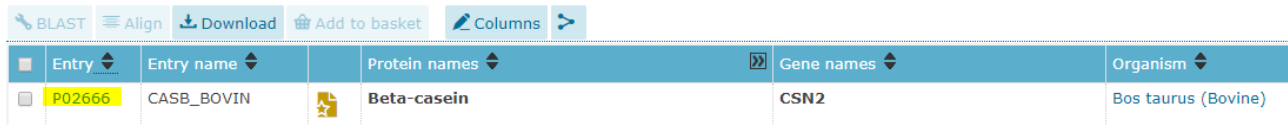


PEPTIDE PREDICTOR: HELP

ENTER UNIPROT.ORG PROTIIN ACCESSION NUMBER

In this field you should enter the six character long protein accession number which can be found at www.uniprot.org. Here highlighted for bovine beta-casein (P02666):



The screenshot shows a web interface with a table. The table has five columns: Entry, Entry name, Protein names, Gene names, and Organism. The first row contains the following data: Entry: P02666 (highlighted in yellow), Entry name: CASB_BOVIN, Protein names: Beta-casein, Gene names: CSN2, Organism: Bos taurus (Bovine). Above the table are several buttons: BLAST, Align, Download, Add to basket, Columns, and a right-pointing arrow.

Entry	Entry name	Protein names	Gene names	Organism
P02666	CASB_BOVIN	Beta-casein	CSN2	Bos taurus (Bovine)

Otherwise you can enter the amino acid sequence (in single amino acid letters).

MASS

Choose either Monoisotopic or Average mass for calculations.

ENZYME CLEAVAGE

Choose the enzyme which you want to hydrolyze the protein with. You can choose more than one enzyme. Below is the list of enzyme patterns that the program uses.

Enzyme	P2'	P1'	P1	P2
Trypsin	-	R or K	Not P	-
GluC	-	D or E	Not P	-
AspN	-	-	D	-
chymotrypsin	-	F,W,Y or L	Not P	-
Pepsin A	-	F or L	-	-
LysC	-	K	-	-
LysN	-	-	K	-
Elastase	-	A,V,I,L,G or R	G,P,A,L or F	-
Protein endopeptidase*	H,K or R	P	Not P	-

Cathepsin D	-	A,V,L,I,P,M,F or W	A,V,L,I,P,M or F	-
Formic acid	-	D	Not P	-
Proteinase K	-	A,E,F,I,L,T,V,W or Y	-	-
Glutamyl endopeptidase	-	E	-	-
Iodosobenzoic acid	-	W	-	-
CNBr	-	M	-	-

EXCLUSION

Contains different options for excluding peptides from the list:

- Excluded the signal and propeptide, as found on uniprot.org.
- Minimum and maximum amino acid length of the peptide. The default minimum value is set to 5, but it can be set as low as 0.
- Excluded peptides containing specific amino acids.

MODIFICATIONS

- Specific post-translation modification
- Modifications to the N and C terminal of the peptides

MASS CALCULATIONS

The mass of the peptides and the mass of its different charges in positive mode is given and calculated based on the following values and formula.

Group	Compound	Monoisotopic mass	Average mass
Amino acids	A	71.03711	71.0788
	R	156.10111	156.1875
	N	114.04293	114.1038
	D	115.02694	115.0886
	C	103.00919	103.1388
	E	129.04259	129.1155
	Q	128.05858	128.1307
	G	57.02146	57.0519
	H	137.05891	137.1411
	I	113.08406	113.1594
	L	113.08406	113.1594
K	128.09496	128.1741	

	M	131.04049	131.1926
	F	147.06841	147.1766
	P	97.05276	97.1167
	S	87.03203	87.0782
	T	101.04768	101.1051
	W	186.07931	186.2132
	Y	163.06333	163.176
	V	99.06841	99.1326
C- and N-terminal	H	1.007825	1.00794
	Acetyl (Ac)	43.0443	43.04524
	Biotin	227.3056	227.3048
	Carbamyl	43.00581	44.03283
	Fmoc	222.0681	223.07602
	OH	17.00274	17.006
	Methyl	14.01565	31.03273
	Amidated	-0.98402	16.02124
Modification	Oxidation (M)	15.995	15.9994
	Phosphorylation (S/T)	79.96633	79.9799
	Deamidation (N/Q)	0.984	0.98476
	Carbamidomethyl (C)	57.021	57.05162

SEARCH MASS

Enter a mass you want to search for within a range of \pm .

PRODUCT ION CALCULATOR

The second column in the result section after pressing submit, contains the amino acids sequence of the resulting peptides. The peptide sequence is also a hyperlink to the product ion calculator for that specific amino acid sequence. The product ion calculator will give an overview of the b, y and a ions with 1-3 charges.