Peptide Property Calculator

Three to One Letter Converter:

Pull down the menu to view the 3 to 1 conversion.[1]

Enter Peptide Sequence in Box (use one letter code)

```
MSLTSNNKYGNTKILTETEKYSVTKLSTDLSFLPGSNGNNNTIDTHHFEGLVDTALQKAL
VNDLDHIYIWNYNSIQKDTPICKISLHDDYSVLSSPPICLFTSSISSTNNDTANYNNNAS
GNINSGKFNNGICIINKKNSQFLYFEDISTINNLYTKLSKSKAHVLDLKLKDNENITSTI
NCEPSGIIIATSLGRVLFITIKDSTGKPKLELKQQLIKPQNSFFFRNLDSSKEIISLKKG
PIVGKGERLLYITTRGGSLQIWQLSINSKSFKRLEINIYEHVLDSLQDLYPFAHGTLAFL
```

Calculate

Hydropathy Plot Window size: 11 HydroPlot

Length: 459 Residues... Molecular Weight: 51610 g/mol

Extinction Coefficient: 41990 cm^{-1} M^{-1}

Approximate Volume: 62448 A^3

BLAST

Three letter code:

```
Met - Ser - Leu - Thr - Ser - Asn - Asn - Lys - Tyr - Gly -
Asn - Thr - Lys - Ile - Leu - Thr - Glu - Thr - Glu - Lys -
Tyr - Ser - Val - Thr - Lys - Leu - Ser - Thr - Asp - Leu -
Ser - Phe - Leu - Pro - Gly - Ser - Asn - Gly - Asn - Asn -
Asn - Thr - Ile - Asp - Thr - His - His - Phe - Glu - Gly -
```

To use this calculator, you must be using Netscape 2.0 or later
or Internet Explorer version 3.0 or later, or another Javascript-capable browser
This page was written in Javascript.

Hydropathy Plot

Hydropathy plots allow for the visualization of hydrophobicity over the length of a peptide sequence. A hydropathy scale which is based on the hydrophobic and hydrophilic properties of the 20 amino acids is used. A moving "window" determines the summed hydropathy at each point in the sequence (Y coordinate). These sums are then plotted against their respective positions (X coordinate). Such plots are useful in determining the hydrophobic interior portions of globular proteins as well as determining membrane spanning regions of membrane bound proteins.
In this calculation the window size has is variable, allowing the user to change the sensitivity of the

calculation. Smaller windows result in "noisier" plots than do larger windows. Window sizes between 7-11 residues were found by Kyte and Doolittle to maximize the information content of the plots. It is advised that the peptide length should be greater than double the window size to get any useful information from the Hydropathy plot.
Reference:Kyte and Doolittle *Jol Mol. Bio. (1982) 157 105-132.*

Extinction Coeffient

UV spectrophotometry is a useful tool for determining protein concentration in a solution. In order to take advantage of this method one needs an accurate measure of the protein of interest's extinction coefficient (molar absorbtion coefficient). Assays that have been used include dry weight calculations, spectral methods, and colorimic techniques (Bradford and Lowry assays). These methods work well but require a fairly large amount of protein, yet modern protein sequencing methods allow us to use sequence data to determine extinction coefficients.

Assumptions:
The primary assumption is the spectral contributions of the tyrosine, tryptophan and cystine at 280 nm do not differ significantly in the native form of the protein, relative to the denatured form. The calculation is based on the Edlehoch model in which proteins are examined in a 6M guanidinium hydrochloride (Gdn-HCl) denaturing solution which allowed for matching of native to denatured forms. Another assumption is that the protein contains no other chromophores (thus those proteins containing prothetic groups absorbing UV and visible portions of the spectrum can't be measured using this calculation).

The calculations is as follows:

$$\mathbf{E_{M,Gdn\text{-}HCl} = aE_{M,Tyr} + bE_{M,Trp} + cE_{M,Cys}}$$

Where a,b,c are the number of tyrosine, trytophan and cystine residues per mole of protein and $E_{residue}$ are the molar extinction rated of the residue at the wavelength used (280 nm). To get the extinction coefficient of the native protein Beer's law is used:

$$\mathbf{Abs_{Gdn\text{-}HCl}/E_{M,Gdn\text{-}HCl} = C_{Den}}$$

which is equivalent to that of the native protein

$$\mathbf{Abs_{nat}/E_{nat} = C_{nat}}$$

since the experimental conditions set the concentrations of both the denature and native form equal. Thus combining the equations above allows one to obtain the extinction coefficient of the native form:

$$\mathbf{(Abs_{nat})(E_{M,Gdn\text{-}HCl})/(Abs_{M,Gdn\text{-}HCl}).}$$

Reference:Gill and von Hipple *Anal Biochem 182,319-326 (1989)*
Extinction Coefficients at 280nm

Residue	Moles^{-1} cm^{-1}
Trp	5690
Tyr	1280

Cys 120

In 6.0 M guanidium hydrochloride, 0.02 M phosphate buffer, pH 6.5.
Reference:Gill and von Hipple *Anal Biochem 182,319-326 (1989)*

Volume

A peptide's volume can be estimated from the molecular weight of the peptide and an average protein partial specific volume. The partial specific volume of a protein is ratio between it's volume and molecular weight.

Assumptions:
The average of experimentally determined partial specific volumes for soluble, globular proteins is approximately 0.73 cm^3/g (average of experimental values from 13 soluble proteins). This value varies from protein to protein, but the range is rather narrow, between 0.70 and 0.75 cm^3/g.

The simple calculation starts from

$$\frac{\textbf{0.73 cm}^3\textbf{/g x 10}^{24}\textbf{A/cm}^3\textbf{ x molecular weight g/mole}}{\textbf{6.02 x 10}^{23}\textbf{ molecules/mole}}$$

and results in a protein volume of approximately:

(1.21 x MW) A^3/molecule

This provides a reasonable estimate for general uses. A recent reference concerning partial specific volumes is: Harpaz, Gerstein and Chothia *(1994) Structure 2, 641-649 (issue of July 15)*.

Amino Acid Table

Amino Acid	3-Letter Code	1-Letter Code	Molecular Weight1	Hydropathy2
Alanine	Ala	A	89.09	6.3
Cysteine	Cys	C	121.16	7.0
Aspartate	Asp	D	133.10	1.0
Glutamate	Glu	E	147.13	1.0
Phenylalanine	Phe	F	165.19	7.2
Glycine	Gly	G	75.07	4.1
Histidine	His	H	155.16	1.3

Isoleucine	Ile	I	131.18	9.0
Lysine	Lys	K	146.19	0.6
Leucine	Leu	L	131.18	8.2
Methionine	Met	M	149.21	6.4
Asparagine	Asn	N	132.12	1.0
Proline	Pro	P	115.13	2.9
Glutamine	Gln	Q	146.15	1.0
Arginine	Arg	R	174.20	0.0
Serine	Ser	S	105.09	3.6
Threonine	The	T	119.12	3.8
Valine	Val	V	117.15	8.7
Tryptophan	Trp	W	204.23	3.6
Tyrosine	Tyr	Y	181.19	3.2
Asaragine or Aspartic acid	Asx	B	132.61	1.0
Glutamine or Glutamic acid	Glx	Z	146.64	1.0

Molecular Weight notes:
The molecular weights above are those of the free acid and not the residue , which is used in the claculations performed by the Peptide Properties Calculator. Subtracting an the weight of a mole of water (18g/mol) yields the molecular weight of the residue. The weights used for Glx and Asx are averages.

Hydropathy Notes:
Hydropathies listed above were taken from the Hydropathy scale derived by Kyte and Doolittle *Jol Mol. Bio. (1982) 157 105-132.*

Adam Chazan e-mail and PH entry.
Center for Biotechnology
Northwestern University
Evanston, IL 60201
Peptide Calculator version 1.00 (Chazan)