

P08574 (CY1_HUMAN): Domain 108 – 209: Cytochrome c

First step: generate tryptic peptides from a given protein sequence

mass	position	peptide sequence: Tryptic peptides
2648.1966	40-63	ELAAEVEVQDGPNEGEMFM RPGK
1914.9384	64-79	LFDYFPKPYPNSEAAR
1716.7291	12-26	QVCASCHSMDFVAYR
1670.8860	80-95	AANNGALPPDLSYIVR
1463.6835	27-39	HLVGVCYTEDEAK
741.3930	6-11	GFQVYK
514.1892	98-102	HGGED

Second step:

Generate a table for each peptide, in which all masses for all species are given for a defined posttranslational modification:

e.g. phosphorylation:

Rules:

1. each phosphorylation increases the mass by 79.9663 Da.
2. The following amino acids can be phosphorylated: D, S, T, Y, H, C

As a result the peptide GFQVYK is listed with the

Sequence + PTM (underlined, bold, italic)	M	[M+H] ⁺	[M+H] ²⁺	[M+H] ³⁺
HLVGVCYTEDEAK	1462,6835	1463,6835	732,34175	488,56117
<u>HL</u> VGVCYTEDEAK	1542,6498	1543,6498	Etc.	Etc.
<u>HL</u> VGVC Y TEDEAK	1622,6161	1623,6161		
<u>HL</u> VGVC C YTEDEAK	1702,5824	1703,5824		
<u>HL</u> VGVC T YTEDEAK	1782,5487	1783,5487		
<u>HL</u> VGVC S YTEDEAK	1862,515	1863,515		
<u>HL</u> VGVC D YTEDEAK	1942,4813	1943,4813		

Third step:

Generate a table for each peptide, in which all masses for all species are given for a further defined posttranslational modification:

e.g. sulfation: occurs on Y and adds a mass of 79,956815 to the amino acid:

Sequence + PTM (underlined, bold, italic)	M	[M+H] ⁺	[M+H] ²⁺	[M+H] ³⁺
HLVGVCYTEDEAK	1462,6835	1463,6835	732,34175	488,56117
HLVGVC <u>Y</u> TEDEAK	1542,640315	1543,640315	Etc.	Etc.

Combine the PTMs:

Rule: every amino acid, which is phosphorylated, can not be sulfated and vice versa

Table: ...