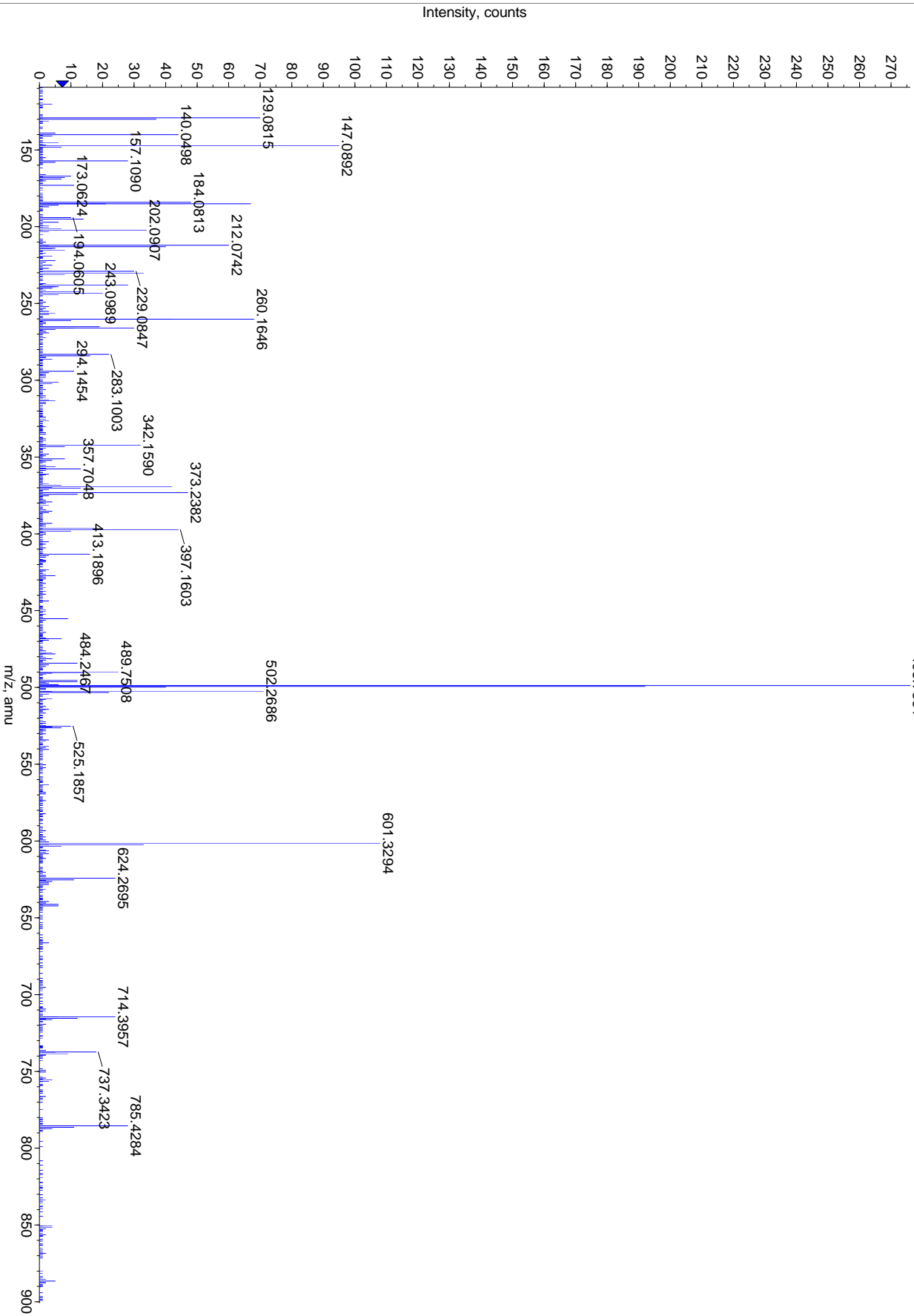


+TOF Product (507.8): Experiment 2, 22.141 min From Sample 2 (060605_BSA-Verdau) of BSA.wiff
a=3.56542312359049760e-004, t0=3.25081628932020980e+001

Max: 276.0 counts.



Mass Spectrum (as measured)

Fragmented peptide ion: m/z 507.76; $z = 2$

Found m/z values, recalibrated, (Noisepeaks where filtered, every signal can be explained!)

129.07	147.11	(212.10)	230.11	260.20	(283.14)
(369.21 ($z = 2$))		373.28	(397.21)	414.23	(434.76 ($z = 2$))
502.32	601.39	(624.34)	642.35	714.48	737.42
785.51	868.51	886.56	1014.61		

Help: (only) one of the ion series (a, b, c, x, y or z) is complete! All ions not marked differently have a charge of one ($z = 1$).

Tasks:

- 1) What is the sequence of the peptide, which was formed after tryptic digestion of a protein?
- 2) Can you assign all the ions according to the nomenclature (e.g. a, b, c, x, y or z, (additional) loss of water/ammonia?)
- 3) Are there problems when assigning the peptide sequence? When can these problems be seen?
- 4) Which method was used for ionization, which one for fragmentation? Explanatory statement!
- 5) Why are there fragment ions with a higher value for m/z than the precursor ion has?

Support (additional to the lecture):

Mass list of the amino acid residues (- H₂O)

symbol	composition	structure	monoisotopic	average
Ala A	Alanine C ₃ H ₅ NO	$\begin{array}{c} \text{CH}_3 \\ \\ \text{-NH-CH-CO-} \end{array}$	71.03711	71.0788
Arg R	Arginine C ₆ H ₁₂ N ₄ O	$\begin{array}{c} \text{CH}_2\text{-(CH}_2\text{)}_2\text{-NH-C-NH}_2 \\ \\ \text{-NH-CH-CO-} \\ \\ \text{NH} \end{array}$	156.10111	156.1876
Asn N	Asparagine C ₄ H ₆ N ₂ O ₂	$\begin{array}{c} \text{CH}_2\text{-CONH}_2 \\ \\ \text{-NH-CH-CO-} \end{array}$	114.04293	114.1039
Asp D	Aspartic Acid C ₄ H ₅ NO ₃	$\begin{array}{c} \text{CH}_2\text{-COOH} \\ \\ \text{-NH-CH-CO-} \end{array}$	115.02694	115.0886
Cys C	Cysteine C ₃ H ₅ NOS	$\begin{array}{c} \text{CH}_2\text{-SH} \\ \\ \text{-NH-CH-CO-} \end{array}$	103.00919	103.1448
Gln Q	Glutamine C ₅ H ₈ N ₂ O ₂	$\begin{array}{c} \text{CH}_2\text{-CH}_2\text{-CONH}_2 \\ \\ \text{-NH-CH-CO-} \end{array}$	128.05858	128.1308
Glu E	Glutamic Acid C ₅ H ₇ NO ₃	$\begin{array}{c} \text{CH}_2\text{-CH}_2\text{-COOH} \\ \\ \text{-NH-CH-CO-} \end{array}$	129.04259	129.1155
Gly G	Glycine C ₂ H ₃ NO	$\text{-NH-CH}_2\text{-CO-}$	57.02146	57.0520
His H	Histidine C ₆ H ₇ N ₃ O		137.05891	137.1412
Ile I	Isoleucine C ₆ H ₁₁ NO	$\begin{array}{c} \text{CH(CH}_3\text{)-CH}_2\text{-CH}_3 \\ \\ \text{-NH-CH-CO-} \end{array}$	113.08406	113.1595
Leu L	Leucine C ₆ H ₁₁ NO	$\begin{array}{c} \text{CH}_2\text{-CH(CH}_3\text{)}_2 \\ \\ \text{-NH-CH-CO-} \end{array}$	113.08406	113.1595
Lys K	Lysine C ₆ H ₁₂ N ₂ O	$\begin{array}{c} \text{CH}_2\text{-(CH}_2\text{)}_3\text{-NH}_2 \\ \\ \text{-NH-CH-CO-} \end{array}$	128.09496	128.1742
Met M	Methionine C ₅ H ₉ NOS	$\begin{array}{c} \text{CH}_2\text{-CH}_2\text{-S-CH}_3 \\ \\ \text{-NH-CH-CO-} \end{array}$	131.04049	131.1986
Phe F	Phenylalanine C ₉ H ₉ NO	$\begin{array}{c} \text{CH}_2\text{-Ph} \\ \\ \text{-NH-CH-CO-} \end{array}$	147.06841	147.1766
Pro P	Proline C ₅ H ₇ NO		97.05276	97.1167
Ser S	Serine C ₃ H ₅ NO ₂	$\begin{array}{c} \text{CH}_2\text{-OH} \\ \\ \text{-NH-CH-CO-} \end{array}$	87.03203	87.0782
Thr T	Threonine C ₄ H ₇ NO ₂	$\begin{array}{c} \text{CH(OH)-CH}_3 \\ \\ \text{-NH-CH-CO-} \end{array}$	101.04768	101.1051
Trp W	Tryptophan C ₁₁ H ₁₀ N ₂ O		186.07931	186.2133
Tyr Y	Tyrosine C ₉ H ₉ NO ₂		163.06333	163.1760
Val V	Valine C ₅ H ₉ NO	$\begin{array}{c} \text{CH(CH}_3\text{)}_2 \\ \\ \text{-NH-CH-CO-} \end{array}$	99.06841	99.1326

More literature and Tools:

<http://www.colby.edu/chemistry/NMR/NMR.html>

http://www.matrixscience.com/help/fragmentation_help.html

<http://prospector.ucsf.edu/>

<http://www.ionsource.com/tutorial/DeNovo/nomenclature.htm> (<http://www.ionsource.com>)