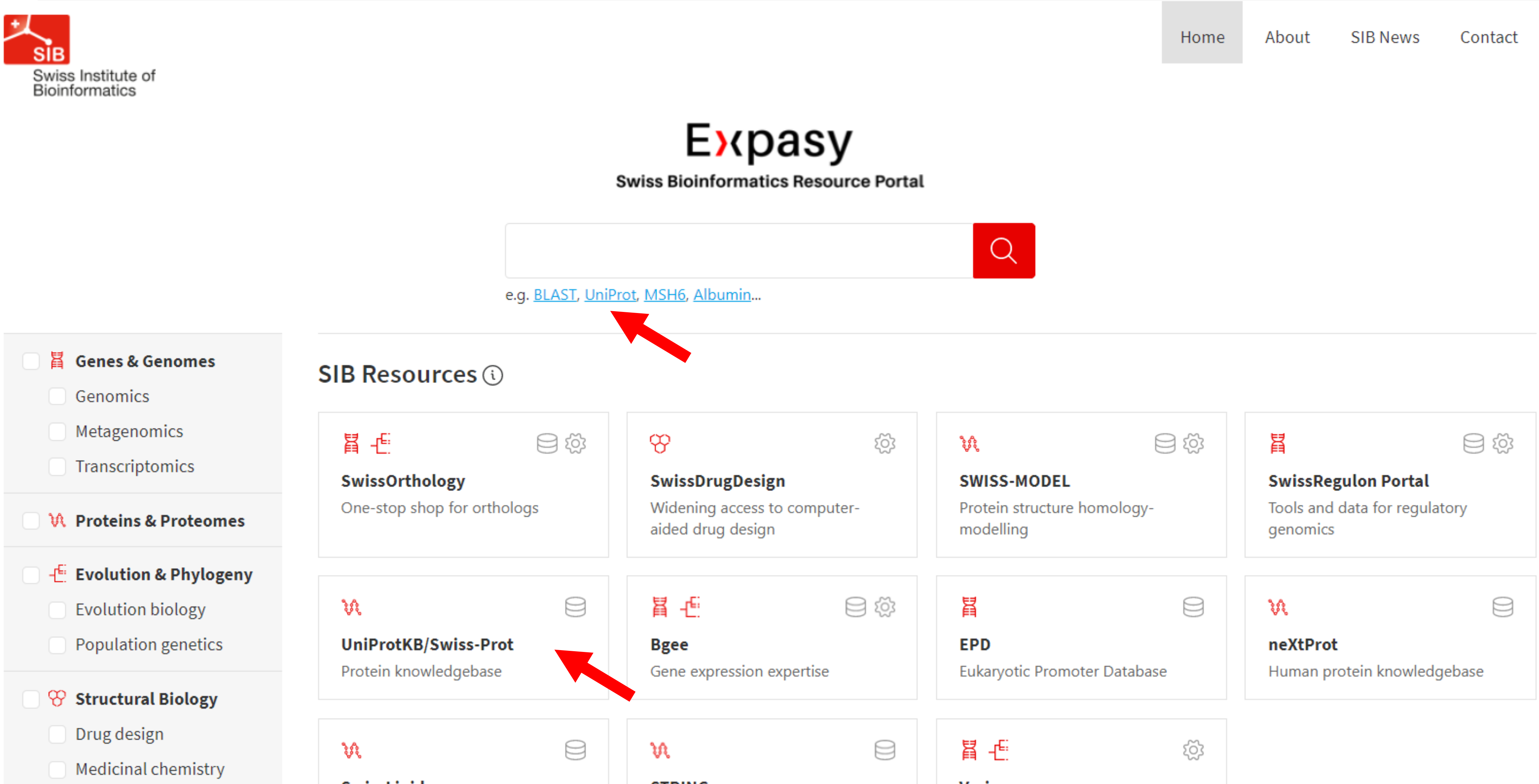
Y	Tyr	Tyrosine	TAC, TAT
Z	Glx	Glutamine or Glutamic acid	CAA, CAG, GAA, GAG

Databases



	Primary database	Secondary database
Synonyms	Archival database	Curated database; knowledgebase
Source of data	Direct submission of experimentally-derived data from researchers	Results of analysis, literature research and interpretation, often of data in primary databases
Examples	• ENA, GenBank and DDBJ (nucleotide sequence) • ArrayExpress Archive and GEO (functional genomics data) • Protein Data Bank (PDB; coordinates of three-dimensional macromolecular structures)	• InterPro (protein families, motifs and domains) • UniProt Knowledgebase (sequence and functional information on proteins) • Ensembl (variation, function, regulation and more layered onto whole genome sequences)

Protein database: Expasy/UniProt



SIB Swiss Institute of Bioinformatics

Home About SIB News Contact

Expasy

Swiss Bioinformatics Resource Portal

e.g. BLAST, UniProt, MSH6, Albumin...

- ☐ **Genes & Genomes**
  - ☐ Genomics
  - ☐ Metagenomics
  - ☐ Transcriptomics
- ☐ **Proteins & Proteomes**
- ☐ **Evolution & Phylogeny**
  - ☐ Evolution biology
  - ☐ Population genetics
- ☐ **Structural Biology**
  - ☐ Drug design
  - ☐ Medicinal chemistry

SIB Resources

SwissOrthology
One-stop shop for orthologs

SwissDrugDesign
Widening access to computer-aided drug design

SWISS-MODEL
Protein structure homology-modelling

SwissRegulon Portal
Tools and data for regulatory genomics

UniProtKB/Swiss-Prot
Protein knowledgebase

Bgee
Gene expression expertise

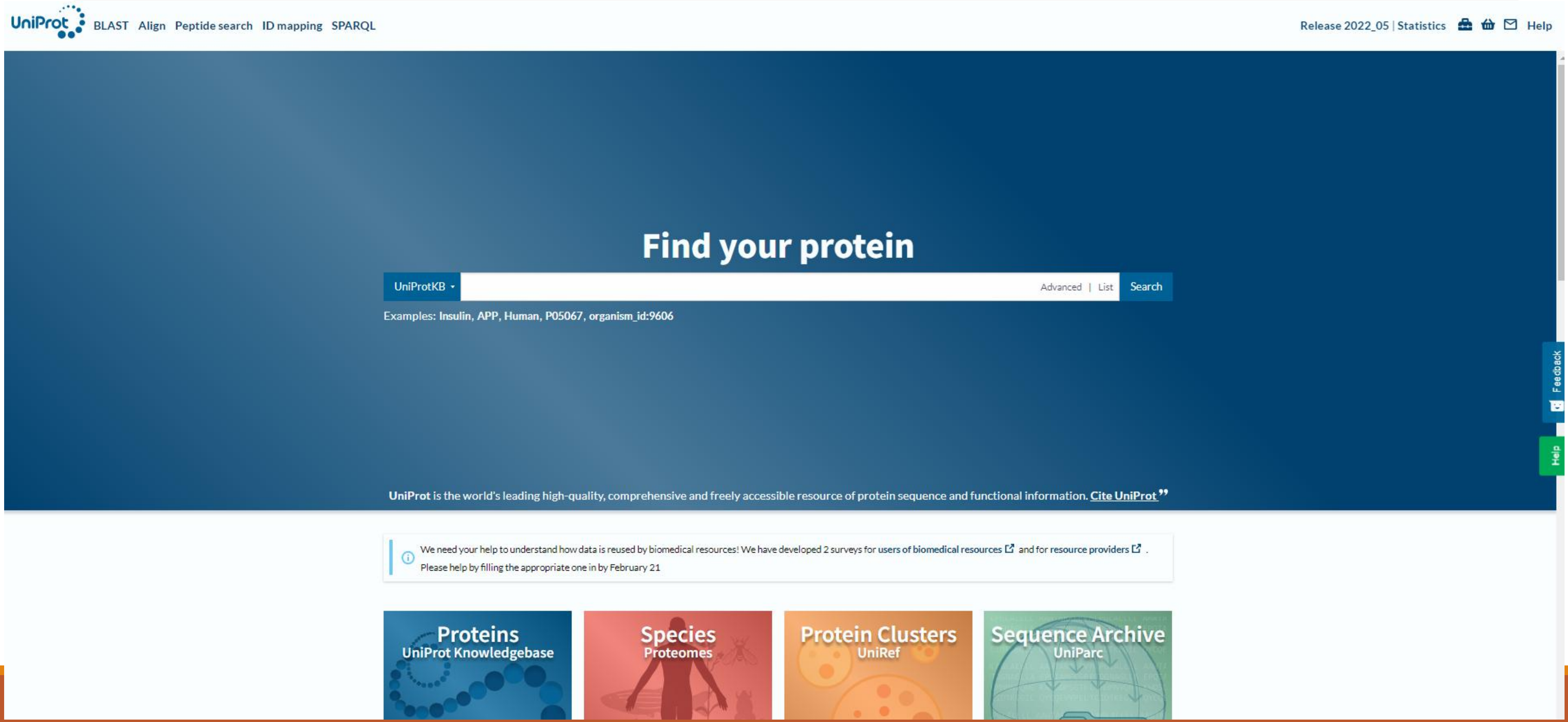
EPD
Eukaryotic Promoter Database

neXtProt
Human protein knowledgebase

http

Protein database: UniProt

http://www.uniprot.org/



Find your protein

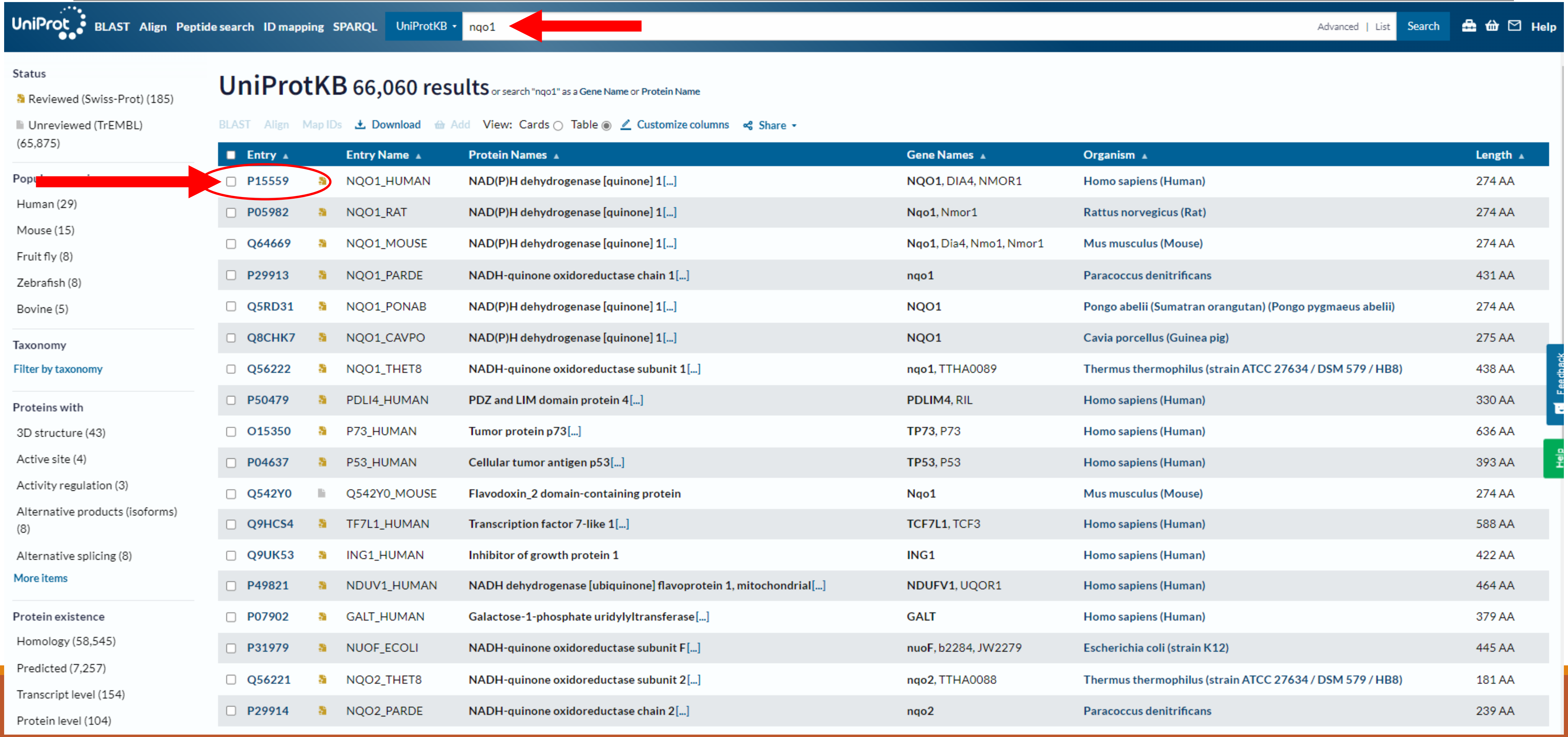
Examples: Insulin, APP, Human, P05067, organism_id:9606

UniProt is the world's leading high-quality, comprehensive and freely accessible resource of protein sequence and functional information. Cite UniProt

We need your help to understand how data is reused by biomedical resources! We have developed 2 surveys for users of biomedical resources and for resource providers. Please help by filling the appropriate one in by February 21

Protein database: UniProt

http://www.uniprot.org/



nqo1

UniProtKB 66,060 results or search "nqo1" as a Gene Name or Protein Name

BLAST Align Map IDs Download Add View: Cards ○ Table ● Customize columns Share ▾

Status

Reviewed (Swiss-Prot) (185)

Unreviewed (TrEMBL) (65,875)

Popu

Human (29)

Mouse (15)

Fruit fly (8)

Zebrafish (8)

Bovine (5)

Taxonomy

Filter by taxonomy

Proteins with

3D structure (43)

Active site (4)

Activity regulation (3)

Alternative products (isoforms) (8)

Alternative splicing (8)

More items

Protein existence

Homology (58,545)

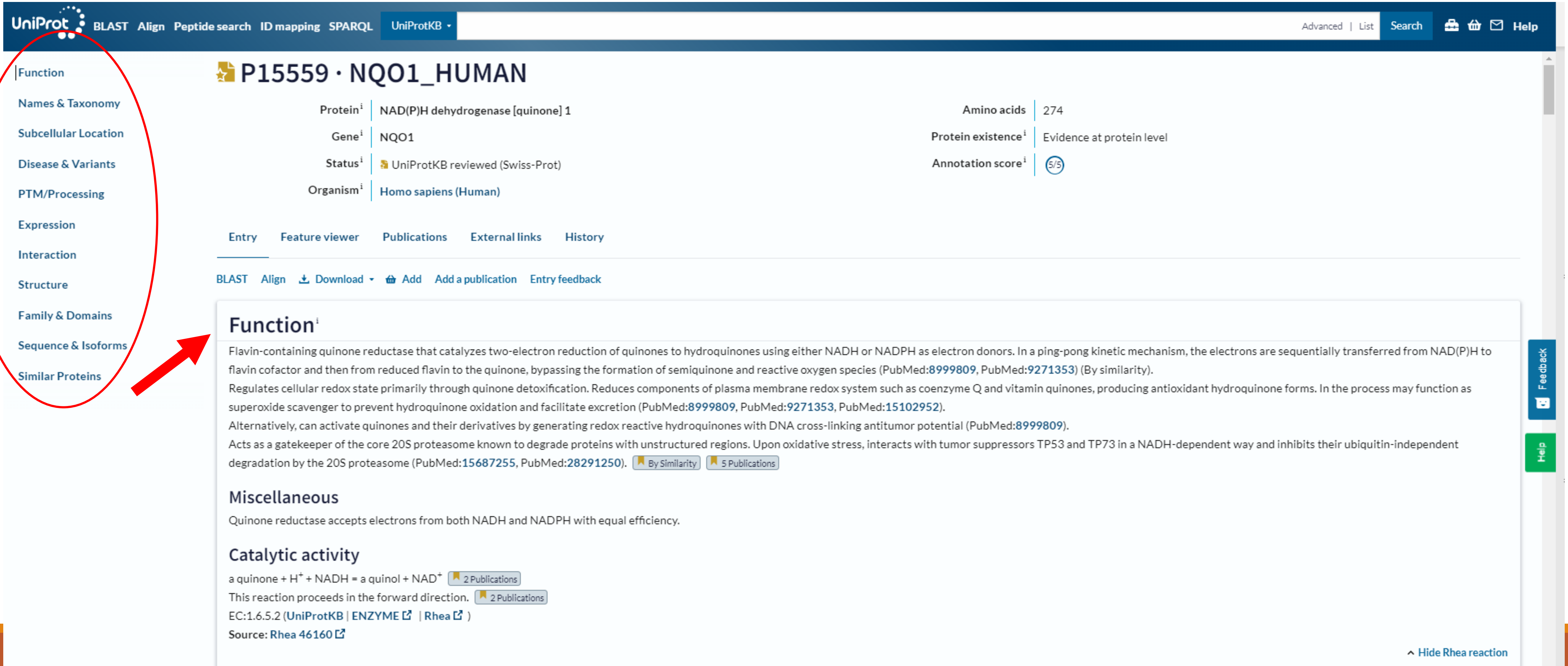
Predicted (7,257)

Transcript level (154)

Protein level (104)

■	Entry ▲	Entry Name ▲	Protein Names ▲	Gene Names ▲	Organism ▲	Length ▲
☐	P15559	NQO1_HUMAN	NAD(P)H dehydrogenase [quinone] 1[...]	NQO1, DIA4, NMOR1	Homo sapiens (Human)	274 AA
☐	P05982	NQO1_RAT	NAD(P)H dehydrogenase [quinone] 1[...]	Nqo1, Nmor1	Rattus norvegicus (Rat)	274 AA
☐	Q64669	NQO1_MOUSE	NAD(P)H dehydrogenase [quinone] 1[...]	Nqo1, Dia4, Nmo1, Nmor1	Mus musculus (Mouse)	274 AA
☐	P29913	NQO1_PARDE	NADH-quinone oxidoreductase chain 1[...]	nqo1	Paracoccus denitrificans	431 AA
☐	Q5RD31	NQO1_PONAB	NAD(P)H dehydrogenase [quinone] 1[...]	NQO1	Pongo abelii (Sumatran orangutan) (Pongo pygmaeus abelii)	274 AA
☐	Q8CHK7	NQO1_CAVPO	NAD(P)H dehydrogenase [quinone] 1[...]	NQO1	Cavia porcellus (Guinea pig)	275 AA
☐	Q56222	NQO1_THET8	NADH-quinone oxidoreductase subunit 1[...]	nqo1, TTHA0089	Thermus thermophilus (strain ATCC 27634 / DSM 579 / HB8)	438 AA
☐	P50479	PDLI4_HUMAN	PDZ and LIM domain protein 4[...]	PDLIM4, RIL	Homo sapiens (Human)	330 AA
☐	O15350	P73_HUMAN	Tumor protein p73[...]	TP73, P73	Homo sapiens (Human)	636 AA
☐	P04637	P53_HUMAN	Cellular tumor antigen p53[...]	TP53, P53	Homo sapiens (Human)	393 AA
☐	Q542Y0	Q542Y0_MOUSE	Flavodoxin_2 domain-containing protein	Nqo1	Mus musculus (Mouse)	274 AA
☐	Q9HCS4	TF7L1_HUMAN	Transcription factor 7-like 1[...]	TCF7L1, TCF3	Homo sapiens (Human)	588 AA
☐	Q9UK53	ING1_HUMAN	Inhibitor of growth protein 1	ING1	Homo sapiens (Human)	422 AA
☐	P49821	NDUV1_HUMAN	NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial[...]	NDUFV1, UQOR1	Homo sapiens (Human)	464 AA
☐	P07902	GALT_HUMAN	Galactose-1-phosphate uridylyltransferase[...]	GALT	Homo sapiens (Human)	379 AA
☐	P31979	NUOF_ECOLI	NADH-quinone oxidoreductase subunit F[...]	nuoF, b2284, JW2279	Escherichia coli (strain K12)	445 AA
☐	Q56221	NQO2_THET8	NADH-quinone oxidoreductase subunit 2[...]	nqo2, TTHA0088	Thermus thermophilus (strain ATCC 27634 / DSM 579 / HB8)	181 AA
☐	P29914	NQO2_PARDE	NADH-quinone oxidoreductase chain 2[...]	nqo2	Paracoccus denitrificans	239 AA

Protein database: UniProt



P15559 · NQO1_HUMAN

Protein: NAD(P)H dehydrogenase [quinone] 1
Gene: NQO1
Status: UniProtKB reviewed (Swiss-Prot)
Organism: Homo sapiens (Human)
Amino acids: 274
Protein existence: Evidence at protein level
Annotation score: 5/5

Function

Flavin-containing quinone reductase that catalyzes two-electron reduction of quinones to hydroquinones using either NADH or NADPH as electron donors. In a ping-pong kinetic mechanism, the electrons are sequentially transferred from NAD(P)H to flavin cofactor and then from reduced flavin to the quinone, bypassing the formation of semiquinone and reactive oxygen species (PubMed:8999809, PubMed:9271353) (By similarity).

Regulates cellular redox state primarily through quinone detoxification. Reduces components of plasma membrane redox system such as coenzyme Q and vitamin quinones, producing antioxidant hydroquinone forms. In the process may function as superoxide scavenger to prevent hydroquinone oxidation and facilitate excretion (PubMed:8999809, PubMed:9271353, PubMed:15102952).

Alternatively, can activate quinones and their derivatives by generating redox reactive hydroquinones with DNA cross-linking antitumor potential (PubMed:8999809).

Acts as a gatekeeper of the core 20S proteasome known to degrade proteins with unstructured regions. Upon oxidative stress, interacts with tumor suppressors TP53 and TP73 in a NADH-dependent way and inhibits their ubiquitin-independent degradation by the 20S proteasome (PubMed:15687255, PubMed:28291250). By Similarity | 5 Publications

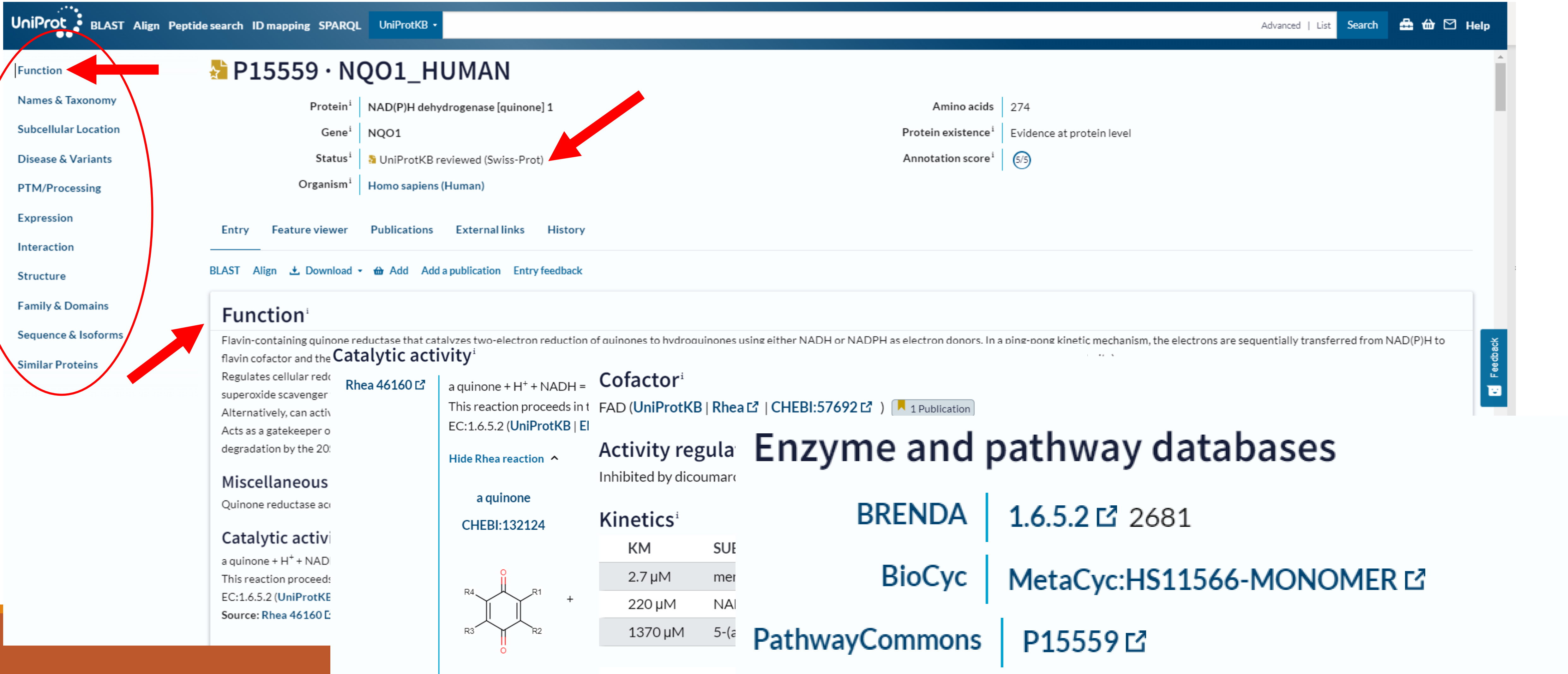
Miscellaneous

Quinone reductase accepts electrons from both NADH and NADPH with equal efficiency.

Catalytic activity

a quinone + H^+ + NADH = a quinol + NAD^+ 2 Publications
This reaction proceeds in the forward direction. 2 Publications
EC:1.6.5.2 (UniProtKB | ENZYME | Rhea)
Source: Rhea 46160

Protein database: UniProt



- Function
- Names & Taxonomy
- Subcellular Location
- Disease & Variants
- PTM/Processing
- Expression
- Interaction
- Structure
- Family & Domains
- Sequence & Isoforms
- Similar Proteins

P15559 · NQO1_HUMAN

Protein	NAD(P)H dehydrogenase [quinone] 1	Amino acids	274
Gene	NQO1	Protein existence	Evidence at protein level
Status	UniProtKB reviewed (Swiss-Prot)	Annotation score	5/5
Organism	Homo sapiens (Human)		

Entry | Feature viewer | Publications | External links | History

BLAST | Align | Download | Add | Add a publication | Entry feedback

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Regulates cellular red

superoxide scavenger

Alternatively, can activ

Acts as a gatekeeper o

degradation by the 20

Miscellaneous

Quinone reductase ac

Catalytic activi

a quinone + H^+ + NAD

This reaction proceeds

EC:1.6.5.2 (UniProtKE

Source: Rhea 46160

Catalytic activity

Rhea 46160

a quinone + H^+ + NADH =

This reaction proceeds in t

EC:1.6.5.2 (UniProtKB | El

Hide Rhea reaction

a quinone

CHEBI:132124

Cofactor

FAD (UniProtKB | Rhea | CHEBI:57692) 1 Publication

Activity regula

Inhibited by dicoumar

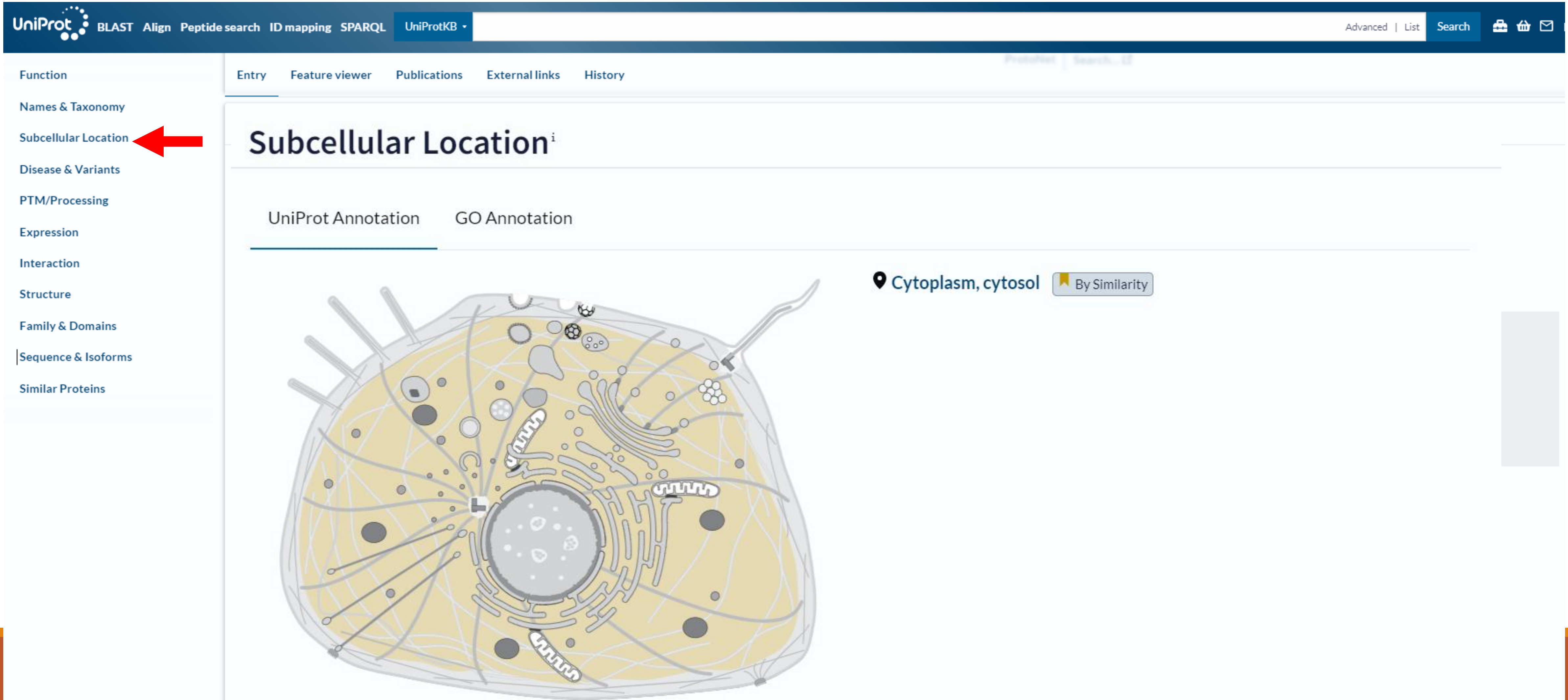
Kinetics

KM	SUE
2.7 μM	mer
220 μM	NAI
1370 μM	5-(a

Enzyme and pathway databases

BRENDA	1.6.5.2 2681
BioCyc	MetaCyc:HS11566-MONOMER
PathwayCommons	P15559

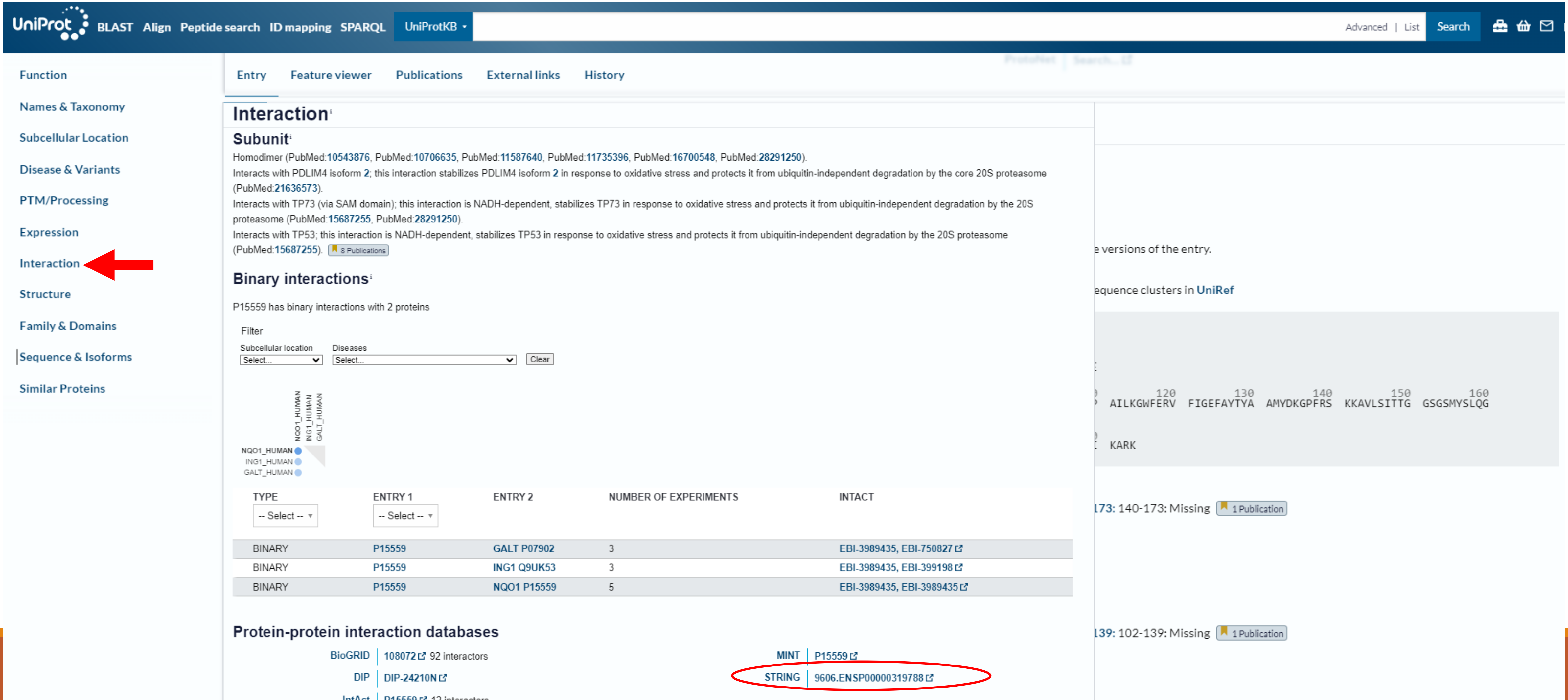
Protein database: UniProt



Subcellular Location

Cytoplasm, cytosol By Similarity

Protein database: UniProt



Interaction

Subunit

Homodimer (PubMed:10543876, PubMed:10706635, PubMed:11587640, PubMed:11735396, PubMed:16700548, PubMed:28291250).

Interacts with PDLIM4 isoform 2; this interaction stabilizes PDLIM4 isoform 2 in response to oxidative stress and protects it from ubiquitin-independent degradation by the core 20S proteasome (PubMed:21636573).

Interacts with TP73 (via SAM domain); this interaction is NADH-dependent, stabilizes TP73 in response to oxidative stress and protects it from ubiquitin-independent degradation by the 20S proteasome (PubMed:15687255, PubMed:28291250).

Interacts with TP53; this interaction is NADH-dependent, stabilizes TP53 in response to oxidative stress and protects it from ubiquitin-independent degradation by the 20S proteasome (PubMed:15687255). 8 Publications

Binary interactions

P15559 has binary interactions with 2 proteins

Filter

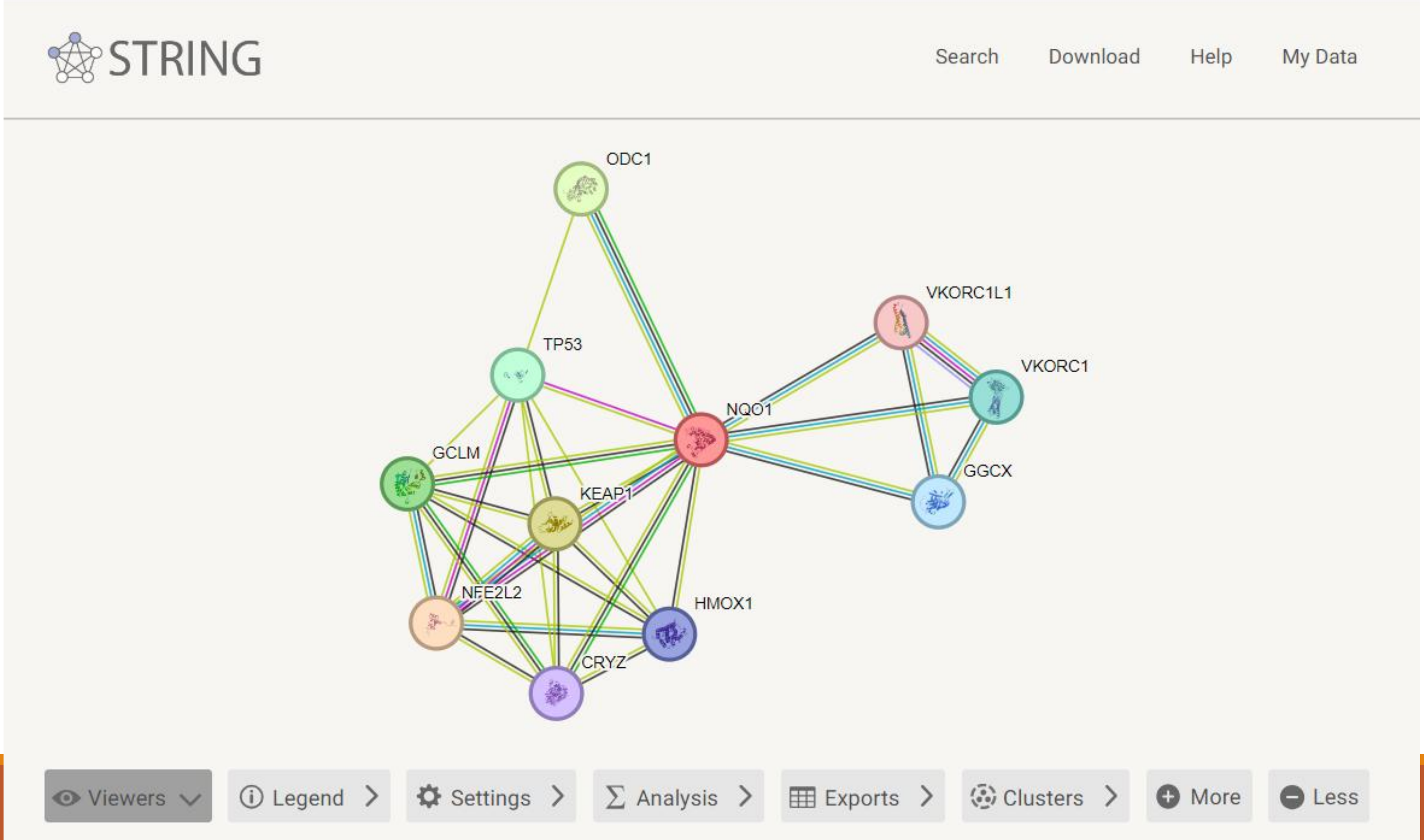
Subcellular location: Select...
Diseases: Select...
Clear

TYPE	ENTRY 1	ENTRY 2	NUMBER OF EXPERIMENTS	INTACT
-- Select --	-- Select --			
BINARY	P15559	GALT P07902	3	EBI-3989435, EBI-750827
BINARY	P15559	ING1 Q9UK53	3	EBI-3989435, EBI-399198
BINARY	P15559	NQO1 P15559	5	EBI-3989435, EBI-3989435

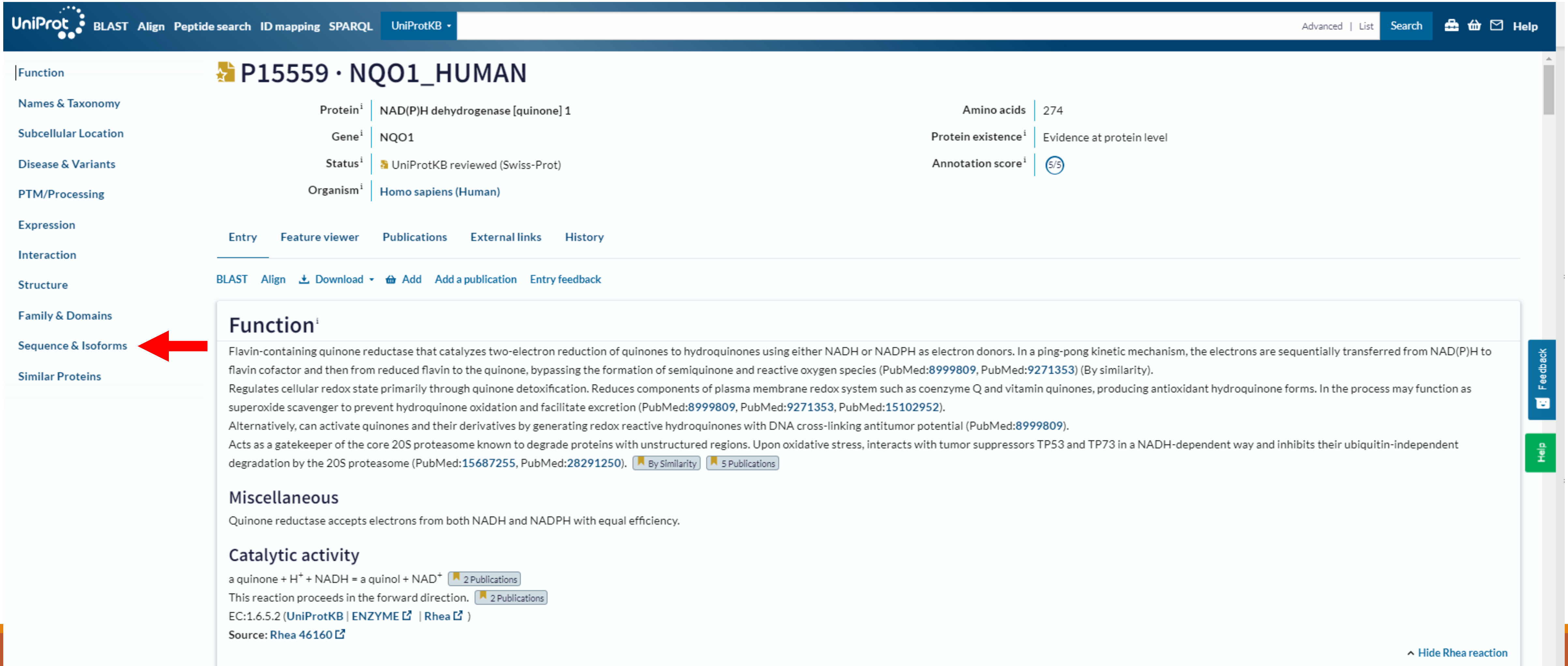
Protein-protein interaction databases

BioGRID	108072 92 interactors	MINT	P15559
DIP	DIP-24210N	STRING	9606.ENSP00000319788
IntAct	P15559 12 interactors		

STRING: protein-protein interaction



Protein database: UniProt



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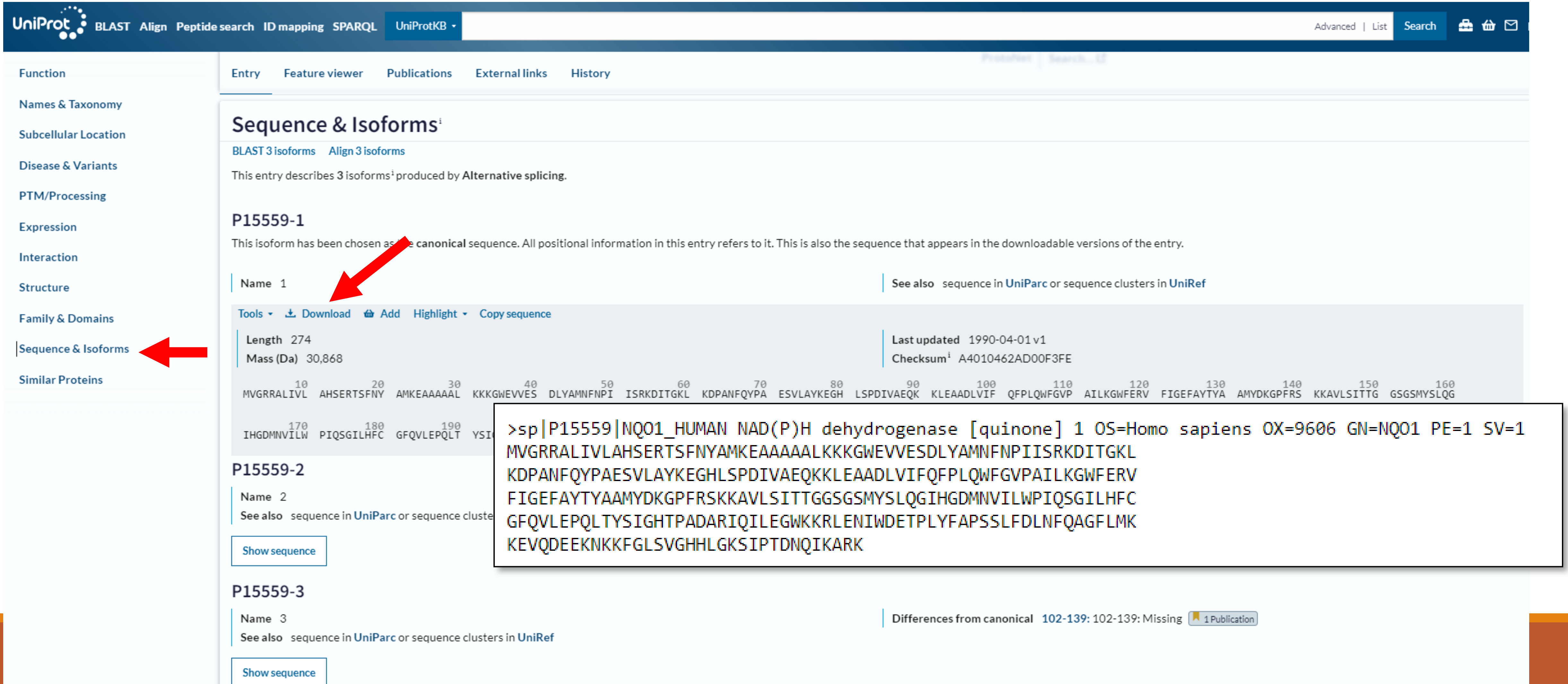
Source: Rhea 46160

Protein database: UniProt



Sequence & Isoforms

BLAST 3 isoforms Align 3 isoforms

This entry describes **3** isoforms produced by **Alternative splicing**.

P15559-1

This isoform has been chosen as the **canonical** sequence. All positional information in this entry refers to it. This is also the sequence that appears in the downloadable versions of the entry.

Name 1

See also sequence in UniParc or sequence clusters in UniRef

Length 274
Mass (Da) 30,868

Last updated 1990-04-01 v1
Checksum A4010462AD00F3FE

```
        10         20         30         40         50         60         70         80         90        100        110        120        130        140        150        160
MVGRRALIVL AHSERTSFNY AMKEAAAAAL KKKGWEVVES DLYAMNFNPI ISRKDITGKL KDPANFQYPA ESVLAYKEGH LSPDIVAEQK KLEAADLVIF QFPLQWFGVP AILKGWFERV FIGEFAYTYA AMYDKGPFRS KKAVLSITTG GSGSMYSLQG

       170        180        190
IHGDMNVILW PIQSGILHFC GFQVLEPQLT YSI
```

```
>sp|P15559|NQO1_HUMAN NAD(P)H dehydrogenase [quinone] 1 OS=Homo sapiens OX=9606 GN=NQO1 PE=1 SV=1
MVGRRALIVLAHSERTSFNYAMKEAAAAALKKKGWEVVESDLYAMNFNPIISRKDITGKL
KDPANFQYPAESVLAYKEGHLSPDIVAEQKKLEAADLVIFQFPLQWFGVPAILKGWFERV
FIGEFAYTYAAMYDKGPFRSKKAVLSITTGGSGSMYSLQGIHGDMNVILWPIQSGILHFC
GFQVLEPQLTYSIGHTPADARIQILEGWKKRLENIWDETPLYFAPSSLFDLNFQAGFLMK
KEVQDEEKNKKFGLSVGHHLGKSIPTDNQIKARK
```

P15559-2

Name 2
See also sequence in UniParc or sequence cluste

P15559-3

Name 3
See also sequence in UniParc or sequence clusters in UniRef

Differences from canonical 102-139: 102-139: Missing 1 Publication

FASTA (and RAW) format

FASTA = popular tool for sequence comparison and database searching

W.R. Pearson a D.J. Lipman 1988

fasta format:

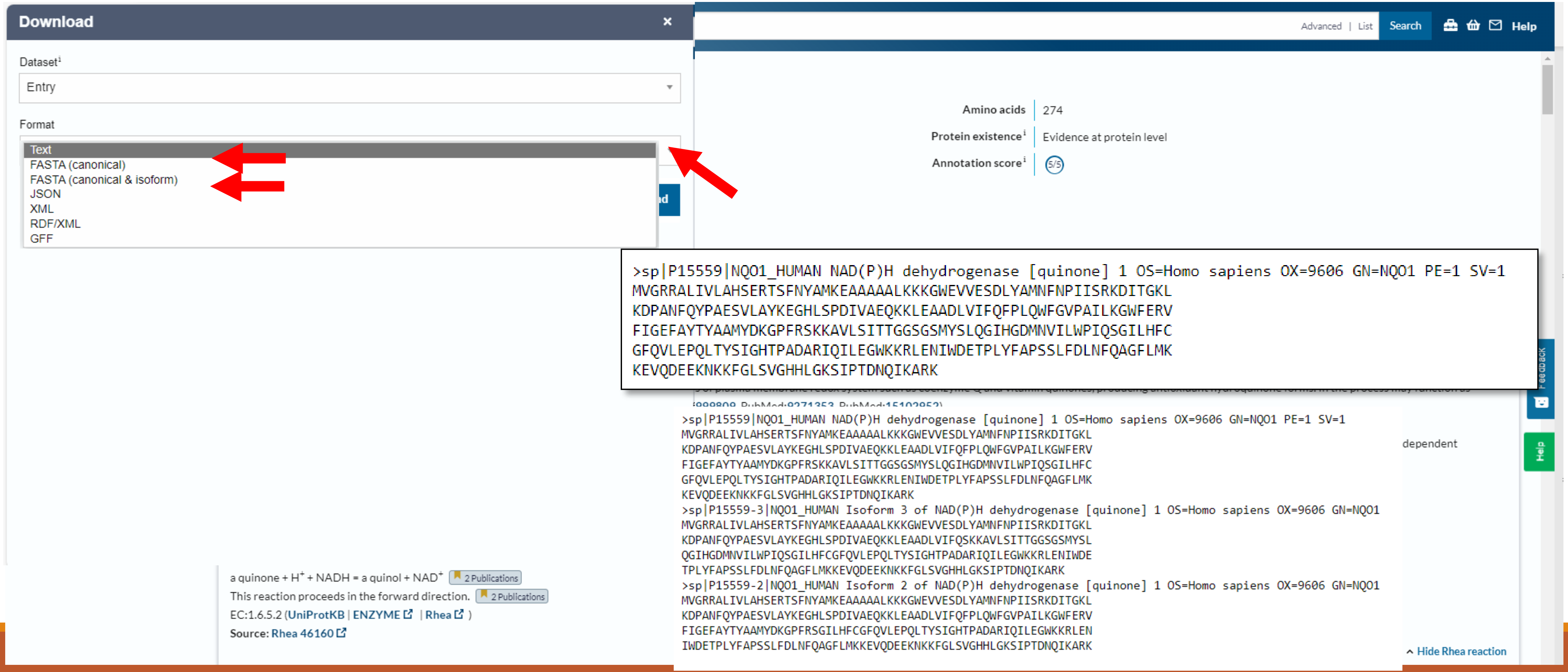
```
>NQO1_homo
MVGRRALIVLAHSERTSFNYAMKEAAAAA
LKKKGWEVVESDLYAMNFNPIISRKDITG
KLKDPANFQYPA
```

```
MVGRRALIVLAHSERTSFNYAMKEAAAAA
LKKKGWEVVESDLYAMNFNPIISRKDITG
KLKDPANFQYPA
```

1. „definition“ line starts with **>** and unique identification follows.

2. line-a sequence (DNA/protein- single letter code).

Protein database: UniProt



Dataset: Entry

Format:
- Text
- FASTA (canonical)
- FASTA (canonical & isoform)
- JSON
- XML
- RDF/XML
- GFF

Amino acids: 274

Protein existence: Evidence at protein level

Annotation score: 5/5

```
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KDPANFQYPAESVLAYKEGHLSPDIVAEQKKLEAADLVIFQFPLQWFGVPAILKGWFERV
FIGEFAYTYAAMYDKGPFRSKKAVLSITTGGSGSMYSLQGIHGDMNVILWPIQSGILHFC
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```
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>sp|P15559-2|NQO1_HUMAN Isoform 2 of NAD(P)H dehydrogenase [quinone] 1 OS=Homo sapiens OX=9606 GN=NQO1
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```

dependent

a quinone + H^+ + NADH = a quinol + NAD^+ 2 Publications

This reaction proceeds in the forward direction. 2 Publications

EC:1.6.5.2 (UniProtKB | ENZYME | Rhea)

Source: Rhea 46160

^ Hide Rhea reaction

Practical part in UniProt

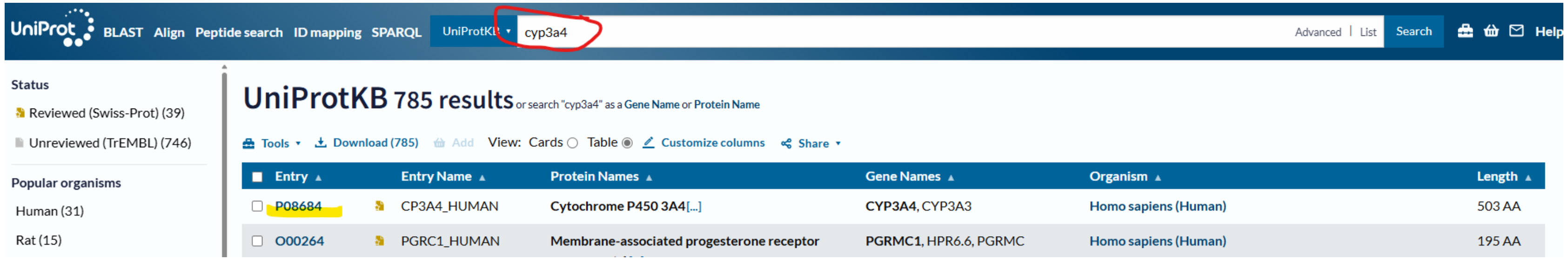
Find the accession number of human cytochrome P450 3A4 (CYP3A4)

What function has and where is locallized protein Q9C0B1?

What function has enzyme O95251 and how many isoforms it has?

Practical part in UniProt

Find the accession number of human cytochrome P450 3A4 (CYP3A4)



cyp3a4

Status
Reviewed (Swiss-Prot) (39)
Unreviewed (TrEMBL) (746)

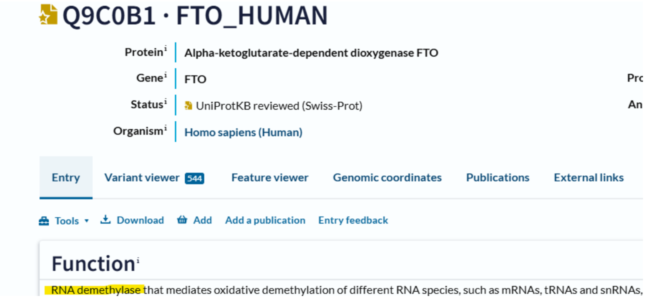
Popular organisms
Human (31)
Rat (15)

UniProtKB 785 results or search "cyp3a4" as a Gene Name or Protein Name

Tools ▾ Download (785) Add View: Cards ○ Table ● Customize columns Share ▾

☐ Entry	Entry Name	Protein Names	Gene Names	Organism	Length
☐ P08684	CP3A4_HUMAN	Cytochrome P450 3A4[...]	CYP3A4, CYP3A3	Homo sapiens (Human)	503 AA
☐ O00264	PGRC1_HUMAN	Membrane-associated progesterone receptor	PGRMC1, HPR6.6, PGRMC	Homo sapiens (Human)	195 AA

What function has and where is locallized protein Q9C0B1?

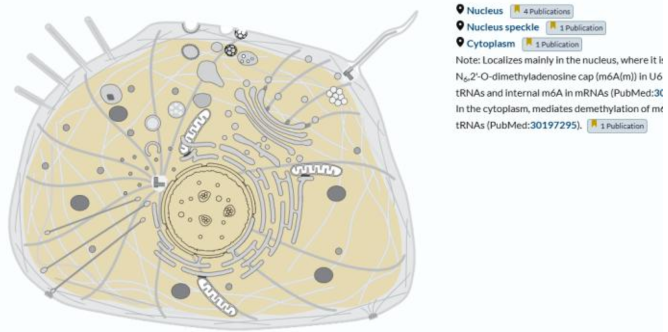


Q9C0B1 · FTO_HUMAN

Protein | Alpha-ketoglutarate-dependent dioxygenase FTO
Gene | FTO
Status | UniProtKB reviewed (Swiss-Prot)
Organism | Homo sapiens (Human)

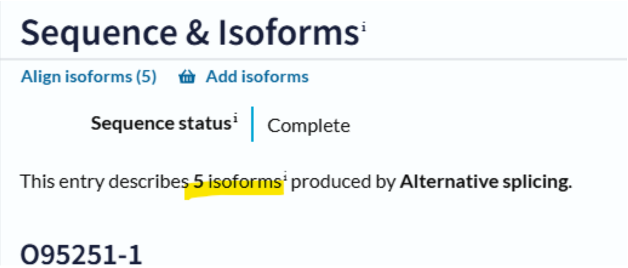
Function

RNA demethylase that mediates oxidative demethylation of different RNA species, such as mRNAs, tRNAs and snRNAs,



Nucleus 4 Publications
Nucleus speckle 1 Publication
Cytoplasm 1 Publication

Note: Localizes mainly in the nucleus, where it i
N_6,2'-O-dimethyladenosine cap (m6A(m)) in U6
tRNAs and internal m6A in mRNAs (PubMed:3
In the cytoplasm, mediates demethylation of m
tRNAs (PubMed:30197295). 1 Publication



Sequence & Isoforms

Sequence status | Complete

This entry describes 5 isoforms produced by **Alternative splicing.**

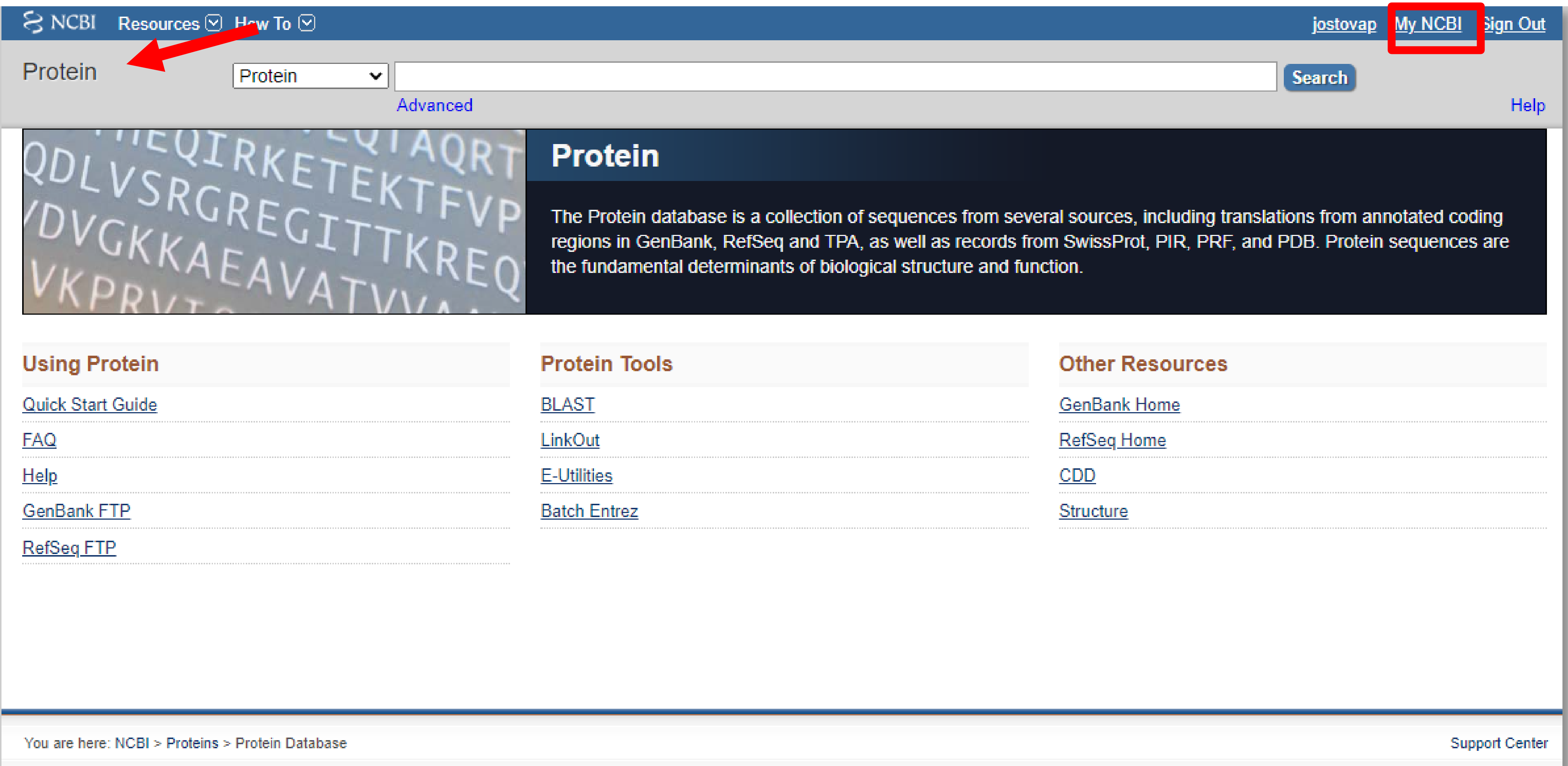
O95251-1

What function has enzyme O95251 and how many isoforms it has?

O95251 · KAT7_HUMAN

Protein | Histone acetyltransferase KAT7

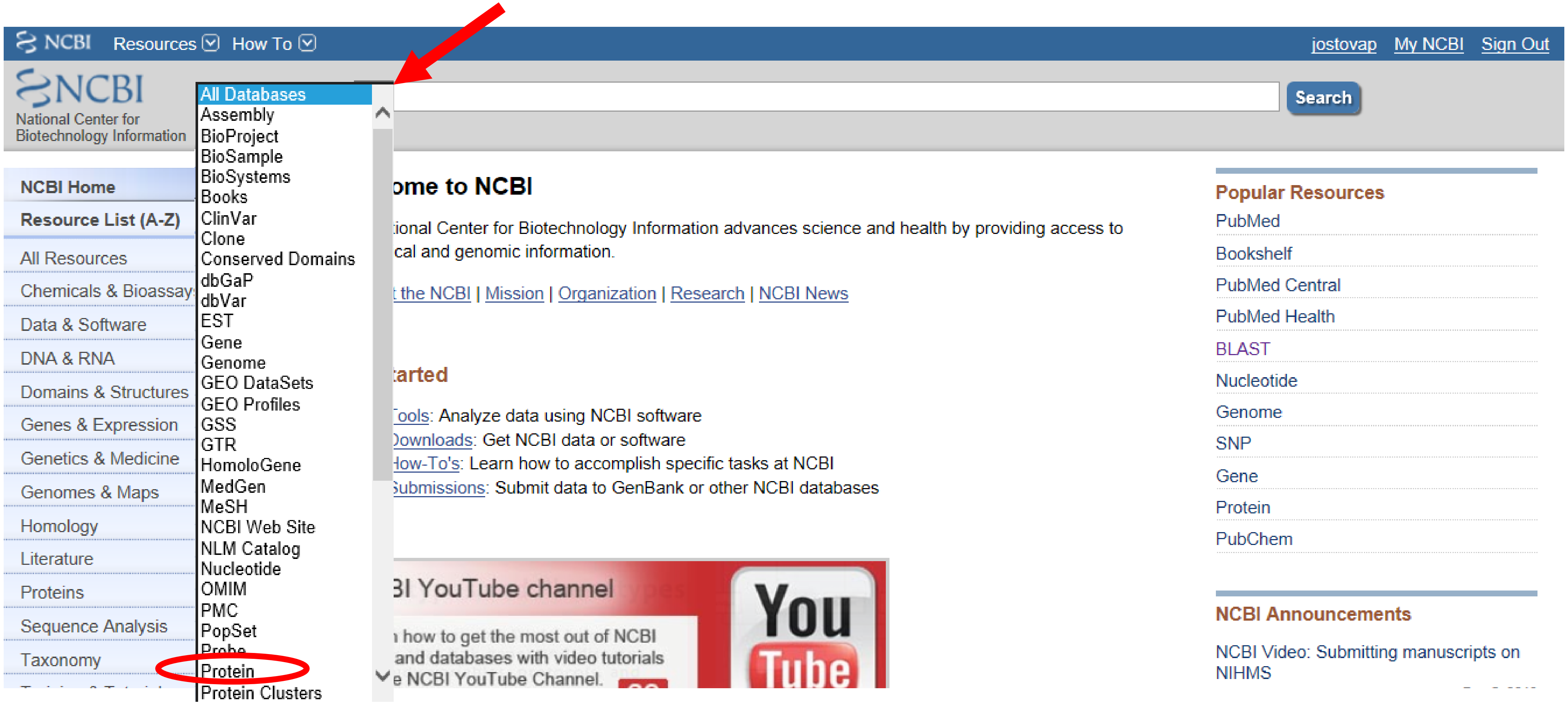
Protein database: NCBI



Protein

The Protein database is a collection of sequences from several sources, including translations from annotated coding regions in GenBank, RefSeq and TPA, as well as records from SwissProt, PIR, PRF, and PDB. Protein sequences are the fundamental determinants of biological structure and function.

Protein database: NCBI



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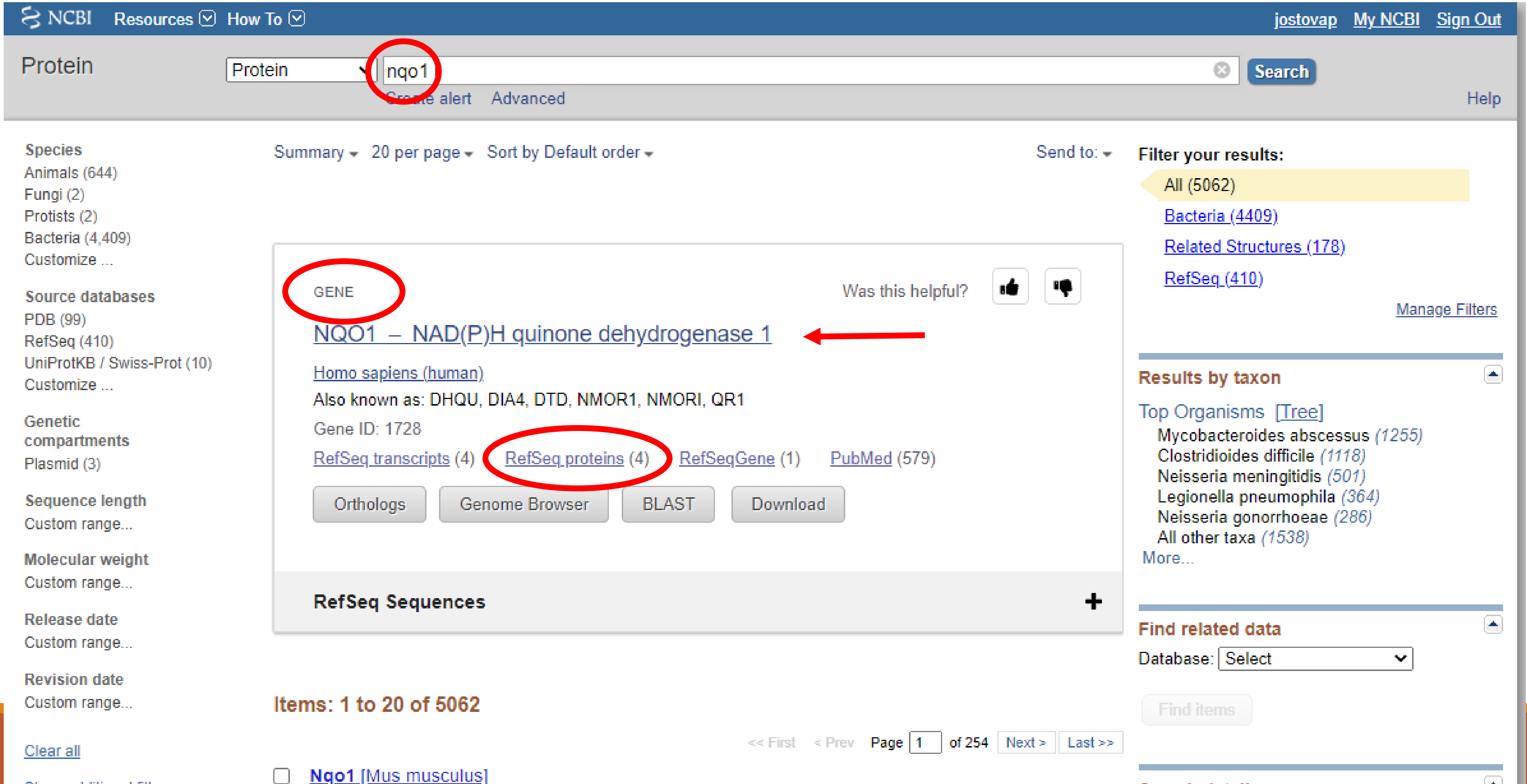
Protein database: NCBI



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Protein

Protein nqo1 Search

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Species
Animals (644)
Fungi (2)
Protists (2)
Bacteria (4,409)
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Source databases
PDB (99)
RefSeq (410)
UniProtKB / Swiss-Prot (10)
Customize ...

Genetic compartments
Plasmid (3)

Sequence length
Custom range...

Molecular weight
Custom range...

Release date
Custom range...

Revision date
Custom range...

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GENE

Was this helpful?

NQO1 – NAD(P)H quinone dehydrogenase 1

Homo sapiens (human)

Also known as: DHQU, DIA4, DTD, NMOR1, NMORI, QR1

Gene ID: 1728

RefSeq transcripts (4) RefSeq proteins (4) RefSeqGene (1) PubMed (579)

Orthologs Genome Browser BLAST Download

RefSeq Sequences

Items: 1 to 20 of 5062

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☐ Ngo1 [Mus musculus]

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Bacteria (4409)
Related Structures (178)
RefSeq (410)
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Clostridioides difficile	(1118)
Neisseria meningitidis	(501)
Legionella pneumophila	(364)
Neisseria gonorrhoeae	(286)
All other taxa	(1538)

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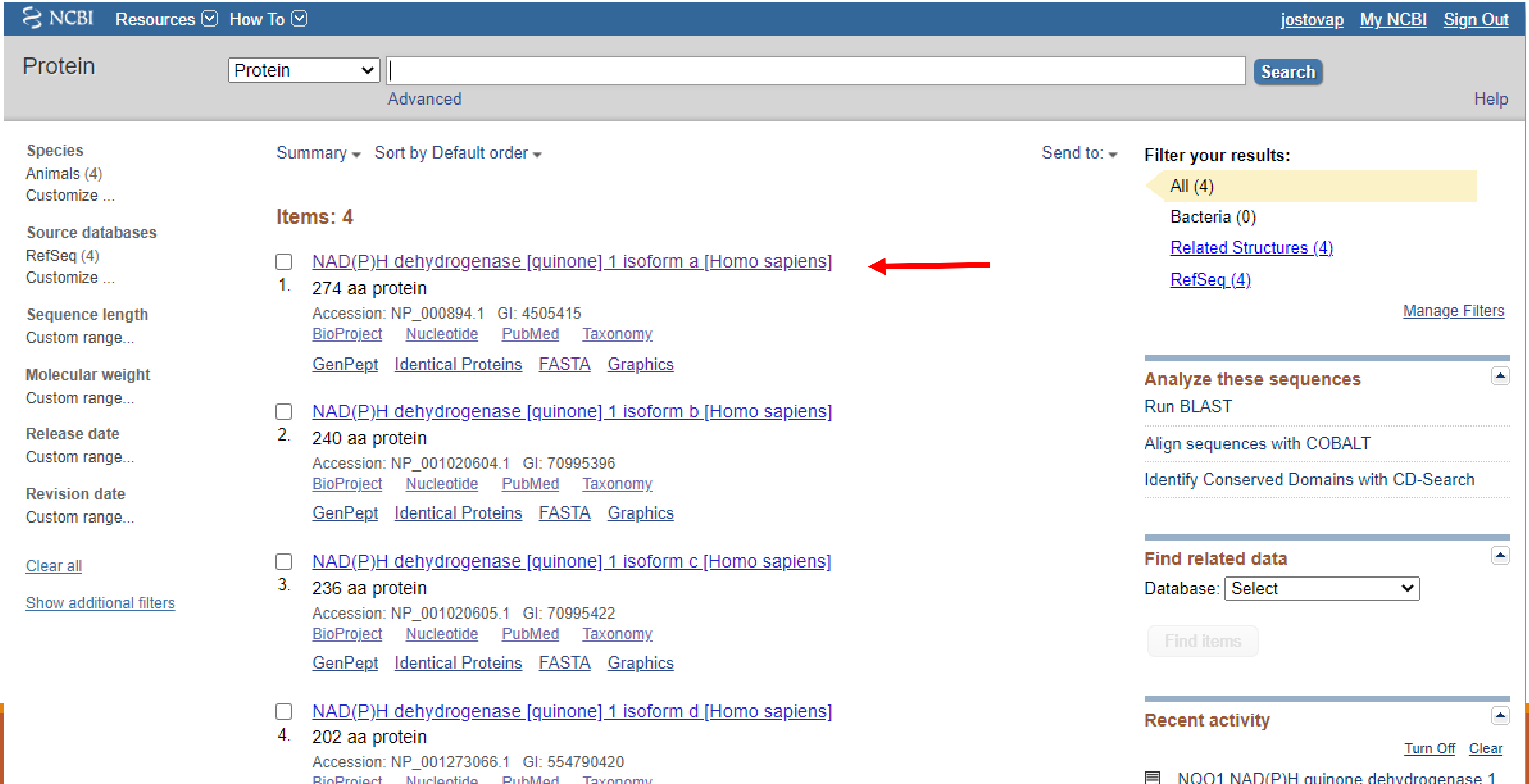
Protein database: NCBI



Items: 4

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   BioProject Nucleotide PubMed Taxonomy
   GenPept Identical Proteins FASTA Graphics
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   GenPept Identical Proteins FASTA Graphics
3. ☐ NAD(P)H dehydrogenase [quinone] 1 isoform c [Homo sapiens]
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   BioProject Nucleotide PubMed Taxonomy
   GenPept Identical Proteins FASTA Graphics
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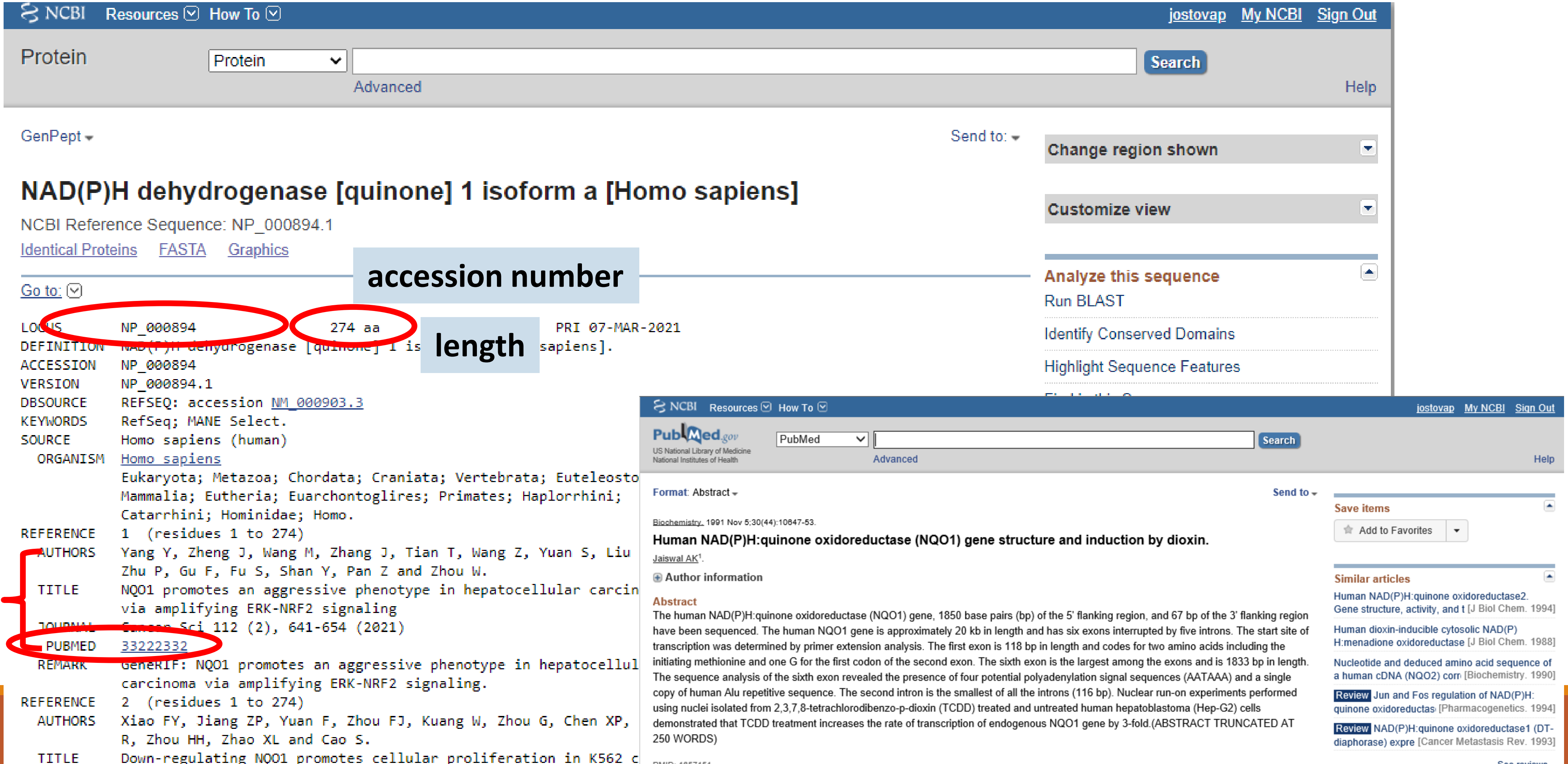
   BioProject Nucleotide PubMed Taxonomy

Protein database: NCBI



NAD(P)H dehydrogenase [quinone] 1 isoform a [Homo sapiens]

NCBI Reference Sequence: NP_000894.1

accession number

length

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VERSION     NP_000894.1
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KEYWORDS    RefSeq; MANE Select.
SOURCE      Homo sapiens (human)
  ORGANISM  Homo sapiens
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            Catarrhini; Hominidae; Homo.
REFERENCE   1  (residues 1 to 274)
  AUTHORS   Yang Y, Zheng J, Wang M, Zhang J, Tian T, Wang Z, Yuan S, Liu
            Zhu P, Gu F, Fu S, Shan Y, Pan Z and Zhou W.
  TITLE     NQO1 promotes an aggressive phenotype in hepatocellular carcin
            via amplifying ERK-NRF2 signaling
  JOURNAL   Cancer Sci 112 (2), 641-654 (2021)
   PUBMED   33222332
  REMARK    GeneRIF: NQO1 promotes an aggressive phenotype in hepatocellul
            carcinoma via amplifying ERK-NRF2 signaling.
REFERENCE   2  (residues 1 to 274)
  AUTHORS   Xiao FY, Jiang ZP, Yuan F, Zhou FJ, Kuang W, Zhou G, Chen XP,
            R, Zhou HH, Zhao XL and Cao S.
  TITLE     Down-regulating NQO1 promotes cellular proliferation in K562 c
```

Biochemistry. 1991 Nov 5;30(44):10647-53.

Human NAD(P)H:quinone oxidoreductase (NQO1) gene structure and induction by dioxin.

Jaiswal AK[1].

Author information

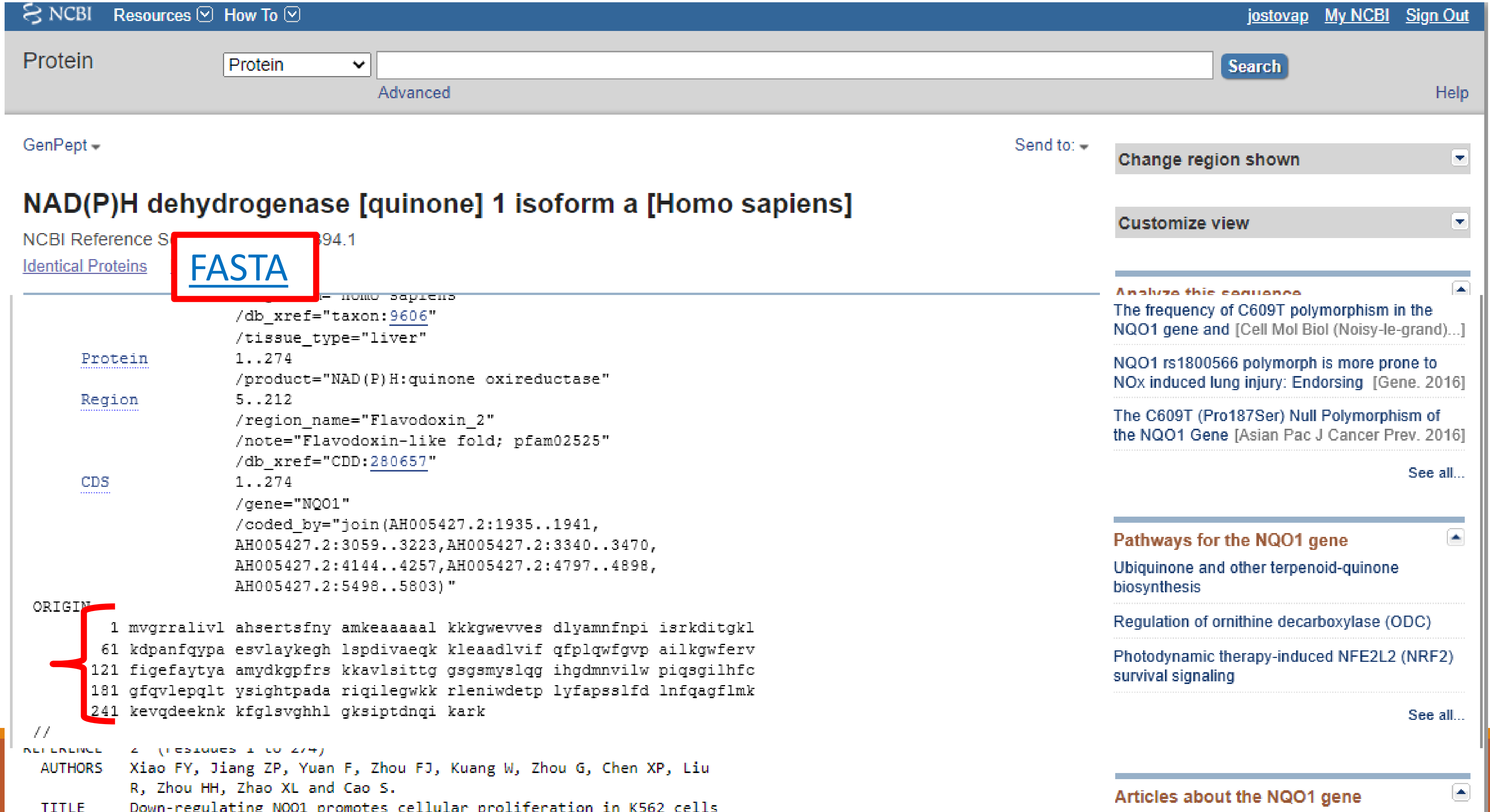
Abstract

The human NAD(P)H:quinone oxidoreductase (NQO1) gene, 1850 base pairs (bp) of the 5' flanking region, and 67 bp of the 3' flanking region have been sequenced. The human NQO1 gene is approximately 20 kb in length and has six exons interrupted by five introns. The start site of transcription was determined by primer extension analysis. The first exon is 118 bp in length and codes for two amino acids including the initiating methionine and one G for the first codon of the second exon. The sixth exon is the largest among the exons and is 1833 bp in length. The sequence analysis of the sixth exon revealed the presence of four potential polyadenylation signal sequences (AATAAA) and a single copy of human Alu repetitive sequence. The second intron is the smallest of all the introns (116 bp). Nuclear run-on experiments performed using nuclei isolated from 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) treated and untreated human hepatoblastoma (Hep-G2) cells demonstrated that TCDD treatment increases the rate of transcription of endogenous NQO1 gene by 3-fold.(ABSTRACT TRUNCATED AT 250 WORDS)

Similar articles

- Human NAD(P)H:quinone oxidoreductase2. Gene structure, activity, and t [J Biol Chem. 1994]
- Human dioxin-inducible cytosolic NAD(P) H:menadione oxidoreductase [J Biol Chem. 1988]
- Nucleotide and deduced amino acid sequence of a human cDNA (NQO2) corr [Biochemistry. 1990]
- Review Jun and Fos regulation of NAD(P)H: quinone oxidoreductas [Pharmacogenetics. 1994]
- Review NAD(P)H:quinone oxidoreductase1 (DT-diaphorase) expre [Cancer Metastasis Rev. 1993]

Protein database: NCBI



NAD(P)H dehydrogenase [quinone] 1 isoform a [Homo sapiens]

NCBI Reference S 94.1

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            R, Zhou HH, Zhao XL and Cao S.
  TITLE     Down-regulating NQO1 promotes cellular proliferation in K562 cells
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Analyze this sequence

The frequency of C609T polymorphism in the NQO1 gene and [Cell Mol Biol (Noisy-le-grand)...]

NQO1 rs1800566 polymorph is more prone to NOx induced lung injury: Endorsing [Gene. 2016]

The C609T (Pro187Ser) Null Polymorphism of the NQO1 Gene [Asian Pac J Cancer Prev. 2016]

See all...

Pathways for the NQO1 gene

Ubiquinone and other terpenoid-quinone biosynthesis

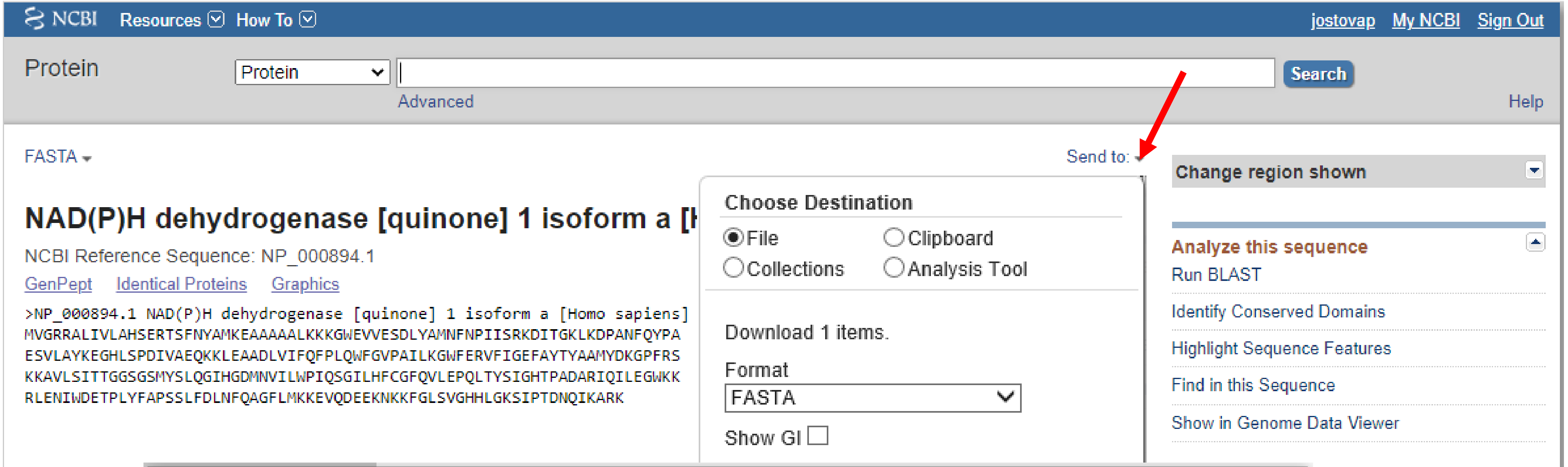
Regulation of ornithine decarboxylase (ODC)

Photodynamic therapy-induced NFE2L2 (NRF2) survival signaling

See all...

Articles about the NQO1 gene

Protein database: NCBI



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NCBI Reference Sequence: NP_000894.1

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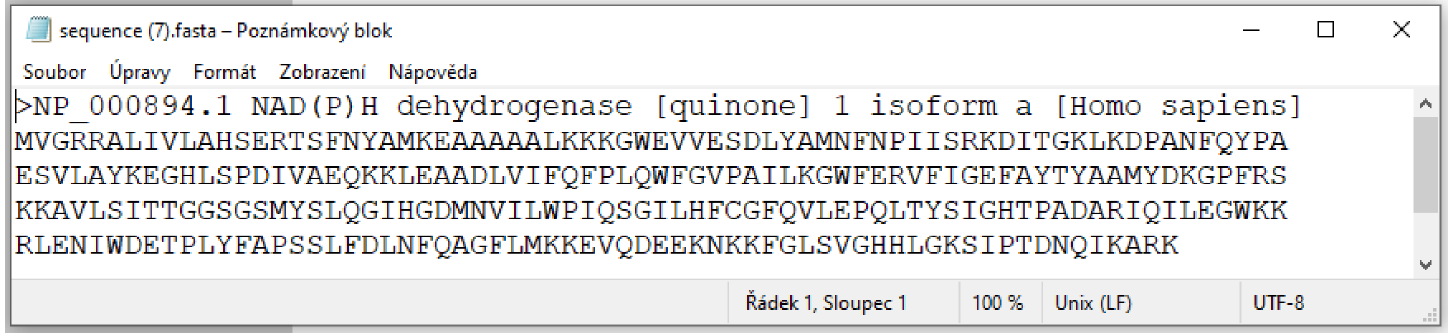

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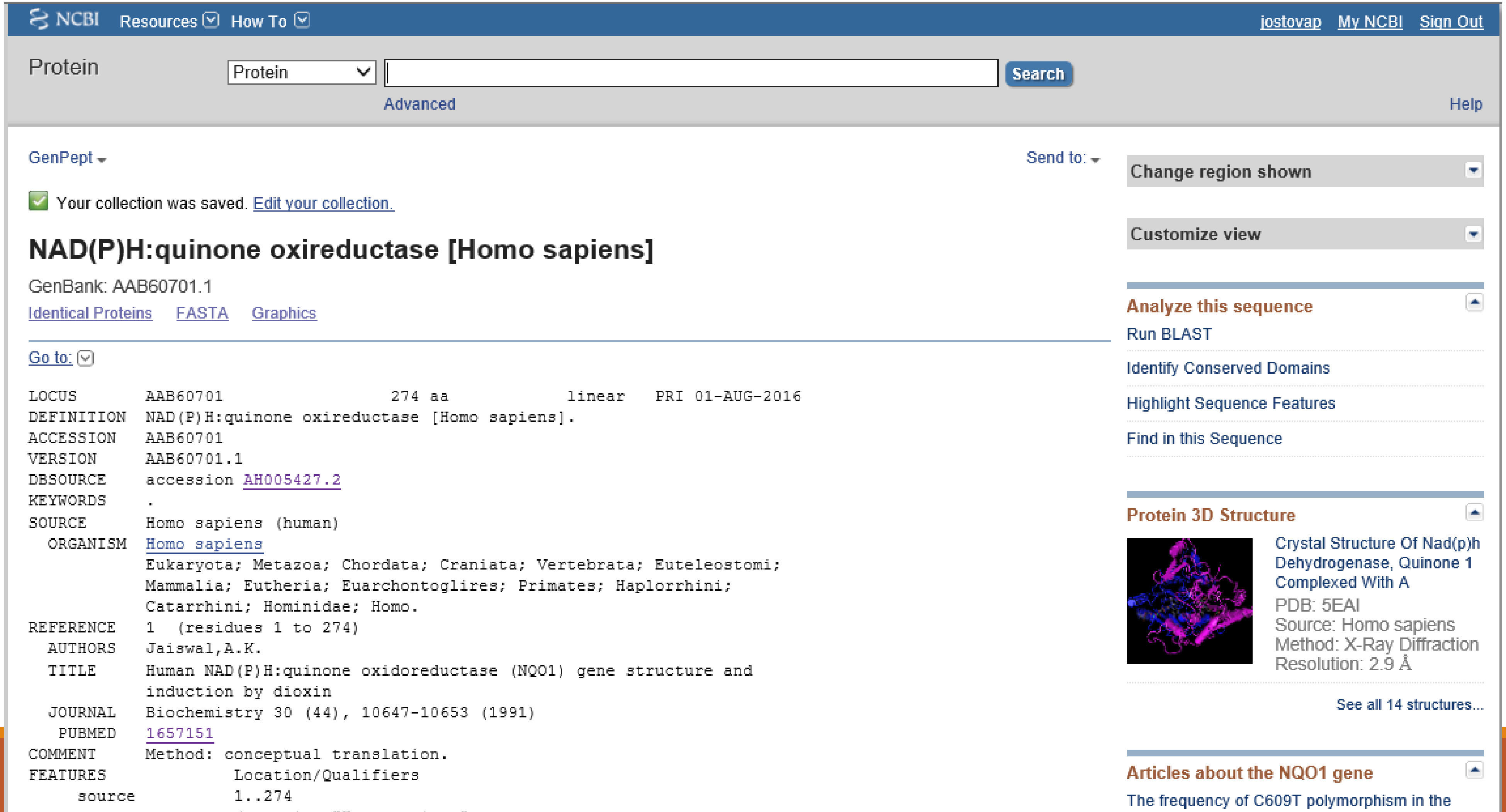
Protein database: NCBI → MyNCBI



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NAD(P)H:quinone oxireductase [Homo sapiens]

GenBank: AAB60701.1

Identical Proteins FASTA Graphics

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DEFINITION  NAD(P)H:quinone oxireductase [Homo sapiens].
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VERSION     AAB60701.1
DBSOURCE    accession AH005427.2
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REFERENCE   1  (residues 1 to 274)
  AUTHORS   Jaiswal,A.K.
  TITLE     Human NAD(P)H:quinone oxidoreductase (NQO1) gene structure and
            induction by dioxin
  JOURNAL   Biochemistry 30 (44), 10647-10653 (1991)
   PUBMED   1657151
COMMENT     Method: conceptual translation.
FEATURES             Location/Qualifiers
     source          1..274
```

Analyze this sequence

Run BLAST

Identify Conserved Domains

Highlight Sequence Features

Find in this Sequence

Protein 3D Structure

Crystal Structure Of Nad(p)h Dehydrogenase, Quinone 1 Complexed With A

PDB: 5EAI

Source: Homo sapiens

Method: X-Ray Diffraction

Resolution: 2.9 Å

See all 14 structures...

Articles about the NQO1 gene

The frequency of C609T polymorphism in the

Protein database: NCBI

NAD(P)H dehydrogenase [quinone] 1 isoform a [Homo sapiens]

NCBI Reference Sequen

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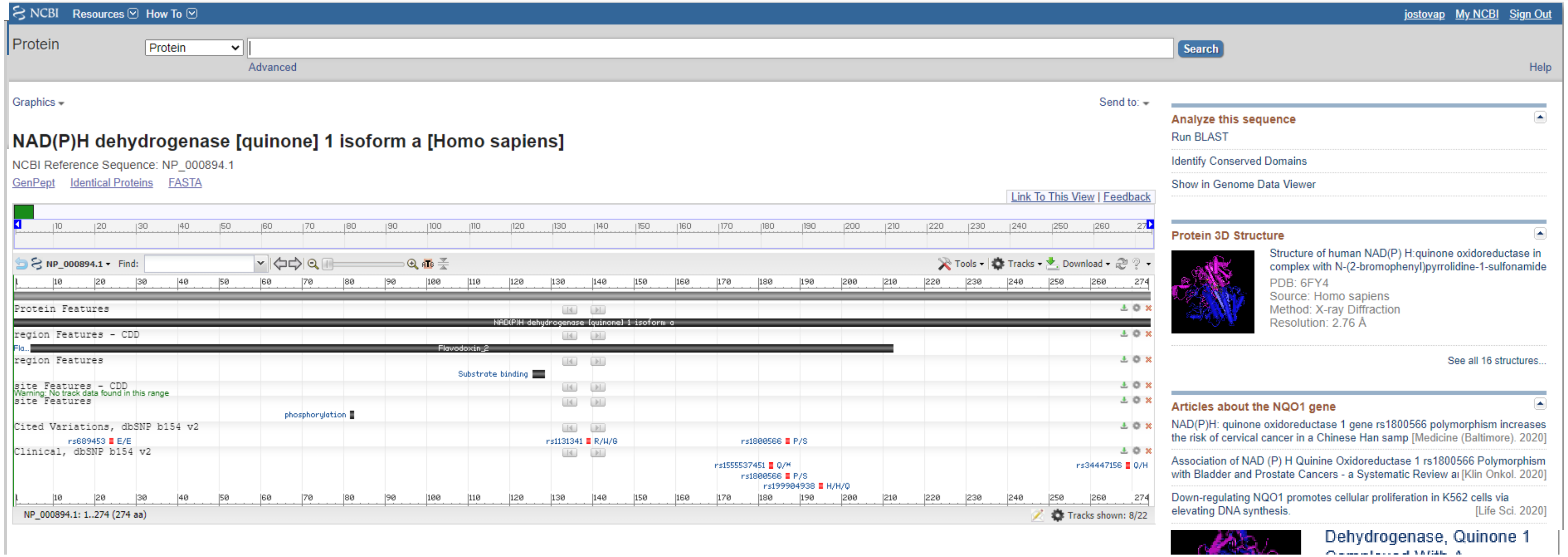
Protein database: NCBI



NAD(P)H dehydrogenase [quinone] 1 isoform a [Homo sapiens]

NCBI Reference Sequence: NP_000894.1

Analyze this sequence

Run BLAST

Identify Conserved Domains

Show in Genome Data Viewer

Protein 3D Structure

Structure of human NAD(P) H:quinone oxidoreductase in complex with N-(2-bromophenyl)pyrrolidine-1-sulfonamide

PDB: 6FY4
Source: Homo sapiens
Method: X-ray Diffraction
Resolution: 2.76 Å

Articles about the NQO1 gene

NAD(P)H: quinone oxidoreductase 1 gene rs1800566 polymorphism increases the risk of cervical cancer in a Chinese Han samp [Medicine (Baltimore). 2020]

Association of NAD (P) H Quinine Oxidoreductase 1 rs1800566 Polymorphism with Bladder and Prostate Cancers - a Systematic Review aı [Klin Onkol. 2020]

Down-regulating NQO1 promotes cellular proliferation in K562 cells via elevating DNA synthesis. [Life Sci. 2020]

Dehydrogenase, Quinone 1

Practical part with NQO1

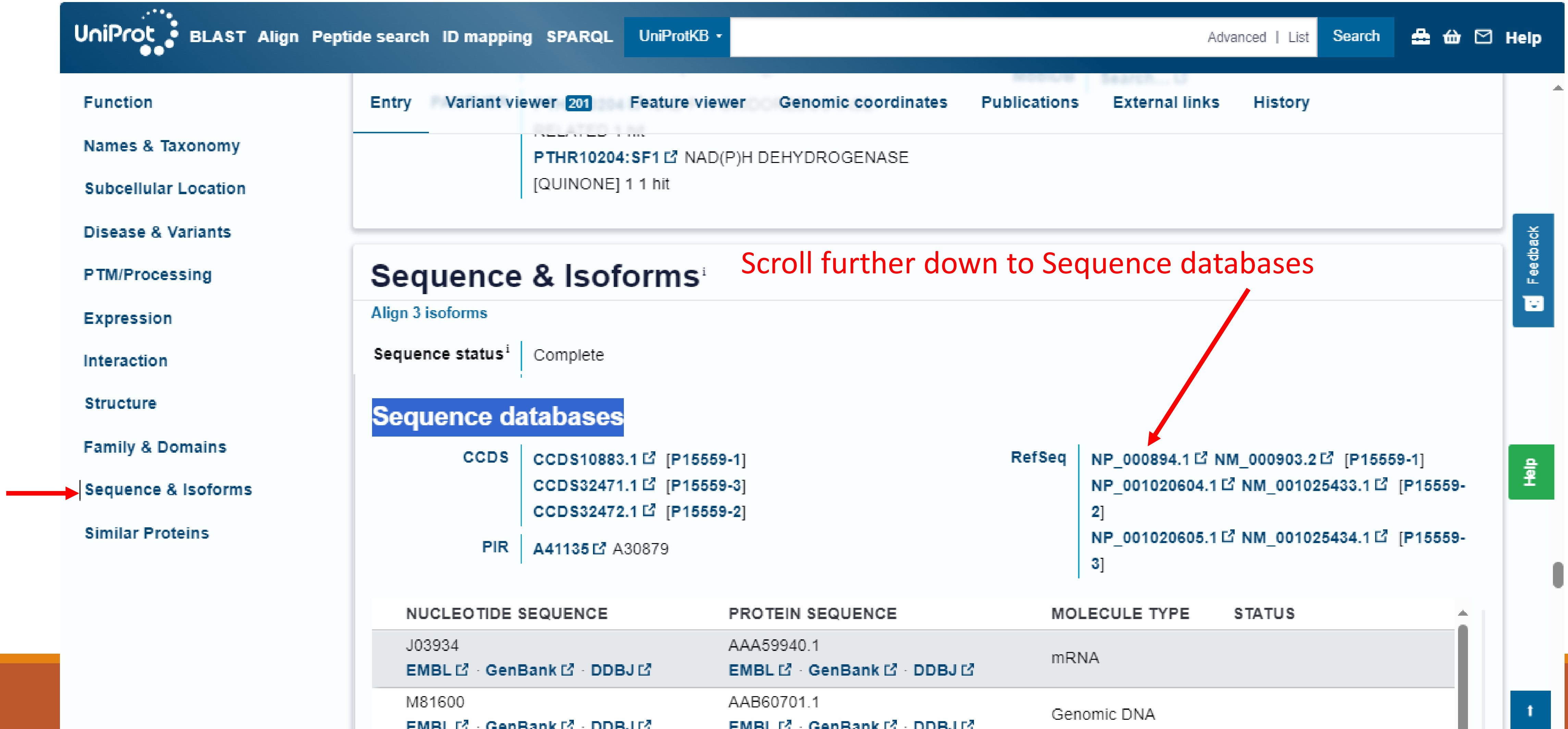
Try Uniprot and protein NCBI:

Find your sequnce

-what is the function of your protein?
-find subcellular location of your protein
-is it involved in any pathology?
-how many amino acids has your sequence?

-try direct search in NCBI
-**try link through Sequence databases → Refseq from Uniprot**

link through Sequence databases → Refseq from Uniprot



PTHR10204:SF1 NAD(P)H DEHYDROGENASE [QUINONE] 1 1 hit

Sequence & Isoforms

Scroll further down to Sequence databases

Align 3 isoforms

Sequence status Complete

Sequence databases

CCDS	CCDS10883.1 [P15559-1] CCDS32471.1 [P15559-3] CCDS32472.1 [P15559-2]	RefSeq	NP_000894.1 NM_000903.2 [P15559-1] NP_001020604.1 NM_001025433.1 [P15559-2] NP_001020605.1 NM_001025434.1 [P15559-3]
PIR	A41135 A30879		

NUCLEOTIDE SEQUENCE	PROTEIN SEQUENCE	MOLECULE TYPE	STATUS
J03934 EMBL · GenBank · DDBJ	AAA59940.1 EMBL · GenBank · DDBJ	mRNA	
M81600 EMBL · GenBank · DDBJ	AAB60701.1 EMBL · GenBank · DDBJ	Genomic DNA	

„Protein bioinformatics I“

Retrieving protein sequences from databases

→ **Computing amino-acids compositions, molecular weight, isoelectric point, and other parameters**

Prediction of proteases cutting

Predicting elements of protein secondary structure, domains

Predicting 3-D structure and the domain organization of proteins

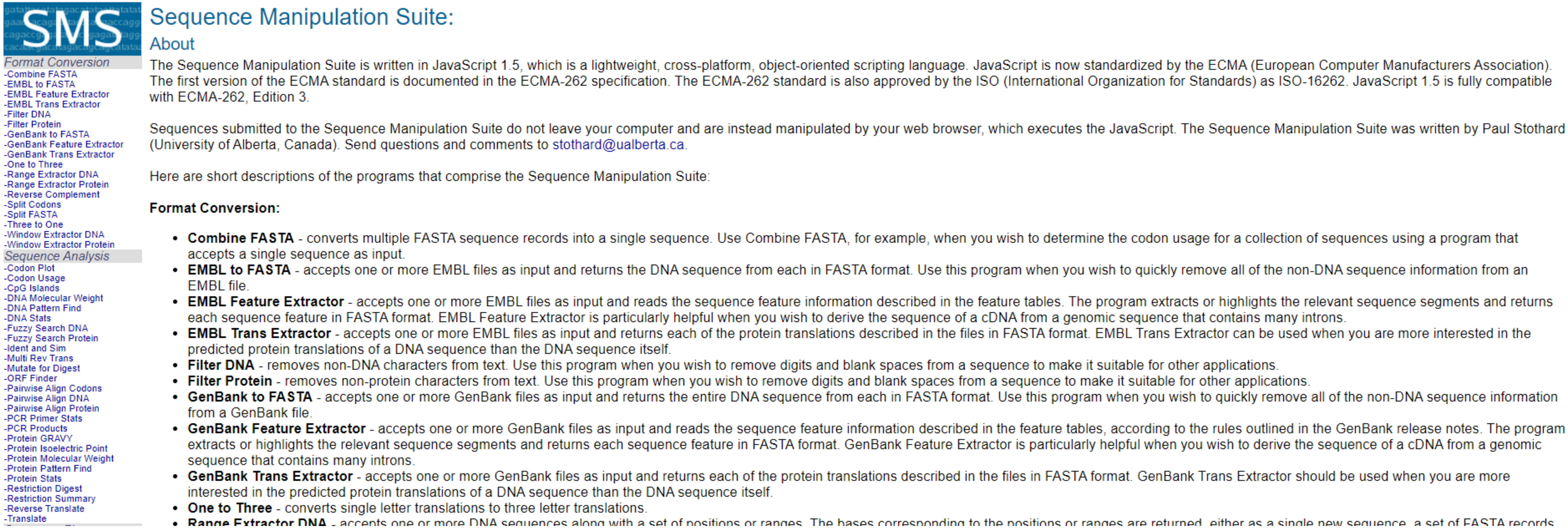
Finding all proteins that share a similar sequence and Classifying proteins into families

Finding evolutionary relationships between proteins, drawing proteins’ family trees

Computing the optimal alignment between two or more protein sequences

…

Protein Sequence Analysis



Sequence Manipulation Suite:

About

The Sequence Manipulation Suite is written in JavaScript 1.5, which is a lightweight, cross-platform, object-oriented scripting language. JavaScript is now standardized by the ECMA (European Computer Manufacturers Association). The first version of the ECMA standard is documented in the ECMA-262 specification. The ECMA-262 standard is also approved by the ISO (International Organization for Standards) as ISO-16262. JavaScript 1.5 is fully compatible with ECMA-262, Edition 3.

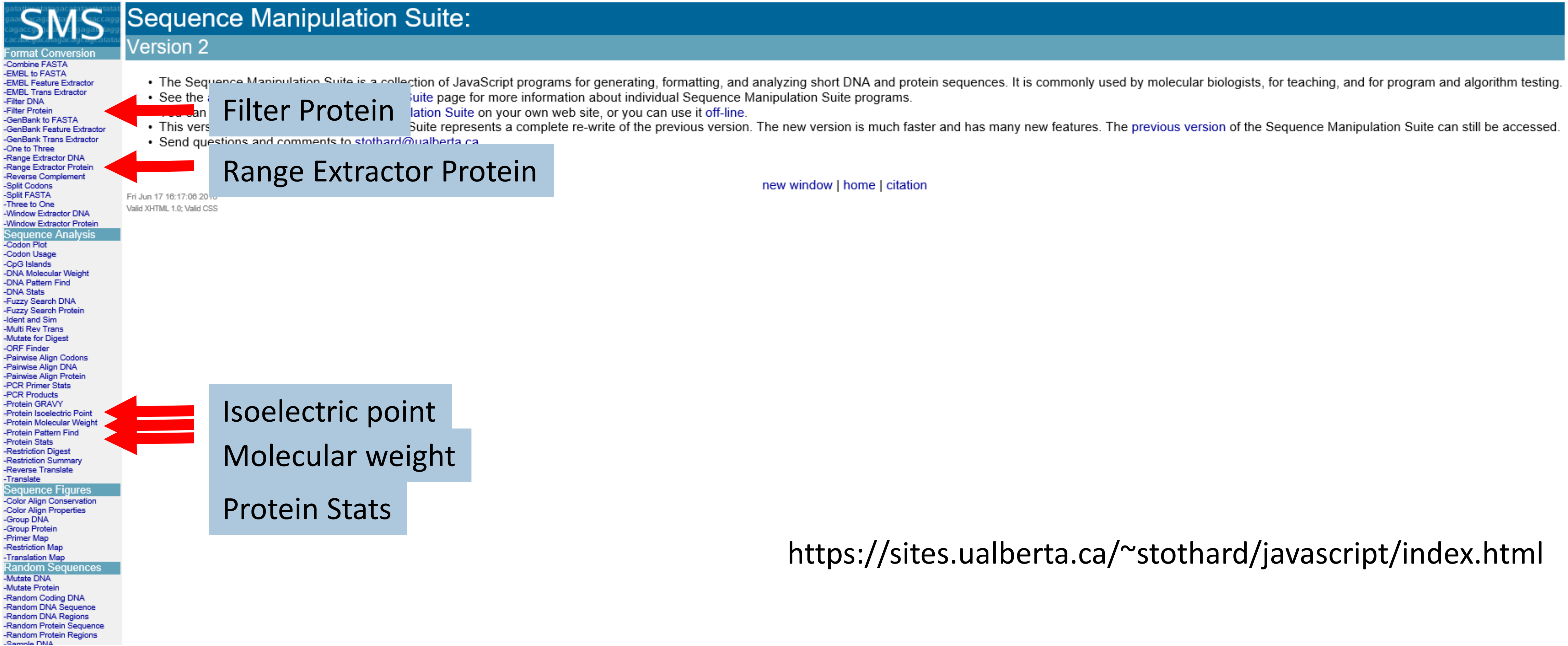
Sequences submitted to the Sequence Manipulation Suite do not leave your computer and are instead manipulated by your web browser, which executes the JavaScript. The Sequence Manipulation Suite was written by Paul Stothard (University of Alberta, Canada). Send questions and comments to stothard@ualberta.ca.

Here are short descriptions of the programs that comprise the Sequence Manipulation Suite:

Format Conversion:

- **Combine FASTA** - converts multiple FASTA sequence records into a single sequence. Use Combine FASTA, for example, when you wish to determine the codon usage for a collection of sequences using a program that accepts a single sequence as input.
- **EMBL to FASTA** - accepts one or more EMBL files as input and returns the DNA sequence from each in FASTA format. Use this program when you wish to quickly remove all of the non-DNA sequence information from an EMBL file.
- **EMBL Feature Extractor** - accepts one or more EMBL files as input and reads the sequence feature information described in the feature tables. The program extracts or highlights the relevant sequence segments and returns each sequence feature in FASTA format. EMBL Feature Extractor is particularly helpful when you wish to derive the sequence of a cDNA from a genomic sequence that contains many introns.
- **EMBL Trans Extractor** - accepts one or more EMBL files as input and returns each of the protein translations described in the files in FASTA format. EMBL Trans Extractor can be used when you are more interested in the predicted protein translations of a DNA sequence than the DNA sequence itself.
- **Filter DNA** - removes non-DNA characters from text. Use this program when you wish to remove digits and blank spaces from a sequence to make it suitable for other applications.
- **Filter Protein** - removes non-protein characters from text. Use this program when you wish to remove digits and blank spaces from a sequence to make it suitable for other applications.
- **GenBank to FASTA** - accepts one or more GenBank files as input and returns the entire DNA sequence from each in FASTA format. Use this program when you wish to quickly remove all of the non-DNA sequence information from a GenBank file.
- **GenBank Feature Extractor** - accepts one or more GenBank files as input and reads the sequence feature information described in the feature tables, according to the rules outlined in the GenBank release notes. The program extracts or highlights the relevant sequence segments and returns each sequence feature in FASTA format. GenBank Feature Extractor is particularly helpful when you wish to derive the sequence of a cDNA from a genomic sequence that contains many introns.
- **GenBank Trans Extractor** - accepts one or more GenBank files as input and returns each of the protein translations described in the files in FASTA format. GenBank Trans Extractor should be used when you are more interested in the predicted protein translations of a DNA sequence than the DNA sequence itself.
- **One to Three** - converts single letter translations to three letter translations.
- **Range Extractor DNA** - accepts one or more DNA sequences along with a set of positions or ranges. The bases corresponding to the positions or ranges are returned, either as a single new sequence, a set of FASTA records

Protein Sequence Analysis



SMS

Format Conversion
-Combine FASTA
-EMBL to FASTA
-EMBL Feature Extractor
-EMBL Trans Extractor
-Filter DNA
-Filter Protein
-GenBank to FASTA
-GenBank Feature Extractor
-GenBank Trans Extractor
-One to Three
-Range Extractor DNA
-Range Extractor Protein
-Reverse Complement
-Split Codons
-Split FASTA
-Three to One
-Window Extractor DNA
-Window Extractor Protein

Sequence Analysis
-Codon Plot
-Codon Usage
-CpG Islands
-DNA Molecular Weight
-DNA Pattern Find
-DNA Stats
-Fuzzy Search DNA
-Fuzzy Search Protein
-Ident and Sim
-Multi Rev Trans
-Mutate for Digest
-ORF Finder
-Pairwise Align Codons
-Pairwise Align DNA
-Pairwise Align Protein
-PCR Primer Stats
-PCR Products
-Protein GRAVY
-Protein Isoelectric Point
-Protein Molecular Weight
-Protein Pattern Find
-Protein Stats
-Restriction Digest
-Restriction Summary
-Reverse Translate
-Translate

Sequence Figures
-Color Align Conservation
-Color Align Properties
-Group DNA
-Group Protein
-Primer Map
-Restriction Map
-Translation Map

Random Sequences
-Mutate DNA
-Mutate Protein
-Random Coding DNA
-Random DNA Sequence
-Random DNA Regions
-Random Protein Sequence
-Random Protein Regions
-Sample DNA

Sequence Manipulation Suite:

Version 2

- The Sequence Manipulation Suite is a collection of JavaScript programs for generating, formatting, and analyzing short DNA and protein sequences. It is commonly used by molecular biologists, for teaching, and for program and algorithm testing.
- See the uite page for more information about individual Sequence Manipulation Suite programs.
- You can lation Suite on your own web site, or you can use it off-line.
- This vers Suite represents a complete re-write of the previous version. The new version is much faster and has many new features. The previous version of the Sequence Manipulation Suite can still be accessed.
- Send questions and comments to stothard@ualberta.ca

new window | home | citation

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Filter Protein

Range Extractor Protein

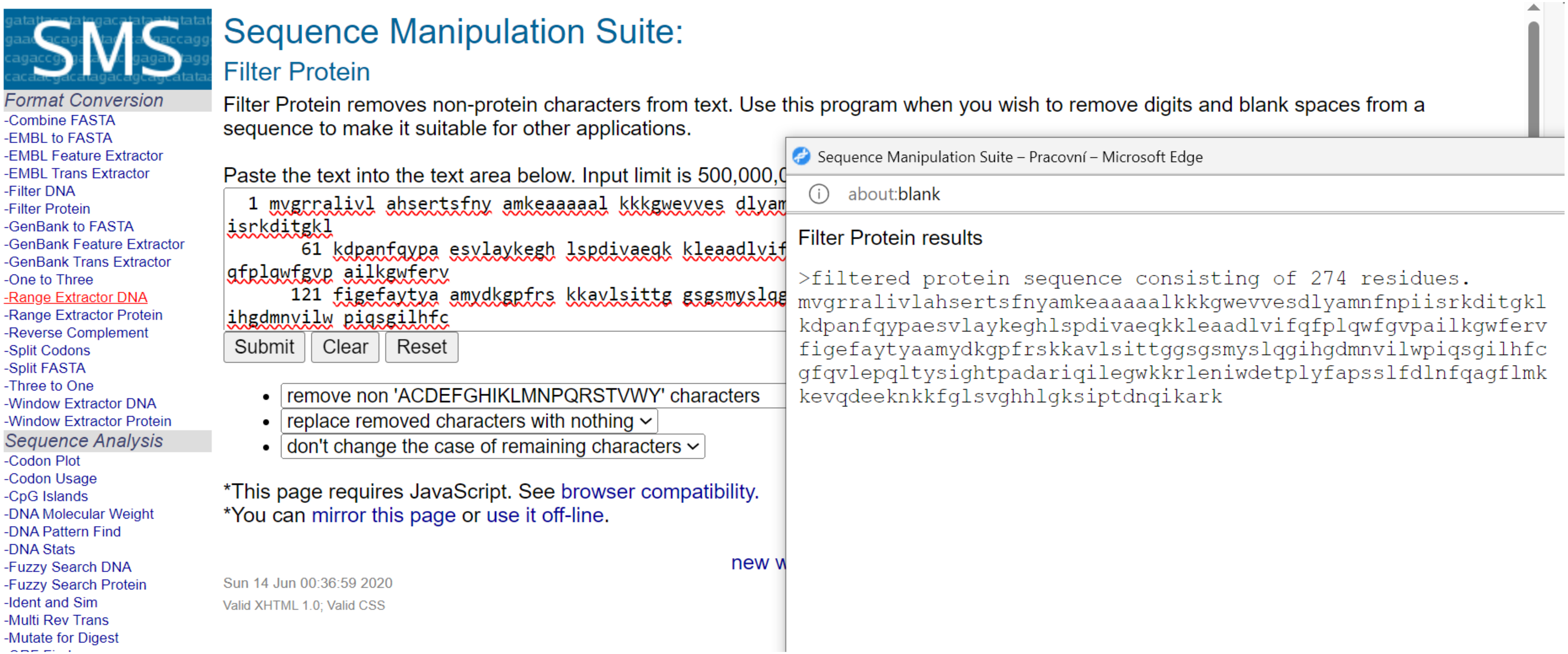
Isoelectric point

Molecular weight

Protein Stats

https://sites.ualberta.ca/~stothard/javascript/index.html

Protein Sequence Analysis



Sequence Manipulation Suite:

Filter Protein

Filter Protein removes non-protein characters from text. Use this program when you wish to remove digits and blank spaces from a sequence to make it suitable for other applications.

Paste the text into the text area below. Input limit is 500,0

```
  1 mvgrralivl ahsertsfny amkeaaaaal kkkgwevves dlyam
isrkditgkl
       61 kdpanfqypa esvlaykegh lspdivaeqk kleaadlvif
qfplqwfgvp ailkgwferv
      121 figefaytya amydkgpfrs kkavlsittg gsgsmyslqg
ihgdmnvilw piqsgilhfc
```

- remove non 'ACDEFGHIKLMNPQRSTVWY' characters
- replace removed characters with nothing
- don't change the case of remaining characters

*This page requires JavaScript. See browser compatibility.
*You can mirror this page or use it off-line.

Sun 14 Jun 00:36:59 2020

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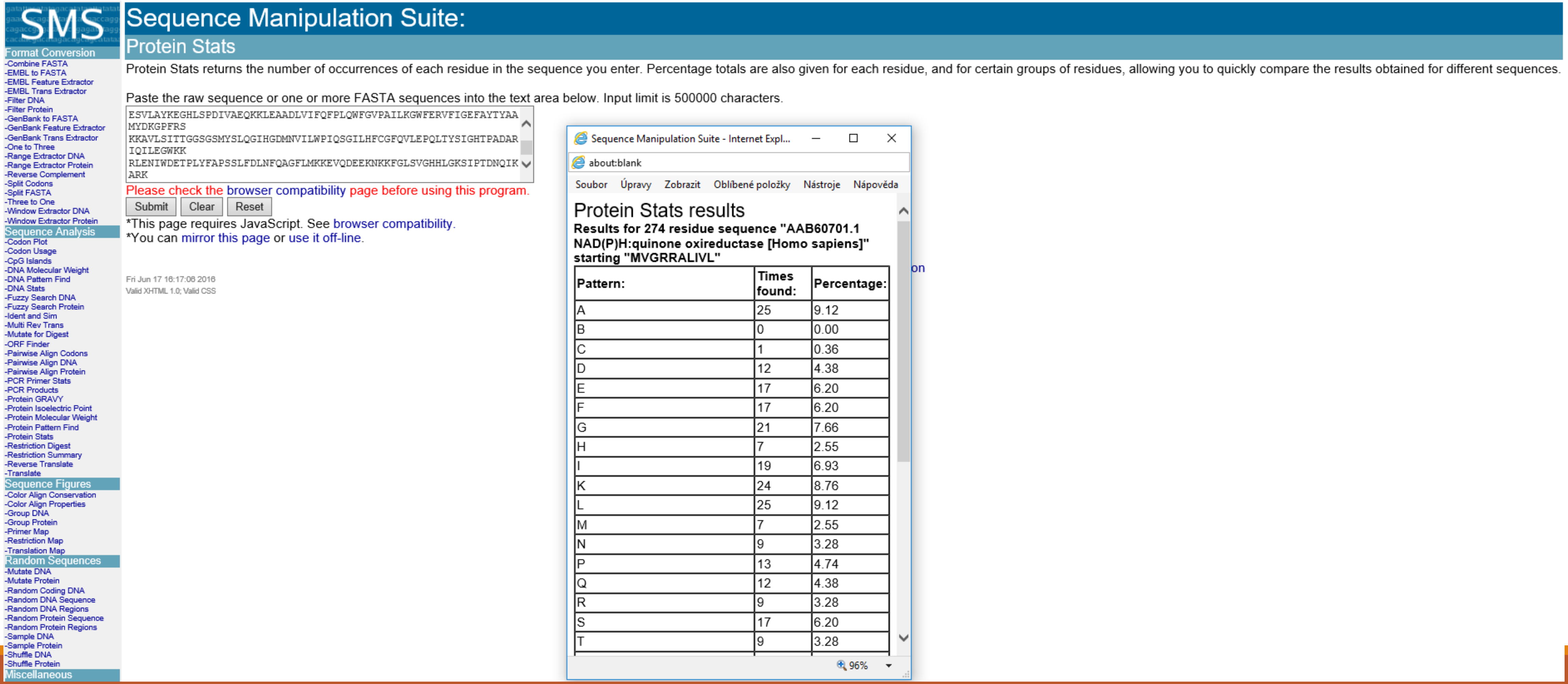
Filter Protein results

```
>filtered protein sequence consisting of 274 residues.
mvgrralivlahsertsfnyamkeaaaaalkkkgwevvesdlyamnfnpiisrkditgkl
kdpanfqypaesvlaykeghlspdivaeqkkleaadlvifqfplqwfgvpailkgwferv
figefaytyaamydkgpfrskkavlsittggsgsmyslqgihgdmnvilwpiqsgilhfc
gfqvlepqltysightpadariqilegwkkrleniwdetplyfapsslfdlnfqagflmk
kevqdeeknkkfglsvghhlgksiptdnqikark
```

Protein Sequence Analysis



Sequence Manipulation Suite:

Protein Stats

Protein Stats returns the number of occurrences of each residue in the sequence you enter. Percentage totals are also given for each residue, and for certain groups of residues, allowing you to quickly compare the results obtained for different sequences.

Paste the raw sequence or one or more FASTA sequences into the text area below. Input limit is 500000 characters.

```
ESVLAYKEGHLSPDIVAEQKKLEAADLVIFQFPLQWFGVPAILKGWFERVFIGEFAYTYAA
MYDKGPFRS
KKAVLSITTGGSGSMYSLQGIHGDMNVILWPIQSGILHFCGFQVLEPQLTYSIGHTPADAR
IQILEGWKK
RLENIWDETPLYFAPSSLFDLNFQAGFLMKKEVQDEEKNKKFGLSVGHHLGKSIPTDNQIK
ARK
```

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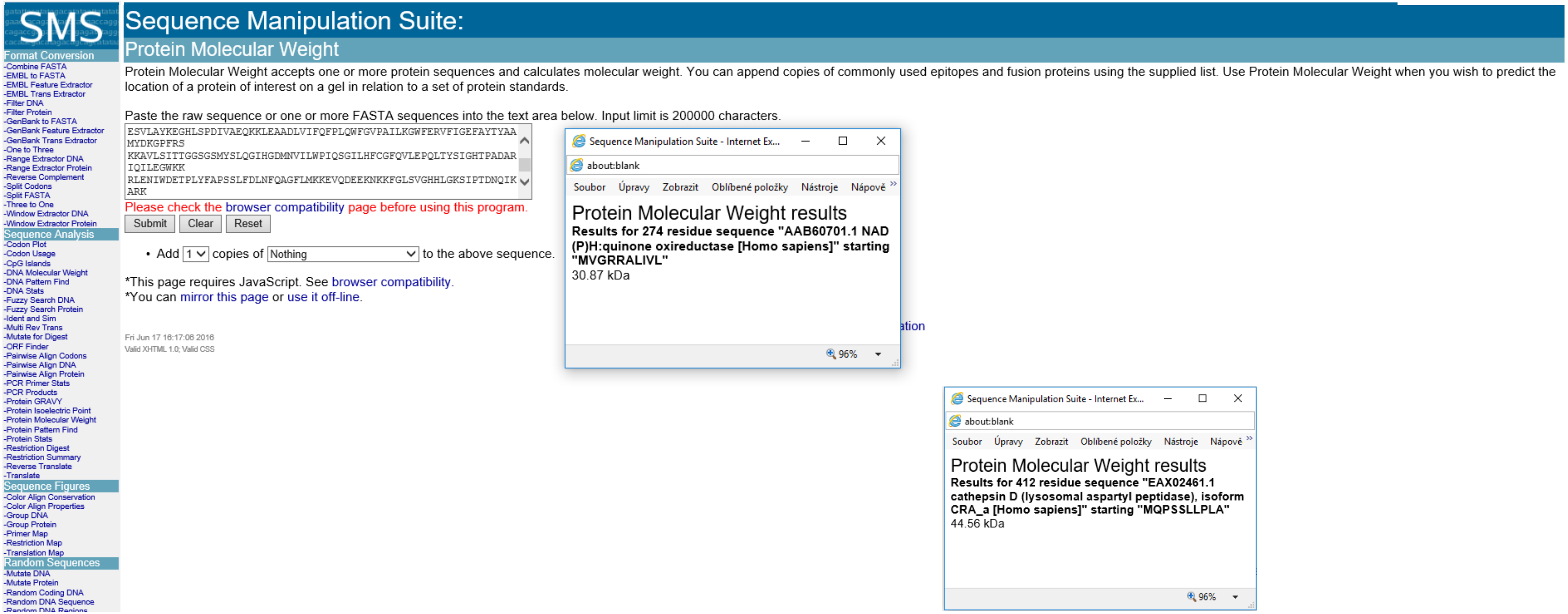
Protein Stats results

Results for 274 residue sequence "AAB60701.1 NAD(P)H:quinone oxireductase [Homo sapiens]" starting "MVGRRALIVL"

Pattern:	Times found:	Percentage:
A	25	9.12
B	0	0.00
C	1	0.36
D	12	4.38
E	17	6.20
F	17	6.20
G	21	7.66
H	7	2.55
I	19	6.93
K	24	8.76
L	25	9.12
M	7	2.55
N	9	3.28
P	13	4.74
Q	12	4.38
R	9	3.28
S	17	6.20
T	9	3.28

Protein Sequence Analysis



Sequence Manipulation Suite:

Protein Molecular Weight

Protein Molecular Weight accepts one or more protein sequences and calculates molecular weight. You can append copies of commonly used epitopes and fusion proteins using the supplied list. Use Protein Molecular Weight when you wish to predict the location of a protein of interest on a gel in relation to a set of protein standards.

Paste the raw sequence or one or more FASTA sequences into the text area below. Input limit is 200000 characters.

```
ESVLAYKEGHLSPDIVAEQKKLEAADLVIFQFPLQWFGVPAILKGWFERVFIGEFAYTYAA
MYDKGPFRS
KKAVLSITTGGSGSMYSLQGIHGDMNVILWPIQSGILHFCGFQVLEPQLTYSIGHTPADAR
IQILEGWKK
RLENIWDETPLYFAPSSLFDLNFQAGFLMKKEVQDEEKNKKFGLSVGHHLGKSIPTDNQIK
ARK
```

Please check the browser compatibility page before using this program.

- Add 1 copies of Nothing to the above sequence.

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ation

Protein Molecular Weight results

Results for 274 residue sequence "AAB60701.1 NAD (P)H:quinone oxireductase [Homo sapiens]" starting "MVGRRALIVL"

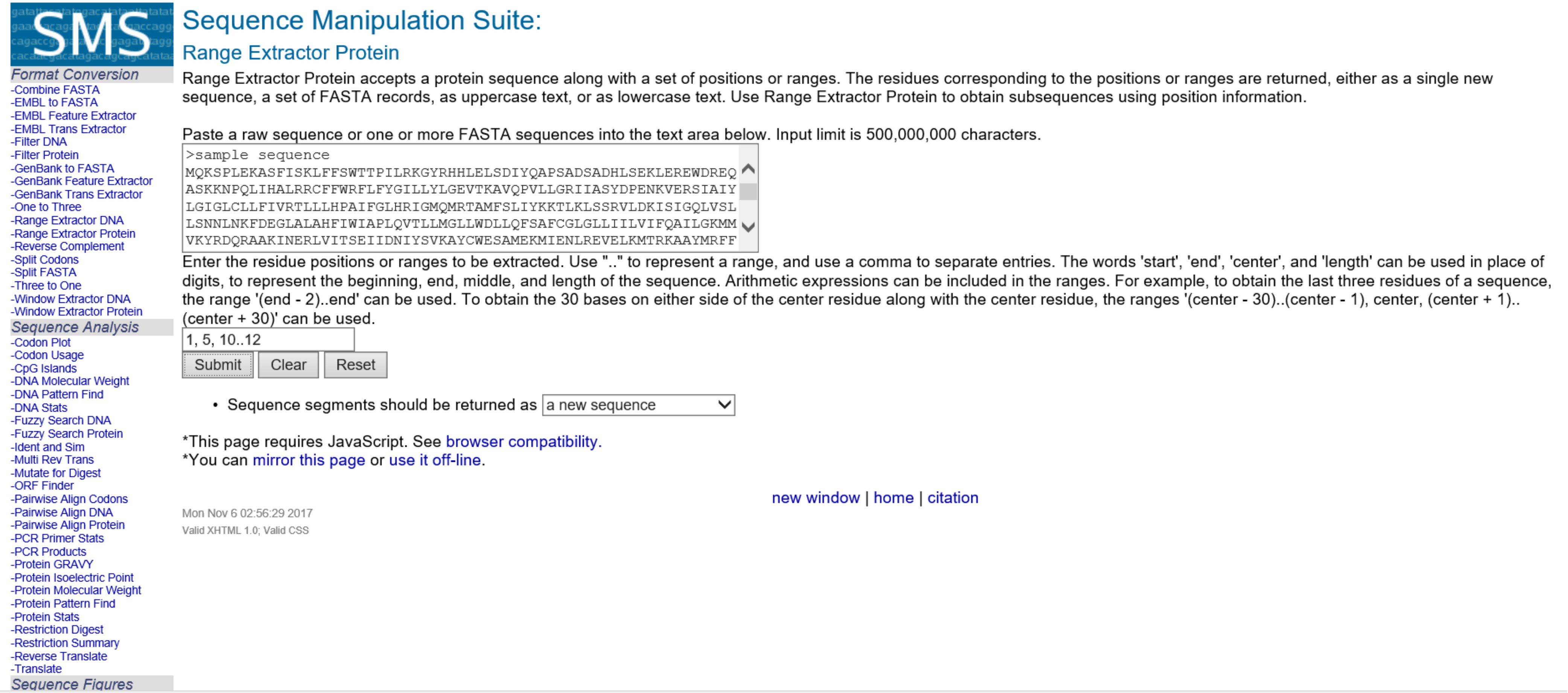
30.87 kDa

Protein Molecular Weight results

Results for 412 residue sequence "EAX02461.1 cathepsin D (lysosomal aspartyl peptidase), isoform CRA_a [Homo sapiens]" starting "MQPSSLLPLA"

44.56 kDa

Protein Sequence Analysis



Sequence Manipulation Suite:

Range Extractor Protein

Range Extractor Protein accepts a protein sequence along with a set of positions or ranges. The residues corresponding to the positions or ranges are returned, either as a single new sequence, a set of FASTA records, as uppercase text, or as lowercase text. Use Range Extractor Protein to obtain subsequences using position information.

Paste a raw sequence or one or more FASTA sequences into the text area below. Input limit is 500,000,000 characters.

```
>sample sequence
MQKSPLEKASFISKLFFSWTTPILRKGYRHHLELSDIYQAPSADSADHLSEKLEREWDREQ
ASKKNPQLIHALRRCFFWRFLFYGILLYLGEVTKAVQPVLLGRIIASYDPENKVERSIAIY
LGIGLCLLFIVRTLLLHPAIFGLHRIGMQMRTAMFSLIYKKTLKLSSRVLDKISIGQLVSL
LSNNLNKFDEGLALAHFIWIAPLQVTLLMGLLWDLLQFSAFCGLGLLIILVIFQAILGKMM
VKYRDQRAAKINERLVITSEIIDNIYSVKAYCWESAMEKMIENLREVELKMTRKAAYMRFF
```

Enter the residue positions or ranges to be extracted. Use ".." to represent a range, and use a comma to separate entries. The words 'start', 'end', 'center', and 'length' can be used in place of digits, to represent the beginning, end, middle, and length of the sequence. Arithmetic expressions can be included in the ranges. For example, to obtain the last three residues of a sequence, the range '(end - 2)..end' can be used. To obtain the 30 bases on either side of the center residue along with the center residue, the ranges '(center - 30)..(center - 1), center, (center + 1)..(center + 30)' can be used.

1, 5, 10..12

- Sequence segments should be returned as: a new sequence

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Try SMS suite

Analyze your sequence
- how many cysteins are in your sequence?

HW2

3) Extract peptide from 10. - 50. amino acid.
4) Count the molecular weight of this (short) peptide.
5) How many cysteins are in your (whole) sequence?

„Protein bioinformatics II“

Retrieving protein sequences from databases

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

→ **Prediction of proteases cutting**

Predicting elements of protein secondary structure, domains

Predicting 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

…

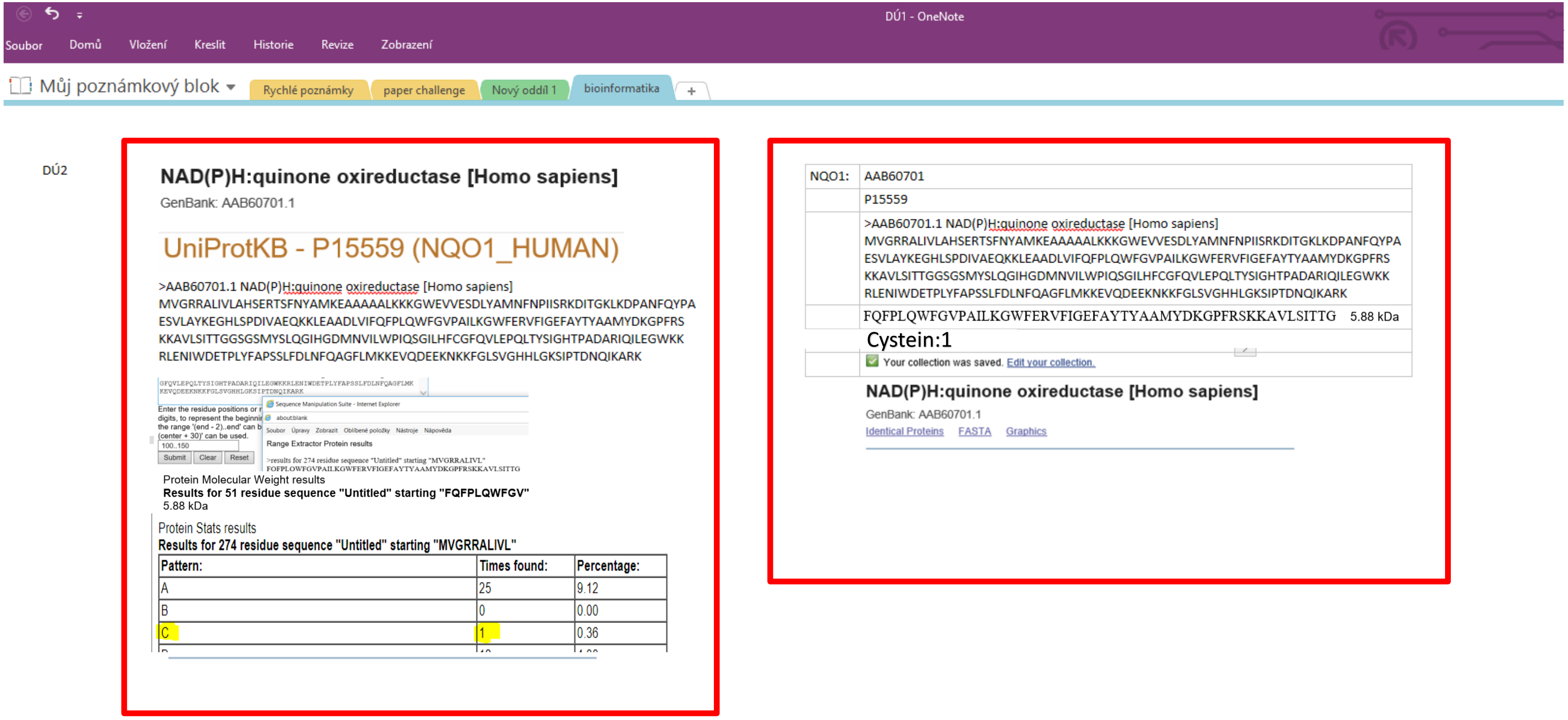
Homework 2

1) find both (Uniprot/NCBI) accession numbers for reference sequence (isoform 1)
2) download your sequence in FASTA format
3) Extract peptide form positions 10 to 50
4) Predict molecular weight of this peptide
5) How many cysteins are in your sequence?

E.g use „výstřižky“ „snipping tool“

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

Homework 2: examples



DÚ2

NAD(P)H:quinone oxireductase [Homo sapiens]

GenBank: AAB60701.1

UniProtKB - P15559 (NQO1_HUMAN)

>AAB60701.1 NAD(P)H:quinone oxireductase [Homo sapiens]
MVGRRALIVLAHSERTSFNYAMKEAAAAALKKKGWEVVESDLYAMNFNPIISRKDITGKLKDPANFQYPA
ESVLAYKEGHLSPDIVAEQKKLEAADLVIFQFPLQWFGVPAILKGWFERVFIGEFAYTYAAMYDKGPFRS
KKAVLSITTGGSGSMYSLQGIHGDMNVILWPIQSGILHFCGFQVLEPQLTYSIGHTPADARIQILEGWKK
RLENIWDETPLYFAPSSLFDLNFQAGFLMKKEVQDEEKNKKFGLSVGHHLGKSIPTDNQIKARK

GFQVLEPQLTYSIGHTPADARIQILEGWKKRLENIWDETPLYFAPSSLFDLNFQAGFLMK
KEVQDEEKNKKFGLSVGHHLGKSIPTDNQIKARK

Enter the residue positions or r
digits, to represent the beginnir
the range '(end - 2)..end' can b
(center + 30)' can be used.

100..150

Range Extractor Protein results

>results for 274 residue sequence "Untitled" starting "MVGRRALIVL"
FQFPLQWFGVPAILKGWFERVFIGEFAYTYAAMYDKGPFRSKKAVLSITTG

Protein Molecular Weight results

Results for 51 residue sequence "Untitled" starting "FQFPLQWFGV"

5.88 kDa

Protein Stats results

Results for 274 residue sequence "Untitled" starting "MVGRRALIVL"

Pattern:	Times found:	Percentage:
A	25	9.12
B	0	0.00
C	1	0.36

NQO1:	AAB60701
	P15559
	>AAB60701.1 NAD(P)H:quinone oxireductase [Homo sapiens] MVGRRALIVLAHSERTSFNYAMKEAAAAALKKKGWEVVESDLYAMNFNPIISRKDITGKLKDPANFQYPA ESVLAYKEGHLSPDIVAEQKKLEAADLVIFQFPLQWFGVPAILKGWFERVFIGEFAYTYAAMYDKGPFRS KKAVLSITTGGSGSMYSLQGIHGDMNVILWPIQSGILHFCGFQVLEPQLTYSIGHTPADARIQILEGWKK RLENIWDETPLYFAPSSLFDLNFQAGFLMKKEVQDEEKNKKFGLSVGHHLGKSIPTDNQIKARK
	FQFPLQWFGVPAILKGWFERVFIGEFAYTYAAMYDKGPFRSKKAVLSITTG 5.88 kDa
	Cystein:1
	✅ Your collection was saved. Edit your collection.

NAD(P)H:quinone oxireductase [Homo sapiens]

GenBank: AAB60701.1