

PIERRE WENSEL

PROTEOMICS: EXERCISE 1-DeNOVO

Open the file `Ex-1-HCD-OT-OT.raw` using the SeeMS software. This data has been acquired with high resolution both in MS1 and MS2 using HCD as fragmentation method.

Go to `scan 326` and determine the sequence of this peptide from the MS2 data. Remember to determine the mass of the peptide from the previous MS1 scan. You have a printout of the MS2 spectrum in the next page and a printout of the previous MS1 scan in case you don't have access to the SeeMS software.

To validate the result use PROSIT (the mass/intensity information is in the `scan326.xlsx` file located in the `evaluation-task-1-denovo` folder)

The output of the exercise is the sequence (this is a mouse fully tryptic peptide with no missed cleavages) and the explanation on how you have deduced the sequence plus the correlation between the experimental spectrum and the predicted spectrum using PROSIT.

<https://prospector.ucsf.edu/prospector/cgi-bin/msform.cgi?form=mspattern>

V[IL]EST[QK]D[IL]GND[IL]AGVMA[IL][QK]R

[←](#) [↻](#) <https://prospector.ucsf.edu/prospector/cgi-bin/mssearch.cgi> [A](#) [☆](#)

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MS-Pattern Search Results

Search completed. 4 sec elapsed. 0 sec remaining.

[\[±\] Parameters](#)

[\[±\] Pre Search Results \(SwissProt.2021.06.18\)](#)

MS-Pattern search selects **2** entries.

Number of Substitutions	Matching Sequence	Start AA	Peptide M+H	MS-Digest Index #	Protein MW (Da)/pI	Accession #	Species	Protein Name
0	(K)VIESTQDLGNDLAGVMALQR(K)	977	2130.0859	451189	274225/5.4	Q62261	MOUSE	Spectrin beta chain, non-erythrocytic 1
3	(K)V V ESTKDLG Q DLAGV I AIR(K)	968	2112.1659	451186	245252/5.2	P15508	MOUSE	Spectrin beta chain, erythrocytic

https://www.uniprot.org/uniprotkb/Q62261/entry

UniProt BLAST Align Peptide search ID mapping SPARQL UniProtKB Advanced | List Search Help

Q62261 · SPTB2_MOUSE

Function

Names & Taxonomy **Protein**ⁱ Spectrin beta chain, non-erythrocytic 1 **Amino acids** 2363 (go to sequence)

Subcellular Location **Gene**ⁱ Sptbn1 **Protein existence**ⁱ Evidence at protein level

Phenotypes & Variants **Status**ⁱ UniProtKB reviewed (Swiss-Prot) **Annotation score**ⁱ 56

PTM/Processing **Organism**ⁱ Mus musculus (Mouse)

Expression **Entry** **Variant viewer** **Feature viewer** **Genomic coordinates** **Publications** **External links** **History**

Interaction **BLAST** **Align** **Download** **Add** **Add a publication** **Entry feedback**

Structure

Family & Domains

Sequence & Isoform

Similar Proteins

Functionⁱ

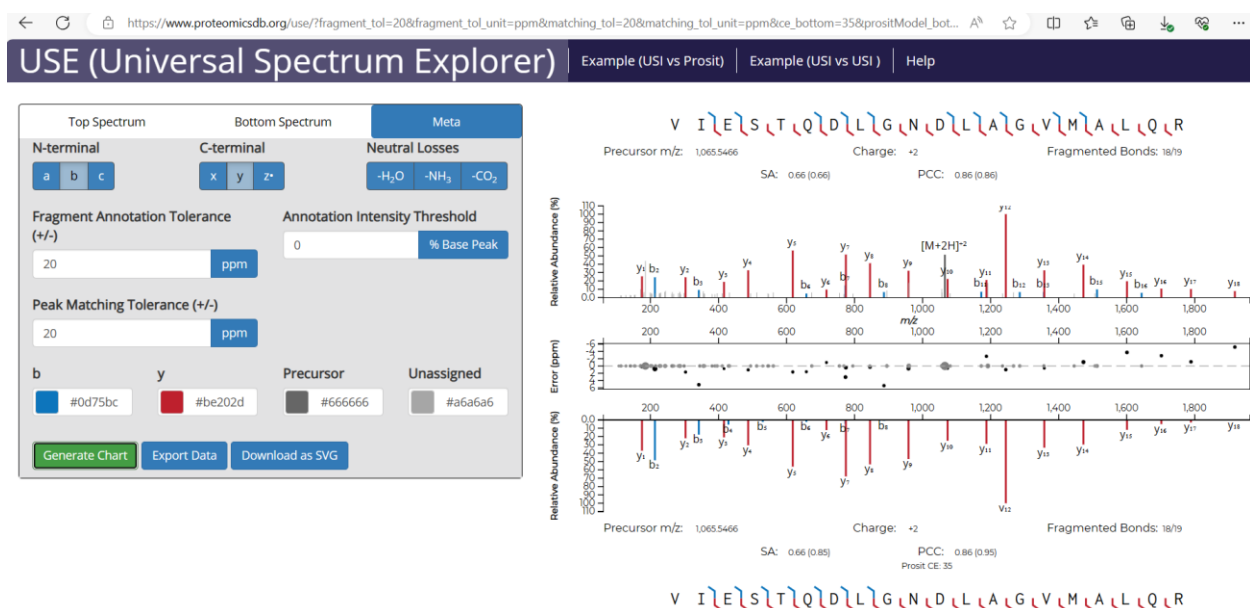
Fodrin, which seems to be involved in secretion, interacts with calmodulin in a calcium-dependent manner and is thus candidate for the calcium-dependent movement of the cytoskeleton at the membrane. Plays a critical role in central nervous system development and function. [1 Publication](#)

GO annotationsⁱ

Access the complete set of GO annotations on QuickGO [↗](#)

Slimming set:
generic

VIESTQDLGNDLAGVMALQR



V I E S T Q D L G N D L A G V M A L Q R

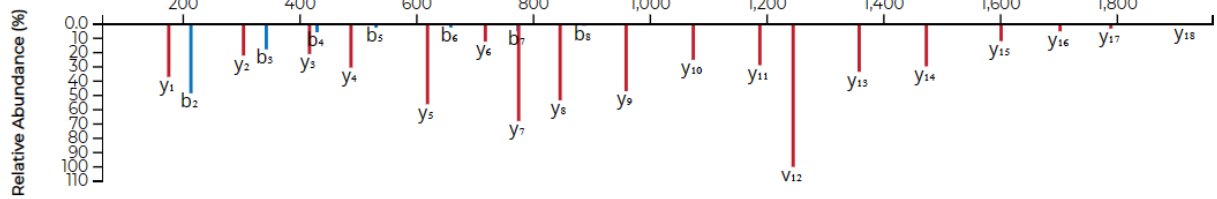
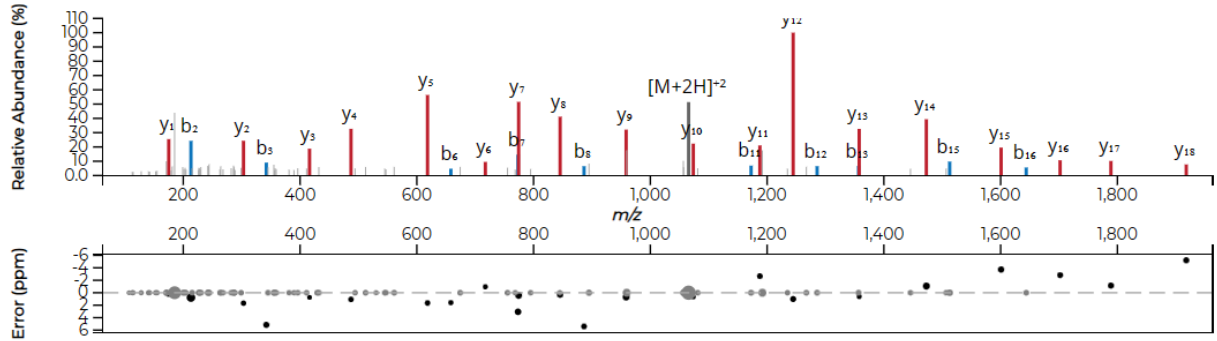
Precursor m/z: 1,065.5466

Charge: +2

Fragmented Bonds: 18/19

SA: 0.66 (0.66)

PCC: 0.86 (0.86)



Precursor m/z: 1,065.5466

Charge: +2

Fragmented Bonds: 18/19

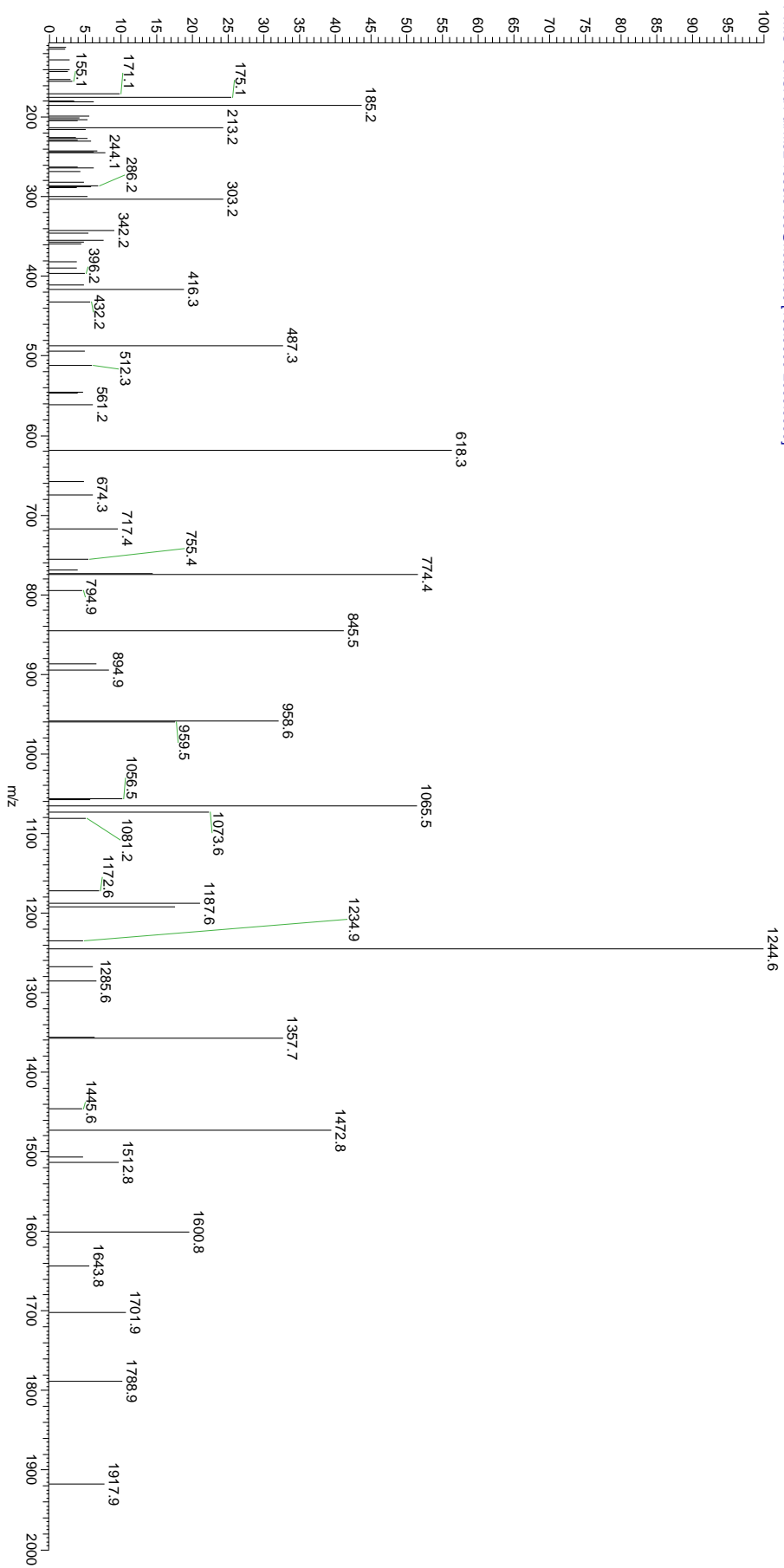
SA: 0.66 (0.85)

PCC: 0.86 (0.95)

Prosit CE: 35

V I E S T Q D L G N D L A G V M A L Q R

EX1-HCD-OT-OT #326 RT: 91.26 AV: 1 NL: 9.23E5
T: FTMS + c NSI d Full ms2 1065.5463@hcd30.00 [106.0000-2000.0000]



EX1-HCD-OT-OT #321 RT: 91.26 AV: 1 NL: 4.87E7
T: FTMS + p NSI Full ms [350.0000-1400.0000]

