Supplementary Material

The Reactivity of Human Serum Albumin towards *trans*-4-Hydroxy-2-nonenal

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Data Analysis Expanded Details

Sequest (version 28, revision 13; Thermo, San Jose, CA, USA) [1], controlled through BioWorks Browser (version 3.3.1, SP1; Thermo), was used to obtain peptide identifications from recorded tandem mass spectra (MS/MS). Scan grouping, when extracting peak lists, was disabled in all cases. For searching linear ion trap MS/MS from the LTQ XL (Thermo) instrument, average masses were used for parent ions while monoisotopic masses were used for fragment ions. For LTQ Orbitrap Velos (Thermo) data, monoisotopic masses were used for both parent and fragment ions. This approach was taken because the LTQ Orbitrap Velos system can, while the LTQ XL linear ion trap system cannot, reliably identify the monoisotopic peak. Only peptides fully conforming to digestion by trypsin were considered. Trypsin was defined as cutting to the C-terminal side of lysine and arginine except when the residue to the C-terminal side of the proposed break was proline. A maximum of two missed cleavages were allowed. For searching linear ion trap MS/MS from the LTQ XL instrument, the parent ion tolerance was set to

±2 AMU while the fragment ion tolerance for all dissociation methods was set to ±1 AMU. For Orbitrap data, the parent ion tolerance was set to ±15 ppm while the fragment ion tolerance for collision-induced dissociation (CID) fragmentation was set to ±1 AMU and for higher-energy C-trap dissociation (HCD) fragmentation was set to ±0.1 AMU (HCD MS/MS were recorded using the Orbitrap while CID MS/MS were recorded in the linear ion trap region of the LTQ Orbitrap Velos instrument). A maximum of three differential modifications were permitted for each peptide. Precise modification mass shifts are listed in Table S1 for experiments without iTRAQ labels (Applied Biosystems, Foster City, CA, USA) and in Table S2 for experiment with iTRAQ labels.

Modification Description	**Modification Composition**	**Monoisotopic Mass Shift**	**Type**
Oxidation at Met	+O	+15.994915	Differential
Iodoacetamide Alkylation at Cys	$+C_2H_3NO$	+57.021464	Fixed
Michael Addition of HNE at Cys, Reduced	$+C_9H_{18}O_2$ −[acetamide cap]	+101.109216	Differential
Michael Addition of HNE at His, Reduced	$+C_9H_{18}O_2$	+158.130680	Differential
Michael Addition of HNE at Lys, Reduced	$+C_9H_{18}O_2$	+158.130680	Differential
Schiff Base Formation with HNE at Lys, Reduced	$+C_9H_{16}O$	+140.120115	Differential

Table S1: Modification mass shifts considered in non-iTRAQ experiments

Modification Description	Modification Composition	Monoisotopic Mass Shift	Type
Oxidation at Met	+O	+15.994915	Differential
Iodoacetamide Alkylation at Cys	$+C_2H_3NO$	+57.021464	Fixed
iTRAQ Label at Lys	$+^{12}C_5{}^{13}C_2{}^{1}H_{12}{}^{14}N_2{}^{18}O$/ $+^{12}C_4{}^{13}C_3{}^{1}H_{12}{}^{14}N^{15}N^{16}O$	+144.103991†	Fixed
iTRAQ Label at Peptide N-terminus	$+^{12}C_5{}^{13}C_2{}^{1}H_{12}{}^{14}N_2{}^{18}O$/ $+^{12}C_4{}^{13}C_3{}^{1}H_{12}{}^{14}N^{15}N^{16}O$	+144.103991†	Fixed
iTRAQ Label at Tyr‡	$+^{12}C_5{}^{13}C_2{}^{1}H_{12}{}^{14}N_2{}^{18}O$/ $+^{12}C_4{}^{13}C_3{}^{1}H_{12}{}^{14}N^{15}N^{16}O$	+144.103991†	Differential
Michael Addition of HNE at Cys, Reduced	$+C_9H_{18}O_2$ −[acetamide cap]	+101.109216	Differential
Michael Addition of HNE at His, Reduced	$+C_9H_{18}O_2$	+158.130680	Differential
Michael Addition of HNE at Lys, Reduced	$+C_9H_{18}O_2$ −[iTRAQ label]	+14.026689	Differential
Schiff Base Formation with HNE at Lys, Reduced	$+C_9H_{16}O$ −[iTRAQ label]	−3.983876	Differential

Table S2: Modification mass shifts considered in iTRAQ experiments; † iTRAQ label mass shift value was the average for the four tags (separation between heavy pair and light pair is circa 0.004 Da, too small to resolve with available instrumentation); ‡ iTRAQ label addition at tyrosine only considered with Orbitrap data and found to be uncommon

Sequest used a protein sequence database that was composed of entries for normal and reversed versions of NCBI RefSeq human sequences and the UniProt porcine trypsin sequence. NCBI RefSeq human sequences were downloaded on November 20, 2010, from ftp://ftp.ncbi.nlm.nih.gov/refseq/H_sapiens/mRNA_Prot/human.protein.faa.gz, while the UniProt porcine trypsin sequence (TRYP_PIG) was obtained on the same day from http://www.uniprot.org/uniprot/P00761. The final database contained 68,040 sequences (normal and reversed versions of 34,019 human and one pig protein).

Initial Sequest output was refined using the Trans-Proteomic Pipeline software package (version 4.4, VUVUZELA, revision 1, build 201010121551, MinGW; Institute for Systems Biology, Seattle, WA, USA). PeptideProphet [2] was operated in semi-

supervised mode [3] so that reversed (decoy) protein sequence entries could be used to improve discrimination between correct and incorrect identifications. At the PeptideProphet stage, repeat runs were combined and iTRAQ reporter ion intensities were extracted and corrected (using the Libra module; isotope corrections were those provided by Applied Biosystems, the iTRAQ kit manufacturer). PeptideProphet output was exported and then manipulated using Microsoft Access database software. Instances where the same MS/MS produces two identifications capable of passing the scoring threshold were removed (can occur in linear ion trap data when MS/MS are searched as potentially resulting from doubly- and triply-charged precursors).

Results Expanded Details

MODIFICATIONS: We report modifications resulting from the exposure of human serum albumin (HSA) to *trans*-4-hydroxy-2-nonenal (HNE) at HNE:HSA ratios of 1:1 and 10:1. For both treatment ratios, five complete repeats were performed. Four were analyzed using the linear ion trap system while one was analyzed using the Orbitrap system. For each preparation, three replicate LC–MS/MS runs were collected. Therefore, a total of twelve runs were performed at each ratio using the LTQ XL and three runs were performed at each ratio using the LTQ Orbitrap Velos. In the main manuscript, Table 1 gives the modifications discovered in terms of a count of runs in which the modification in question was detected by (i) CID MS/MS using the LTQ XL, (ii) electron-transfer dissociation (ETD) MS/MS using the LTQ XL and (iii) CID MS/MS using the LTQ Orbitrap Velos. In this document, Tables S3 and S4 give the peptides that support the modification identifications given in Table 1. Results are presented as counts of runs in

which the peptide in question was detected in Table S3 and as simple detection counts in Table S4 (counts for the fragmentation methods and instrumental platforms are given in the same way as found in Table 1). Using a PeptideProphet score threshold of 0.9, 38 modified peptides were initially proposed from the LTQ XL CID scans while 31 were proposed from the LTQ XL ETD scans. After manual scrutiny, 35 peptides from the LTQ XL CID scans and 27 peptides from the LTQ XL ETD scans were accepted. Naturally, there was considerable overlap, resulting in a total of 39 accepted peptides from the LTQ XL. Using the same PeptideProphet scoring threshold, 18 modified peptides were initially identified using the LTQ Orbitrap Velos. After inspection, 17 were accepted. Example MS/MS for all accepted peptides, from all fragmentation methods and instrumental platforms, are provided at the end of this document.

Modified Peptide (with flanking residues)	Modification Site or Sites (MA indicates Michael addition; SB indicates Schiff base formation)	Counts of LC–MS/MS runs in which the modified peptide was identified using LTQ XL CID scans (maximum = 12)/LTQ XL ETD scans (maximum = 12)/LTQ Orbitrap Velos CID scans associated with high mass accuracy Orbitrap precursor ion mass measurements (maximum = 3)	
		1:1 HNE to HSA Ratio	10:1 HNE to HSA Ratio
K.DLGEENFKALVLIAFAQYLQQC#PFEDHVK.L	Cys-034 (MA)	not detected	0/0/1
K.ALVLIAFAQYLQQC#PFEDHVK.L	Cys-034 (MA)	9/1/0	9/3/3
K.SLH@TLFGDK.L	His-067 (MA)	12/0/3	12/5/3
K.SLHTLFGDK^LCTVATLR.E	Lys-073 (MA)	not detected	3/0/0
R.NECFLQHK~DDNPNLPR.L	Lys-106 (SB)	not detected	0/1/0
R.LVRPEVDVMCTAFH@DNEETFLK.K	His-128 (MA)	0/2/0	2/3/0
K.K^YLYEIAR.R	Lys-137 (MA)	not detected	1/0/0
R.RH@PYFYAPELLFFAK.R	His-146 (MA)	12/11/0	12/12/3
R.RH@PYFYAPELLFFAKR.Y	His-146 (MA)	not detected	1/0/0
R.RH@PYFYAPELLFFAK^R.Y	His-146 (MA) & Lys-159 (MA)	not detected	0/2/1
R.YK^AAFTECCQAADK.A	Lys-162 (MA)	not detected	12/2/2
R.YK~AAFTECCQAADK.A	Lys-162 (SB)	not detected	10/1/0
R.LK^CASLQK.F	Lys-199 (MA)	6/0/2	11/0/3
R.AFK^AWAVAR.L	Lys-212 (MA)	not detected	12/0/1
K.AEFAEVSK^LVTDLTK.V	Lys-233 (MA)	not detected	9/4/0
K.LVTDLTK^VH@TECCHGDLLECADDR.A	Lys-240 (MA) & His-242 (MA)	8/0/0	3/0/0
K.VH@TECCHGDLLECADDR.A	His-242 (MA)	0/7/0	0/7/0
K.VH@TECCH@GDLLECADDR.A	His-242 (MA) & His-247 (MA)	not detected	9/4/0
K.VH@TECCH@GDLLECADDRADLAK.Y	His-242 (MA) & His-247 (MA)	not detected	3/7/0
R.ADLAK^YICENQDSISSK.L	Lys-262 (MA)	not detected	5/3/0
K.SH@CIAEVENDEMPADLPSLAADFVESK.D	His-288 (MA)	10/0/0	12/1/3
K.SH@CIAEVENDEM*PADLPSLAADFVESK.D	His-288 (MA)	1/0/0	11/1/1
R.RH@PDYSVVLLLR.L	His-338 (MA)	4/0/0	12/3/3
R.H@PDYSVVLLLR.L	His-338 (MA)	not detected	2/0/0
R.H@PDYSVVLLLRLAKTYETTLEK.C	His-338 (MA)	0/6/0	1/9/0
R.LAK^TYETTLEK.C	Lys-351 (MA)	10/0/0	9/0/0
R.LAK~TYETTLEK.C	Lys-351 (SB)	not detected	3/1/0
K.TYETTLEK^CCAAADPHECYAK.V	Lys-359 (MA)	not detected	1/3/0
K.CCAAADPH@ECYAK.V	His-367 (MA)	not detected	9/0/0
K.VFDEFK^PLVEEPQNLIK.Q	Lys-378 (MA)	not detected	5/1/0
K.QNCELFEQLGEYK^FQNALLVR.Y	Lys-402 (MA)	not detected	4/0/2
K.K^VPQVSTPTLVEVSR.N	Lys-414 (MA)	not detected	11/1/3
K.K~VPQVSTPTLVEVSR.N	Lys-414 (SB)	8/0/0	12/1/3
R.VTK^CCTESLVNR.R	Lys-475 (MA)	not detected	1/0/0
K.EFNAETFTFH@ADICTLSEK.E	His-510 (MA)	1/8/0	12/11/0
K.EFNAETFTFHADICTLSEK^ER.Q	Lys-519 (MA)	not detected	1/0/0
K.K^QTALVELVK.H	Lys-525 (MA)	not detected	0/1/3
K.K~QTALVELVK.H	Lys-525 (SB)	3/0/3	8/3/3
K.EQLK^AVMDDFAAFVEK.C	Lys-545 (MA)	4/7/0	11/11/3
K.EQLK~AVMDDFAAFVEK.C	Lys-545 (SB)	not detected	4/7/0

Table S3: Counts of LC–MS/MS runs in which the indicated modified peptide was identified. The PeptideProphet score threshold was 0.9. Five independent preparations were made for each HNE:HSA ratio. For each ratio, four preparations were analyzed using a Thermo LTQ XL linear ion trap mass spectrometer and one preparation was analyzed using a Thermo LTQ Orbitrap Velos instrument. In all cases, three replicate LC–MS/MS runs were recorded for each preparation. For the LTQ XL runs, one collision-induced dissocation (CID) and one electron-transfer dissociation (ETD) MS/MS were recorded for each precursor ion selected for fragmentation; resulting CID and ETD spectrum counts are presented separately. For the LTQ Orbitrap Velos runs, only CID MS/MS were recorded. C# indicates HNE Michael addition at Cys followed by reduction; H@ indicates HNE Michael addition at His followed by reduction; K^ indicates HNE Michael addition at Lys followed by reduction; K~ indicates Schiff base formation with HNE at Lys followed by reduction; M* indicates oxidation at Met.

Modified Peptide (with flanking residues)	Modification Site or Sites (MA indicates Michael addition; SB indicates Schiff base formation)	Counts of spectra that pased the PeptideProphet score threshold obtained using LTQ XL CID scans (from 12 LC–MS/MS runs)/LTQ XL ETD scans (from 12 LC–MS/MS runs)/LTQ Orbitrap Velos CID scans associated with high mass accuracy Orbitrap precursor ion mass measurements (from 3 LC–MS/MS runs)	
		1:1 HNE to HSA Ratio	10:1 HNE to HSA Ratio
K.DLGEENFKALVLIAFAQYLQQC#PFEDHVK.L	Cys-034 (MA)	not detected	0/0/1
K.ALVLIAFAQYLQQC#PFEDHVK.L	Cys-034 (MA)	13/1/0	16/3/10
K.SLH@TLFGDK.L	His-067 (MA)	16/0/8	68/23/30
K.SLHTLFGDK^LCTVATLR.E	Lys-073 (MA)	not detected	3/0/0
R.NECFLQHK~DDNPNLPR.L	Lys-106 (SB)	not detected	0/1/0
R.LVRPEVDVMCTAFH@DNEETFLK.K	His-128 (MA)	0/2/0	2/4/0
K.K^YLYEIAR.R	Lys-137 (MA)	not detected	1/0/0
R.RH@PYFYAPELLFFAK.R	His-146 (MA)	27/24/0	157/130/26
R.RH@PYFYAPELLFFAKR.Y	His-146 (MA)	not detected	1/0/0
R.RH@PYFYAPELLFFAK^R.Y	His-146 (MA) & Lys-159 (MA)	not detected	0/2/1
R.YK^AAFTECCQAADK.A	Lys-162 (MA)	not detected	20/2/4
R.YK~AAFTECCQAADK.A	Lys-162 (SB)	not detected	10/1/0
R.LK^CASLQK.F	Lys-199 (MA)	6/0/4	11/0/6
R.AFK^AWAVAR.L	Lys-212 (MA)	not detected	12/0/2
K.AEFAEVSK^LVTDLTK.V	Lys-233 (MA)	not detected	9/4/0
K.LVTDLTK^VH@TECCHGDLLECADDR.A	Lys-240 (MA) & His-242 (MA)	8/0/0	3/0/0
K.VH@TECCHGDLLECADDR.A	His-242 (MA)	0/7/0	0/10/0
K.VH@TECCH@GDLLECADDR.A	His-242 (MA) & His-247 (MA)	not detected	11/4/0
K.VH@TECCH@GDLLECADDRADLAK.Y	His-242 (MA) & His-247 (MA)	not detected	3/7/0
R.ADLAK^YICENQDSISSK.L	Lys-262 (MA)	not detected	6/3/0
K.SH@CIAEVENDEMPADLPSLAADFVESK.D	His-288 (MA)	10/0/0	86/8/6
K.SH@CIAEVENDEM*PADLPSLAADFVESK.D	His-288 (MA)	1/0/0	16/2/1
R.RH@PDYSVVLLLR.L	His-338 (MA)	4/0/0	46/3/21
R.H@PDYSVVLLLR.L	His-338 (MA)	not detected	2/0/0
R.H@PDYSVVLLLRLAKTYETTLEK.C	His-338 (MA)	0/6/0	1/9/0
R.LAK^TYETTLEK.C	Lys-351 (MA)	10/0/0	9/0/0
R.LAK~TYETTLEK.C	Lys-351 (SB)	not detected	3/1/0
K.TYETTLEK^CCAAADPHECYAK.V	Lys-359 (MA)	not detected	1/3/0
K.CCAAADPH@ECYAK.V	His-367 (MA)	not detected	9/0/0
K.VFDEFK^PLVEEPQNLIK.Q	Lys-378 (MA)	not detected	5/1/0
K.QNCELFEQLGEYK^FQNALLVR.Y	Lys-402 (MA)	not detected	4/0/4
K.K^VPQVSTPTLVEVSR.N	Lys-414 (MA)	not detected	25/4/5
K.K~VPQVSTPTLVEVSR.N	Lys-414 (SB)	8/0/0	36/4/17
R.VTK^CCTESLVNR.R	Lys-475 (MA)	not detected	1/0/0
K.EFNAETFTFH@ADICTLSEK.E	His-510 (MA)	1/8/0	20/21/0
K.EFNAETFTFHADICTLSEK^ER.Q	Lys-519 (MA)	not detected	1/0/0
K.K^QTALVELVK.H	Lys-525 (MA)	not detected	0/1/7
K.K~QTALVELVK.H	Lys-525 (SB)	3/0/8	8/5/17
K.EQLK^AVMDDFAAFVEK.C	Lys-545 (MA)	4/7/0	19/21/6
K.EQLK~AVMDDFAAFVEK.C	Lys-545 (SB)	not detected	4/7/0

Table S4: Counts of MS/MS supporting the indicated modified peptides. The PeptideProphet score threshold was 0.9. Five independent preparations were made for each HNE:HSA ratio. For each ratio, four preparations were analyzed using a Thermo LTQ XL linear ion trap mass spectrometer and one preparation was analyzed using a Thermo LTQ Orbitrap Velos instrument. In all cases, three replicate LC–MS/MS runs were recorded for each preparation. For the LTQ XL runs, one collision-induced dissocation (CID) and one electron-transfer dissociation (ETD) MS/MS were recorded for each precursor ion selected for fragmentation; resulting CID and ETD spectrum counts are presented separately. For the LTQ Orbitrap Velos runs, only CID MS/MS were recorded. C# indicates HNE Michael addition at Cys followed by reduction; H@ indicates HNE Michael addition at His followed by reduction; K^ indicates HNE Michael addition at Lys followed by reduction; K~ indicates Schiff base formation with HNE at Lys followed by reduction; M* indicates oxidation at Met.

MASS LIST: Measurements of iTRAQ reporter ion intensities obtained using pulsed-Q dissociation (PQD) in a linear ion trap system are not very precise, so a targeted mass list was used to increase the number of measurements obtained. The targeted mass list was also used for iTRAQ experiments performed using the LTQ Orbitrap Velos instrument. Those peptides that appeared to be most important from the initial survey runs and from previously published studies [4,5] were included in the mass list. The mass list contains *m/z* ratios for singly-, doubly- and triply-charged ions falling within the analyzed *m/z* window (300–2000). Both modified peptides and unmodified versions of the same peptide were included. In cases where HNE addition was indicated at lysine, the full length peptide, which now contains a missed cleavage, and the two shorter peptides covering the same sequence that would result from cleavage with trypsin were included (provided they were long enough to be efficiently detected). The mass list was constructed with the aim of covering eighteen modification sites and contained 138 entries. The *m/z* ratio window around the listed masses that was accepted was ±2. Approximately 27% of the *m/z* ratio window from which precursor ions were selected was covered. The complete targeted mass list is presented as Table S5 while a shorter list of targeted modified peptides is provided as Table 2 in the main manuscript.

Modification Site or Modification Site(s) Associated with Unmodified Peptide (MA indicates Michael addition; SB indicates Schiff base formation)	Peptide	Mass List Constituents		
		$[M+H]^{+}$	$[M+2H]^{2+}$	$[M+3H]^{3+}$
Cys-034 (MA)	ALVLIAFAQYLQQC#PFEDHVK	2879.60	1440.31	960.54
Cys-034-associated	ALVLIAFAQYLQQCPFEDHVK	2778.49	1389.75	926.84
Lys-051 (MA)	LVNEVTEFAK^TCVAD	1998.06	999.53	666.69
Lys-051-associated	LVNEVTEFAKTCVAD	1984.03	992.52	662.02
Lys-051-associated	LVNEVTEFAK	1437.82	719.42	479.95
Lys-051-associated	TCVAD	709.33	355.17	237.12
His-067 (MA)	SLH@TLFGDK	1463.88	732.44	488.63
His-067-associated	SLHTLFGDK	1305.74	653.38	435.92
His-105 (MA)	NECFLQH@K	1521.84	761.42	507.95
His-105-associated	NECFLQHK	1363.71	682.36	455.24
Lys-162 (MA)	YK^AAFTECCQAADK	2109.06	1055.04	703.69
Lys-162-associated	YKAAFTECCQAADK	2095.04	1048.02	699.02
Lys-162-associated	AAFTECCQAADK	1659.78	830.39	553.93
Lys-199 (MA)	LK^CASLQK	1393.87	697.44	465.30
Lys-199-associated	LKCASLQK	1379.85	690.43	460.62
Lys-199-associated	CASLQK	994.56	497.79	332.19
Lys-212 (MA)	AFK^AWAVAR	1321.81	661.41	441.28
Lys-212-associated	AFKAWAVAR	1307.79	654.40	436.60
Lys-212-associated	AWAVAR	817.48	409.25	273.17
Lys-233 (MA)	AEFAEVSK^LVTDLTK	2097.23	1049.12	699.75
Lys-233-associated	AEFAEVSKLVTDLTK	2083.21	1042.11	695.07
Lys-233-associated	AEFAEVSK	1168.65	584.83	390.22
Lys-233-associated	LVTDLTK	1077.68	539.34	359.90
His-242 (MA)	VH@TECCHGDLLECADDR	2389.07	1195.04	797.03
His-247 (MA)	VHTECCH@GDLLECADDR	2389.07	1195.04	797.03
His-242-associated & His-247-associated	VHTECCHGDLLECADDR	2230.94	1115.97	744.32
Lys-262 (MA)	ADLAK^YICENQDSISSK	2388.26	1194.63	796.76
Lys-262-associated	ADLAKYICENQDSISSK	2374.23	1187.62	792.08
Lys-262-associated	ADLAK	805.51	403.26	269.17
Lys-262-associated	YICENQDSISSK	1731.85	866.43	577.96
His-288 (MA)	SH@CIAEVENDEM*PADLPSLAADFVESK	3436.68	1718.84	1146.23
His-288 (MA)	SH@CIAEVENDEMPADLPSLAADFVESK	3420.68	1710.85	1140.90
His-288-associated	SHCIAEVENDEM*PADLPSLAADFVESK	3278.55	1639.78	1093.52
His-288-associated	SHCIAEVENDEMPADLPSLAADFVESK	3262.55	1631.78	1088.19
Lys-351 (MA)	LAK^TYETTLEK	1743.04	872.03	581.69
Lys-351-associated	LAKTYETTLEK	1729.02	865.01	577.01
Lys-351-associated	TYETTLEK	1272.70	636.85	424.90
His-367 (MA)	CCAAADPH@ECYAK	1998.94	999.97	666.98
His-367-associated	CCAAADPHECYAK	1840.81	920.91	614.27
Lys-378 (MA)	VFDEFK^PLVEEPQNLIK	2491.43	1246.22	831.15
Lys-378-associated	VFDEFKPLVEEPQNLIK	2477.41	1239.21	826.47
Lys-378-associated	VFDEFK	1072.60	536.80	358.20
Lys-378-associated	PLVEEPQNLIK	1567.93	784.47	523.32
Residue 403-410 peptide	FQNALLVR	1104.67	552.84	368.89
Lys-414 (MA)	K^VPQVSTPTLVEVSR	1942.17	971.59	648.06
Lys-414 (SB)	K~VPQVSTPTLVEVSR	1924.16	962.59	642.06
Lys-414-associated	KVPQVSTPTLVEVSR	1928.15	964.58	643.39
Lys-414-associated	VPQVSTPTLVEVSR	1655.95	828.48	552.65
His-510 (MA)	EFNAETFTFH@ADICTLSEK	2706.36	1353.68	902.79
His-510-associated	EFNAETFTFHADICTLSEK	2548.23	1274.62	850.08
Lys-525 (MA)	K^QTALVELVK	1575.04	788.02	525.68
Lys-525 (SB)	K~QTALVELVK	1557.03	779.02	519.68
Lys-525-associated	KQTALVELVK	1561.01	781.01	521.01
Lys-525-associated	QTALVELVK	1288.81	644.91	430.28

Table S5: List of targeted peptides and associated monoisotopic mass-to-charge ratios that were used as a targeted mass list for chosing parent ions for fragmentation. Mass-to-charge ratios in gray are outside the analyzed range (300-2000). Targeted peptides are grouped by modification site. C# indicates HNE Michael addition at Cys followed by reduction; H@ indicates HNE Michael addition at His followed by reduction; K^ indicates HNE Michael addition at Lys followed by reduction; K~ indicates Schiff base formation with HNE at Lys followed by reduction; M* indicates oxidation at Met. Eighteen sites were targeted and both Schiff base formation and Michael addition were considered at two of these sites (Lys-414 and Lys-525). The peptide, FQNALLVR, was included in error and is listed here for completeness. In total, the mass list contained 138 entries.

RELATIVE ABUNDANCE MEASUREMENTS: Changes in relative abundance for HNE-modified and corresponding unmodified HSA peptides were measured using the iTRAQ approach. The targeted mass list was used in all cases. Table S6 gives relative abundances for a comparison of no added HNE with applied HNE:HSA ratios of 50:1 and 100:1. A single repeat experiment was performed and three replicate LC–MS/MS runs were collected using PQD fragmentation on the LTQ XL system. Only mass list peptides are reported in the table. Bolded peptides were used in constructing Figure 1 in the main document. Tables S7 and S8 give the results of an experiment in which incubation time was varied at the 100:1 HNE:HSA ratio. Incubation times of 0, 1, 3, and 24 h were investigated. Three complete repeats were performed. For each repeat, three replicate LC–MS/MS runs were collected using PQD fragmentation on the LTQ XL system and three further replicates were recorded using HCD fragmentation on the LTQ Orbitrap Velos system. Linear ion trap/PQD results are given as Table S7 and Orbitrap/HCD results are given as Table S8. Together, these results were used to construct Figures 2 and 3 in the main document (Figure 2 displays results for the histidines while Figure 3 does the same for the lysines). Bolded entries in the tables indicate those peptides used in constructing the main document figures. Where more than one peptide was available to represent a site (most common for the unmodified peptides corresponding to the lysine modification sites), the most frequently-detected peptide was used. As can be seen from Tables S6–S8, the same peptides were chosen for use in constructing the main document figures in all cases. For peptide identification acceptance, a PeptideProphet score of 0.9 or greater was required and MS/MS for which all four iTRAQ reporter ion intensities were zero were discarded.

Modification	Peptide	Detection Count	No HNE Added	50:1 HNE:HSA	100:1 HNE:HSA
Cys-034-associated	*ALVLIAFAQYLQQCPFEDHVK*	*412*	*78.9%*	*11.0%*	*10.2%*
Cys-034 (MA)	*ALVLIAFAQYLQQC#PFEDHVK*	*2*	*15.0%*	*0.0%*	*85.0%*
His-067-associated	**SLHTLFGDK**	**795**	**70.8%**	**18.6%**	**10.7%**
His-105-associated	**NECFLQHK**	**345**	**50.1%**	**27.8%**	**22.0%**
His-242- & His-247-associated	*VHTECCHGDLLECADDR*	*239*	*65.3%*	*19.0%*	*15.7%*
His-288-associated	*SHCIAEVENDEMPADLPSLAADFVESK*	*433*	*84.0%*	*10.9%*	*5.0%*
His-367-associated	**CCAAADPHECYAK**	**642**	**54.4%**	**28.4%**	**17.1%**
His-510-associated	**EFNAETFTFHADICTLSEK**	**748**	**75.5%**	**17.6%**	**6.9%**
His-067 (MA)	**SLH@TLFGDK**	**916**	**1.3%**	**51.2%**	**47.5%**
His-105 (MA)	**NECFLQH@K**	**89**	**1.2%**	**42.7%**	**56.1%**
His-367 (MA)	**CCAAADPH@ECYAK**	**326**	**2.1%**	**42.6%**	**55.2%**
His-510 (MA)	**EFNAETFTFH@ADICTLSEK**	**126**	**2.7%**	**34.4%**	**62.8%**
Lys-051-associated	*LVNEVTEFAK*	*1356*	*46.6%*	*31.2%*	*22.3%*
Lys-162-associated	**AAFTECCQAADK**	**527**	**49.7%**	**30.4%**	**19.9%**
Lys-199-associated	**CASLQK**	**21**	**82.2%**	**14.2%**	**3.6%**
Lys-233-associated	**AEFAEVSK**	**1018**	**44.2%**	**29.7%**	**26.2%**
Lys-233-associated	*LVTDLTK*	*313*	*42.4%*	*30.6%*	*27.1%*
Lys-262-associated	*ADLAK*	*6*	*47.2%*	*25.5%*	*27.4%*
Lys-262-associated	**YICENQDSISSK**	**1195**	**47.6%**	**29.6%**	**22.8%**
Lys-351-associated	**TYETTLEK**	**212**	**59.2%**	**26.7%**	**14.1%**
Lys-378-associated	**VFDEFKPLVEEPQNLIK**	**895**	**46.5%**	**29.4%**	**24.1%**
Lys-414-associated	**KVPQVSTPTLVEVSR**	**778**	**46.5%**	**32.0%**	**21.5%**
Lys-414-associated	*VPQVSTPTLVEVSR*	*575*	*37.4%*	*36.5%*	*26.1%*
Lys-525-associated	*KQTALVELVK*	*174*	*79.4%*	*15.9%*	*4.7%*
Lys-525-associated	**QTALVELVK**	**794**	**70.1%**	**18.4%**	**11.5%**
Lys-162 (MA)	**YK^AAFTECCQAADK**	**44**	**1.6%**	**44.0%**	**54.4%**
Lys-199 (MA)	**LK^CASLQK**	**1**	**0.0%**	**41.2%**	**58.8%**
Lys-233 (MA)	**AEFAEVSK^LVTDLTK**	**79**	**1.7%**	**28.6%**	**69.6%**
Lys-262 (MA)	**ADLAK^YICENQDSISSK**	**2**	**0.0%**	**13.0%**	**87.0%**
Lys-351 (MA)	**LAK^TYETTLEK**	**43**	**1.2%**	**44.8%**	**54.1%**
Lys-378 (MA)	**VFDEFK^PLVEEPQNLIK**	**43**	**21.3%**	**27.6%**	**51.0%**
Lys-414 (MA)	**K^VPQVSTPTLVEVSR**	**248**	**10.5%**	**45.9%**	**43.6%**
Lys-414 (SB)	**K~VPQVSTPTLVEVSR**	**118**	**12.5%**	**43.9%**	**43.7%**
Lys-525 (MA)	**K^QTALVELVK**	**135**	**1.0%**	**54.1%**	**44.9%**
Lys-525 (SB)	**K~QTALVELVK**	**12**	**2.2%**	**70.3%**	**27.5%**

Table S6: Change in relative abundance for HNE-modified and corresponding unmodiifed HSA peptides in response to HNE-exposure at stated HNE:HSA molar ratios. Raw iTRAQ reporter ion intensities for each MS/MS are converted to relative percentages and then averaged for each peptide; since the control was duplicated, raw intensity for the two control signals was averaged before relative percentages were calculated. iTRAQ reporter ion intensities were obtained using pulsed-Q dissociation (PQD) in a linear ion trap mass spectrometer. This dataset is the result of a single repeat preparation subjected to three replicate LC–MS/MS runs. Incubation time with HNE was 3 h. The mass list described in Table S5 was used and only mass list peptides are included in this table. Bolded entries were used in constructing Figure 1 while italicized entries were not used. For a peptide identification to be accepted, a PeptideProphet score of 0.9 or greater was required. MS/MS where all four iTRAQ reporter ion intensities were zero were discarded. C# indicates HNE Michael addition at Cys followed by reduction; H@ indicates HNE Michael addition at His followed by reduction; K^ indicates HNE Michael addition at Lys followed by reduction; K~ indicates Schiff base formation with HNE at Lys followed by reduction; M* indicates oxidation at Met.

Modification	Peptide	Detection Count	Repeat Count	100:1 HNE:HSA for 0 h	100:1 HNE:HSA for 1 h	100:1 HNE:HSA for 3 h	100:1 HNE:HSA for 24 h
Cys-034-associated	*ALVLIAFAQYLQQCPFEDHVK*	*342*	*3*	*31.6%*	*20.2%*	*19.1%*	*29.1%*
Cys-034 (MA)	*ALVLIAFAQYLQQC#PFEDHVK*	*70*	*1*	*3.2%*	*32.4%*	*24.2%*	*40.3%*
His-067-associated	**SLHTLFGDK**	**953**	**3**	**52.4%**	**28.4%**	**13.6%**	**5.5%**
His-105-associated	**NECFLQHK**	**437**	**3**	**33.2%**	**28.1%**	**24.5%**	**14.1%**
His-242- & His-247-associated	**VHTECCHGDLLECADDR**	**353**	**3**	**51.4%**	**15.6%**	**21.0%**	**12.0%**
His-288-associated	*SHCIAEVENDEM*PADLPSLAADFVESK*	*857*	*2*	*14.4%*	*57.8%*	*15.1%*	*12.7%*
His-288-associated	**SHCIAEVENDEMPADLPSLAADFVESK**	**866**	**3**	**60.2%**	**17.7%**	**13.3%**	**8.8%**
His-367-associated	**CCAAADPHECYAK**	**966**	**3**	**35.5%**	**30.2%**	**22.1%**	**12.2%**
His-510-associated	**EFNAETFTFHADICTLSEK**	**2204**	**3**	**48.0%**	**27.8%**	**13.9%**	**10.4%**
His-067 (MA)	**SLH@TLFGDK**	**3622**	**3**	**0.9%**	**28.2%**	**37.6%**	**33.3%**
His-105 (MA)	**NECFLQH@K**	**260**	**3**	**0.9%**	**24.9%**	**27.5%**	**46.7%**
His-242 (MA)	**VH@TECCHGDLLECADDR**	**8**	**3**	**0.4%**	**26.4%**	**43.5%**	**29.7%**
His-288 (MA)	*SH@CIAEVENDEM*PADLPSLAADFVESK*	*834*	*2*	*1.2%*	*13.8%*	*45.7%*	*39.4%*
His-288 (MA)	**SH@CIAEVENDEMPADLPSLAADFVESK**	**2751**	**2**	**2.2%**	**13.6%**	**45.1%**	**39.1%**
His-367 (MA)	**CCAAADPH@ECYAK**	**1401**	**3**	**1.2%**	**14.8%**	**23.8%**	**60.2%**
His-510 (MA)	**EFNAETFTFH@ADICTLSEK**	**1722**	**3**	**1.2%**	**23.8%**	**36.9%**	**38.2%**
Lys-051-associated	*LVNEVTEFAK*	*2442*	*3*	*26.4%*	*27.4%*	*23.9%*	*22.3%*
Lys-162-associated	**AAFTECCQAADK**	**1052**	**3**	**32.2%**	**29.4%**	**23.3%**	**15.1%**
Lys-199-associated	**CASLQK**	**29**	**2**	**79.8%**	**6.0%**	**6.6%**	**7.6%**
Lys-233-associated	**AEFAEVSK**	**1404**	**3**	**26.5%**	**27.7%**	**24.1%**	**21.6%**
Lys-233-associated	*AEFAEVSKLVTDLTK*	*1*	*1*	*6.3%*	*39.7%*	*24.5%*	*29.5%*
Lys-233-associated	*LVTDLTK*	*499*	*3*	*27.1%*	*26.7%*	*25.2%*	*21.1%*
Lys-262-associated	*ADLAK*	*5*	*2*	*35.0%*	*17.7%*	*19.6%*	*27.7%*
Lys-262-associated	**YICENQDSISSK**	**1803**	**3**	**26.2%**	**26.4%**	**23.8%**	**23.6%**
Lys-351-associated	**TYETTLEK**	**344**	**3**	**39.4%**	**26.8%**	**19.1%**	**14.7%**
Lys-378-associated	**VFDEFKPLVEEPQNLIK**	**6292**	**3**	**24.2%**	**28.2%**	**25.0%**	**22.6%**
Lys-414-associated	**KVPQVSTPTLVEVSR**	**1293**	**3**	**32.1%**	**27.0%**	**22.9%**	**18.0%**
Lys-414-associated	*VPQVSTPTLVEVSR*	*1052*	*3*	*19.8%*	*36.5%*	*24.8%*	*18.9%*
Lys-525-associated	*KQTALVELVK*	*270*	*3*	*62.9%*	*13.9%*	*12.5%*	*10.7%*
Lys-525-associated	**QTALVELVK**	**1020**	**3**	**48.5%**	**17.5%**	**16.6%**	**17.3%**
Lys-162 (MA)	**YK^AAFTECCQAADK**	**210**	**3**	**1.3%**	**32.1%**	**38.5%**	**28.1%**
Lys-199 (MA)	**LK^CASLQK**	**33**	**3**	**1.1%**	**26.7%**	**38.3%**	**33.9%**
Lys-212 (MA)	**AFK^AWAVAR**	**48**	**2**	**9.2%**	**14.4%**	**21.2%**	**55.2%**
Lys-233 (MA)	**AEFAEVSK^LVTDLTK**	**355**	**3**	**0.9%**	**11.2%**	**21.2%**	**66.7%**
Lys-262 (MA)	**ADLAK^YICENQDSISSK**	**120**	**3**	**0.9%**	**18.0%**	**26.8%**	**54.4%**
Lys-351 (MA)	**LAK^TYETTLEK**	**222**	**3**	**2.2%**	**20.7%**	**38.4%**	**38.7%**
Lys-378 (MA)	**VFDEFK^PLVEEPQNLIK**	**357**	**3**	**11.6%**	**22.0%**	**24.8%**	**41.6%**
Lys-414 (MA)	**K^VPQVSTPTLVEVSR**	**501**	**3**	**6.4%**	**33.4%**	**26.5%**	**33.7%**
Lys-414 (SB)	**K~VPQVSTPTLVEVSR**	**145**	**3**	**11.7%**	**44.6%**	**28.2%**	**15.5%**
Lys-525 (MA)	**K^QTALVELVK**	**345**	**3**	**1.1%**	**20.2%**	**30.8%**	**47.8%**
Lys-525 (SB)	**K~QTALVELVK**	**1**	**1**	**0.0%**	**0.0%**	**20.2%**	**79.8%**

Table S7: Change in relative abundance for HNE-modified and corresponding unmodiifed HSA peptides in response to HNE-exposure time at a 100:1 HNE:HSA molar ratio. Raw iTRAQ reporter ion intensities for each MS/MS are converted to relative percentages and then averaged for each peptide. iTRAQ reporter ion intensities were obtained using pulsed-Q dissociation (PQD) in a linear ion trap mass spectrometer. This dataset is the result of a three repeat preparations subjected to three replicate LC–MS/MS runs each. The Repeat Count column gives a count of repeats in which the peptide in question was identified. The same set of three repeat preparations was analyzed using the LTQ Orbitrap Velos system (see Table S8). The mass list described in Table S5 was used and only mass list peptides are included in this table. Bolded entries were used in constructing Figures 2 and 3 while italicized entries were not used. For a peptide identification to be accepted, a PeptideProphet score of 0.9 or greater was required. MS/MS where all four iTRAQ reporter ion intensities were zero were discarded. C# indicates HNE Michael addition at Cys followed by reduction; H@ indicates HNE Michael addition at His followed by reduction; K^ indicates HNE Michael addition at Lys followed by reduction; K~ indicates Schiff base formation with HNE at Lys followed by reduction; M* indicates oxidation at Met.

Modification	Peptide	Detection Count	Repeat Count	100:1 HNE:HSA for 0 h	100:1 HNE:HSA for 1 h	100:1 HNE:HSA for 3 h	100:1 HNE:HSA for 24 h
Cys-034-associated	*ALVLIAFAQYLQQCPFEDHVK*	*587*	*3*	*36.2%*	*19.3%*	*20.0%*	*24.6%*
Cys-034 (MA)	*ALVLIAFAQYLQQC#PFEDHVK*	*42*	*3*	*0.1%*	*28.0%*	*29.4%*	*42.5%*
His-067-associated	**SLHTLFGDK**	**415**	**3**	**52.7%**	**26.6%**	**14.4%**	**6.2%**
His-105-associated	**NECFLQHK**	**136**	**3**	**32.6%**	**26.6%**	**24.7%**	**16.1%**
His-242- & His-247-associated	**VHTECCHGDLLECADDR**	**165**	**3**	**67.1%**	**6.5%**	**15.4%**	**11.0%**
His-288-associated	*SHCIAEVENDEM*PADLPSLAADFVESK*	*427*	*3*	*58.2%*	*23.1%*	*8.1%*	*10.5%*
His-288-associated	**SHCIAEVENDEMPADLPSLAADFVESK**	**447**	**3**	**63.8%**	**8.5%**	**9.2%**	**18.5%**
His-367-associated	**CCAAADPHECYAK**	**242**	**3**	**35.5%**	**29.2%**	**22.9%**	**12.4%**
His-510-associated	**EFNAETFTFHADICTLSEK**	**3968**	**3**	**53.1%**	**25.3%**	**12.5%**	**9.2%**
His-067 (MA)	**SLH@TLFGDK**	**1726**	**3**	**0.7%**	**27.6%**	**37.6%**	**34.0%**
His-105 (MA)	**NECFLQH@K**	**144**	**3**	**0.3%**	**17.3%**	**24.1%**	**58.4%**
His-242 (MA)	**VH@TECCHGDLLECADDR**	**1**	**1**	**0.0%**	**5.8%**	**26.3%**	**67.9%**
His-288 (MA)	*SH@CIAEVENDEM*PADLPSLAADFVESK*	*432*	*3*	*0.7%*	*18.2%*	*44.0%*	*37.2%*
His-288 (MA)	**SH@CIAEVENDEMPADLPSLAADFVESK**	**517**	**3**	**0.9%**	**17.0%**	**45.8%**	**36.3%**
His-367 (MA)	**CCAAADPH@ECYAK**	**300**	**3**	**1.6%**	**14.6%**	**23.8%**	**60.0%**
His-510 (MA)	**EFNAETFTFH@ADICTLSEK**	**1709**	**3**	**0.3%**	**24.6%**	**37.3%**	**37.8%**
Lys-051-associated	*LVNEVTEFAK*	*1711*	*3*	*26.3%*	*25.8%*	*24.0%*	*23.9%*
Lys-162-associated	**AAFTECCQAADK**	**326**	**3**	**32.9%**	**27.2%**	**23.4%**	**16.5%**
Lys-199-associated	**CASLQK**	**3**	**1**	**84.3%**	**0.9%**	**5.8%**	**9.0%**
Lys-212-associated	**AWAVAR**	**18**	**2**	**25.8%**	**26.4%**	**27.0%**	**20.8%**
Lys-233-associated	**AEFAEVSK**	**1405**	**3**	**25.5%**	**25.9%**	**25.2%**	**23.4%**
Lys-233-associated	*LVTDLTK*	*83*	*2*	*21.4%*	*25.2%*	*28.1%*	*25.3%*
Lys-262-associated	*ADLAK*	*33*	*2*	*21.1%*	*24.3%*	*26.7%*	*27.9%*
Lys-262-associated	**YICENQDSISSK**	**433**	**3**	**25.7%**	**26.5%**	**24.3%**	**23.6%**
Lys-351-associated	*LAKTYETTLEK*	*3*	*1*	*40.2%*	*23.5%*	*23.3%*	*13.0%*
Lys-351-associated	**TYETTLEK**	**318**	**3**	**38.4%**	**25.2%**	**20.3%**	**16.1%**
Lys-378-associated	**VFDEFKPLVEEPQNLIK**	**3490**	**3**	**25.0%**	**26.8%**	**24.8%**	**23.4%**
Lys-414-associated	**KVPQVSTPTLVEVSR**	**2689**	**3**	**34.2%**	**23.8%**	**21.9%**	**20.0%**
Lys-414-associated	*VPQVSTPTLVEVSR*	*335*	*3*	*24.3%*	*20.2%*	*24.5%*	*30.9%*
Lys-525-associated	*KQTALVELVK*	*105*	*3*	*64.5%*	*11.2%*	*13.0%*	*11.3%*
Lys-525-associated	**QTALVELVK**	**337**	**3**	**49.7%**	**14.0%**	**17.4%**	**18.9%**
Lys-162 (MA)	**YK^AAFTECCQAADK**	**109**	**3**	**1.2%**	**30.3%**	**38.9%**	**29.5%**
Lys-199 (MA)	**LK^CASLQK**	**82**	**3**	**1.3%**	**27.5%**	**37.7%**	**33.5%**
Lys-212 (MA)	**AFK^AWAVAR**	**183**	**3**	**1.3%**	**10.7%**	**21.2%**	**66.8%**
Lys-233 (MA)	**AEFAEVSK^LVTDLTK**	**259**	**3**	**0.0%**	**7.5%**	**18.8%**	**73.6%**
Lys-262 (MA)	**ADLAK^YICENQDSISSK**	**221**	**3**	**0.8%**	**14.1%**	**24.8%**	**60.2%**
Lys-351 (MA)	**LAK^TYETTLEK**	**358**	**3**	**1.3%**	**23.9%**	**34.4%**	**40.3%**
Lys-378 (MA)	**VFDEFK^PLVEEPQNLIK**	**222**	**3**	**11.0%**	**18.4%**	**23.1%**	**47.5%**
Lys-414 (MA)	**K^VPQVSTPTLVEVSR**	**168**	**3**	**8.5%**	**30.2%**	**26.9%**	**34.4%**
Lys-414 (SB)	**K~VPQVSTPTLVEVSR**	**139**	**3**	**13.0%**	**40.3%**	**29.7%**	**17.0%**
Lys-525 (MA)	**K^QTALVELVK**	**269**	**3**	**0.6%**	**23.9%**	**33.3%**	**42.3%**
Lys-525 (SB)	**K~QTALVELVK**	**150**	**3**	**0.7%**	**54.6%**	**33.8%**	**10.8%**

Table S8: Change in relative abundance for HNE-modified and corresponding unmodiifed HSA peptides in response to HNE-exposure time at a 100:1 HNE:HSA molar ratio. Raw iTRAQ reporter ion intensities for each MS/MS are converted to relative percentages and then averaged for each peptide. iTRAQ reporter ion intensities were obtained using higher-energy C-trap dissociation (HCD) in an Orbitrap mass spectrometer. This dataset is the result of a three repeat preparations subjected to three replicate LC–MS/MS runs each. The Repeat Count column gives a count of repeats in which the peptide in question was identified. The same set of three repeat preparations was analyzed using the LTQ XL system (see Table S7). The mass list described in Table S5 was used and only mass list peptides are included in this table. Bolded entries were used in constructing Figures 2 and 3 while italicized entries were not used. For a peptide identification to be accepted, a PeptideProphet score of 0.9 or greater was required. MS/MS where all four iTRAQ reporter ion intensities were zero were discarded. C# indicates HNE Michael addition at Cys followed by reduction; H@ indicates HNE Michael addition at His followed by reduction; K^ indicates HNE Michael addition at Lys followed by reduction; K~ indicates Schiff base formation with HNE at Lys followed by reduction; M* indicates oxidation at Met.

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[5] M.E. Szapacs, J.N. Riggins, L.J. Zimmerman, D.C. Liebler, Covalent Adduction of Human Serum Albumin by 4-Hydroxy-2-nonenal: Kinetic Analysis of Competing Alkylation Reactions, Biochemistry 45 (2006) 10521-10528.

Index of Example LTQ XL Linear Ion Trap Tandem Mass Spectra

Modified Peptide (with flanking residues)	Modification Site or Sites (MA indicates Michael addition; SB indicates Schiff base formation)	Type	Sequest Xcorr	Sequest DeltaCn	Sequest RankSp	Peptide Prophet Score	Page Number
K.ALVLIAFAQYLQQC#PFEDHVK.L	Cys-034 (MA)	CID	4.873	0.477	1	1.0000	17
K.ALVLIAFAQYLQQC#PFEDHVK.L	Cys-034 (MA)	ETD	5.488	0.458	1	1.0000	18
K.SLH@TLFGDK.L	His-067 (MA)	CID	3.949	0.302	1	0.9999	19
K.SLH@TLFGDK.L	His-067 (MA)	ETD	3.687	0.287	1	0.9998	20
K.SLHTLFGDK^LCTVATLR.E	Lys-073 (MA)	CID	2.956	0.391	1	0.9770	21
R.NECFLQHK~DDNPNLPR.L	Lys-106 (SB)	ETD	4.241	0.372	1	0.9982	22
R.LVRPEVDVMCTAFH@DNEETFLK.K	His-128 (MA)	CID	5.787	0.436	1	1.0000	23
R.LVRPEVDVMCTAFH@DNEETFLK.K	His-128 (MA)	ETD	5.225	0.457	1	1.0000	24
K.K^YLYEIAR.R	Lys-137 (MA)	CID	3.041	0.312	1	0.9919	25
R.RH@PYFYAPELLFFAK.R	His-146 (MA)	CID	4.582	0.501	1	1.0000	26
R.RH@PYFYAPELLFFAK.R	His-146 (MA)	ETD	5.467	0.433	1	1.0000	27
R.RH@PYFYAPELLFFAKR.Y	His-146 (MA)	CID	6.144	0.446	1	1.0000	28
R.RH@PYFYAPELLFFAK^R.Y	His-146 (MA) & Lys-159 (MA)	ETD	5.282	0.353	1	0.9999	29
R.YK^AAFTECCQAADK.A	Lys-162 (MA)	CID	5.758	0.560	1	1.0000	30
R.YK^AAFTECCQAADK.A	Lys-162 (MA)	ETD	5.303	0.489	1	1.0000	31
R.YK~AAFTECCQAADK.A	Lys-162 (SB)	CID	4.249	0.331	1	0.9970	32
R.YK~AAFTECCQAADK.A	Lys-162 (SB)	ETD	4.803	0.354	1	0.9980	33
R.LK^CASLQK.F	Lys-199 (MA)	CID	4.196	0.261	1	0.9961	34
R.AFK^AWAVAR.L	Lys-212 (MA)	CID	3.815	0.257	2	0.9782	35
K.AEFAEVSK^LVTDLTK.V	Lys-233 (MA)	CID	3.979	0.313	1	0.9931	36
K.AEFAEVSK^LVTDLTK.V	Lys-233 (MA)	ETD	3.436	0.371	1	1.0000	37
K.LVTDLTK^VH@TECCHGDLLECADDR.A	Lys-240 (MA) & His-242 (MA)	CID	4.775	0.319	1	0.9843	38
K.VH@TECCHGDLLECADDR.A	His-242 (MA)	ETD	4.505	0.274	1	0.9997	39
K.VH@TECCH@GDLLECADDR.A	His-242 (MA) & His-247 (MA)	CID	4.561	0.419	1	1.0000	40
K.VH@TECCH@GDLLECADDR.A	His-242 (MA) & His-247 (MA)	ETD	3.321	0.329	1	0.9995	41
K.VH@TECCH@GDLLECADDRADLAK.Y	His-242 (MA) & His-247 (MA)	CID	4.297	0.361	1	0.9923	42
K.VH@TECCH@GDLLECADDRADLAK.Y	His-242 (MA) & His-247 (MA)	ETD	5.437	0.432	1	0.9996	43
R.ADLAK^YICENQDSISSK.L	Lys-262 (MA)	CID	4.947	0.447	1	0.9999	44
R.ADLAK^YICENQDSISSK.L	Lys-262 (MA)	ETD	4.260	0.427	1	0.9978	45
K.SH@CIAEVENDEMPADLPSLAADFVESK.D	His-288 (MA)	CID	6.548	0.471	1	1.0000	46
K.SH@CIAEVENDEMPADLPSLAADFVESK.D	His-288 (MA)	ETD	5.269	0.555	1	1.0000	47
K.SH@CIAEVENDEM*PADLPSLAADFVESK.D	His-288 (MA)	CID	7.038	0.576	1	1.0000	48
K.SH@CIAEVENDEM*PADLPSLAADFVESK.D	His-288 (MA)	ETD	3.552	0.224	1	0.9868	49
R.RH@PDYSVVLLLR.L	His-338 (MA)	CID	4.528	0.420	1	1.0000	50
R.RH@PDYSVVLLLR.L	His-338 (MA)	ETD	4.562	0.432	1	1.0000	51
R.H@PDYSVVLLLR.L	His-338 (MA)	CID	4.439	0.250	1	0.9997	52
R.H@PDYSVVLLLRLAKTYETTLEK.C	His-338 (MA)	CID	3.784	0.360	1	0.9821	53
R.H@PDYSVVLLLRLAKTYETTLEK.C	His-338 (MA)	ETD	6.466	0.463	1	0.9962	54
R.LAK^TYETTLEK.C	Lys-351 (MA)	CID	4.137	0.420	1	0.9998	55
R.LAK~TYETTLEK.C	Lys-351 (SB)	CID	3.265	0.311	2	0.9704	56
R.LAK~TYETTLEK.C	Lys-351 (SB)	ETD	3.874	0.412	1	0.9988	57
K.TYETTLEK^CCAAADPHECYAK.V	Lys-359 (MA)	CID	5.601	0.527	1	1.0000	58
K.TYETTLEK^CCAAADPHECYAK.V	Lys-359 (MA)	ETD	4.199	0.381	1	0.9957	59
K.CCAAADPH@ECYAK.V	His-367 (MA)	CID	4.350	0.460	1	0.9987	60
K.VFDEFK^PLVEEPQNLIK.Q	Lys-378 (MA)	CID	4.943	0.479	1	1.0000	61
K.VFDEFK^PLVEEPQNLIK.Q	Lys-378 (MA)	ETD	2.804	0.178	2	0.9295	62
K.QNCELFEQLGEYK^FQNALLVR.Y	Lys-402 (MA)	CID	3.700	0.442	1	0.9991	63
K.K^VPQVSTPTLVEVSR.N	Lys-414 (MA)	CID	4.007	0.435	1	1.0000	64
K.K^VPQVSTPTLVEVSR.N	Lys-414 (MA)	ETD	4.331	0.346	1	0.9999	65
K.K~VPQVSTPTLVEVSR.N	Lys-414 (SB)	CID	4.161	0.488	1	1.0000	66
K.K~VPQVSTPTLVEVSR.N	Lys-414 (SB)	ETD	4.454	0.297	1	0.9998	67
R.VTK^CCTESLVNR.R	Lys-475 (MA)	CID	3.635	0.402	1	0.9991	68
K.EFNAETFTFH@ADICTLSEK.E	His-510 (MA)	CID	5.059	0.588	1	1.0000	69
K.EFNAETFTFH@ADICTLSEK.E	His-510 (MA)	ETD	3.799	0.404	1	0.9997	70
K.EFNAETFTFHADICTLSEK^ER.Q	Lys-519 (MA)	CID	4.686	0.393	1	0.9992	71
K.K^QTALVELVK.H	Lys-525 (MA)	ETD	2.547	0.293	5	0.9961	72
K.K~QTALVELVK.H	Lys-525 (SB)	CID	4.406	0.189	1	0.9991	73
K.K~QTALVELVK.H	Lys-525 (SB)	ETD	4.142	0.197	2	0.9988	74
K.EQLK^AVMDDFAAFVEK.C	Lys-545 (MA)	CID	5.270	0.512	1	1.0000	75
K.EQLK^AVMDDFAAFVEK.C	Lys-545 (MA)	ETD	6.854	0.527	1	1.0000	76
K.EQLK~AVMDDFAAFVEK.C	Lys-545 (SB)	CID	3.975	0.414	1	0.9993	77
K.EQLK~AVMDDFAAFVEK.C	Lys-545 (SB)	ETD	5.433	0.552	1	1.0000	78

Iodoacetamide addition to cysteine is highlighted in the following Trans-Proteomic Pipeline screenshots, but not in this table (all cysteines were assumed to have been alkylated with iodoacetamide unless HNE addition occurred). C# indicates HNE Michael addition at Cys followed by reduction; H@ indicates HNE Michael addition at His followed by reduction; K^ indicates HNE Michael addition at Lys followed by reduction; K~ indicates Schiff base formation with HNE at Lys followed by reduction; M* indicates oxidation at Met.

Index of Example LTQ Orbitrap Velos Linear Ion Trap Tandem Mass Spectra

Modified Peptide (with flanking residues)	Modification Site or Sites (MA indicates Michael addition; SB indicates Schiff base formation)	Type	Sequest Xcorr	Sequest DeltaCn	Sequest RankSp	Peptide Prophet Score	Page Number
K.DLGEENFKALVLIAFAQYLQQC#PFEDHVK.L	Cys-034 (MA)	CID	4.225	0.329	1	0.9248	79
K.ALVLIAFAQYLQQC#PFEDHVK.L	Cys-034 (MA)	CID	5.397	0.355	1	0.9953	80
K.SLH@TLFGDK.L	His-067 (MA)	CID	3.033	0.459	1	0.9988	81
R.RH@PYFYAPELLFFAK.R	His-146 (MA)	CID	6.258	0.597	1	1.0000	82
R.RH@PYFYAPELLFFAK^R.Y	His-146 (MA) & Lys-159 (MA)	CID	4.641	0.460	1	0.9989	83
R.YK^AAFTECCQAADK.A	Lys-162 (MA)	CID	4.453	0.480	1	0.9919	84
R.LK^CASLQK.F	Lys-199 (MA)	CID	4.123	0.387	1	0.9845	85
R.AFK^AWAVAR.L	Lys-212 (MA)	CID	3.733	0.488	1	0.9926	86
K.SH@CIAEVENDEMPADLPSLAADFVESK.D	His-288 (MA)	CID	6.444	0.592	1	1.0000	87
K.SH@CIAEVENDEM*PADLPSLAADFVESK.D	His-288 (MA)	CID	6.357	0.610	1	1.0000	88
R.RH@PDYSVVLLLR.L	His-338 (MA)	CID	5.221	0.449	1	0.9997	89
K.QNCELFEQLGEYK^FQNALLVR.Y	Lys-402 (MA)	CID	4.428	0.489	1	0.9881	90
K.K^VPQVSTPTLVEVSR.N	Lys-414 (MA)	CID	3.622	0.470	1	0.9990	91
K.K~VPQVSTPTLVEVSR.N	Lys-414 (SB)	CID	4.254	0.580	1	0.9998	92
K.K^QTALVELVK.H	Lys-525 (MA)	CID	3.197	0.298	1	0.9854	93
K.K~QTALVELVK.H	Lys-525 (SB)	CID	5.027	0.366	1	0.9993	94
K.EQLK^AVMDDFAAFVEK.C	Lys-545 (MA)	CID	4.783	0.438	1	0.9868	95

Iodoacetamide addition to cysteine is highlighted in the following Trans-Proteomic Pipeline screenshots, but not in this table (all cysteines were assumed to have been alkylated with iodoacetamide unless HNE addition occurred). C# indicates HNE Michael addition at Cys followed by reduction; H@ indicates HNE Michael addition at His followed by reduction; K^ indicates HNE Michael addition at Lys followed by reduction; K~ indicates Schiff base formation with HNE at Lys followed by reduction; M* indicates oxidation at Met.

X-range: 200 - 1400
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MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

a	[ ] +	[ ] 2+	[ ] 3+
b	[x] +	[x] 2+	[ ] 3+
c	[ ] +	[ ] 2+	[ ] 3+
x	[ ] +	[ ] 2+	[ ] 3+
y	[x] +	[x] 2+	[x] 3+
z	[ ] +	[ ] 2+	[ ] 3+

hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

ALVLIAFAQYLQQCPFEDHVK, MH+ 2591.5244, m/z 864.5130
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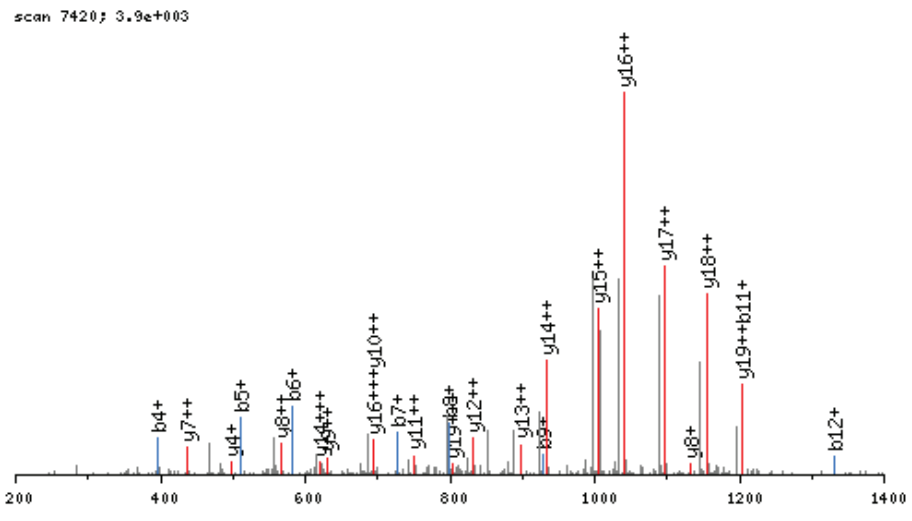
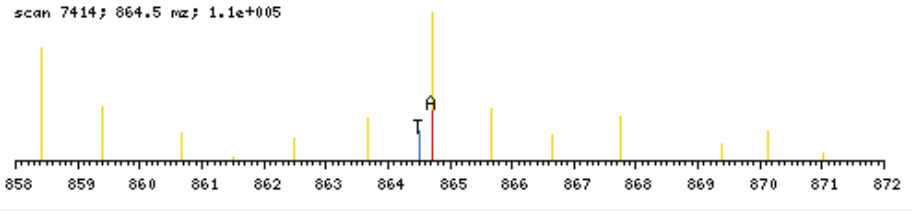


click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
72.0449	36.5264	1	A	21			
185.1290	93.0684	2	L	20	2520.4873	1260.7476	840.8343
284.1974	142.6026	3	V	19	2407.4032	**1204.2055**	**803.1396**
397.2815	199.1447	4	L	18	2308.3348	**1154.6713**	770.1168
510.3655	255.6867	5	I	17	2195.2507	**1098.1293**	732.4221
581.4027	291.2052	6	A	16	2082.1667	**1041.5873**	**694.7274**
728.4711	364.7394	7	F	15	2011.1296	**1006.0687**	671.0484
799.5082	400.2580	8	A	14	1864.0611	**932.5345**	**622.0256**
927.5668	464.2873	9	Q	13	1793.0240	**897.0159**	598.3466
1090.6301	545.8190	10	Y	12	1664.9655	**832.9866**	555.6604
1203.7142	602.3610	11	L	11	1501.9021	**751.4550**	501.3059
1331.7727	666.3903	12	Q	10	1388.8181	**694.9129**	463.6112
1459.8313	730.4196	13	Q	9	1260.7595	**630.8837**	420.9250
1721.1008	861.0543	14	C	8	**1132.7009**	**566.8544**	378.2389
1818.1536	909.5807	15	P	7	871.4314	**436.2196**	291.1490
1965.2220	983.1149	16	F	6	774.3786	387.6932	258.7981
2094.2646	1047.6362	17	E	5	627.3102	314.1590	209.7753
2209.2915	1105.1497	18	D	4	**498.2676**	249.6377	166.7611
2346.3505	1173.6791	19	H	3	383.2407	192.1243	128.4188
2445.4189	1223.2133	20	V	2	246.1818	123.5948	82.7325
		21	K	1	147.1134	74.0606	49.7097

C(14):+261.27

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MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
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Label: I M -
Ions:

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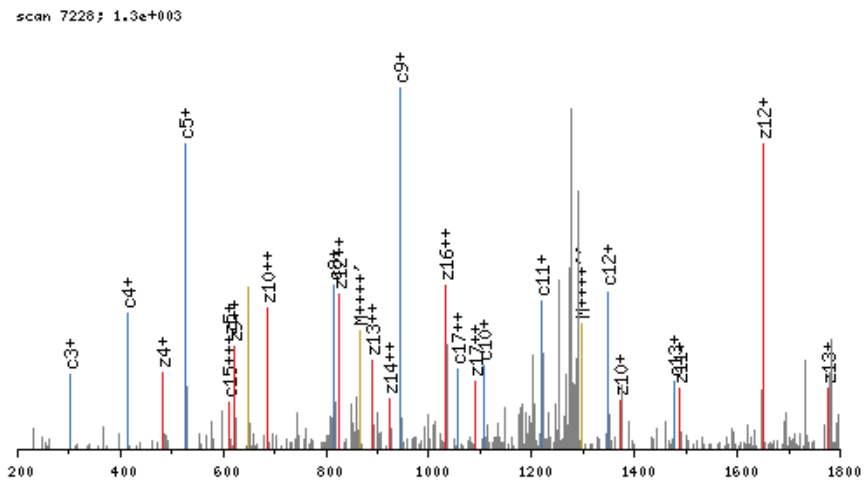
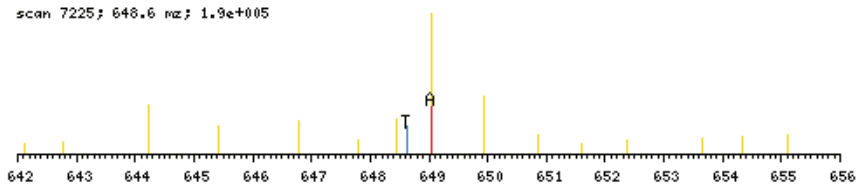
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

ALVLIAFAQYLQQCPFEDHVK, MH+ 2591.5244, m/z 648.6366
10HNE-1HSA-37Trypsin2-LTQ1.7228.7228.4.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	c^{3+}	#	AA	#	z^+	z^{2+}	z^{3+}
89.0715	45.0397	30.3624	1	A	21			
202.1556	101.5817	68.0571	2	L	20	2504.4686	1252.7382	835.4947
301.2240	151.1159	101.0799	3	V	19	2391.3845	1196.1962	797.8000
414.3080	207.6579	138.7746	4	L	18	2292.3161	1146.6620	764.7772
527.3921	264.2000	176.4692	5	I	17	2179.2320	**1090.1199**	727.0826
598.4292	299.7185	200.1483	6	A	16	2066.1480	**1033.5779**	689.3879
745.4976	373.2527	249.1711	7	F	15	1995.1108	998.0593	665.7088
816.5347	408.7713	272.8501	8	A	14	1848.0424	**924.5251**	616.6860
944.5933	472.8006	315.5363	9	Q	13	**1777.0053**	**889.0066**	593.0070
1107.6566	554.3322	369.8908	10	Y	12	**1648.9467**	**824.9773**	550.3208
1220.7407	610.8743	407.5855	11	L	11	**1485.8834**	743.4456	495.9664
1348.7993	674.9036	450.2716	12	Q	10	**1372.7993**	**686.9036**	458.2717
1476.8579	738.9328	492.9578	13	Q	9	1244.7408	**622.8743**	415.5855
1738.1274	869.5676	580.0477	14	C	8	1116.6822	558.8450	372.8993
1835.1801	918.0940	**612.3986**	15	P	7	855.4127	428.2102	285.8094
1982.2486	991.6282	661.4214	16	F	6	758.3599	379.6839	253.4585
2111.2911	**1056.1495**	704.4356	17	E	5	**611.2915**	306.1497	204.4357
2226.3181	1113.6630	742.7779	18	D	4	**482.2489**	241.6284	161.4215
2363.3770	1182.1924	788.4642	19	H	3	367.2220	184.1149	123.0792
2462.4454	1231.7266	821.4870	20	V	2	230.1630	115.5854	77.3929
			21	K	1	131.0946	66.0512	44.3701

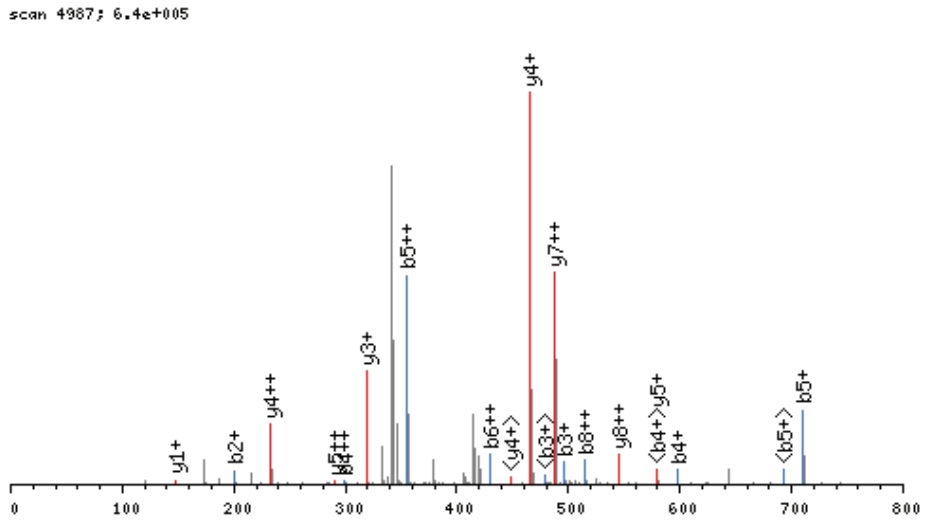
C(14):+261.27

X-range:
0 - 0
MassTol: Y-zoom:
0.950 1.00
ImageSize:
(•) Sm ( ) Lg
MassType:
( ) AVG (•) MONO
Axis:
(•) 1 ( ) 2
Label:
(•) I ( ) M ( ) -
Ions:

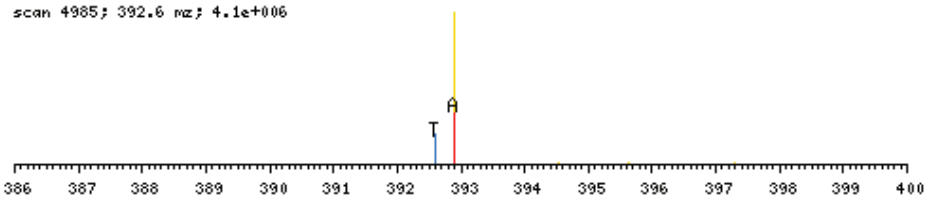
a	☐ +	☐ 2+	☐ 3+
b	☑ +	☑ 2+	☐ 3+
c	☐ +	☐ 2+	☐ 3+
x	☐ +	☐ 2+	☐ 3+
y	☑ +	☑ 2+	☑ 3+
z	☐ +	☐ 2+	☐ 3+

hide H_2O/NH_3 ☐
zoom 112-122 ☐
zoom 124-133 ☐
GO

SLHTLFGDK, MH+ 1175.7498, m/z 392.5881
10HNE-1HSA-37Trypsin3-LTQ1.4987.4987.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
88.0399	44.5238	1	S	9			
201.1239	101.0659	2	L	8	1088.7178	**544.8628**	363.5778
496.3957	248.7018	3	H	7	975.6337	**488.3208**	325.8831
597.4434	**299.2256**	4	T	6	680.3619	340.6849	227.4592
710.5274	**355.7676**	5	L	5	**579.3142**	**290.1610**	193.7766
857.5959	**429.3018**	6	F	4	**466.2302**	**233.6190**	156.0819
914.6173	457.8126	7	G	3	**319.1618**	160.0848	107.0591
1029.6443	**515.3260**	8	D	2	262.1403	131.5741	88.0520
		9	K	1	**147.1134**	74.0606	49.7097

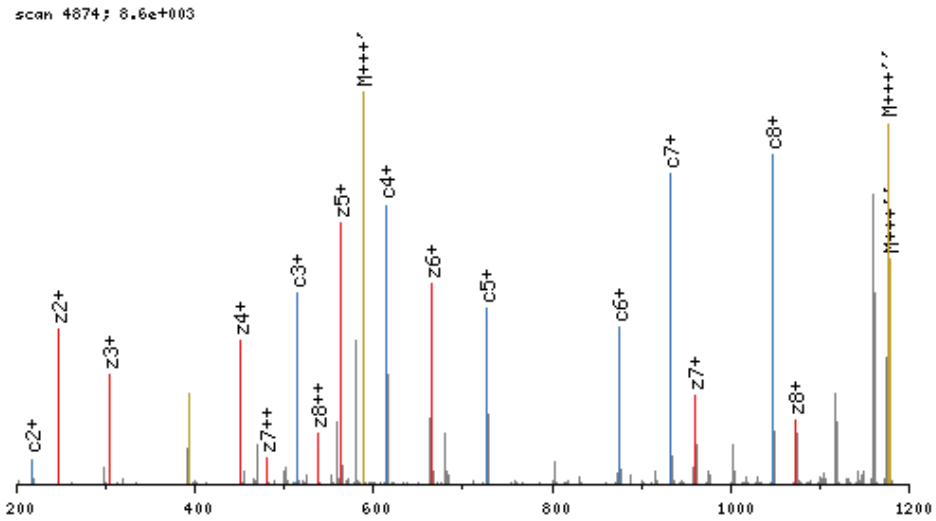
H(3):+295.27

X-range: 200 - 1200
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

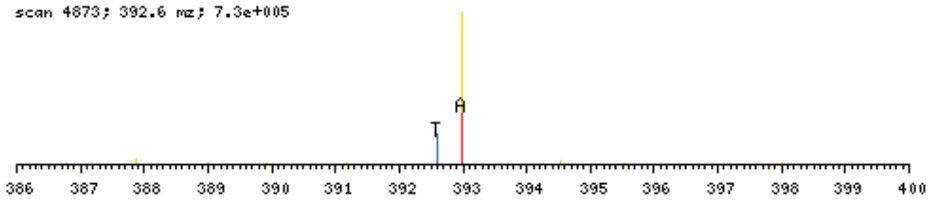
a	☐ +	☐ 2+	☐ 3+
b	☐ +	☐ 2+	☐ 3+
c	☑ +	☑ 2+	☐ 3+
x	☐ +	☐ 2+	☐ 3+
y	☐ +	☐ 2+	☐ 3+
z	☑ +	☑ 2+	☑ 3+

hide H_2O/NH_3 ☐
zoom 112-122 ☐
zoom 124-133 ☐
GO

SLHTLFGDK, MH+ 1175.7498, m/z 392.5881
10HNE-1HSA-37Trypsin3-LTQ3.4874.4874.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



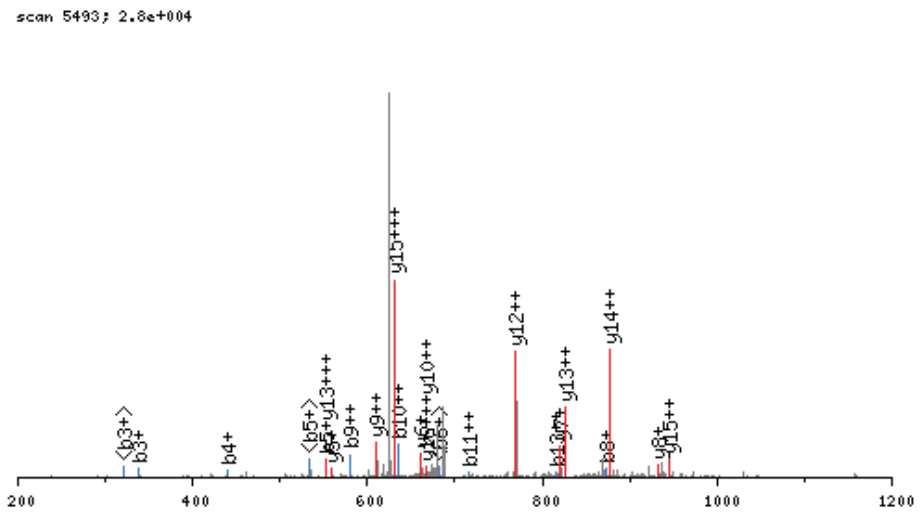
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
105.0664	53.0371	1	S	9			
218.1505	109.5791	2	L	8	1072.6990	536.8534	358.2382
513.4222	257.2150	3	H	7	959.6150	480.3114	320.5435
614.4699	307.7389	4	T	6	664.3432	332.6755	222.1196
727.5540	364.2809	5	L	5	563.2955	282.1517	188.4371
874.6224	437.8151	6	F	4	450.2114	225.6096	150.7424
931.6439	466.3258	7	G	3	303.1430	152.0754	101.7196
1046.6708	523.8393	8	D	2	246.1216	123.5647	82.7124
		9	K	1	131.0946	66.0512	44.3701

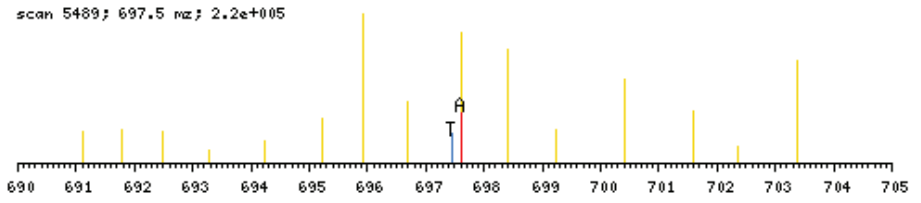
H(3):+295.27

X-range: 200 - 1200
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

SLHTLFGDKLCTVATLR, MH+ 2090.3772, m/z 697.4639
10HNE-1HSA-37Trypsin5-LTQ3.5493.5493.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



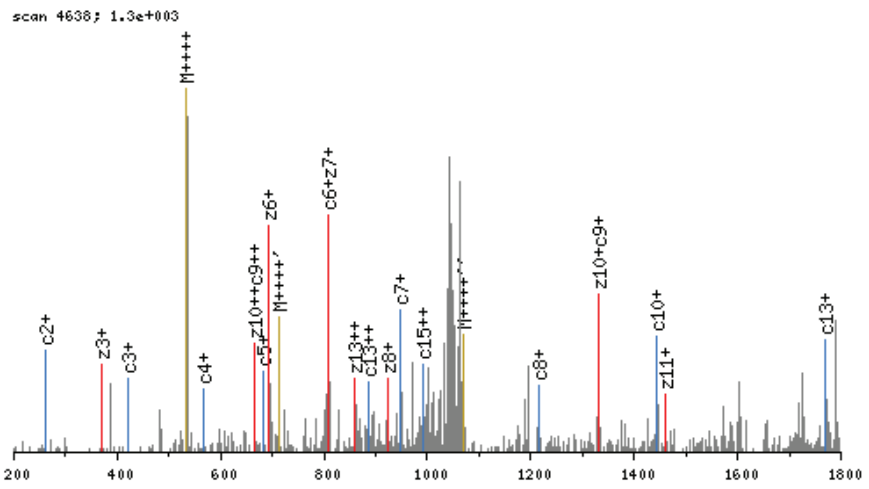
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
88.0399	44.5238	1	S	17			
201.1239	101.0659	2	L	16	2003.3451	1002.1765	**668.4536**
338.1828	169.5953	3	H	15	1890.2611	**945.6344**	**630.7589**
439.2305	220.1192	4	T	14	1753.2022	**877.1050**	585.0726
552.3146	276.6612	5	L	13	1652.1545	**826.5812**	**551.3900**
699.3830	350.1954	6	F	12	1539.0704	**770.0391**	513.6954
756.4044	378.7061	7	G	11	1392.0020	696.5049	464.6726
871.4314	436.2196	8	D	10	1334.9805	**667.9942**	445.6654
1157.7362	**579.3720**	9	K	9	1219.9536	**610.4807**	407.3231
1270.8202	**635.9140**	10	L	8	**933.6488**	467.3283	311.8882
1430.9805	**715.9942**	11	C	7	**820.5647**	410.7863	274.1935
1532.0282	766.5180	12	T	6	**660.4044**	330.7061	220.8067
1631.0966	**816.0522**	13	V	5	**559.3568**	280.1823	187.1241
1702.1337	851.5708	14	A	4	460.2884	230.6481	154.1013
1803.1814	902.0946	15	T	3	389.2512	195.1295	130.4223
1916.2655	958.6367	16	L	2	288.2036	144.6057	96.7397
		17	R	1	175.1195	88.0637	59.0451

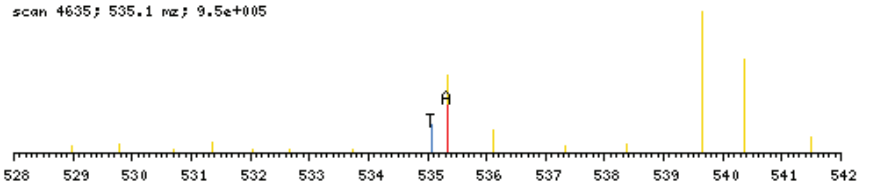
K(9):+286.30 C(11):+160.16

X-range: 200 - 1800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

NECFLQHKDDNPNLPR, MH+ 2137.2588, m/z 535.0702
10HNE-1HSA-37Trypsin2-LTQ2.4638.4638.4.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	c^{3+}	#	AA	#	z^+	z^{2+}	z^{3+}
132.0773	66.5426	44.6977	1	N	16			
261.1199	131.0639	87.7118	2	E	15	2007.1972	1004.1025	669.7376
421.2802	211.1440	141.0986	3	C	14	1878.1546	939.5812	626.7234
568.3486	284.6782	190.1214	4	F	13	1717.9943	**859.5011**	573.3366
681.4327	341.2202	227.8161	5	L	12	1570.9259	785.9669	524.3138
809.4913	405.2495	270.5023	6	Q	11	**1457.8418**	729.4248	486.6192
946.5502	473.7790	316.1886	7	H	10	**1329.7832**	**665.3955**	443.9330
1214.8444	607.9261	405.6200	8	K	9	1192.7243	596.8661	398.2467
1329.8713	**665.4396**	443.9623	9	D	8	**924.4301**	462.7190	308.8153
1444.8983	722.9530	482.3046	10	D	7	**809.4032**	405.2055	270.4729
1558.9412	779.9745	520.3189	11	N	6	**694.3762**	347.6920	232.1306
1655.9940	828.5009	552.6699	12	P	5	580.3333	290.6706	194.1163
1770.0369	**885.5224**	590.6842	13	N	4	483.2805	242.1442	161.7654
1883.1209	942.0644	628.3789	14	L	3	**369.2376**	185.1227	123.7511
1980.1737	**990.5908**	660.7298	15	P	2	256.1535	128.5807	86.0564
			16	R	1	159.1008	80.0543	53.7055

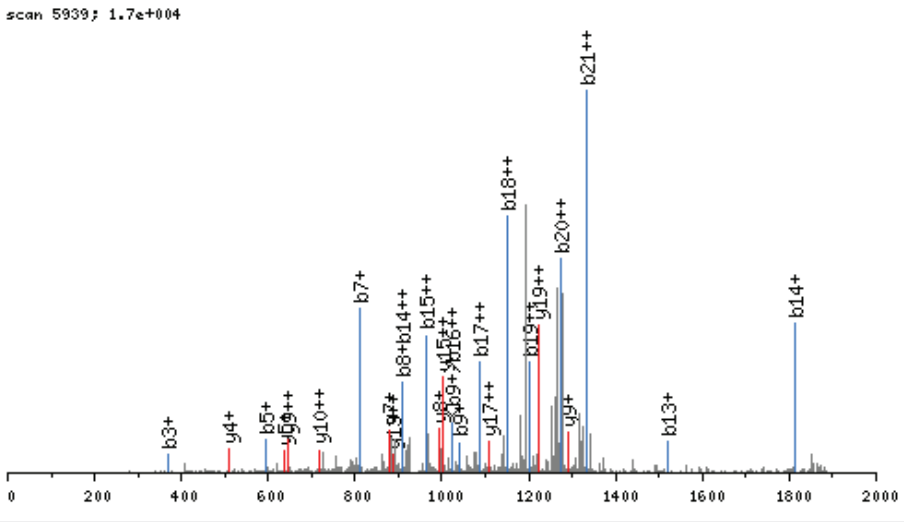
C(3):+160.16 K(8):+268.29

X-range: 0 - 0
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

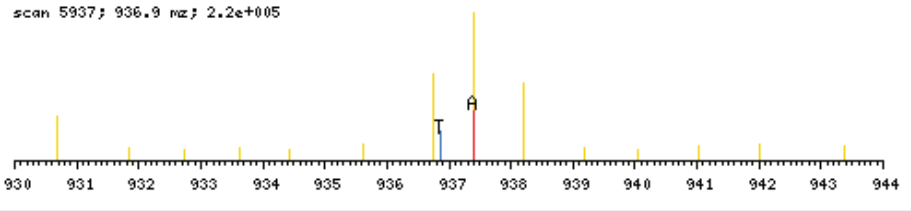
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

LVRPEVDVMCTAFHDNEETFLK, MH+ 2808.6071, m/z 936.8739
10HNE-1HSA-37Trypsin2-LTQ3.5939.5939.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
114.0919	57.5499	1	L	22			
213.1603	107.0841	2	V	21	2695.5230	1348.2654	899.1795
369.2614	185.1346	3	R	20	2596.4546	1298.7312	866.1567
466.3142	233.6610	4	P	19	2440.3535	1220.6806	814.1230
595.3568	298.1823	5	E	18	2343.3007	1172.1543	781.7721
694.4252	347.7165	6	V	17	2214.2581	1107.6330	738.7579
809.4521	405.2300	7	D	16	2115.1897	1058.0988	705.7351
908.5205	454.7642	8	V	15	2000.1628	1000.5853	667.3928
1039.5610	520.2844	9	M	14	1901.0943	951.0511	634.3700
1199.7213	600.3646	10	C	13	1770.0539	885.5308	590.6898
1300.7690	650.8884	11	T	12	1609.8936	805.4507	537.3031
1371.8061	686.4070	12	A	11	1508.8459	754.9268	503.6205
1518.8745	759.9412	13	F	10	1437.8088	719.4083	479.9415
1814.1463	907.5771	14	H	9	1290.7403	645.8741	430.9187
1929.1733	965.0905	15	D	8	995.4686	498.2382	332.4947
2043.2162	1022.1120	16	N	7	880.4416	440.7247	294.1524
2172.2588	1086.6333	17	E	6	766.3987	383.7033	256.1381
2301.3014	1151.1546	18	E	5	637.3561	319.1820	213.1239
2402.3490	1201.6784	19	T	4	508.3135	254.6607	170.1097
2549.4175	1275.2126	20	F	3	407.2658	204.1368	136.4272
2662.5015	1331.7547	21	L	2	260.1974	130.6026	87.4044
		22	K	1	147.1134	74.0606	49.7097

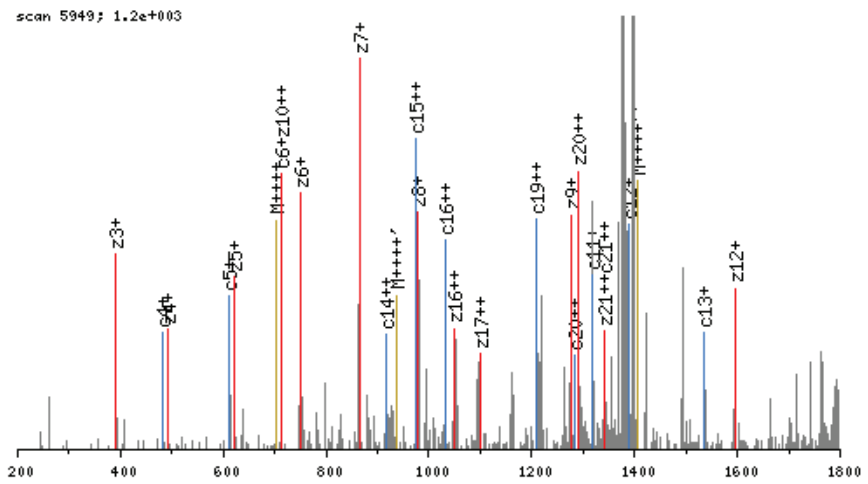
C(10):+160.16 H(14):+295.27

X-range: 200 - 1800
MassTol: 0.950 Y-zoom: 2.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

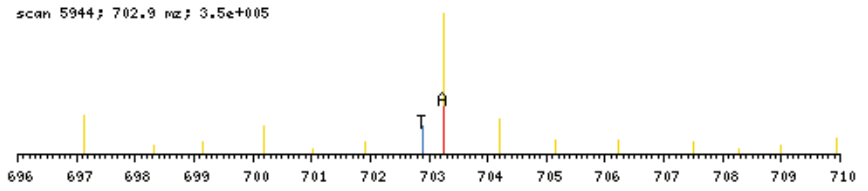
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

LVRPEVDVMCTAFHDNEETFLK, MH+ 2808.6071, m/z 702.9072
10HNE-1HSA-37Trypsin3-LTQ3.5949.5949.4.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	c^{3+}	#	AA	#	z^+	z^{2+}	z^{3+}
131.1184	66.0631	44.3780	1	L	22			
230.1869	115.5973	77.4008	2	V	21	2679.5043	1340.2560	893.8400
386.2880	193.6479	129.4345	3	R	20	2580.4359	1290.7218	860.8172
483.3407	242.1743	161.7855	4	P	19	2424.3347	1212.6713	808.7835
612.3833	306.6956	204.7997	5	E	18	2327.2820	1164.1449	776.4325
711.4517	356.2298	237.8225	6	V	17	2198.2394	1099.6236	733.4183
826.4787	413.7433	276.1648	7	D	16	2099.1710	1050.0894	700.3955
925.5471	463.2775	309.1876	8	V	15	1984.1440	992.5759	662.0532
1056.5876	528.7977	352.8677	9	M	14	1885.0756	943.0417	629.0304
1216.7479	608.8779	406.2545	10	C	13	1754.0351	877.5215	585.3503
1317.7956	659.4017	439.9371	11	T	12	1593.8748	797.4413	531.9635
1388.8327	694.9202	463.6161	12	A	11	1492.8271	746.9175	498.2809
1535.9011	768.4545	512.6389	13	F	10	1421.7900	711.3989	474.6019
1831.1729	916.0903	611.0628	14	H	9	1274.7216	637.8647	425.5791
1946.1998	973.6038	649.4052	15	D	8	979.4498	490.2288	327.1552
2060.2427	1030.6253	687.4195	16	N	7	864.4229	432.7154	288.8128
2189.2853	1095.1466	730.4337	17	E	6	750.3800	375.6939	250.7985
2318.3279	1159.6679	773.4479	18	E	5	621.3374	311.1726	207.7843
2419.3756	1210.1917	807.1304	19	T	4	492.2948	246.6513	164.7701
2566.4440	1283.7259	856.1532	20	F	3	391.2471	196.1275	131.0876
2679.5281	1340.2680	893.8479	21	L	2	244.1787	122.5933	82.0648
			22	K	1	131.0946	66.0512	44.3701

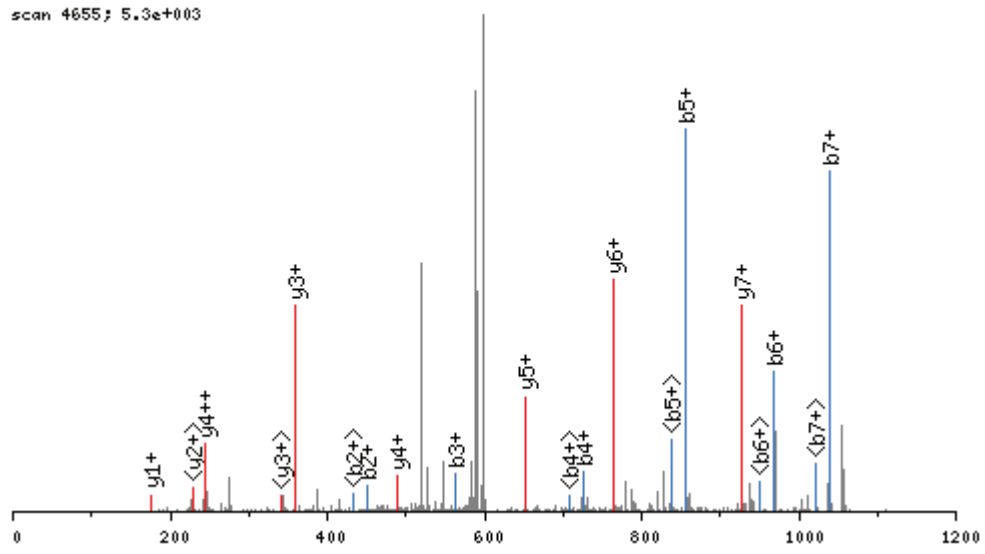
C(10):+160.16 H(14):+295.27

X-range: 0 - 1200
MassTol: 0.950 Y-zoom: 4.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

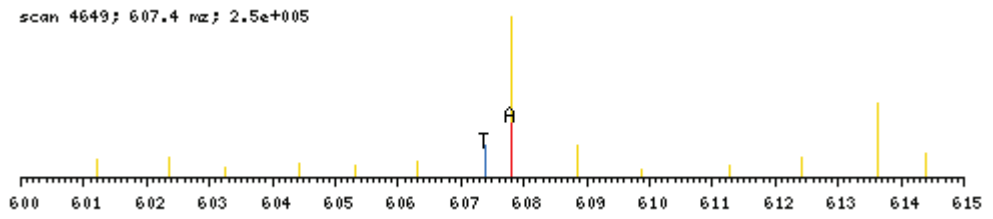
a	[ ] +	[ ] 2+	[ ] 3+
b	[x] +	[ ] 2+	[ ] 3+
c	[ ] +	[ ] 2+	[ ] 3+
x	[ ] +	[ ] 2+	[ ] 3+
y	[x] +	[x] 2+	[ ] 3+
z	[ ] +	[ ] 2+	[ ] 3+

hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

KYLYEIAR, MH+ 1213.7988, m/z 607.4030
10HNE-1HSA-37Trypsin4-LTQ2.4655.4655.2.dta



click image to zoom in; click top corners to zoom out [precursor±]



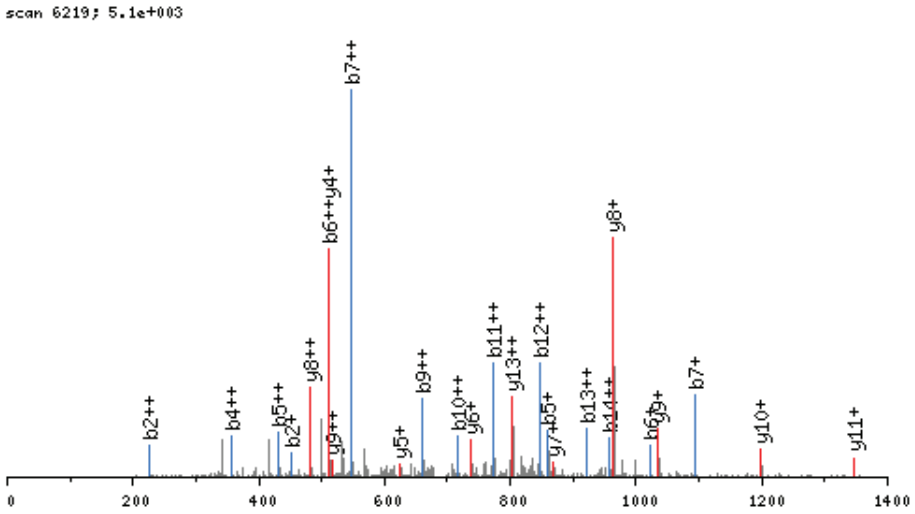
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	#	AA	#	y^+	y^{2+}
287.3126	1	K	8		
450.3759	2	Y	7	927.4940	464.2509
563.4600	3	L	6	764.4307	382.7192
726.5233	4	Y	5	651.3466	326.1772
855.5659	5	E	4	488.2833	244.6455
968.6500	6	I	3	359.2407	180.1243
1039.6871	7	A	2	246.1566	123.5822
	8	R	1	175.1195	88.0637

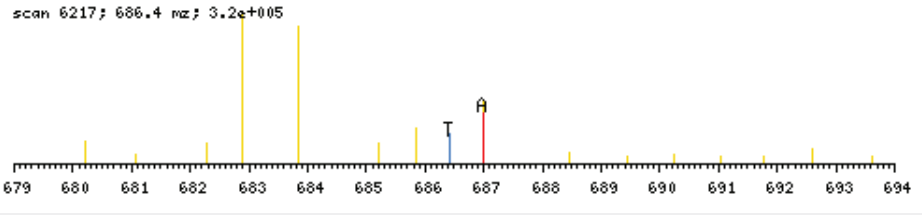
K(1):+286.30

X-range: 0 - 0
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

RHPYFYAPELLFFAK, MH+ 2057.2086, m/z 686.4077
10HNE-1HSA-37Trypsin5-LTQ3.6219.6219.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
157.1089	79.0584	1	R	15			
452.3807	226.6943	2	H	14	1901.1075	951.0577	634.3744
549.4335	275.2207	3	P	13	1605.8357	803.4218	535.9505
712.4968	356.7523	4	Y	12	1508.7830	754.8954	503.5995
859.5652	430.2865	5	F	11	1345.7196	673.3637	449.2451
1022.6286	511.8182	6	Y	10	1198.6512	599.8295	400.2223
1093.6657	547.3367	7	A	9	1035.5879	518.2979	345.8678
1190.7184	595.8631	8	P	8	964.5508	482.7793	322.1888
1319.7610	660.3844	9	E	7	867.4980	434.2529	289.8379
1432.8451	716.9265	10	L	6	738.4554	369.7316	246.8237
1545.9291	773.4685	11	L	5	625.3714	313.1896	209.1290
1692.9976	847.0027	12	F	4	512.2873	256.6476	171.4343
1840.0660	920.5369	13	F	3	365.2189	183.1134	122.4115
1911.1031	956.0555	14	A	2	218.1505	109.5791	73.3887
		15	K	1	147.1134	74.0606	49.7097

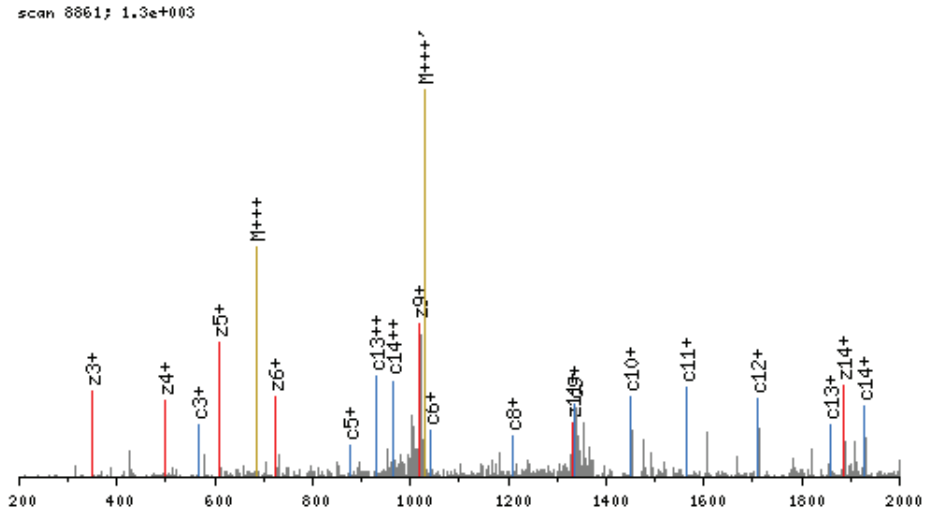
H(2):+295.27

X-range: 200 - 2000
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

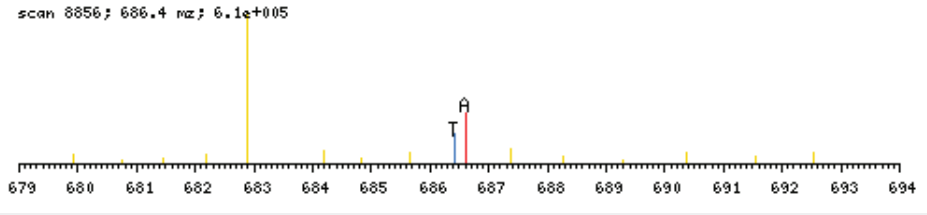
	+	2+	3+
a	☐	☐	☐
b	☐	☐	☐
c	☑	☑	☐
x	☐	☐	☐
y	☐	☐	☐
z	☑	☑	☑

hide H_2O/NH_3 ☐
zoom 112-122 ☐
zoom 124-133 ☐
GO

RHPYFYAPELLFFAK, MH+ 2057.2086, m/z 686.4077
10HNE-1HSA-37Trypsin5-LTQ4.8861.8861.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
174.1355	87.5717	1	R	15			
469.4073	235.2075	2	H	14	1885.0888	943.0483	629.0348
566.4600	283.7339	3	P	13	1589.8170	795.4124	530.6109
729.5234	365.2656	4	Y	12	1492.7642	746.8860	498.2600
876.5918	438.7998	5	F	11	1329.7009	665.3544	443.9055
1039.6551	520.3315	6	Y	10	1182.6325	591.8202	394.8827
1110.6922	555.8500	7	A	9	1019.5692	510.2885	340.5283
1207.7450	604.3764	8	P	8	948.5321	474.7699	316.8492
1336.7876	668.8977	9	E	7	851.4793	426.2436	284.4983
1449.8716	725.4397	10	L	6	722.4367	361.7223	241.4841
1562.9557	781.9818	11	L	5	609.3526	305.1802	203.7894
1710.0241	855.5160	12	F	4	496.2686	248.6382	166.0947
1857.0925	929.0502	13	F	3	349.2002	175.1040	117.0719
1928.1296	964.5687	14	A	2	202.1317	101.5698	68.0491
		15	K	1	131.0946	66.0512	44.3701

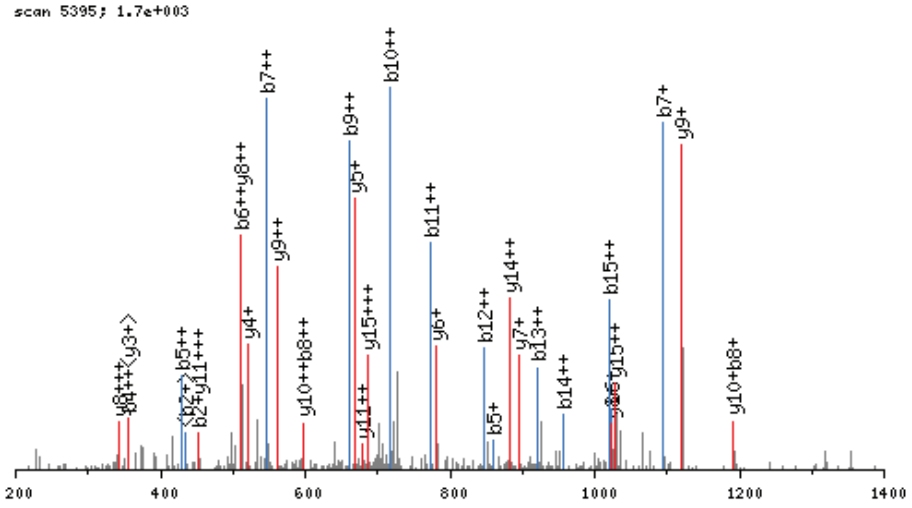
H(2):+295.27

X-range: 200 - 1400
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

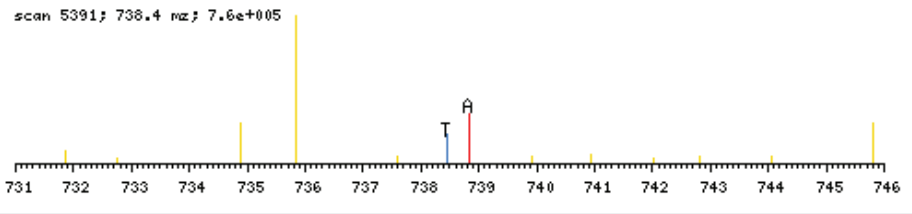
a	[ ] +	[ ] 2+	[ ] 3+
b	[x] +	[x] 2+	[ ] 3+
c	[ ] +	[ ] 2+	[ ] 3+
x	[ ] +	[ ] 2+	[ ] 3+
y	[x] +	[x] 2+	[x] 3+
z	[ ] +	[ ] 2+	[ ] 3+

hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

RHPYFYAPELLFFAKR, MH+ 2213.3097, m/z 738.4414
10HNE-1HSA-37Trypsin5-LTQ1.5395.5395.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
157.1089	79.0584	1	R	16			
452.3807	226.6943	2	H	15	2057.2086	**1029.1082**	**686.4081**
549.4335	275.2207	3	P	14	1761.9368	**881.4723**	587.9842
712.4968	**356.7523**	4	Y	13	1664.8841	832.9460	555.6332
859.5652	**430.2865**	5	F	12	1501.8207	751.4143	501.2788
1022.6286	**511.8182**	6	Y	11	1354.7523	**677.8801**	**452.2560**
1093.6657	**547.3367**	7	A	10	**1191.6890**	**596.3484**	397.9016
1190.7184	**595.8631**	8	P	9	**1120.6519**	**560.8299**	374.2225
1319.7610	**660.3844**	9	E	8	**1023.5991**	**512.3035**	**341.8716**
1432.8451	**716.9265**	10	L	7	**894.5565**	447.7822	298.8574
1545.9291	**773.4685**	11	L	6	**781.4725**	391.2401	261.1627
1692.9976	**847.0027**	12	F	5	**668.3884**	334.6981	223.4680
1840.0660	**920.5369**	13	F	4	**521.3200**	261.1639	174.4452
1911.1031	**956.0555**	14	A	3	374.2516	187.6297	125.4224
2039.1981	**1020.1029**	15	K	2	303.2145	152.1111	101.7434
		16	R	1	175.1195	88.0637	59.0451

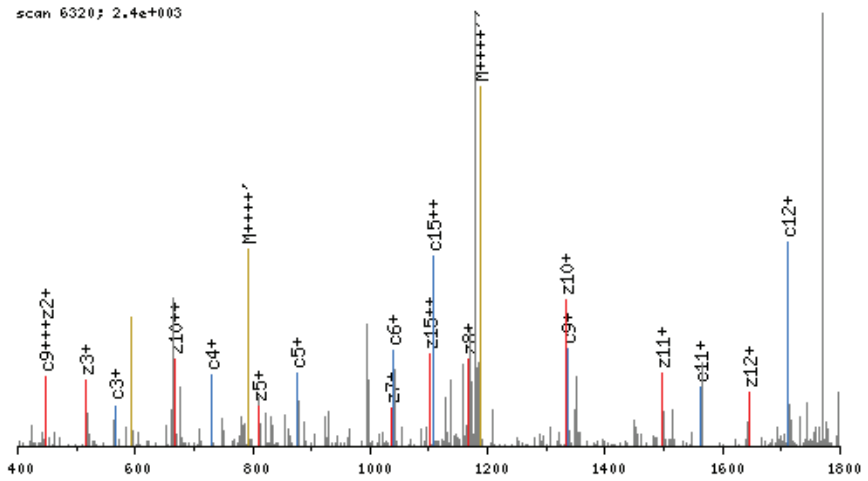
H(2):+295.27

X-range: 400 - 1800
MassTol: 0.950 Y-zoom: 1.70
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

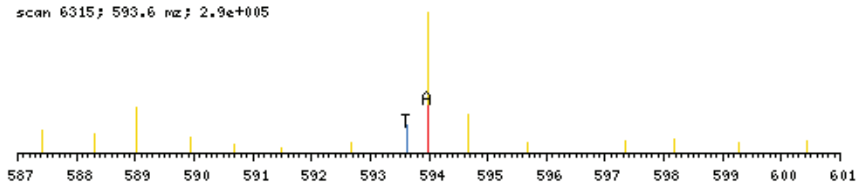
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

RHPYFYAPELLFFAKR, MH+ 2371.5195, m/z 593.6353
10HNE-1HSA-37Trypsin3-LTQ2.6320.6320.4.dta



click image to zoom in; click top corners to zoom out [precursor±]



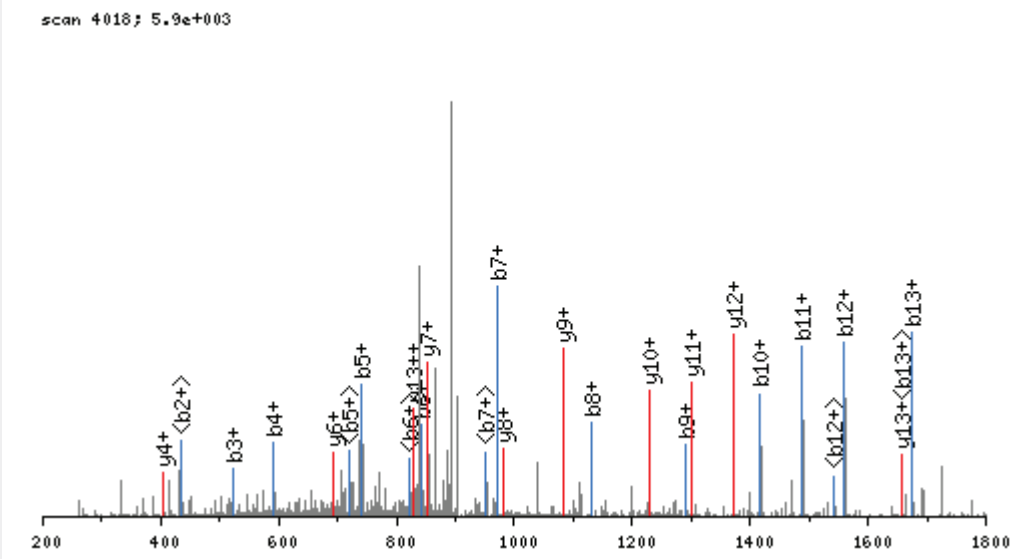
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	c^{3+}	#	AA	#	z^+	z^{2+}	z^{3+}
174.1355	87.5717	58.7170	1	R	16			
469.4073	235.2075	157.1410	2	H	15	2199.3997	1100.2038	733.8051
566.4600	283.7339	189.4919	3	P	14	1904.1279	952.5679	635.3812
729.5234	365.2656	243.8463	4	Y	13	1807.0752	904.0415	603.0303
876.5918	438.7998	292.8691	5	F	12	1644.0118	822.5098	548.6758
1039.6551	520.3315	347.2236	6	Y	11	1496.9434	748.9756	499.6530
1110.6922	555.8500	370.9026	7	A	10	1333.8801	667.4440	445.2986
1207.7450	604.3764	403.2535	8	P	9	1262.8430	631.9254	421.6195
1336.7876	668.8977	446.2677	9	E	8	1165.7902	583.3990	389.2686
1449.8716	725.4397	483.9624	10	L	7	1036.7476	518.8777	346.2544
1562.9557	781.9818	521.6571	11	L	6	923.6636	462.3357	308.5597
1710.0241	855.5160	570.6799	12	F	5	810.5795	405.7937	270.8650
1857.0925	929.0502	619.7027	13	F	4	663.5111	332.2595	221.8422
1928.1296	964.5687	643.3818	14	A	3	516.4427	258.7252	172.8194
2214.4344	1107.7211	738.8167	15	K	2	445.4056	223.2067	149.1404
			16	R	1	159.1008	80.0543	53.7055

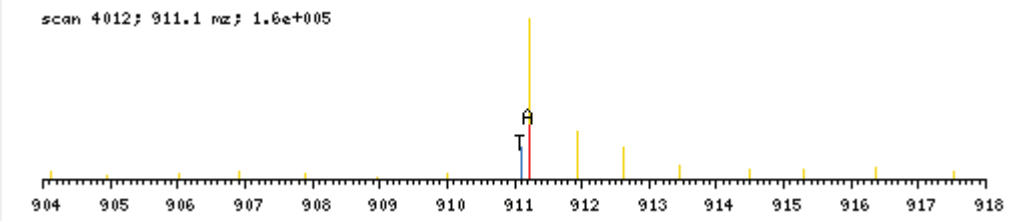
H(2):+295.27 K(15):+286.30

X-range: 200 - 1800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

YKAAFTECCQAADK, MH+ 1821.1947, m/z 911.1010
10HNE-1HSA-37Trypsin4-LTQ3.4018.4018.2.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	#	AA	#	y^+	y^{2+}
164.0712	1	Y	14		
450.3759	2	K	13	1658.1314	829.5696
521.4130	3	A	12	1371.8266	686.4172
592.4502	4	A	11	1300.7895	650.8987
739.5186	5	F	10	1229.7524	615.3801
840.5663	6	T	9	1082.6840	541.8459
969.6088	7	E	8	981.6363	491.3221
1129.7691	8	C	7	852.5937	426.8008
1289.9294	9	C	6	692.4334	346.7206
1417.9880	10	Q	5	532.2731	266.6405
1489.0251	11	A	4	404.2145	202.6112
1560.0623	12	A	3	333.1774	167.0926
1675.0892	13	D	2	262.1403	131.5741
	14	K	1	147.1134	74.0606

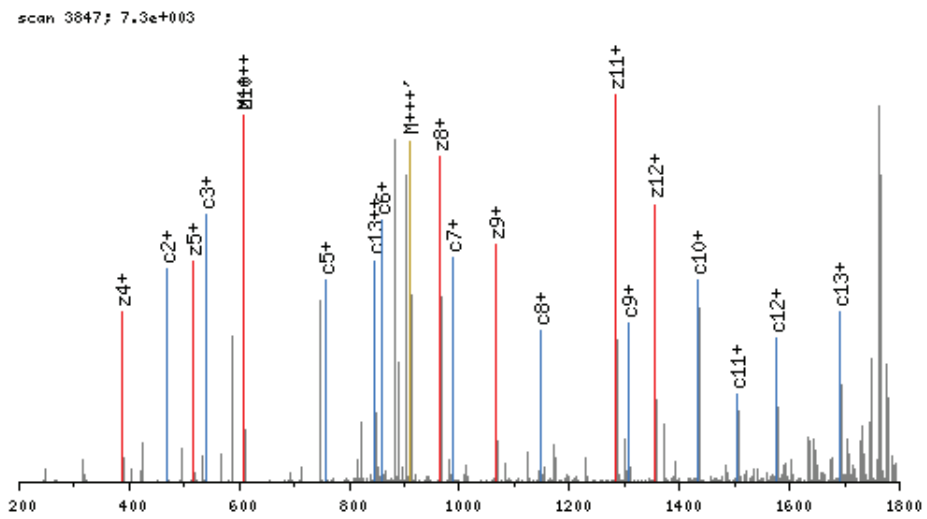
K(2):+286.30 C(8):+160.16 C(9):+160.16

X-range: 200 - 1800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

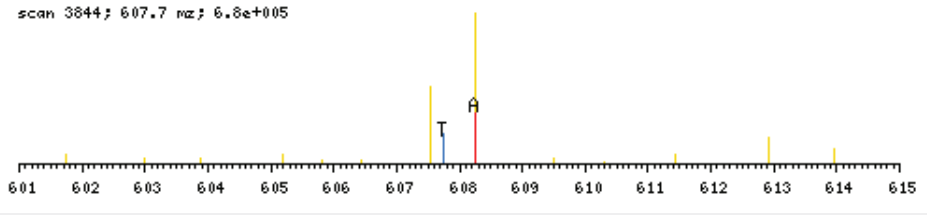
a	☐ +	☐ 2+	☐ 3+
b	☐ +	☐ 2+	☐ 3+
c	☑ +	☑ 2+	☐ 3+
x	☐ +	☐ 2+	☐ 3+
y	☐ +	☐ 2+	☐ 3+
z	☑ +	☑ 2+	☑ 3+

hide H_2O/NH_3 ☐
zoom 112-122 ☐
zoom 124-133 ☐
GO

YKAAFTECCQAADK, MH+ 1821.1947, m/z 607.7364
10HNE-1HSA-37Trypsin2-LTQ1.3847.3847.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



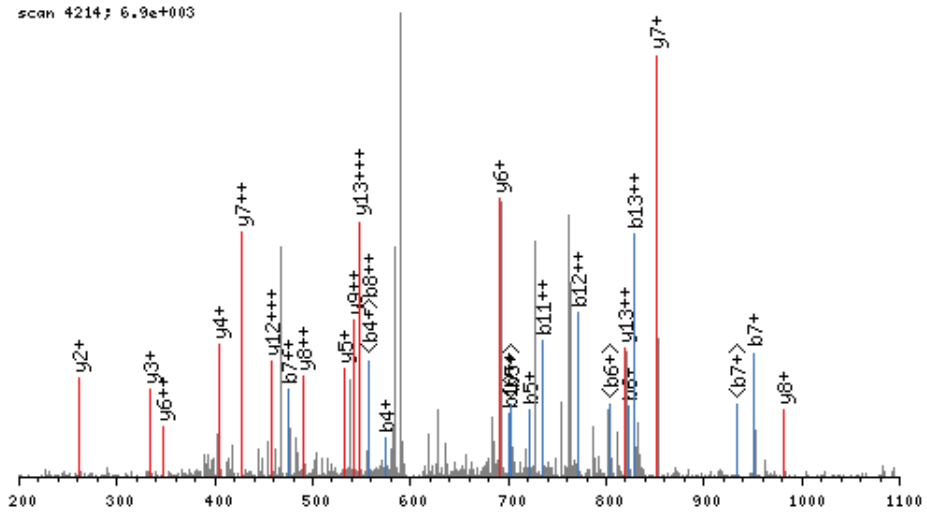
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
181.0977	91.0528	1	Y	14			
467.4025	234.2052	2	K	13	1642.1127	821.5602	548.0428
538.4396	269.7237	3	A	12	**1355.8079**	678.4079	452.6078
609.4767	305.2423	4	A	11	**1284.7708**	642.8893	428.9288
756.5451	378.7765	5	F	10	1213.7337	**607.3707**	405.2498
857.5928	429.3003	6	T	9	**1066.6652**	533.8365	356.2270
986.6354	493.8216	7	E	8	**965.6176**	483.3127	322.5444
1146.7957	573.9018	8	C	7	836.5750	418.7914	279.5302
1306.9560	653.9819	9	C	6	676.4147	338.7113	226.1434
1435.0146	718.0112	10	Q	5	**516.2544**	258.6311	172.7567
1506.0517	753.5298	11	A	4	**388.1958**	194.6018	130.0705
1577.0888	789.0483	12	A	3	317.1587	159.0833	106.3914
1692.1157	**846.5618**	13	D	2	246.1216	123.5647	82.7124
		14	K	1	131.0946	66.0512	44.3701

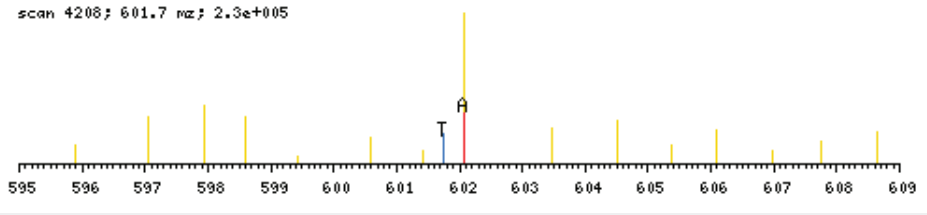
K(2):+286.30 C(8):+160.16 C(9):+160.16

X-range: 200 - 1100
MassTol: 0.950 Y-zoom: 4.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

YKAAFTECCQAADK, MH+ 1803.1842, m/z 601.7329
10HNE-1HSA-37Trypsin3-LTQ2.4214.4214.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
164.0712	82.5395	1	Y	14			
432.3654	216.6866	2	K	13	1640.1208	**820.5643**	**547.3788**
503.4025	252.2052	3	A	12	1371.8266	686.4172	**457.9474**
574.4396	287.7237	4	A	11	1300.7895	650.8987	434.2684
721.5080	361.2579	5	F	10	1229.7524	615.3801	410.5893
822.5557	411.7818	6	T	9	1082.6840	**541.8459**	361.5665
951.5983	**476.3031**	7	E	8	**981.6363**	**491.3221**	327.8840
1111.7586	**556.3832**	8	C	7	**852.5937**	**426.8008**	284.8698
1271.9189	636.4634	9	C	6	**692.4334**	**346.7206**	231.4830
1399.9775	**700.4926**	10	Q	5	**532.2731**	266.6405	178.0963
1471.0146	**736.0112**	11	A	4	**404.2145**	202.6112	135.4101
1542.0517	**771.5298**	12	A	3	**333.1774**	167.0926	111.7310
1657.0786	**829.0432**	13	D	2	**262.1403**	131.5741	88.0520
		14	K	1	147.1134	74.0606	49.7097

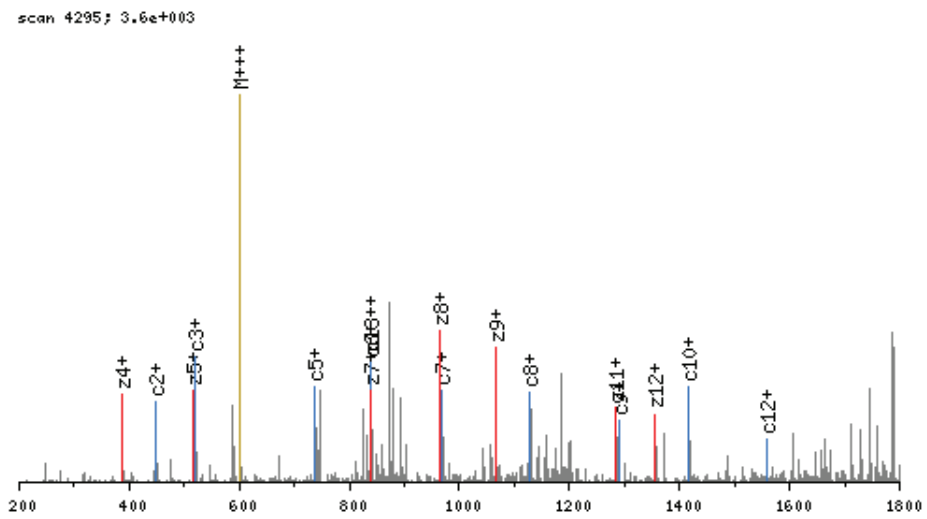
K(2):+268.29 C(8):+160.16 C(9):+160.16

X-range: 200 - 1800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

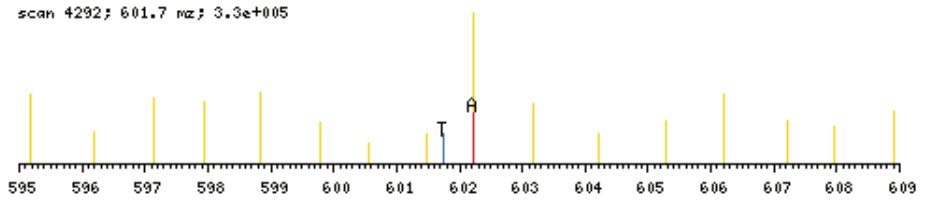
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

YKAAFTECCQAADK, MH+ 1803.1842, m/z 601.7329
10HNE-1HSA-37Trypsin5-LTQ4.4295.4295.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
181.0977	91.0528	1	Y	14			
449.3919	225.1999	2	K	13	1624.1021	812.5550	542.0393
520.4290	260.7184	3	A	12	1355.8079	678.4079	452.6078
591.4661	296.2370	4	A	11	1284.7708	642.8893	428.9288
738.5346	369.7712	5	F	10	1213.7337	607.3707	405.2498
839.5822	420.2950	6	T	9	1066.6652	533.8365	356.2270
968.6248	484.8163	7	E	8	965.6176	483.3127	322.5444
1128.7851	564.8965	8	C	7	836.5750	418.7914	279.5302
1288.9454	644.9766	9	C	6	676.4147	338.7113	226.1434
1417.0040	709.0059	10	Q	5	516.2544	258.6311	172.7567
1488.0411	744.5245	11	A	4	388.1958	194.6018	130.0705
1559.0782	780.0430	12	A	3	317.1587	159.0833	106.3914
1674.1052	837.5565	13	D	2	246.1216	123.5647	82.7124
		14	K	1	131.0946	66.0512	44.3701

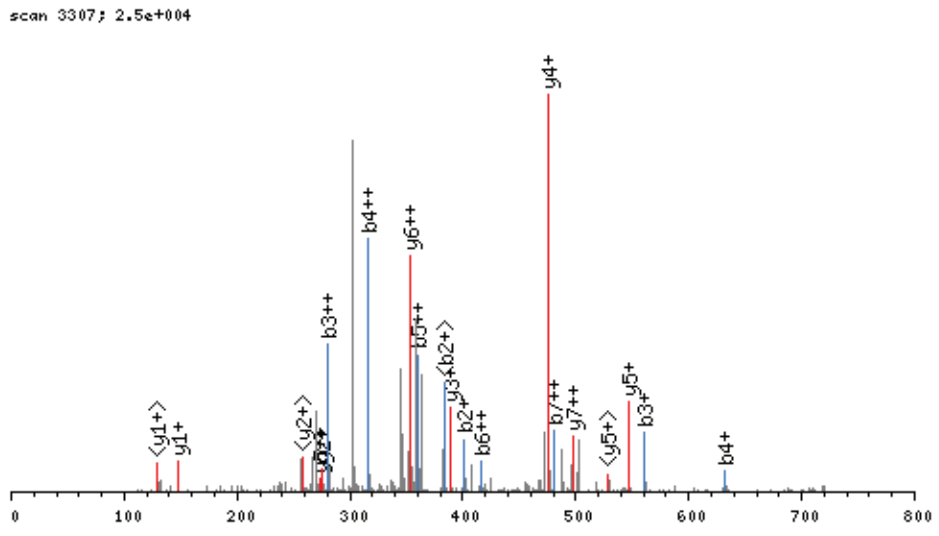
K(2):+268.29 C(8):+160.16 C(9):+160.16

X-range:
0 - 0
MassTol: Y-zoom:
0.950 1.00
ImageSize:
(•) Sm ( ) Lg
MassType:
( ) AVG (•) MONO
Axis:
(•) 1 ( ) 2
Label:
(•) I ( ) M ( ) -
Ions:

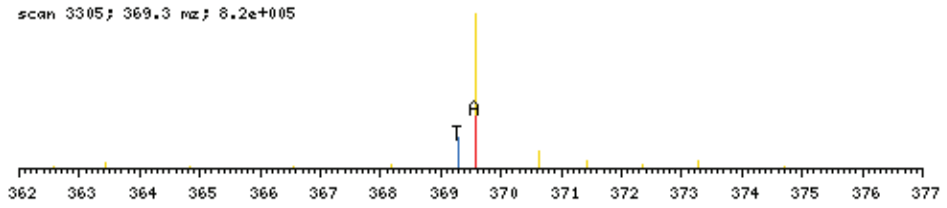
a	☐ +	☐ 2+	☐ 3+
b	☑ +	☑ 2+	☐ 3+
c	☐ +	☐ 2+	☐ 3+
x	☐ +	☐ 2+	☐ 3+
y	☑ +	☑ 2+	☑ 3+
z	☐ +	☐ 2+	☐ 3+

hide H_2O/NH_3 ☐
zoom 112-122 ☐
zoom 124-133 ☐
GO

LKCASLQK, MH+ 1105.8743, m/z 369.2963
10HNE-1HSA-37Trypsin5-LTQ4.3307.3307.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
114.0919	57.5499	1	L	8			
400.3967	200.7022	2	K	7	992.7902	**496.8990**	331.6020
560.5570	**280.7824**	3	C	6	706.4854	**353.7466**	236.1670
631.5941	**316.3010**	4	A	5	**546.3251**	**273.6665**	182.7803
718.6261	**359.8170**	5	S	4	**475.2880**	238.1479	159.1012
831.7102	**416.3590**	6	L	3	**388.2560**	194.6319	130.0905
959.7688	**480.3883**	7	Q	2	**275.1719**	138.0899	92.3959
		8	K	1	**147.1134**	74.0606	49.7097

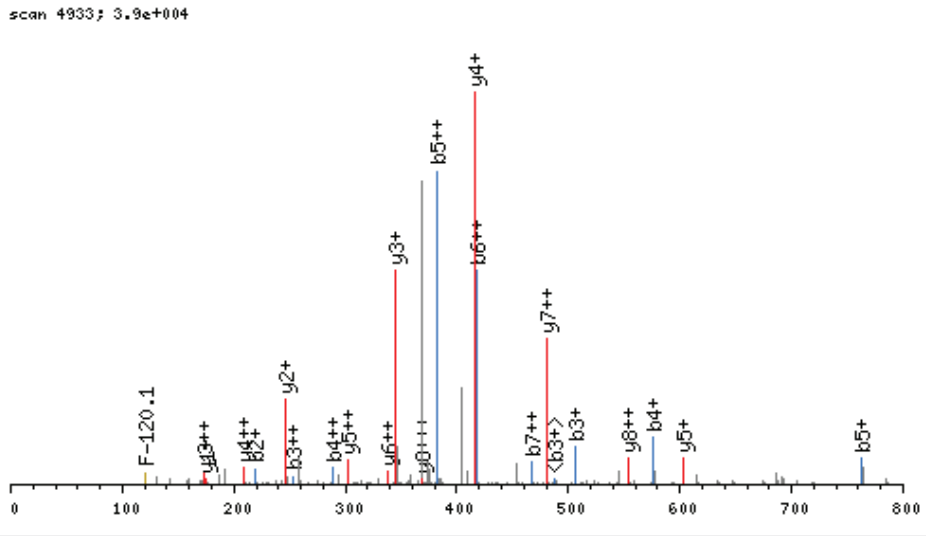
K(2):+286.30 C(3):+160.16

X-range:
0 - 0
MassTol: Y-zoom:
0.950 1.00
ImageSize:
(•) Sm ( ) Lg
MassType:
( ) AVG (•) MONO
Axis:
(•) 1 ( ) 2
Label:
(•) I ( ) M ( ) -
Ions:

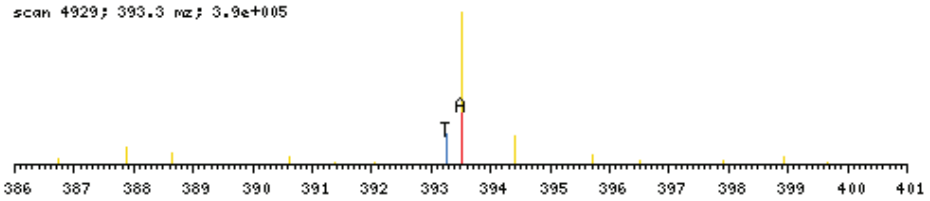
a	☐ +	☐ 2+	☐ 3+
b	☑ +	☑ 2+	☐ 3+
c	☐ +	☐ 2+	☐ 3+
x	☐ +	☐ 2+	☐ 3+
y	☑ +	☑ 2+	☑ 3+
z	☐ +	☐ 2+	☐ 3+

hide H_2O/NH_3 ☐
zoom 112-122 ☐
zoom 124-133 ☐
GO

AFKAWAVAR, MH+ 1177.7889, m/z 393.2678
10HNE-1HSA-37Trypsin5-LTQ4.4933.4933.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



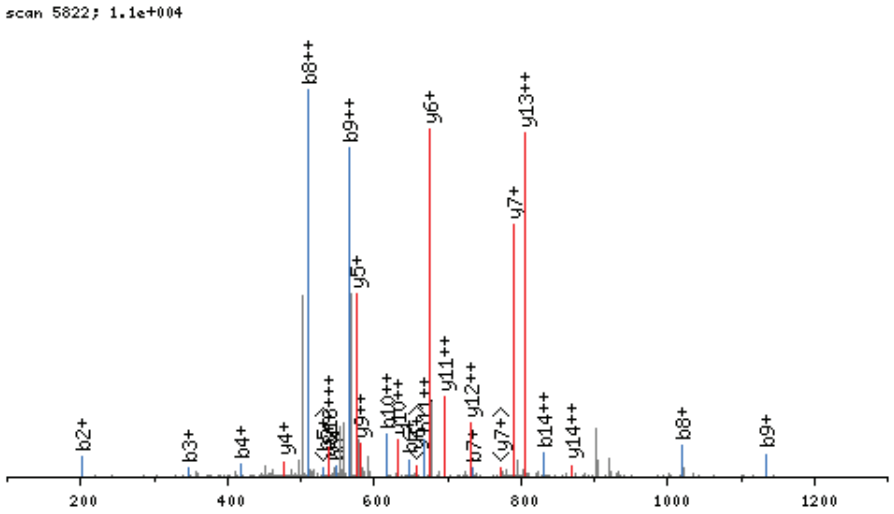
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
72.0449	36.5264	1	A	9			
219.1134	110.0606	2	F	8	1106.7518	**553.8798**	**369.5891**
505.4181	**253.2130**	3	K	7	959.6833	**480.3456**	320.5663
576.4552	**288.7315**	4	A	6	673.3786	**337.1932**	225.1314
762.5346	**381.7712**	5	W	5	**602.3415**	**301.6746**	201.4524
833.5717	**417.2897**	6	A	4	**416.2621**	**208.6350**	139.4259
932.6401	**466.8240**	7	V	3	**345.2250**	**173.1164**	115.7469
1003.6772	502.3425	8	A	2	**246.1566**	123.5822	82.7241
		9	R	1	**175.1195**	88.0637	59.0451

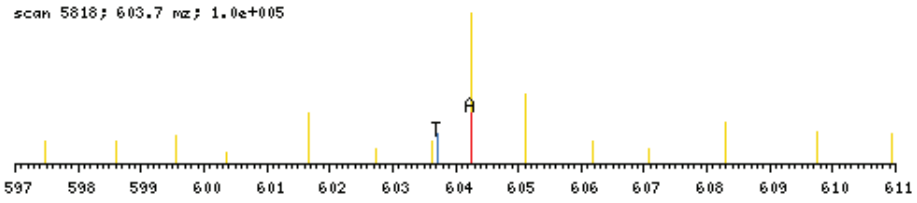
K(3):+286.30

X-range: 100 - 1300
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

AEFAEVSKLVTDLTK, MH+ 1809.1052, m/z 603.7066
10HNE-1HSA-37Trypsin5-LTQ1.5822.5822.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
72.0449	36.5264	1	A	15			
201.0875	101.0477	2	E	14	1738.0681	869.5380	580.0279
348.1559	174.5819	3	F	13	1609.0255	805.0167	537.0137
419.1931	210.1004	4	A	12	1461.9571	731.4825	487.9909
548.2357	274.6217	5	E	11	1390.9200	695.9639	464.3119
647.3041	324.1559	6	V	10	1261.8774	631.4426	421.2977
734.3361	367.6720	7	S	9	1162.8090	581.9084	388.2749
1020.6409	510.8244	8	K	8	1075.7770	538.3924	359.2642
1133.7249	567.3664	9	L	7	789.4722	395.2400	263.8293
1232.7934	616.9006	10	V	6	676.3881	338.6980	226.1346
1333.8410	667.4244	11	T	5	577.3197	289.1638	193.1118
1448.8680	724.9379	12	D	4	476.2720	238.6399	159.4292
1561.9520	781.4799	13	L	3	361.2451	181.1265	121.0869
1662.9997	832.0038	14	T	2	248.1610	124.5844	83.3922
		15	K	1	147.1134	74.0606	49.7097

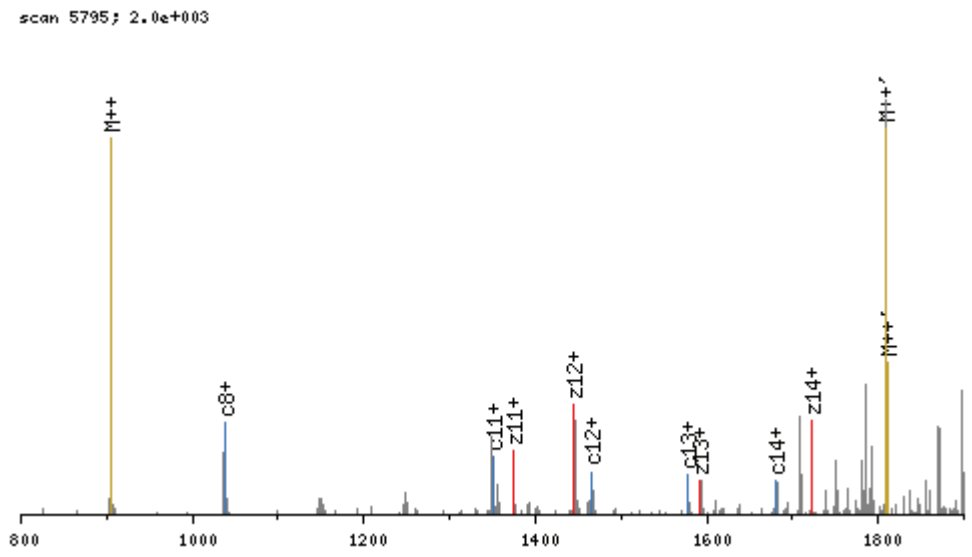
K(8):+286.30

X-range:
800 - 1900
MassTol: Y-zoom:
0.950 1.00
ImageSize:
(•) Sm ( ) Lg
MassType:
( ) AVG (•) MONO
Axis:
(•) 1 ( ) 2
Label:
(•) I ( ) M ( ) -
Ions:

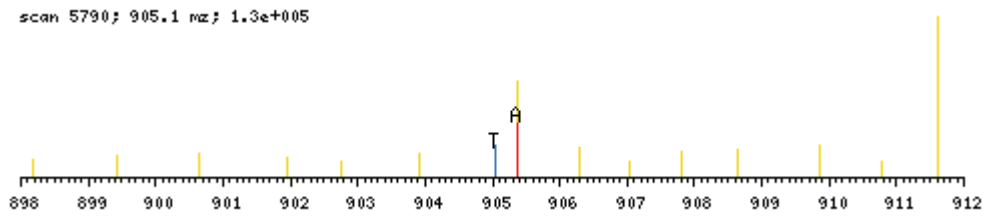
a	[ ] +	[ ] 2+	[ ] 3+
b	[ ] +	[ ] 2+	[ ] 3+
c	[x] +	[ ] 2+	[ ] 3+
x	[ ] +	[ ] 2+	[ ] 3+
y	[ ] +	[ ] 2+	[ ] 3+
z	[x] +	[x] 2+	[ ] 3+

hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

AEFAEVSKLVTDLTK, MH+ 1809.1052, m/z 905.0563
10HNE-1HSA-37Trypsin4-LTQ1.5795.5795.2.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	#	AA	#	z^+	z^{2+}
89.0715	1	A	15		
218.1141	2	E	14	**1722.0494**	861.5286
365.1825	3	F	13	**1593.0068**	797.0073
436.2196	4	A	12	**1445.9384**	723.4731
565.2622	5	E	11	**1374.9013**	687.9546
664.3306	6	V	10	1245.8587	623.4333
751.3626	7	S	9	1146.7903	573.8991
1037.6674	8	K	8	1059.7583	530.3830
1150.7515	9	L	7	773.4535	387.2306
1249.8199	10	V	6	660.3694	330.6886
1350.8676	11	T	5	561.3010	281.1544
1465.8945	12	D	4	460.2533	230.6306
1578.9786	13	L	3	345.2264	173.1171
1680.0263	14	T	2	232.1423	116.5751
	15	K	1	131.0946	66.0512

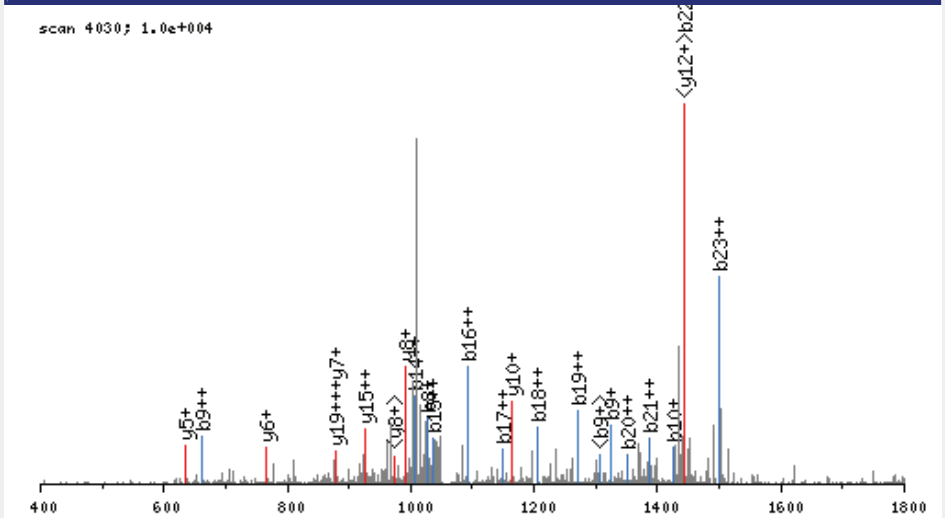
K(8):+286.30

X-range: 400 - 1800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

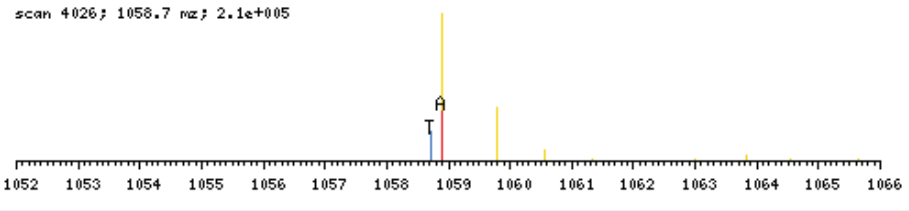
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

LVTDLTKVHTECCHGDLLECADDR, MH+ 3174.1035, m/z 1058.7060
10HNE-1HSA-37Trypsin4-LTQ2.4030.4030.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
114.0919	57.5499	1	L	24			
213.1603	107.0841	2	V	23	3061.0195	1531.0136	1021.0117
314.2080	157.6079	3	T	22	2961.9511	1481.4794	987.9889
429.2349	215.1214	4	D	21	2860.9034	1430.9556	954.3063
542.3190	271.6634	5	L	20	2745.8764	1373.4421	915.9640
643.3667	322.1872	6	T	19	2632.7924	1316.9001	**878.2693**
929.6714	465.3396	7	K	18	2531.7447	1266.3763	844.5868
1028.7399	514.8738	8	V	17	2245.4399	1123.2239	749.1519
1324.0116	**662.5097**	9	H	16	2146.3715	1073.6897	716.1290
1425.0593	713.0336	10	T	15	1851.0997	**926.0538**	617.7051
1554.1019	777.5549	11	E	14	1750.0520	875.5299	584.0226
1714.2622	857.6350	12	C	13	1621.0094	811.0086	541.0084
1874.4225	937.7152	13	C	12	1460.8491	730.9285	487.6216
2011.4814	**1006.2446**	14	H	11	1300.6888	650.8483	434.2348
2068.5029	**1034.7554**	15	G	10	**1163.6299**	582.3189	388.5485
2183.5298	**1092.2688**	16	D	9	1106.6085	553.8081	369.5414
2296.6139	**1148.8109**	17	L	8	**991.5815**	496.2947	331.1991
2409.6980	**1205.3529**	18	L	7	**878.4975**	439.7526	293.5044
2538.7406	**1269.8742**	19	E	6	**765.4134**	383.2106	255.8097
2698.9009	**1349.9543**	20	C	5	**636.3708**	318.6893	212.7955
2769.9380	**1385.4729**	21	A	4	476.2105	238.6092	159.4087
2884.9649	**1442.9864**	22	D	3	405.1734	203.0906	135.7297
2999.9919	**1500.4998**	23	D	2	290.1464	145.5771	97.3874
		24	R	1	175.1195	88.0637	59.0451

K(7):+286.30 H(9):+295.27 C(12):+160.16 C(13):+160.16 C(20):+160.16

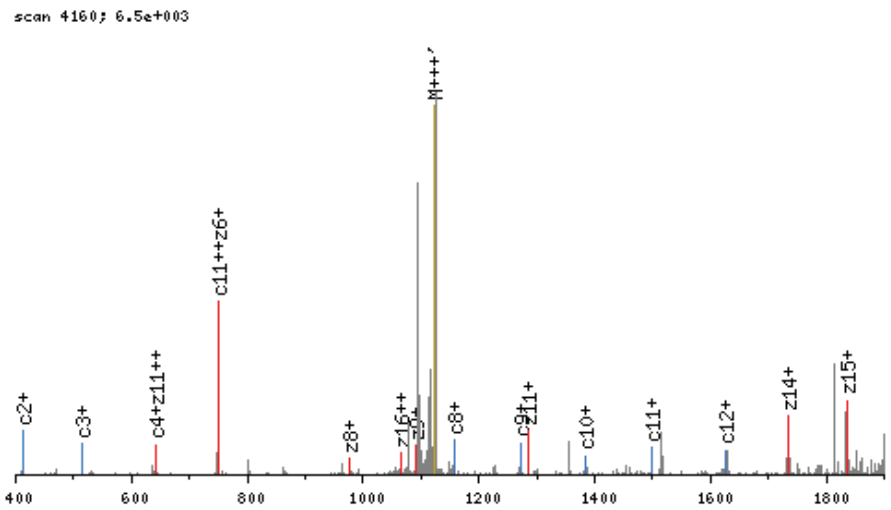
COMET Spectrum View by J.Eng (c) ISB 2001
(TPP v4.4 VUVUZELA rev 1, Build 201010121551 (MinGW))

X-range: 400 - 1900
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

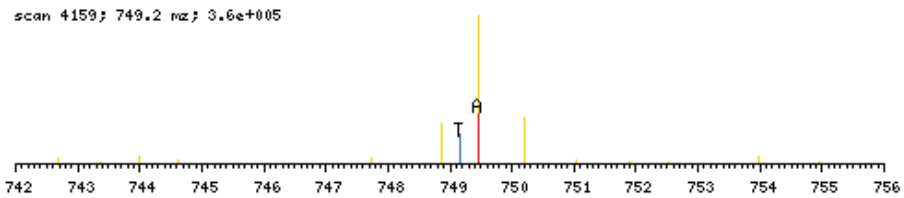
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

VHTECCHGDLLECADDR, MH+ 2245.4399, m/z 749.1515
10HNE-1HSA-37Trypsin2-LTQ2.4160.4160.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
117.1028	59.0553	1	V	17			
412.3746	206.6912	2	H	16	2130.3528	1065.6803	710.7895
513.4222	257.2150	3	T	15	1835.0810	918.0444	612.3655
642.4648	321.7363	4	E	14	1734.0333	867.5206	578.6830
802.6251	401.8165	5	C	13	1604.9907	802.9993	535.6688
962.7854	481.8966	6	C	12	1444.8304	722.9191	482.2820
1099.8444	550.4261	7	H	11	1284.6701	642.8390	428.8953
1156.8658	578.9368	8	G	10	1147.6112	574.3095	383.2090
1271.8928	636.4503	9	D	9	1090.5897	545.7988	364.2018
1384.9768	692.9923	10	L	8	975.5628	488.2853	325.8595
1498.0609	749.5344	11	L	7	862.4787	431.7433	288.1648
1627.1035	814.0557	12	E	6	749.3947	375.2012	250.4701
1787.2638	894.1358	13	C	5	620.3521	310.6800	207.4559
1858.3009	929.6544	14	A	4	460.1918	230.5998	154.0691
1973.3278	987.1678	15	D	3	389.1547	195.0812	130.3901
2088.3548	1044.6813	16	D	2	274.1277	137.5678	92.0478
		17	R	1	159.1008	80.0543	53.7055

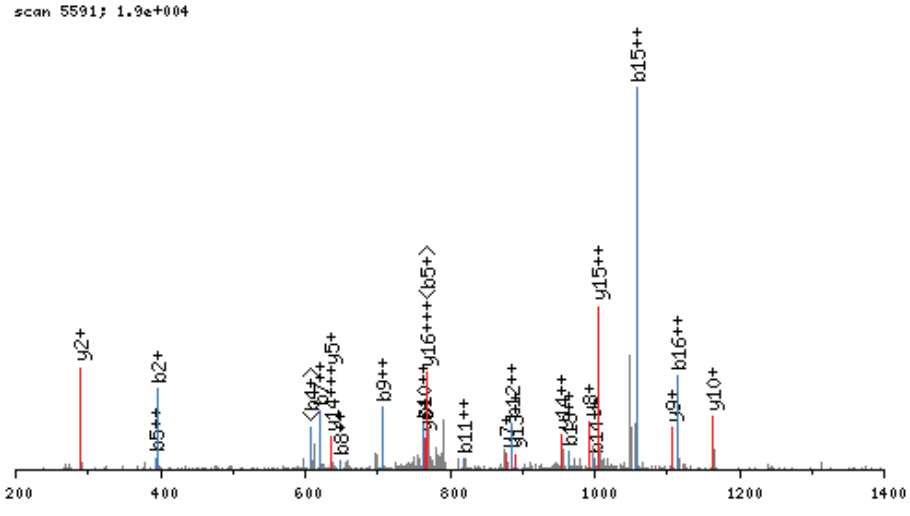
H(2):+295.27 C(5):+160.16 C(6):+160.16 C(13):+160.16

X-range: 200 - 1400
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

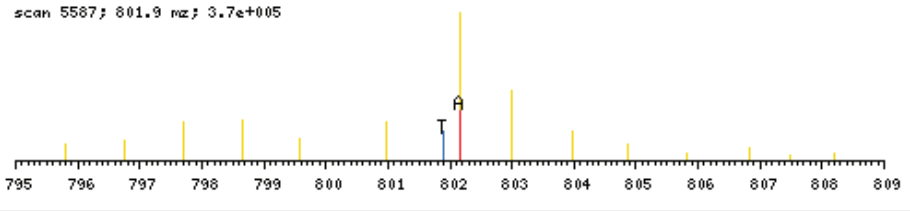
a	☐ +	☐ 2+	☐ 3+
b	☑ +	☑ 2+	☐ 3+
c	☐ +	☐ 2+	☐ 3+
x	☐ +	☐ 2+	☐ 3+
y	☑ +	☑ 2+	☑ 3+
z	☐ +	☐ 2+	☐ 3+

hide H_2O/NH_3 ☐
zoom 112-122 ☐
zoom 124-133 ☐
GO

VHTECCHGDLLECADDR, MH+ 2403.6528, m/z 801.8891
10HNE-1HSA-37Trypsin5-LTQ4.5591.5591.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



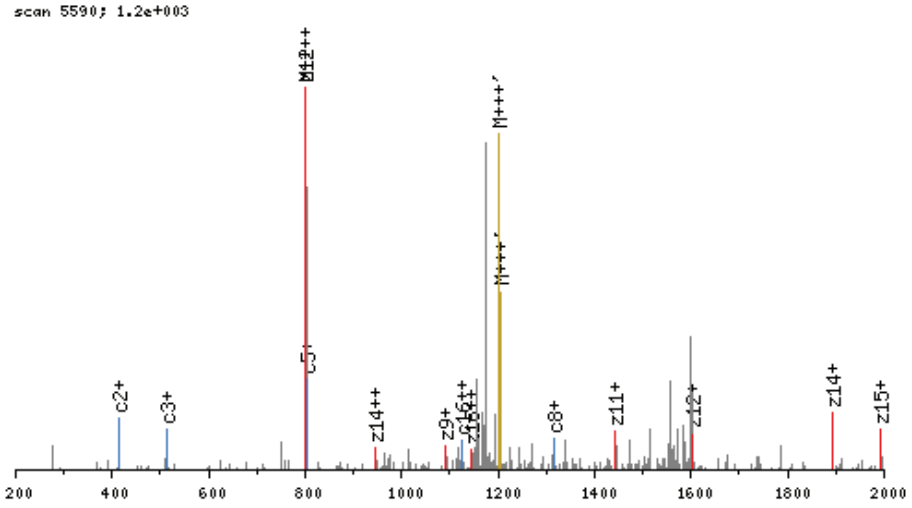
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
100.0762	50.5420	1	V	17			
395.3480	198.1779	2	H	16	2304.5844	1152.7961	**768.8667**
496.3957	248.7018	3	T	15	2009.3126	**1005.1602**	670.4427
625.4383	313.2231	4	E	14	1908.2649	**954.6364**	**636.7602**
785.5986	**393.3032**	5	C	13	1779.2223	**890.1151**	593.7460
945.7589	473.3834	6	C	12	1619.0620	810.0349	540.3592
1241.0307	**621.0192**	7	H	11	1458.9017	729.9548	486.9725
1298.0521	**649.5300**	8	G	10	**1163.6299**	582.3189	388.5485
1413.0791	**707.0435**	9	D	9	**1106.6085**	553.8081	369.5414
1526.1631	**763.5855**	10	L	8	**991.5815**	496.2947	331.1991
1639.2472	**820.1275**	11	L	7	**878.4975**	439.7526	293.5044
1768.2898	**884.6488**	12	E	6	**765.4134**	383.2106	255.8097
1928.4501	**964.7290**	13	C	5	**636.3708**	318.6893	212.7955
1999.4872	**1000.2475**	14	A	4	476.2105	238.6092	159.4087
2114.5142	**1057.7610**	15	D	3	405.1734	203.0906	135.7297
2229.5411	**1115.2745**	16	D	2	**290.1464**	145.5771	97.3874
		17	R	1	175.1195	88.0637	59.0451

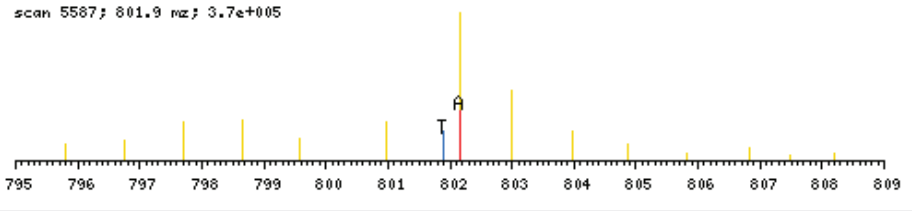
H(2):+295.27 C(5):+160.16 C(6):+160.16 H(7):+295.27
C(13):+160.16

X-range: 200 - 2000
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:
a [ ] + [ ] 2+ [ ] 3+
b [ ] + [ ] 2+ [ ] 3+
c [x] + [x] 2+ [ ] 3+
x [ ] + [ ] 2+ [ ] 3+
y [ ] + [ ] 2+ [ ] 3+
z [x] + [x] 2+ [x] 3+
hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

VHTECCHGDLLECADDR, MH+ 2403.6528, m/z 801.8891
10HNE-1HSA-37Trypsin5-LTQ4.5590.5590.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
117.1028	59.0553	1	V	17			
412.3746	206.6912	2	H	16	2288.5656	**1144.7867**	763.5271
513.4222	257.2150	3	T	15	**1993.2939**	997.1508	665.1032
642.4648	321.7363	4	E	14	**1892.2462**	**946.6270**	631.4206
802.6251	401.8165	5	C	13	1763.2036	882.1057	588.4064
962.7854	481.8966	6	C	12	**1603.0433**	**802.0256**	535.0196
1258.0572	629.5325	7	H	11	**1442.8830**	721.9454	481.6329
1315.0787	658.0433	8	G	10	1147.6112	574.3095	383.2090
1430.1056	715.5567	9	D	9	**1090.5897**	545.7988	364.2018
1543.1897	772.0988	10	L	8	975.5628	488.2853	325.8595
1656.2738	828.6408	11	L	7	862.4787	431.7433	288.1648
1785.3163	893.1621	12	E	6	749.3947	375.2012	250.4701
1945.4766	973.2422	13	C	5	620.3521	310.6800	207.4559
2016.5138	1008.7608	14	A	4	460.1918	230.5998	154.0691
2131.5407	1066.2743	15	D	3	389.1547	195.0812	130.3901
2246.5676	**1123.7877**	16	D	2	274.1277	137.5678	92.0478
		17	R	1	159.1008	80.0543	53.7055

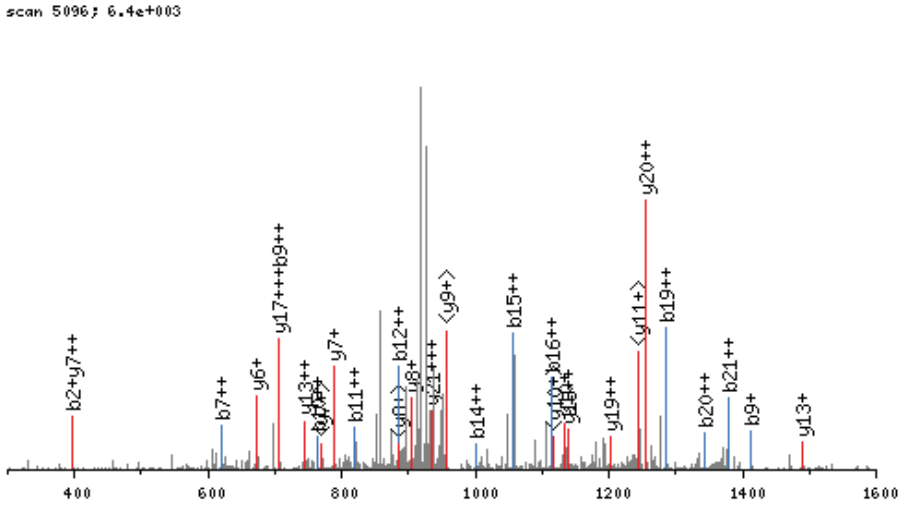
H(2):+295.27 C(5):+160.16 C(6):+160.16 H(7):+295.27
C(13):+160.16

X-range: 300 - 1600
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

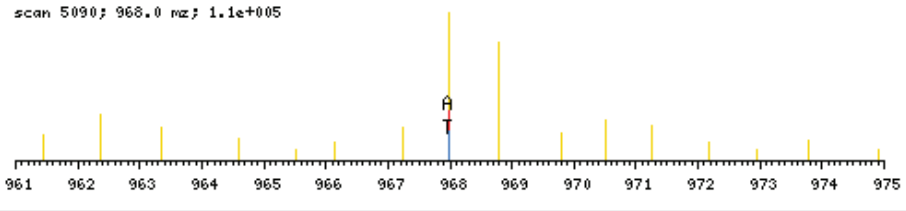
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

VHTECCHGDLLECADDRADLAK, MH+ 2901.9330, m/z 967.9825
10HNE-1HSA-37Trypsin4-LTQ3.5096.5096.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
100.0762	50.5420	1	V	22			
395.3480	198.1779	2	H	21	2802.8646	1401.9362	**934.9601**
496.3957	248.7018	3	T	20	2507.5928	**1254.3003**	836.5361
625.4383	313.2231	4	E	19	2406.5451	**1203.7765**	802.8536
785.5986	393.3032	5	C	18	2277.5025	**1139.2552**	759.8394
945.7589	473.3834	6	C	17	2117.3422	1059.1750	**706.4526**
1241.0307	**621.0192**	7	H	16	1957.1819	979.0949	653.0659
1298.0521	649.5300	8	G	15	1661.9101	831.4590	554.6419
1413.0791	**707.0435**	9	D	14	1604.8887	802.9482	535.6348
1526.1631	**763.5855**	10	L	13	**1489.8617**	**745.4348**	497.2925
1639.2472	**820.1275**	11	L	12	1376.7777	688.8927	459.5978
1768.2898	**884.6488**	12	E	11	1263.6936	632.3507	421.9031
1928.4501	964.7290	13	C	10	**1134.6510**	567.8294	378.8889
1999.4872	**1000.2475**	14	A	9	974.4907	487.7493	325.5021
2114.5142	**1057.7610**	15	D	8	**903.4536**	452.2307	301.8231
2229.5411	**1115.2745**	16	D	7	**788.4266**	**394.7172**	263.4808
2385.6422	1193.3250	17	R	6	**673.3997**	337.2038	225.1384
2456.6793	1228.8436	18	A	5	517.2986	259.1532	173.1047
2571.7063	**1286.3570**	19	D	4	446.2615	223.6346	149.4257
2684.7903	**1342.8991**	20	L	3	331.2345	166.1212	111.0834
2755.8274	**1378.4176**	21	A	2	218.1505	109.5791	73.3887
		22	K	1	147.1134	74.0606	49.7097

H(2):+295.27 C(5):+160.16 C(6):+160.16 H(7):+295.27
C(13):+160.16

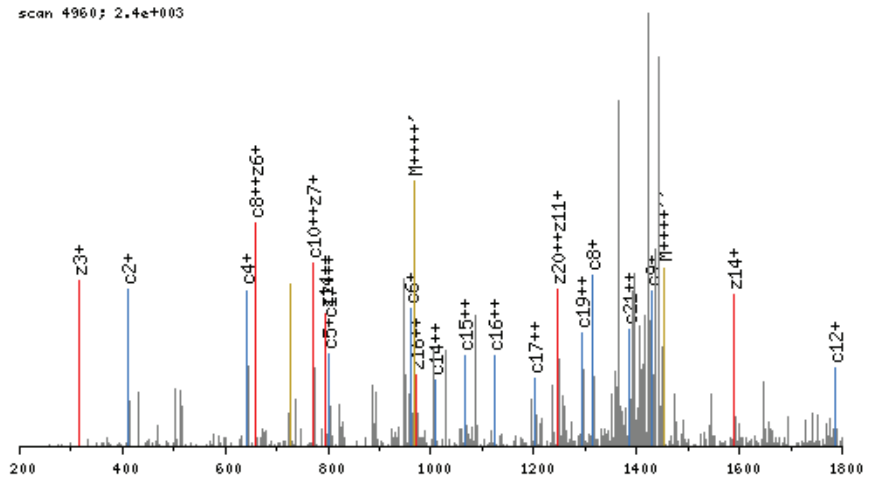
COMET Spectrum View by J.Eng (c) ISB 2001
(TPP v4.4 VUVUZELA rev 1, Build 201010121551 (MinGW))

X-range: 200 - 1800
MassTol: 0.950 Y-zoom: 2.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

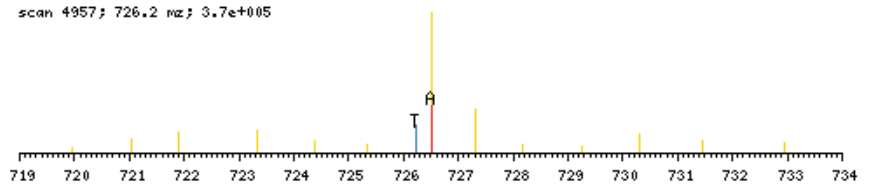
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

VHTECCHGDLLECADDRADLAK, MH+ 2901.9330, m/z 726.2387
10HNE-1HSA-37Trypsin3-LTQ1.4960.4960.4.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	c^{3+}	#	AA	#	z^+	z^{2+}	z^{3+}
117.1028	59.0553	39.7061	1	V	22			
412.3746	206.6912	138.1301	2	H	21	2786.8458	1393.9268	929.6205
513.4222	257.2150	171.8126	3	T	20	2491.5741	1246.2909	831.1966
642.4648	321.7363	214.8268	4	E	19	2390.5264	1195.7671	797.5140
802.6251	401.8165	268.2136	5	C	18	2261.4838	1131.2458	754.4998
962.7854	481.8966	321.6004	6	C	17	2101.3235	1051.1657	701.1130
1258.0572	629.5325	420.0243	7	H	16	1941.1632	971.0855	647.7263
1315.0787	658.0433	439.0314	8	G	15	1645.8914	823.4496	549.3024
1430.1056	715.5567	477.3738	9	D	14	1588.8699	794.9389	530.2952
1543.1897	772.0988	515.0684	10	L	13	1473.8430	737.4254	491.9529
1656.2738	828.6408	552.7631	11	L	12	1360.7589	680.8834	454.2582
1785.3163	893.1621	595.7773	12	E	11	1247.6749	624.3413	416.5635
1945.4766	973.2422	649.1641	13	C	10	1118.6323	559.8200	373.5493
2016.5138	1008.7608	672.8431	14	A	9	958.4720	479.7399	320.1625
2131.5407	1066.2743	711.1855	15	D	8	887.4349	444.2213	296.4835
2246.5676	1123.7877	749.5278	16	D	7	772.4079	386.7079	258.1412
2402.6688	1201.8383	801.5615	17	R	6	657.3810	329.1944	219.7989
2473.7059	1237.3568	825.2405	18	A	5	501.2799	251.1438	167.7652
2588.7328	1294.8703	863.5828	19	D	4	430.2427	215.6253	144.0861
2701.8169	1351.4124	901.2775	20	L	3	315.2158	158.1118	105.7438
2772.8540	1386.9309	924.9565	21	A	2	202.1317	101.5698	68.0491
			22	K	1	131.0946	66.0512	44.3701

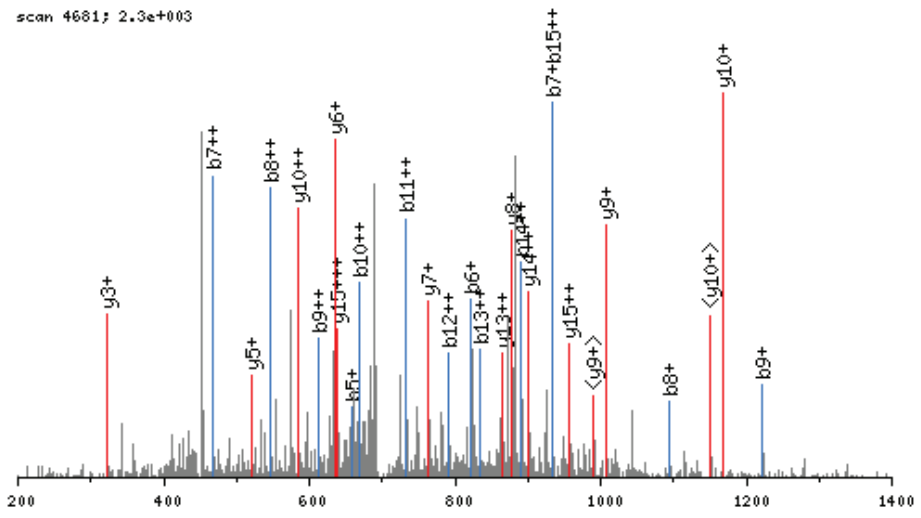
H(2):+295.27 C(5):+160.16 C(6):+160.16 H(7):+295.27 C(13):+160.16

X-range: 200 - 1400
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

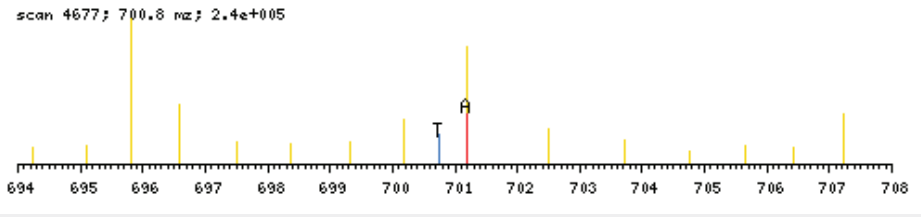
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

ADLAKYICENQDSISSK, MH+ 2100.2623, m/z 700.7589
10HNE-1HSA-37Trypsin5-LTQ3.4681.4681.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
72.0449	36.5264	1	A	17			
187.0719	94.0399	2	D	16	2029.2251	1015.1165	677.0803
300.1559	150.5819	3	L	15	1914.1982	**957.6030**	**638.7379**
371.1931	186.1004	4	A	14	1801.1141	**901.0610**	601.0433
657.4978	329.2528	5	K	13	1730.0770	**865.5424**	577.3642
820.5612	410.7845	6	Y	12	1443.7722	722.3900	481.9293
933.6452	**467.3265**	7	I	11	1280.7089	640.8584	427.5749
1093.8055	**547.4067**	8	C	10	**1167.6248**	**584.3163**	389.8802
1222.8481	**611.9280**	9	E	9	**1007.4645**	504.2362	336.4934
1336.8911	**668.9494**	10	N	8	**878.4220**	439.7149	293.4792
1464.9496	**732.9787**	11	Q	7	**764.3790**	382.6934	255.4649
1579.9766	**790.4922**	12	D	6	**636.3204**	318.6641	212.7787
1667.0086	**834.0082**	13	S	5	**521.2935**	261.1507	174.4364
1780.0927	**890.5502**	14	I	4	434.2615	217.6346	145.4257
1867.1247	**934.0663**	15	S	3	**321.1774**	161.0926	107.7310
1954.1567	977.5823	16	S	2	234.1454	117.5766	78.7203
		17	K	1	147.1134	74.0606	49.7097

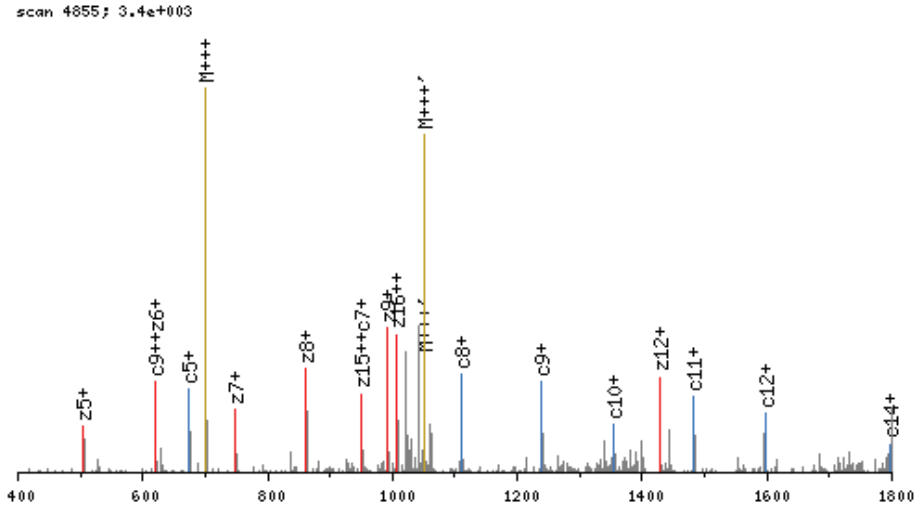
K(5):+286.30 C(8):+160.16

X-range: 400 - 1800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

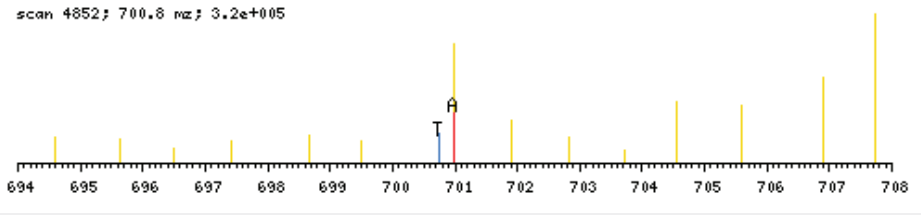
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

ADLAKYICENQDSISSK, MH+ 2100.2623, m/z 700.7589
10HNE-1HSA-37Trypsin3-LTQ2.4855.4855.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



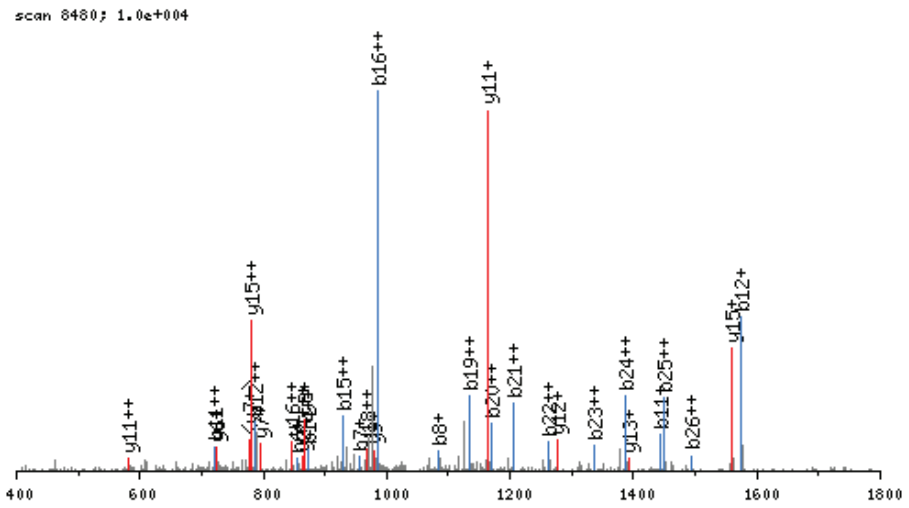
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
89.0715	45.0397	1	A	17			
204.0984	102.5531	2	D	16	2013.2064	**1007.1071**	671.7407
317.1825	159.0952	3	L	15	1898.1795	**949.5936**	633.3984
388.2196	194.6137	4	A	14	1785.0954	893.0516	595.7037
674.5244	337.7661	5	K	13	1714.0583	857.5331	572.0246
837.5877	419.2978	6	Y	12	**1427.7535**	714.3807	476.5897
950.6718	475.8398	7	I	11	1264.6902	632.8490	422.2353
1110.8321	555.9200	8	C	10	1151.6061	576.3070	384.5406
1239.8747	**620.4412**	9	E	9	**991.4458**	496.2268	331.1538
1353.9176	677.4627	10	N	8	**862.4032**	431.7055	288.1396
1481.9762	741.4920	11	Q	7	**748.3603**	374.6841	250.1253
1597.0031	799.0055	12	D	6	**620.3017**	310.6548	207.4391
1684.0352	842.5215	13	S	5	**505.2748**	253.1413	169.0968
1797.1192	899.0635	14	I	4	418.2427	209.6253	140.0861
1884.1512	942.5795	15	S	3	305.1587	153.0833	102.3914
1971.1833	986.0955	16	S	2	218.1267	109.5672	73.3808
		17	K	1	131.0946	66.0512	44.3701

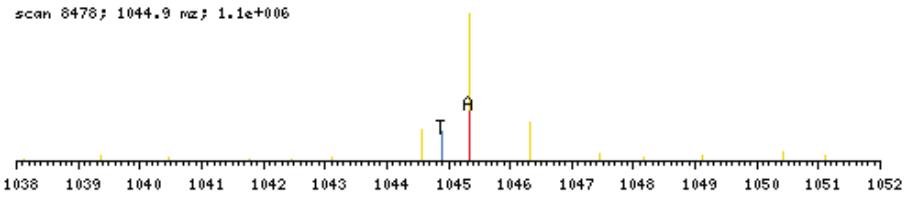
K(5):+286.30 C(8):+160.16

X-range: 400 - 1800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:
a [ ] + [ ] 2+ [ ] 3+
b [x] + [x] 2+ [ ] 3+
c [ ] + [ ] 2+ [ ] 3+
x [ ] + [ ] 2+ [ ] 3+
y [x] + [x] 2+ [x] 3+
z [ ] + [ ] 2+ [ ] 3+
hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

SHCIAEVENDEMPADLPSLAADFVESK, MH+ 3132.6875, m/z 1044.9007
10HNE-1HSA-37Trypsin5-LTQ4.8480.8480.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



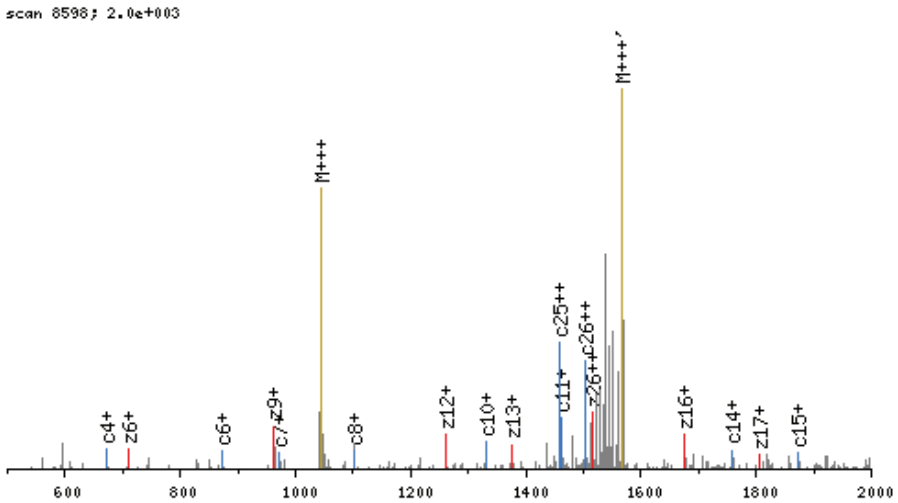
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
88.0399	44.5238	1	S	27			
383.3116	192.1597	2	H	26	3045.6555	1523.3317	1015.8904
543.4719	272.2399	3	C	25	2750.3837	1375.6958	917.4665
656.5560	328.7819	4	I	24	2590.2234	1295.6156	**864.0797**
727.5931	364.3005	5	A	23	2477.1394	1239.0736	826.3850
856.6357	428.8218	6	E	22	2406.1023	1203.5550	802.7060
955.7041	478.3560	7	V	21	2277.0597	1139.0337	759.6918
1084.7467	542.8773	8	E	20	2177.9913	1089.4995	726.6690
1198.7896	599.8987	9	N	19	2048.9487	1024.9782	683.6548
1313.8166	657.4122	10	D	18	1934.9057	**967.9568**	645.6405
1442.8592	**721.9335**	11	E	17	1819.8788	910.4433	607.2981
1573.8997	**787.4537**	12	M	16	1690.8362	**845.9220**	564.2839
1670.9524	835.9801	13	P	15	**1559.7957**	**780.4018**	520.6038
1741.9895	**871.4987**	14	A	14	1462.7430	731.8754	488.2529
1857.0165	**929.0122**	15	D	13	**1391.7058**	696.3568	464.5738
1970.1005	**985.5542**	16	L	12	**1276.6789**	638.8434	426.2315
2067.1533	1034.0806	17	P	11	**1163.5948**	**582.3013**	388.5368
2154.1853	1077.5966	18	S	10	1066.5421	533.7749	356.1859
2267.2694	**1134.1386**	19	L	9	**979.5100**	490.2589	327.1752
2338.3065	**1169.6572**	20	A	8	**866.4260**	433.7169	289.4805
2409.3436	**1205.1757**	21	A	7	**795.3889**	398.1983	265.8015
2524.3706	**1262.6892**	22	D	6	**724.3517**	362.6798	242.1225
2671.4390	**1336.2234**	23	F	5	609.3248	305.1663	203.7802
2770.5074	**1385.7576**	24	V	4	462.2564	231.6321	154.7573
2899.5500	**1450.2789**	25	E	3	363.1880	182.0979	121.7345
2986.5820	**1493.7949**	26	S	2	234.1454	117.5766	78.7203
		27	K	1	147.1134	74.0606	49.7097

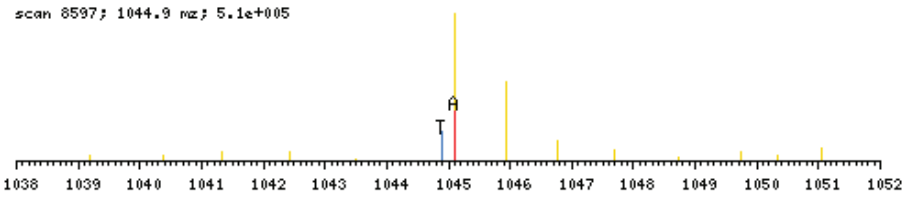
H(2):+295.27 C(3):+160.16

X-range: 500 - 2000
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

SHCIAEVENDEMPADLPSLAADFVESK, MH+ 3132.6875, m/z 1044.9007
10HNE-1HSA-37Trypsin5-LTQ4.8598.8598.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



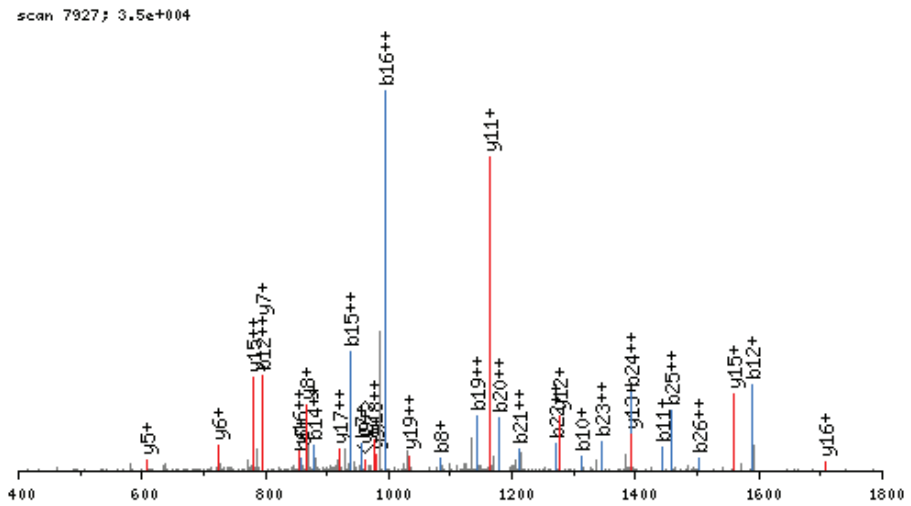
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
105.0664	53.0371	1	S	27			
400.3382	200.6730	2	H	26	3029.6368	1515.3223	1010.5508
560.4985	280.7532	3	C	25	2734.3650	1367.6864	912.1269
673.5825	337.2952	4	I	24	2574.2047	1287.6063	858.7401
744.6197	372.8137	5	A	23	2461.1207	1231.0642	821.0454
873.6623	437.3350	6	E	22	2390.0835	1195.5457	797.3664
972.7307	486.8692	7	V	21	2261.0409	1131.0244	754.3522
1101.7733	551.3905	8	E	20	2161.9725	1081.4902	721.3294
1215.8162	608.4120	9	N	19	2032.9299	1016.9689	678.3152
1330.8431	665.9255	10	D	18	1918.8870	959.9474	640.3009
1459.8857	730.4468	11	E	17	1803.8601	902.4339	601.9586
1590.9262	795.9670	12	M	16	1674.8175	837.9126	558.9444
1687.9790	844.4934	13	P	15	1543.7770	772.3924	515.2642
1759.0161	880.0120	14	A	14	1446.7242	723.8660	482.9133
1874.0430	937.5254	15	D	13	1375.6871	688.3475	459.2343
1987.1271	994.0675	16	L	12	1260.6602	630.8340	420.8919
2084.1799	1042.5938	17	P	11	1147.5761	574.2920	383.1973
2171.2119	1086.1099	18	S	10	1050.5233	525.7656	350.8463
2284.2960	1142.6519	19	L	9	963.4913	482.2496	321.8357
2355.3331	1178.1704	20	A	8	850.4072	425.7075	284.1410
2426.3702	1213.6890	21	A	7	779.3701	390.1890	260.4619
2541.3971	1271.2025	22	D	6	708.3330	354.6704	236.7829
2688.4655	1344.7367	23	F	5	593.3061	297.1570	198.4406
2787.5339	1394.2709	24	V	4	446.2377	223.6227	149.4178
2916.5765	1458.7922	25	E	3	347.1693	174.0885	116.3950
3003.6086	1502.3082	26	S	2	218.1267	109.5672	73.3808
		27	K	1	131.0946	66.0512	44.3701

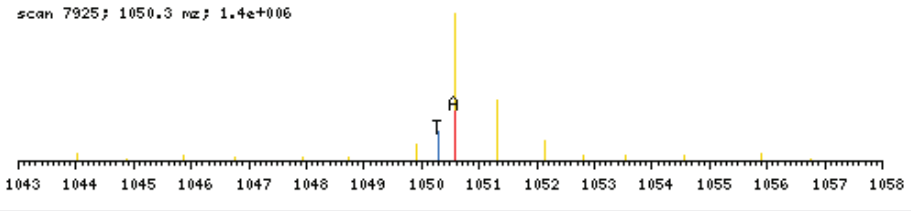
H(2):+295.27 C(3):+160.16

X-range: 400 - 1800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:
a [ ] + [ ] 2+ [ ] 3+
b [x] + [x] 2+ [ ] 3+
c [ ] + [ ] 2+ [ ] 3+
x [ ] + [ ] 2+ [ ] 3+
y [x] + [x] 2+ [x] 3+
z [ ] + [ ] 2+ [ ] 3+
hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

SHCIAEVENDEMPADLPSLAADFVESK, MH+ 3148.8346, m/z 1050.2830
10HNE-1HSA-37Trypsin5-LTQ4.7927.7927.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
88.0399	44.5238	1	S	27			
383.3116	192.1597	2	H	26	3061.8026	1531.4052	1021.2727
543.4719	272.2399	3	C	25	2766.5308	1383.7693	922.8488
656.5560	328.7819	4	I	24	2606.3705	1303.6891	869.4620
727.5931	364.3005	5	A	23	2493.2864	1247.1471	831.7674
856.6357	428.8218	6	E	22	2422.2493	1211.6286	808.0883
955.7041	478.3560	7	V	21	2293.2067	1147.1073	765.0741
1084.7467	542.8773	8	E	20	2194.1383	1097.5731	732.0513
1198.7896	599.8987	9	N	19	2065.0957	1033.0518	689.0371
1313.8166	657.4122	10	D	18	1951.0528	976.0303	651.0228
1442.8592	721.9335	11	E	17	1836.0258	918.5168	612.6805
1590.0467	795.5273	12	M	16	1706.9832	853.9955	569.6663
1687.0995	844.0536	13	P	15	1559.7957	780.4018	520.6038
1758.1366	879.5722	14	A	14	1462.7430	731.8754	488.2529
1873.1635	937.0857	15	D	13	1391.7058	696.3568	464.5738
1986.2476	993.6277	16	L	12	1276.6789	638.8434	426.2315
2083.3003	1042.1541	17	P	11	1163.5948	582.3013	388.5368
2170.3324	1085.6701	18	S	10	1066.5421	533.7749	356.1859
2283.4164	1142.2121	19	L	9	979.5100	490.2589	327.1752
2354.4535	1177.7307	20	A	8	866.4260	433.7169	289.4805
2425.4907	1213.2492	21	A	7	795.3889	398.1983	265.8015
2540.5176	1270.7627	22	D	6	724.3517	362.6798	242.1225
2687.5860	1344.2969	23	F	5	609.3248	305.1663	203.7802
2786.6544	1393.8311	24	V	4	462.2564	231.6321	154.7573
2915.6970	1458.3524	25	E	3	363.1880	182.0979	121.7345
3002.7291	1501.8684	26	S	2	234.1454	117.5766	78.7203
		27	K	1	147.1134	74.0606	49.7097

H(2):+295.27 C(3):+160.16 M(12):+147.19

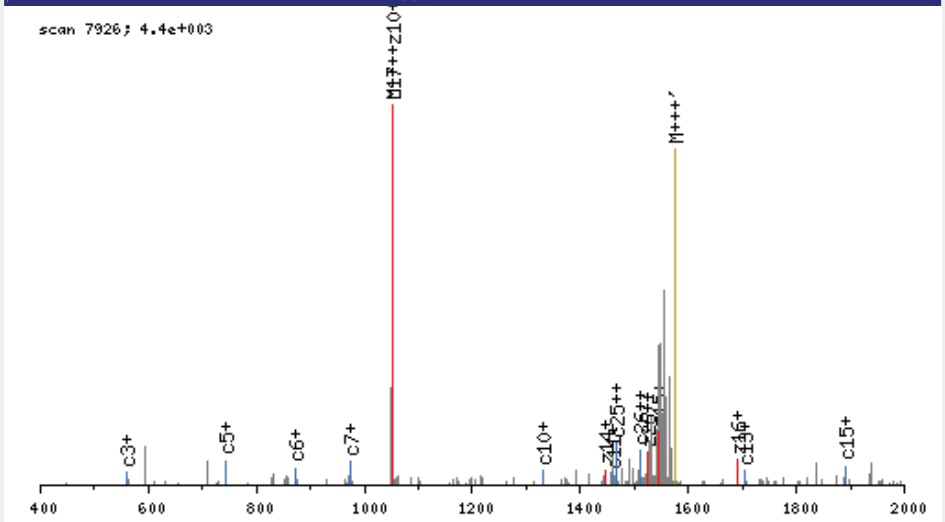
COMET Spectrum View by J.Eng (c) ISB 2001
(TPP v4.4 VUVUZELA rev 1, Build 201010121551 (MinGW))

X-range: 400 - 2000
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

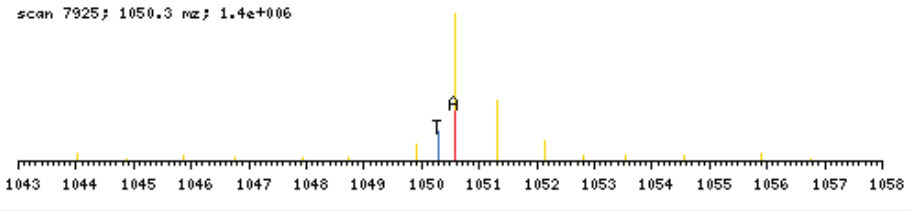
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

SHCIAEVENDEMPADLPSLAADFVESK, MH+ 3148.8346, m/z 1050.2830
10HNE-1HSA-37Trypsin5-LTQ4.7926.7926.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
105.0664	53.0371	1	S	27			
400.3382	200.6730	2	H	26	3045.7838	1523.3958	1015.9332
560.4985	280.7532	3	C	25	2750.5120	1375.7599	917.5092
673.5825	337.2952	4	I	24	2590.3517	1295.6798	864.1225
744.6197	372.8137	5	A	23	2477.2677	1239.1378	826.4278
873.6623	437.3350	6	E	22	2406.2306	1203.6192	802.7487
972.7307	486.8692	7	V	21	2277.1880	1139.0979	759.7345
1101.7733	551.3905	8	E	20	2178.1196	1089.5637	726.7117
1215.8162	608.4120	9	N	19	2049.0770	1025.0424	683.6975
1330.8431	665.9255	10	D	18	1935.0340	968.0209	645.6832
1459.8857	730.4468	11	E	17	1820.0071	910.5075	607.3409
1607.0732	804.0405	12	M	16	1690.9645	845.9862	564.3267
1704.1260	852.5669	13	P	15	1543.7770	772.3924	515.2642
1775.1631	888.0855	14	A	14	1446.7242	723.8660	482.9133
1890.1901	945.5989	15	D	13	1375.6871	688.3475	459.2343
2003.2741	1002.1410	16	L	12	1260.6602	630.8340	420.8919
2100.3269	1050.6674	17	P	11	1147.5761	574.2920	383.1973
2187.3589	1094.1834	18	S	10	1050.5233	525.7656	350.8463
2300.4430	1150.7254	19	L	9	963.4913	482.2496	321.8357
2371.4801	1186.2440	20	A	8	850.4072	425.7075	284.1410
2442.5172	1221.7625	21	A	7	779.3701	390.1890	260.4619
2557.5442	1279.2760	22	D	6	708.3330	354.6704	236.7829
2704.6126	1352.8102	23	F	5	593.3061	297.1570	198.4406
2803.6810	1402.3444	24	V	4	446.2377	223.6227	149.4178
2932.7236	1466.8657	25	E	3	347.1693	174.0885	116.3950
3019.7556	1510.3817	26	S	2	218.1267	109.5672	73.3808
		27	K	1	131.0946	66.0512	44.3701

H(2):+295.27 C(3):+160.16 M(12):+147.19

COMET Spectrum View by J.Eng (c) ISB 2001
(TPP v4.4 VUVUZELA rev 1, Build 201010121551 (MinGW))

X-range: 0 - 0

MassTol: 0.950 Y-zoom: 1.00

ImageSize: Sm Lg

MassType: AVG MONO

Axis: 1 2

Label: I M -

Ions:

a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

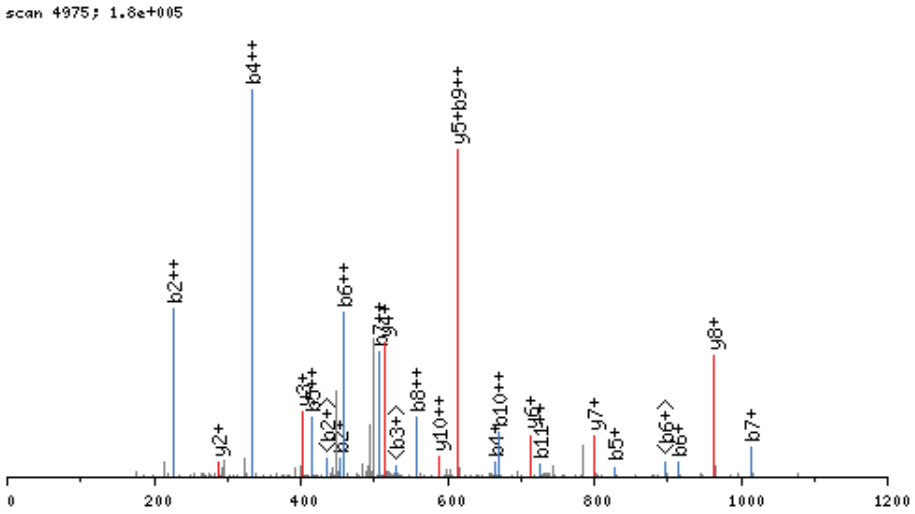
hide H_2O/NH_3

zoom 112-122

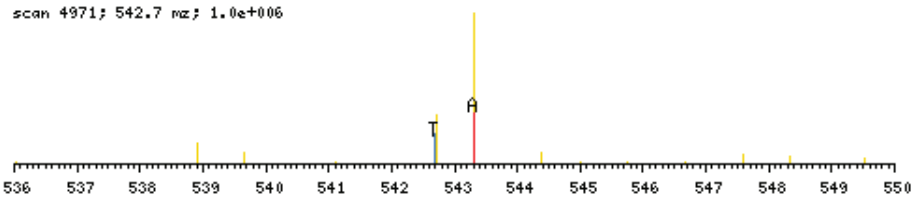
zoom 124-133

GO

RHPDYSVVLLLR, MH+ 1626.0565, m/z 542.6903
10HNE-1HSA-37Trypsin5-LTQ3.4975.4975.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
157.1089	79.0584	1	R	12			
452.3807	226.6943	2	H	11	1469.9554	735.4816	490.6570
549.4335	275.2207	3	P	10	1174.6836	587.8457	392.2331
664.4604	332.7341	4	D	9	1077.6308	539.3193	359.8822
827.5238	414.2658	5	Y	8	962.6039	481.8059	321.5398
914.5558	457.7818	6	S	7	799.5405	400.2742	267.1854
1013.6242	507.3160	7	V	6	712.5085	356.7582	238.1747
1112.6926	556.8502	8	V	5	613.4401	307.2240	205.1519
1225.7767	613.3922	9	L	4	514.3717	257.6898	172.1291
1338.8607	669.9343	10	L	3	401.2876	201.1477	134.4344
1451.9448	726.4763	11	L	2	288.2036	144.6057	96.7397
		12	R	1	175.1195	88.0637	59.0451

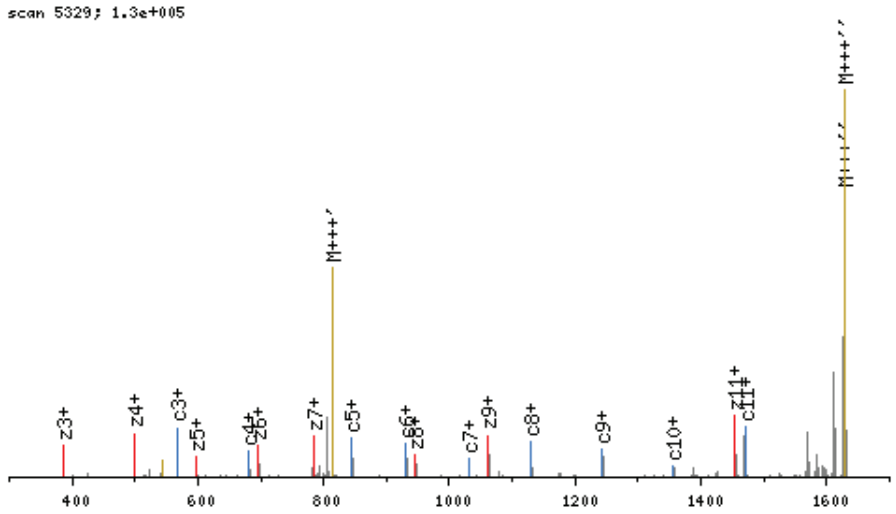
H(2):+295.27

X-range: 300 - 1700
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

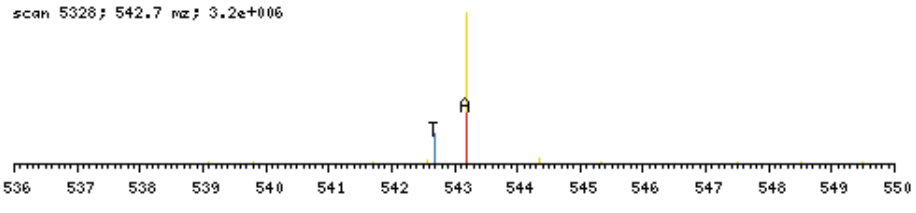
a	[ ] +	[ ] 2+	[ ] 3+
b	[ ] +	[ ] 2+	[ ] 3+
c	[x] +	[x] 2+	[ ] 3+
x	[ ] +	[ ] 2+	[ ] 3+
y	[ ] +	[ ] 2+	[ ] 3+
z	[x] +	[x] 2+	[x] 3+

hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

RHPDYSVVLLLR, MH+ 1626.0565, m/z 542.6903
10HNE-1HSA-37Trypsin3-LTQ3.5329.5329.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



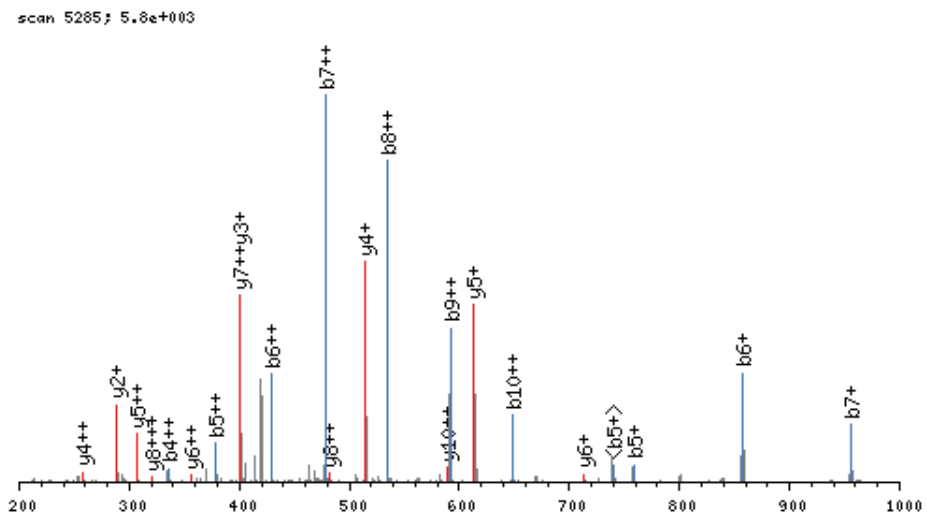
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
174.1355	87.5717	1	R	12			
469.4073	235.2075	2	H	11	1453.9366	727.4722	485.3174
566.4600	283.7339	3	P	10	1158.6649	579.8363	386.8935
681.4870	341.2474	4	D	9	1061.6121	531.3100	354.5426
844.5503	422.7791	5	Y	8	946.5852	473.7965	316.2003
931.5823	466.2951	6	S	7	783.5218	392.2648	261.8458
1030.6507	515.8293	7	V	6	696.4898	348.7488	232.8351
1129.7192	565.3635	8	V	5	597.4214	299.2146	199.8123
1242.8032	621.9055	9	L	4	498.3530	249.6804	166.7895
1355.8873	678.4476	10	L	3	385.2689	193.1384	129.0949
1468.9713	734.9896	11	L	2	272.1848	136.5963	91.4002
		12	R	1	159.1008	80.0543	53.7055

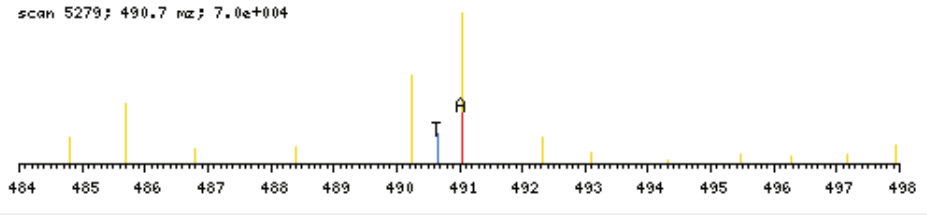
H(2):+295.27

X-range: 200 - 1000
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

HPDYSVVLLLR, MH+ 1469.9554, m/z 490.6566
10HNE-1HSA-37Trypsin4-LTQ1.5285.5285.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
296.2796	148.6437	1	H	11			
393.3324	197.1701	2	P	10	1174.6836	**587.8457**	392.2331
508.3593	254.6836	3	D	9	1077.6308	539.3193	359.8822
671.4226	**336.2152**	4	Y	8	962.6039	**481.8059**	**321.5398**
758.4547	**379.7312**	5	S	7	799.5405	**400.2742**	267.1854
857.5231	**429.2655**	6	V	6	**712.5085**	**356.7582**	238.1747
956.5915	**478.7997**	7	V	5	**613.4401**	**307.2240**	205.1519
1069.6756	**535.3417**	8	L	4	**514.3717**	**257.6898**	172.1291
1182.7596	**591.8837**	9	L	3	**401.2876**	201.1477	134.4344
1295.8437	**648.4258**	10	L	2	**288.2036**	144.6057	96.7397
		11	R	1	175.1195	88.0637	59.0451

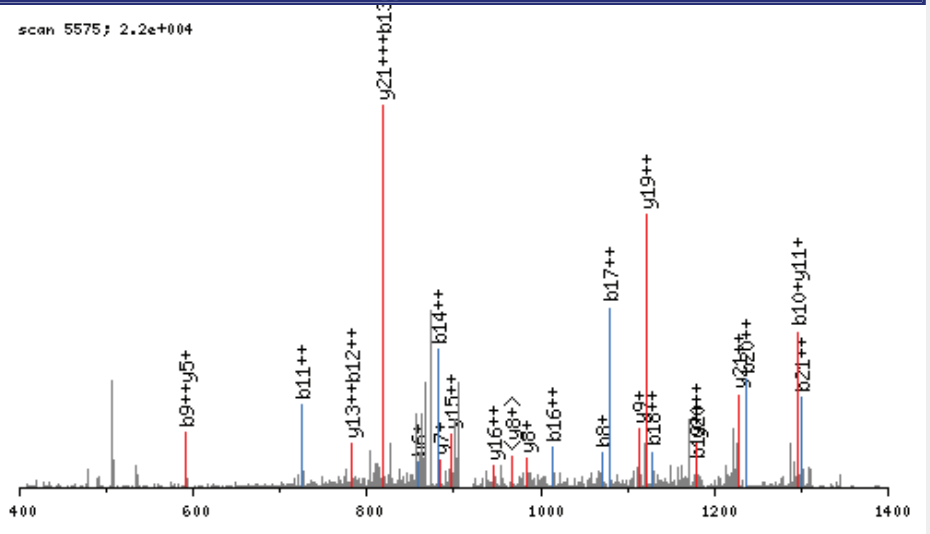
H(1):+295.27

X-range: 400 - 1400
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

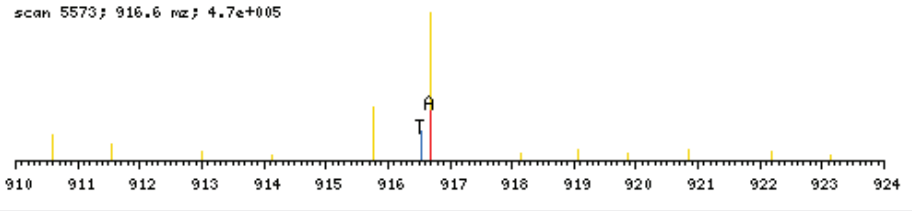
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

HPDYSVVLLLRLAKTYETTLEK, MH+ 2747.6421, m/z 916.5522
10HNE-1HSA-37Trypsin5-LTQ1.5575.5575.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
296.2796	148.6437	1	H	22			
393.3324	197.1701	2	P	21	2452.3703	**1226.6891**	**818.1287**
508.3593	254.6836	3	D	20	2355.3175	**1178.1627**	785.7777
671.4226	336.2152	4	Y	19	2240.2906	**1120.6492**	747.4354
758.4547	379.7312	5	S	18	2077.2273	1039.1175	693.0810
857.5231	429.2655	6	V	17	1990.1952	995.6015	664.0703
956.5915	478.7997	7	V	16	1891.1268	**946.0673**	631.0475
1069.6756	535.3417	8	L	15	1792.0584	**896.5331**	598.0247
1182.7596	**591.8837**	9	L	14	1678.9743	839.9911	560.3300
1295.8437	648.4258	10	L	13	1565.8903	**783.4491**	522.6353
1451.9448	**726.4763**	11	R	12	1452.8062	726.9070	484.9406
1565.0289	**783.0183**	12	L	11	**1296.7051**	648.8565	432.9069
1636.0660	**818.5369**	13	A	10	1183.6210	592.3144	395.2122
1764.1609	**882.5844**	14	K	9	**1112.5839**	556.7959	371.5332
1865.2086	933.1082	15	T	8	**984.4890**	492.7484	328.8349
2028.2719	**1014.6399**	16	Y	7	**883.4413**	442.2246	295.1523
2157.3145	**1079.1612**	17	E	6	720.3780	360.6929	240.7979
2258.3622	**1129.6850**	18	T	5	**591.3354**	296.1716	197.7837
2359.4099	**1180.2089**	19	T	4	490.2877	245.6478	164.1011
2472.4940	**1236.7509**	20	L	3	389.2400	195.1239	130.4186
2601.5366	**1301.2722**	21	E	2	276.1559	138.5819	92.7239
		22	K	1	147.1134	74.0606	49.7097

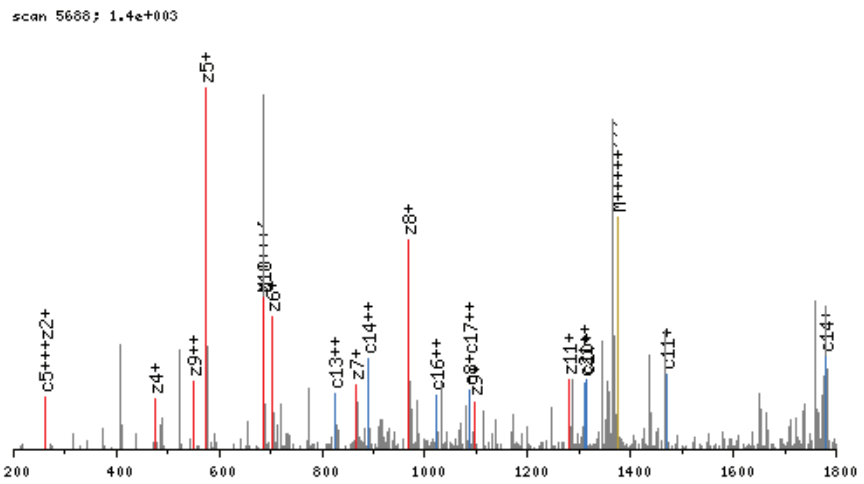
H(1):+295.27

X-range: 200 - 1800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

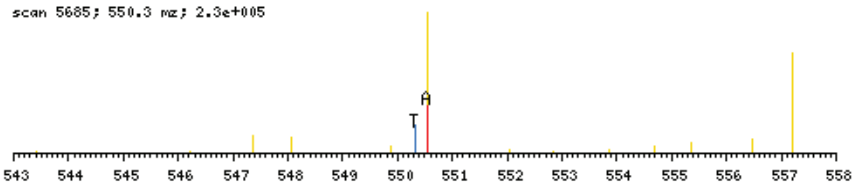
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

HPDYSVVLLLRLAKTYETTLEK, MH+ 2747.6421, m/z 550.3342
1HNE-1HSA-37Trypsin4-LTQ2.5688.5688.5.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

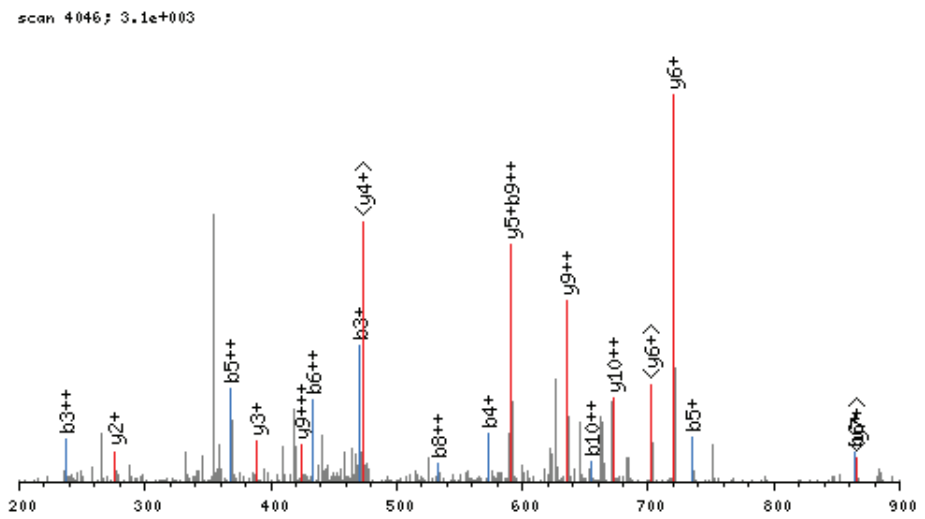
c^+	c^{2+}	c^{3+}	#	AA	#	z^+	z^{2+}	z^{3+}
313.3062	157.1570	105.1073	1	H	22			
410.3589	205.6834	137.4582	2	P	21	2436.3516	1218.6797	812.7891
525.3859	263.1968	175.8005	3	D	20	2339.2988	1170.1533	780.4382
688.4492	344.7285	230.1549	4	Y	19	2224.2719	1112.6398	742.0958
775.4812	388.2445	**259.1656**	5	S	18	2061.2085	1031.1082	**687.7414**
874.5496	437.7787	292.1884	6	V	17	1974.1765	987.5922	658.7307
973.6180	487.3129	325.2112	7	V	16	1875.1081	938.0580	625.7079
1086.7021	543.8550	362.9059	8	L	15	1776.0397	888.5238	592.6851
1199.7862	600.3970	400.6006	9	L	14	1662.9556	831.9817	554.9904
1312.8702	656.9390	438.2953	10	L	13	1549.8716	775.4397	517.2957
1468.9713	734.9896	490.3290	11	R	12	1436.7875	718.8977	479.6010
1582.0554	791.5316	528.0237	12	L	11	**1280.6864**	640.8471	427.5673
1653.0925	**827.0502**	551.7027	13	A	10	1167.6023	584.3051	389.8727
1781.1875	**891.0977**	594.4010	14	K	9	**1096.5652**	**548.7865**	366.1936
1882.2352	941.6215	628.0836	15	T	8	**968.4702**	484.7390	323.4953
2045.2985	**1023.1532**	682.4380	16	Y	7	**867.4226**	434.2152	289.8127
2174.3411	**1087.6745**	725.4522	17	E	6	**704.3592**	352.6835	235.4583
2275.3888	1138.1983	759.1348	18	T	5	**575.3166**	288.1622	192.4441
2376.4364	1188.7221	792.8174	19	T	4	**474.2690**	237.6384	158.7615
2489.5205	1245.2642	830.5121	20	L	3	373.2213	187.1146	125.0790
2618.5631	**1309.7855**	873.5263	21	E	2	**260.1372**	130.5725	87.3843
			22	K	1	131.0946	66.0512	44.3701

H(1):+295.27

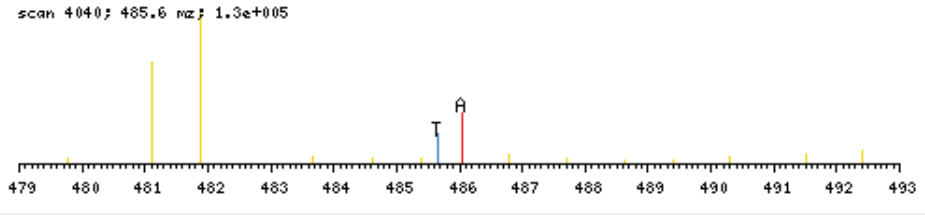
COMET Spectrum View by J.Eng (c) ISB 2001
(TPP v4.4 VUVUZELA rev 1, Build 201010121551 (MinGW))

X-range: 200 - 900
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

LAKTYETTLEK, MH+ 1454.9149, m/z 485.6432
1HNE-1HSA-37Trypsin5-LTQ1.4046.4046.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



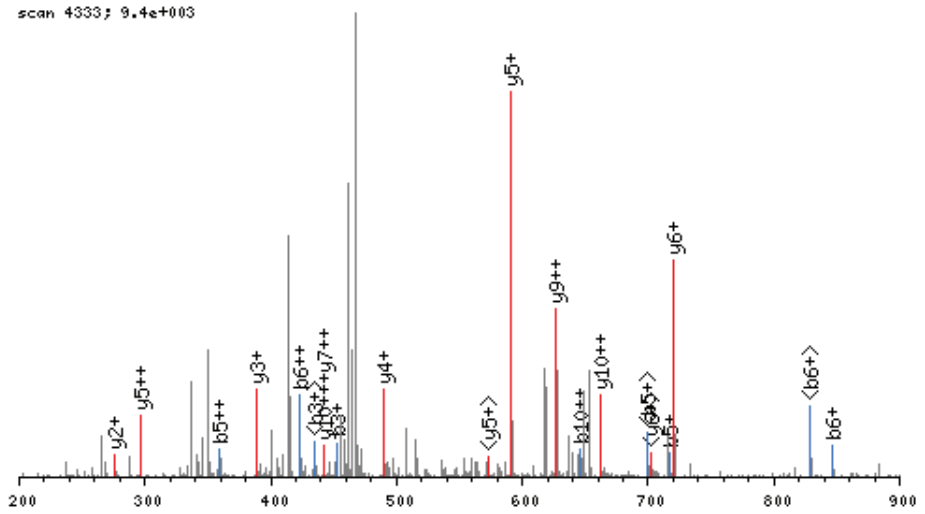
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
114.0919	57.5499	1	L	11			
185.1290	93.0684	2	A	10	1341.8309	671.4193	447.9488
471.4338	236.2208	3	K	9	1270.7937	635.9008	424.2698
572.4815	286.7446	4	T	8	984.4890	492.7484	328.8349
735.5448	368.2763	5	Y	7	883.4413	442.2246	295.1523
864.5874	432.7976	6	E	6	720.3780	360.6929	240.7979
965.6351	483.3214	7	T	5	591.3354	296.1716	197.7837
1066.6827	533.8453	8	T	4	490.2877	245.6478	164.1011
1179.7668	590.3873	9	L	3	389.2400	195.1239	130.4186
1308.8094	654.9086	10	E	2	276.1559	138.5819	92.7239
		11	K	1	147.1134	74.0606	49.7097

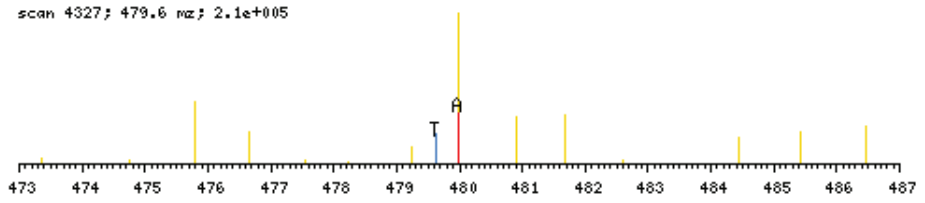
K(3):+286.30

X-range: 200 - 900
MassTol: 0.950 Y-zoom: 6.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

LAKTYETTLEK, MH+ 1436.9044, m/z 479.6396
10HNE-1HSA-37Trypsin3-LTQ2.4333.4333.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
114.0919	57.5499	1	L	11			
185.1290	93.0684	2	A	10	1323.8203	**662.4141**	**441.9453**
453.4232	227.2155	3	K	9	1252.7832	**626.8955**	418.2663
554.4709	277.7394	4	T	8	984.4890	492.7484	328.8349
717.5342	**359.2710**	5	Y	7	883.4413	**442.2246**	295.1523
846.5768	**423.7923**	6	E	6	**720.3780**	360.6929	240.7979
947.6245	474.3162	7	T	5	**591.3354**	**296.1716**	197.7837
1048.6722	524.8400	8	T	4	**490.2877**	245.6478	164.1011
1161.7562	581.3820	9	L	3	**389.2400**	195.1239	130.4186
1290.7988	**645.9033**	10	E	2	**276.1559**	138.5819	92.7239
		11	K	1	147.1134	74.0606	49.7097

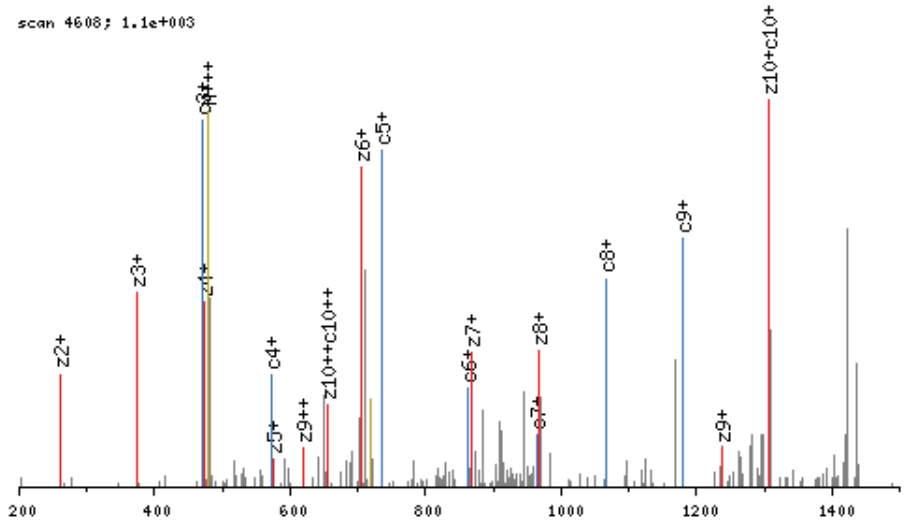
K(3):+268.29

X-range: 200 - 1500
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

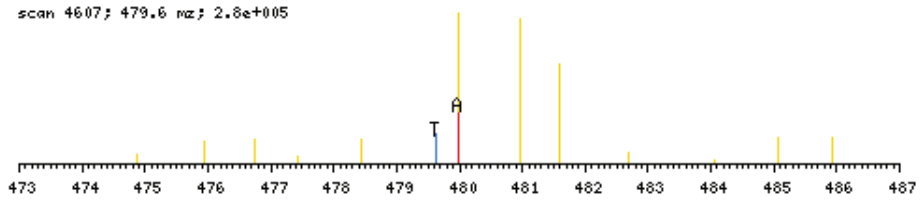
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

LAKTYETTLEK, MH+ 1436.9044, m/z 479.6396
10HNE-1HSA-37Trypsin5-LTQ4.4608.4608.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
131.1184	66.0631	1	L	11			
202.1556	101.5817	2	A	10	1307.8016	654.4047	436.6057
470.4498	235.7288	3	K	9	1236.7645	618.8861	412.9267
571.4974	286.2526	4	T	8	968.4702	484.7390	323.4953
734.5608	367.7843	5	Y	7	867.4226	434.2152	289.8127
863.6034	432.3056	6	E	6	704.3592	352.6835	235.4583
964.6510	482.8294	7	T	5	575.3166	288.1622	192.4441
1065.6987	533.3533	8	T	4	474.2690	237.6384	158.7615
1178.7828	589.8953	9	L	3	373.2213	187.1146	125.0790
1307.8254	654.4166	10	E	2	260.1372	130.5725	87.3843
		11	K	1	131.0946	66.0512	44.3701

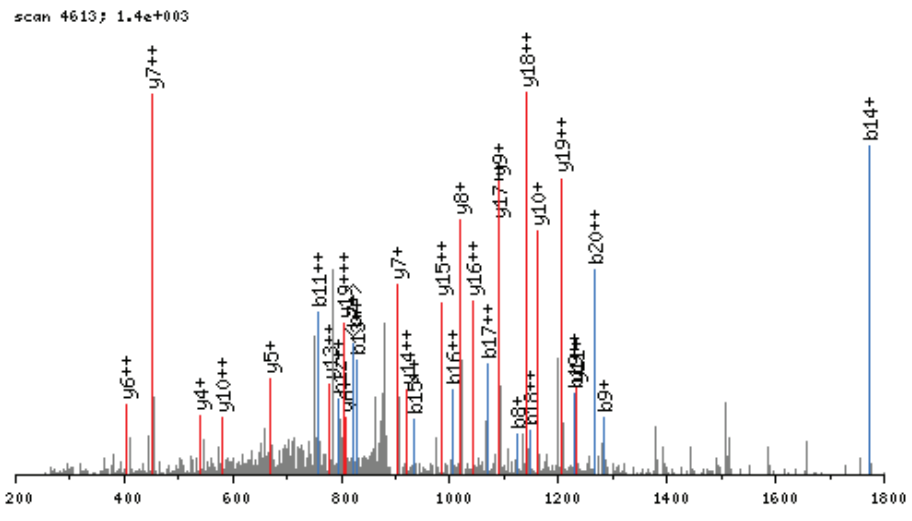
K(3):+268.29

X-range: 200 - 1800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

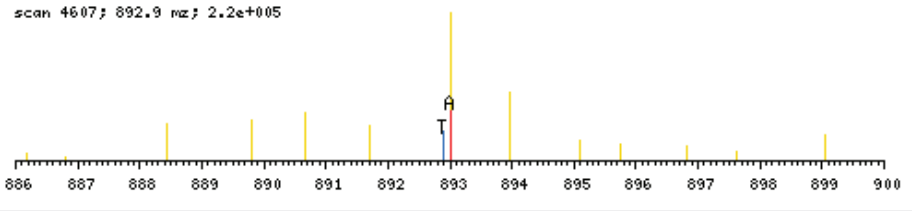
a	☐ +	☐ 2+	☐ 3+
b	☑ +	☑ 2+	☐ 3+
c	☐ +	☐ 2+	☐ 3+
x	☐ +	☐ 2+	☐ 3+
y	☑ +	☑ 2+	☑ 3+
z	☐ +	☐ 2+	☐ 3+

hide H_2O/NH_3 ☐
zoom 112-122 ☐
zoom 124-133 ☐
GO

TYETTLEKCCAAADPHECYAK, MH+ 2676.6676, m/z 892.8941
10HNE-1HSA-37Trypsin5-LTQ4.4613.4613.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
102.0555	51.5317	1	T	21			
265.1188	133.0633	2	Y	20	2575.6200	1288.3139	859.2119
394.1614	197.5846	3	E	19	2412.5566	**1206.7822**	**804.8574**
495.2091	248.1085	4	T	18	2283.5140	**1142.2609**	761.8432
596.2568	298.6323	5	T	17	2182.4664	**1091.7371**	728.1607
709.3408	355.1743	6	L	16	2081.4187	**1041.2133**	694.4781
838.3834	419.6956	7	E	15	1968.3346	**984.6712**	656.7834
1124.6882	562.8480	8	K	14	1839.2920	**920.1499**	613.7692
1284.8485	642.9282	9	C	13	1552.9872	**776.9975**	518.3343
1445.0088	723.0083	10	C	12	1392.8269	696.9174	464.9475
1516.0459	**758.5269**	11	A	11	**1232.6666**	616.8372	411.5608
1587.0830	**794.0454**	12	A	10	**1161.6295**	**581.3187**	387.8817
1658.1202	**829.5640**	13	A	9	**1090.5924**	545.8001	364.2027
1773.1471	887.0775	14	D	8	**1019.5553**	510.2816	340.5237
1870.1999	**935.6038**	15	P	7	**904.5284**	**452.7681**	302.1813
2007.2588	**1004.1333**	16	H	6	**807.4756**	**404.2417**	269.8304
2136.3014	**1068.6546**	17	E	5	**670.4167**	335.7123	224.1441
2296.4617	**1148.7347**	18	C	4	**541.3741**	271.1910	181.1299
2459.5250	**1230.2664**	19	Y	3	381.2138	191.1108	127.7431
2530.5621	**1265.7850**	20	A	2	218.1505	109.5791	73.3887
		21	K	1	147.1134	74.0606	49.7097

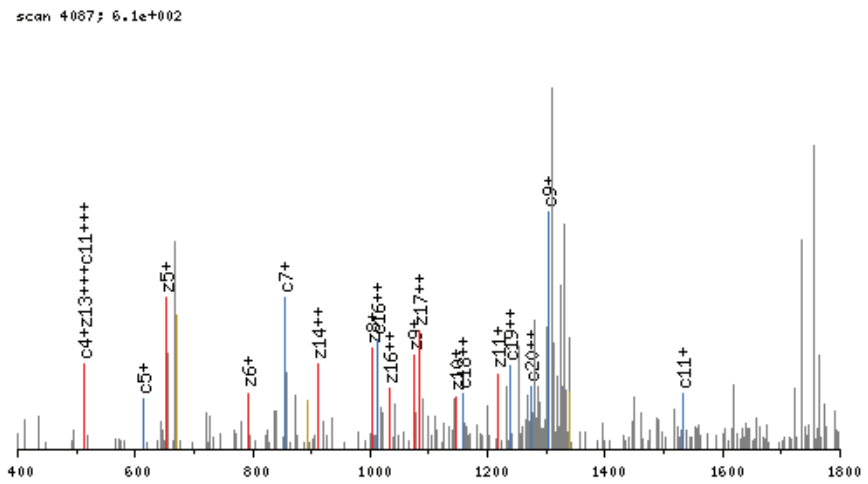
K(8):+286.30 C(9):+160.16 C(10):+160.16 C(18):+160.16

X-range: 400 - 1800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

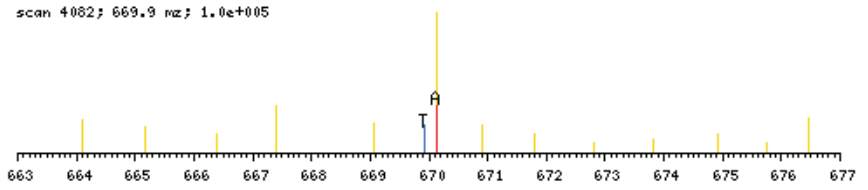
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

TYETTLEKCCAAADPHECYAK, MH+ 2676.6676, m/z 669.9224
10HNE-1HSA-37Trypsin3-LTQ3.4087.4087.4.dta



click image to zoom in; click top corners to zoom out [precursor±]



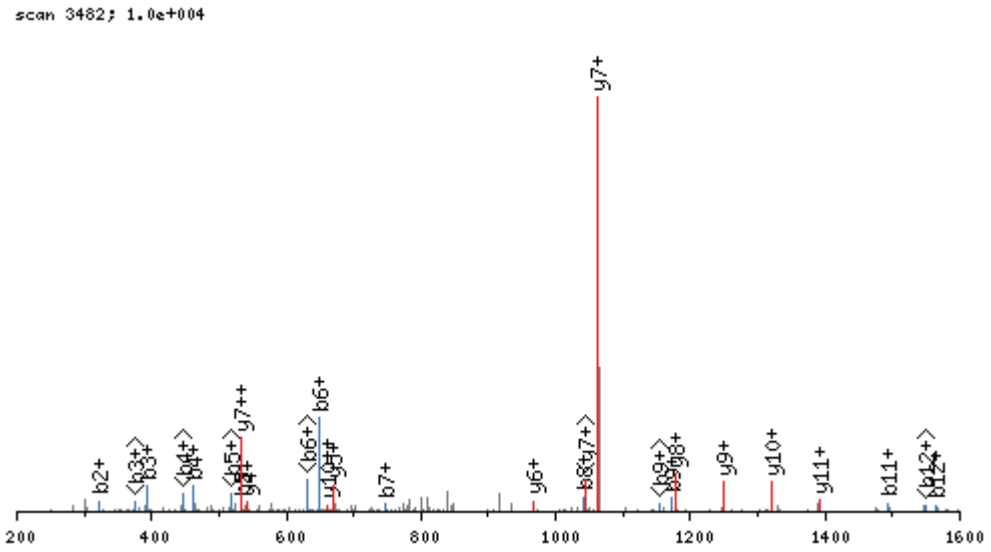
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	c^{3+}	#	AA	#	z^+	z^{2+}	z^{3+}
119.0821	60.0449	40.3659	1	T	21			
282.1454	141.5766	94.7203	2	Y	20	2559.6012	1280.3045	853.8723
411.1880	206.0979	137.7345	3	E	19	2396.5379	1198.7729	799.5179
512.2357	256.6217	171.4171	4	T	18	2267.4953	1134.2516	756.5037
613.2833	307.1456	205.0997	5	T	17	2166.4476	**1083.7277**	722.8211
726.3674	363.6876	242.7943	6	L	16	2065.4000	**1033.2039**	689.1385
855.4100	428.2089	285.8085	7	E	15	1952.3159	976.6619	651.4438
1141.7148	571.3613	381.2435	8	K	14	1823.2733	**912.1406**	608.4297
1301.8751	651.4414	434.6302	9	C	13	1536.9685	768.9882	**512.9947**
1462.0354	731.5216	488.0170	10	C	12	1376.8082	688.9080	459.6080
1533.0725	767.0402	**511.6960**	11	A	11	**1216.6479**	608.8279	406.2212
1604.1096	802.5587	535.3751	12	A	10	**1145.6108**	573.3093	382.5422
1675.1467	838.0773	559.0541	13	A	9	**1074.5737**	537.7908	358.8631
1790.1737	895.5907	597.3964	14	D	8	**1003.5366**	502.2722	335.1841
1887.2264	944.1171	629.7474	15	P	7	888.5096	444.7587	296.8418
2024.2853	**1012.6466**	675.4337	16	H	6	**791.4569**	396.2324	264.4908
2153.3279	1077.1679	718.4479	17	E	5	**654.3980**	327.7029	218.8045
2313.4882	**1157.2480**	771.8346	18	C	4	525.3554	263.1816	175.7903
2476.5516	**1238.7797**	826.1891	19	Y	3	365.1951	183.1014	122.4036
2547.5887	**1274.2982**	849.8681	20	A	2	202.1317	101.5698	68.0491
			21	K	1	131.0946	66.0512	44.3701

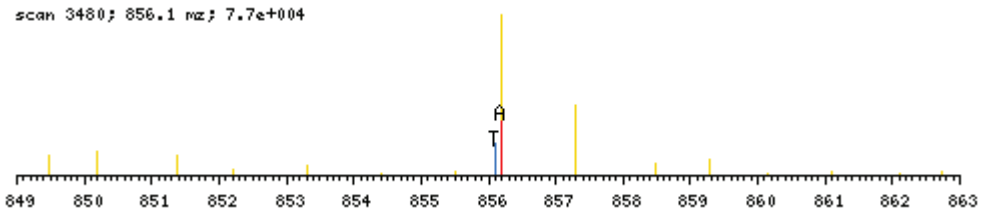
K(8):+286.30 C(9):+160.16 C(10):+160.16 C(18):+160.16

X-range: 200 - 1600
MassTol: Y-zoom: 0.950 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:
a [ ] + [ ] 2+ [ ] 3+
b [x] + [ ] 2+ [ ] 3+
c [ ] + [ ] 2+ [ ] 3+
x [ ] + [ ] 2+ [ ] 3+
y [x] + [x] 2+ [ ] 3+
z [ ] + [ ] 2+ [ ] 3+
hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

CCAAADPHECYAK, MH+ 1711.2001, m/z 856.1037
10HNE-1HSA-37Trypsin2-LTQ1.3482.3482.2.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	#	AA	#	y^+	y^{2+}
161.1681	1	C	13		
321.3284	2	C	12	1551.0398	776.0238
392.3655	3	A	11	1390.8795	695.9437
463.4027	4	A	10	1319.8424	660.4251
534.4398	5	A	9	1248.8053	624.9066
649.4667	6	D	8	1177.7682	589.3880
746.5195	7	P	7	1062.7412	531.8745
1041.7913	8	H	6	965.6885	483.3481
1170.8338	9	E	5	670.4167	335.7123
1330.9941	10	C	4	541.3741	271.1910
1494.0575	11	Y	3	381.2138	191.1108
1565.0946	12	A	2	218.1505	109.5791
	13	K	1	147.1134	74.0606

C(1):+160.16 C(2):+160.16 H(8):+295.27
C(10):+160.16

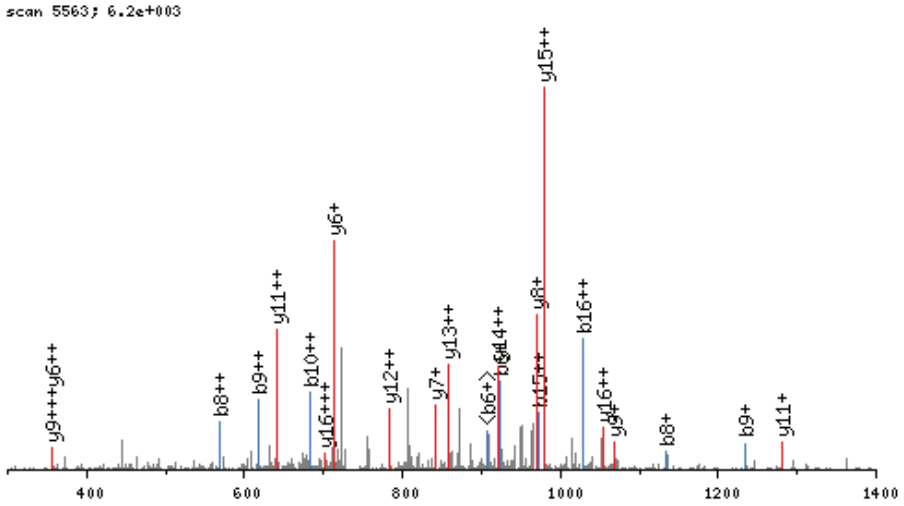
COMET Spectrum View by J.Eng (c) ISB 2001
(TPP v4.4 VUVUZELA rev 1, Build 201010121551 (MinGW))

X-range: 300 - 1400
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

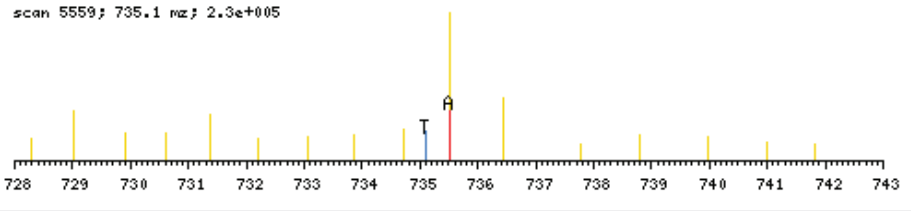
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

VFDEFKPLVEEPQNLIK, MH+ 2203.3057, m/z 735.1068
10HNE-1HSA-37Trypsin4-LTQ1.5563.5563.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
100.0762	50.5420	1	V	17			
247.1447	124.0762	2	F	16	2104.2373	**1052.6226**	**702.0843**
362.1716	181.5897	3	D	15	1957.1689	**979.0884**	653.0615
491.2142	246.1110	4	E	14	1842.1420	**921.5749**	614.7192
638.2826	319.6452	5	F	13	1713.0994	**857.0536**	571.7050
924.5874	462.7976	6	K	12	1566.0310	**783.5194**	522.6822
1021.6401	511.3240	7	P	11	**1279.7262**	**640.3670**	427.2473
1134.7242	**567.8660**	8	L	10	1182.6734	591.8406	394.8964
1233.7926	**617.4002**	9	V	9	**1069.5893**	535.2986	**357.2017**
1362.8352	**681.9215**	10	E	8	**970.5209**	485.7644	324.1789
1491.8778	746.4428	11	E	7	**841.4783**	421.2431	281.1647
1588.9306	794.9692	12	P	6	**712.4357**	**356.7218**	238.1505
1716.9892	858.9985	13	Q	5	615.3830	308.1954	205.7995
1831.0321	916.0200	14	N	4	487.3244	244.1661	163.1134
1944.1161	**972.5620**	15	L	3	373.2815	187.1447	125.0990
2057.2002	**1029.1040**	16	I	2	260.1974	130.6026	87.4044
		17	K	1	147.1134	74.0606	49.7097

K(6):+286.30

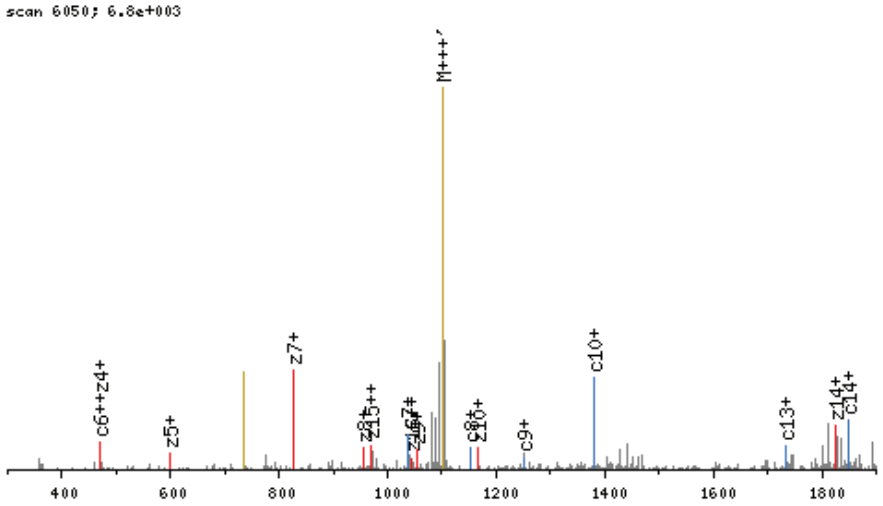
COMET Spectrum View by J.Eng (c) ISB 2001
(TPP v4.4 VUVUZELA rev 1, Build 201010121551 (MinGW))

X-range: 300 - 1900
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

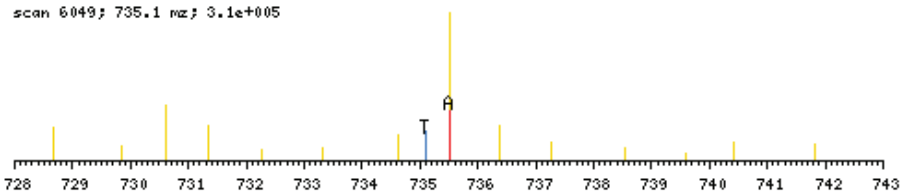
a	[ ] +	[ ] 2+	[ ] 3+
b	[ ] +	[ ] 2+	[ ] 3+
c	[x] +	[x] 2+	[ ] 3+
x	[ ] +	[ ] 2+	[ ] 3+
y	[ ] +	[ ] 2+	[ ] 3+
z	[x] +	[x] 2+	[x] 3+

hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

VFDEFKPLVEEPQNLIK, MH+ 2203.3057, m/z 735.1068
10HNE-1HSA-37Trypsin3-LTQ3.6050.6050.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
117.1028	59.0553	1	V	17			
264.1712	132.5895	2	F	16	2088.2186	**1044.6132**	696.7447
379.1981	190.1030	3	D	15	1941.1502	**971.0790**	647.7219
508.2407	254.6243	4	E	14	**1826.1232**	913.5655	609.3796
655.3092	328.1585	5	F	13	1697.0806	849.0442	566.3654
941.6139	**471.3109**	6	K	12	1550.0122	775.5100	517.3426
1038.6667	519.8373	7	P	11	1263.7075	632.3576	421.9077
1151.7508	576.3793	8	L	10	**1166.6547**	583.8313	389.5568
1250.8192	625.9135	9	V	9	**1053.5706**	527.2892	351.8621
1379.8618	690.4348	10	E	8	**954.5022**	477.7550	318.8393
1508.9044	754.9561	11	E	7	**825.4596**	413.2337	275.8251
1605.9571	803.4825	12	P	6	696.4170	348.7124	232.8109
1734.0157	867.5118	13	Q	5	**599.3643**	300.1860	200.4600
1848.0586	924.5332	14	N	4	**471.3057**	236.1568	157.7738
1961.1427	981.0753	15	L	3	357.2628	179.1353	119.7595
2074.2268	1037.6173	16	I	2	244.1787	122.5933	82.0648
		17	K	1	131.0946	66.0512	44.3701

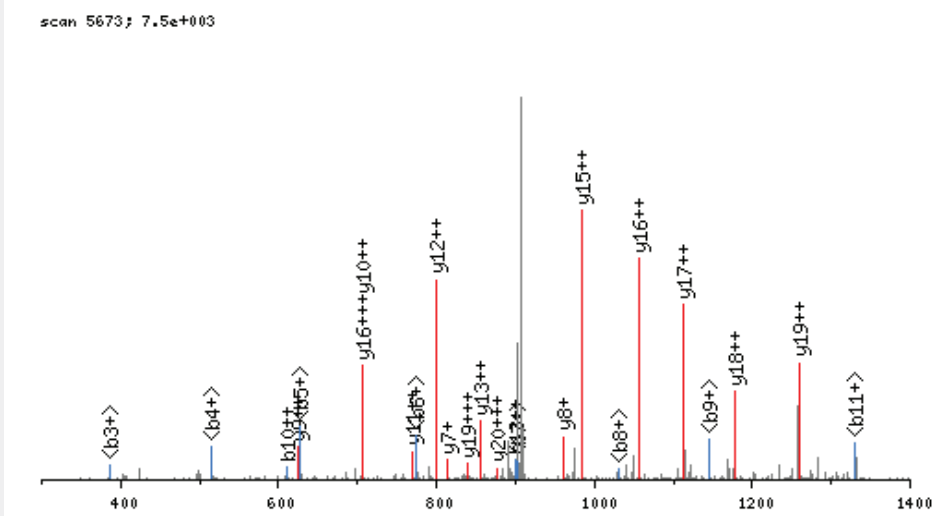
K(6):+286.30

X-range: 300 - 1400
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

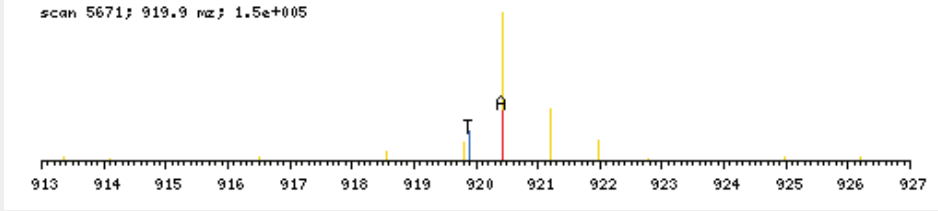
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

QNCELFEQLGEYKFQNALLVR, MH+ 2757.6374, m/z 919.8840
10HNE-1HSA-37Trypsin4-LTQ1.5673.5673.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



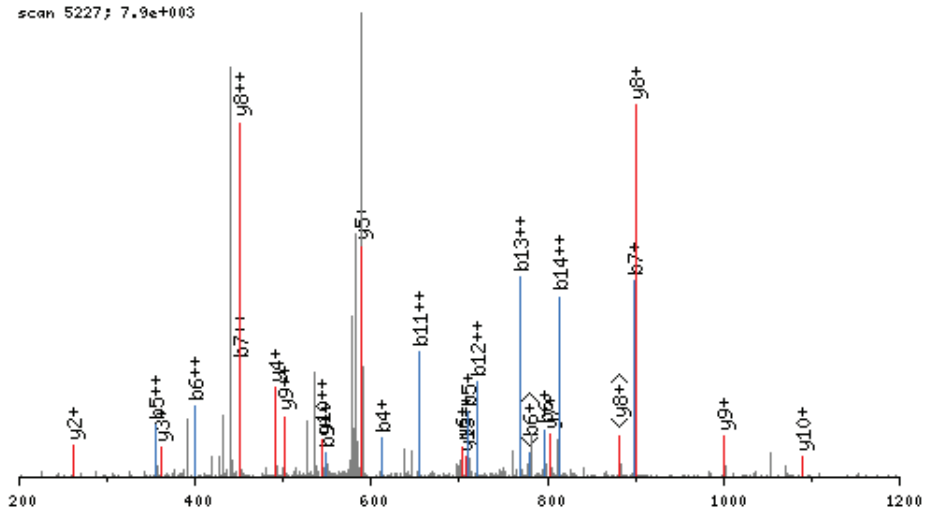
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
129.0664	65.0371	1	Q	21			
243.1093	122.0586	2	N	20	2629.5788	1315.2933	**877.1981**
403.2696	202.1387	3	C	19	2515.5358	**1258.2718**	**839.1838**
532.3122	266.6600	4	E	18	2355.3755	**1178.1917**	785.7971
645.3963	323.2021	5	L	17	2226.3330	**1113.6704**	742.7829
792.4647	396.7363	6	F	16	2113.2489	**1057.1284**	**705.0882**
921.5073	461.2576	7	E	15	1966.1805	**983.5942**	656.0654
1049.5659	525.2868	8	Q	14	1837.1379	919.0729	613.0512
1162.6499	581.8289	9	L	13	1709.0793	**855.0436**	570.3650
1219.6714	**610.3396**	10	G	12	1595.9952	**798.5015**	532.6703
1348.7140	674.8609	11	E	11	1538.9738	**769.9908**	513.6631
1511.7773	756.3926	12	Y	10	1409.9312	**705.4695**	470.6489
1798.0821	**899.5450**	13	K	9	1246.8679	**623.9378**	416.2945
1945.1505	973.0792	14	F	8	**960.5631**	480.7855	320.8596
2073.2091	1037.1085	15	Q	7	**813.4947**	407.2512	271.8368
2187.2520	1094.1299	16	N	6	685.4361	343.2220	229.1506
2258.2891	1129.6485	17	A	5	571.3932	286.2005	191.1363
2371.3732	1186.1905	18	L	4	500.3560	250.6819	167.4572
2484.4573	1242.7325	19	L	3	387.2720	194.1399	129.7625
2583.5257	1292.2668	20	V	2	274.1879	137.5979	92.0679
		21	R	1	175.1195	88.0637	59.0451

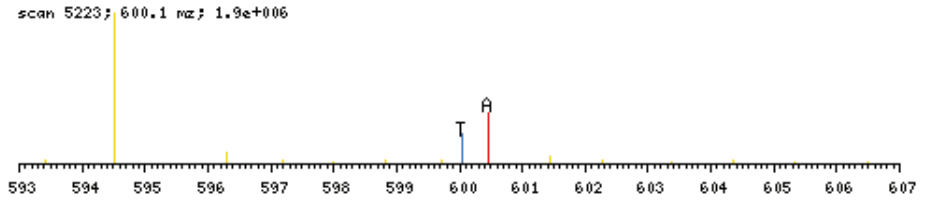
C(3):+160.16 K(13):+286.30

X-range: 200 - 1200
MassTol: 0.950 Y-zoom: 7.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

KVPQVSTPTLVEVSR, MH+ 1798.1481, m/z 600.0542
10HNE-1HSA-37Trypsin4-LTQ2.5227.5227.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
287.3126	144.1602	1	K	15			
386.3810	193.6944	2	V	14	1511.8433	756.4256	504.6197
483.4338	242.2208	3	P	13	1412.7749	706.8914	471.5969
611.4924	306.2501	4	Q	12	1315.7222	658.3650	439.2459
710.5608	355.7843	5	V	11	1187.6636	594.3357	396.5597
797.5928	399.3003	6	S	10	1088.5952	544.8015	363.5369
898.6405	449.8242	7	T	9	1001.5631	501.2855	334.5263
995.6932	498.3505	8	P	8	900.5155	450.7616	300.8437
1096.7409	548.8744	9	T	7	803.4627	402.2353	268.4928
1209.8250	605.4164	10	L	6	702.4150	351.7114	234.8102
1308.8934	654.9506	11	V	5	589.3310	295.1694	197.1155
1437.9360	719.4719	12	E	4	490.2625	245.6352	164.0927
1537.0044	769.0061	13	V	3	361.2199	181.1139	121.0785
1624.0364	812.5221	14	S	2	262.1515	131.5797	88.0557
		15	R	1	175.1195	88.0637	59.0451

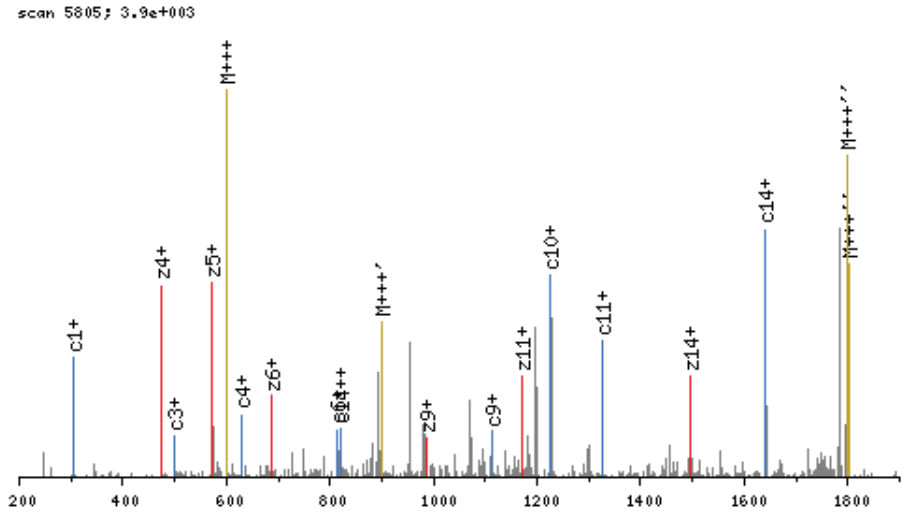
K(1):+286.30

X-range: 200 - 1900
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

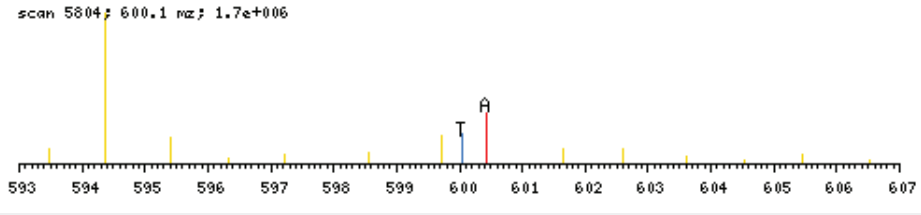
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

KVPQVSTPTLVEVSR, MH+ 1798.1481, m/z 600.0542
10HNE-1HSA-37Trypsin5-LTQ4.5805.5805.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



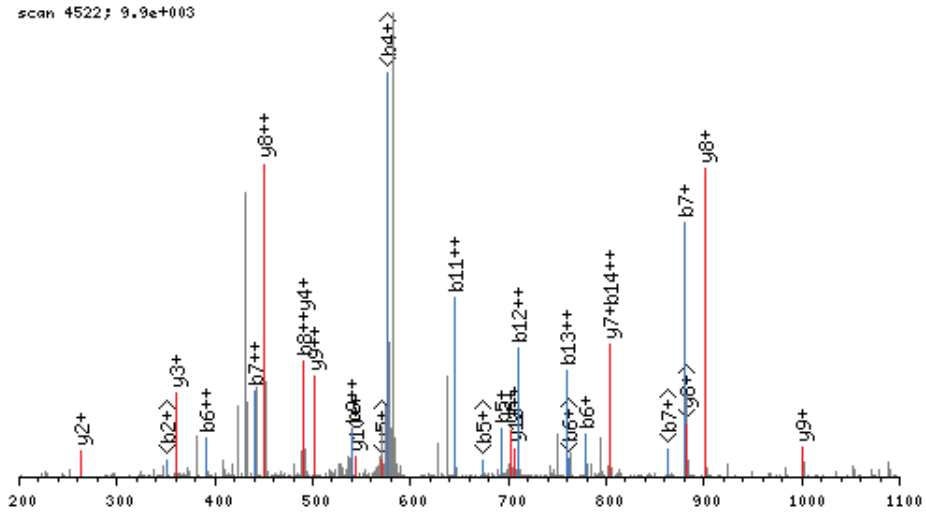
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
304.3392	152.6735	1	K	15			
403.4076	202.2077	2	V	14	1495.8246	748.4162	499.2801
500.4603	250.7341	3	P	13	1396.7562	698.8820	466.2573
628.5189	314.7634	4	Q	12	1299.7034	650.3556	433.9064
727.5873	364.2976	5	V	11	1171.6449	586.3263	391.2202
814.6194	407.8136	6	S	10	1072.5764	536.7921	358.1974
915.6670	458.3374	7	T	9	985.5444	493.2761	329.1867
1012.7198	506.8638	8	P	8	884.4967	442.7523	295.5041
1113.7675	557.3876	9	T	7	787.4440	394.2259	263.1532
1226.8515	613.9297	10	L	6	686.3963	343.7021	229.4706
1325.9200	663.4639	11	V	5	573.3122	287.1600	191.7760
1454.9625	727.9852	12	E	4	474.2438	237.6258	158.7532
1554.0310	777.5194	13	V	3	345.2012	173.1045	115.7390
1641.0630	821.0354	14	S	2	246.1328	123.5703	82.7162
		15	R	1	159.1008	80.0543	53.7055

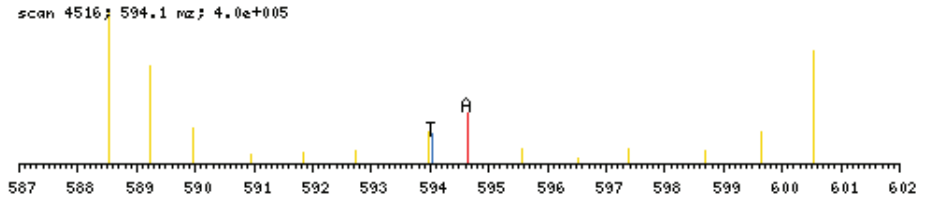
K(1):+286.30

X-range: 200 - 1100
MassTol: 0.950 Y-zoom: 7.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

KVPQVSTPTLVEVSR, MH+ 1780.1375, m/z 594.0507
10HNE-1HSA-37Trypsin5-LTQ1.4522.4522.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
269.3020	135.1549	1	K	15			
368.3705	184.6891	2	V	14	1511.8433	756.4256	504.6197
465.4232	233.2155	3	P	13	1412.7749	**706.8914**	471.5969
593.4818	297.2448	4	Q	12	1315.7222	658.3650	439.2459
692.5502	346.7790	5	V	11	1187.6636	594.3357	396.5597
779.5822	**390.2950**	6	S	10	1088.5952	**544.8015**	363.5369
880.6299	**440.8189**	7	T	9	**1001.5631**	**501.2855**	334.5263
977.6827	**489.3453**	8	P	8	**900.5155**	**450.7616**	300.8437
1078.7304	**539.8691**	9	T	7	**803.4627**	402.2353	268.4928
1191.8144	596.4111	10	L	6	**702.4150**	351.7114	234.8102
1290.8828	**645.9453**	11	V	5	589.3310	295.1694	197.1155
1419.9254	**710.4666**	12	E	4	**490.2625**	245.6352	164.0927
1518.9938	**760.0008**	13	V	3	**361.2199**	181.1139	121.0785
1606.0259	**803.5168**	14	S	2	**262.1515**	131.5797	88.0557
		15	R	1	175.1195	88.0637	59.0451

K(1):+268.29

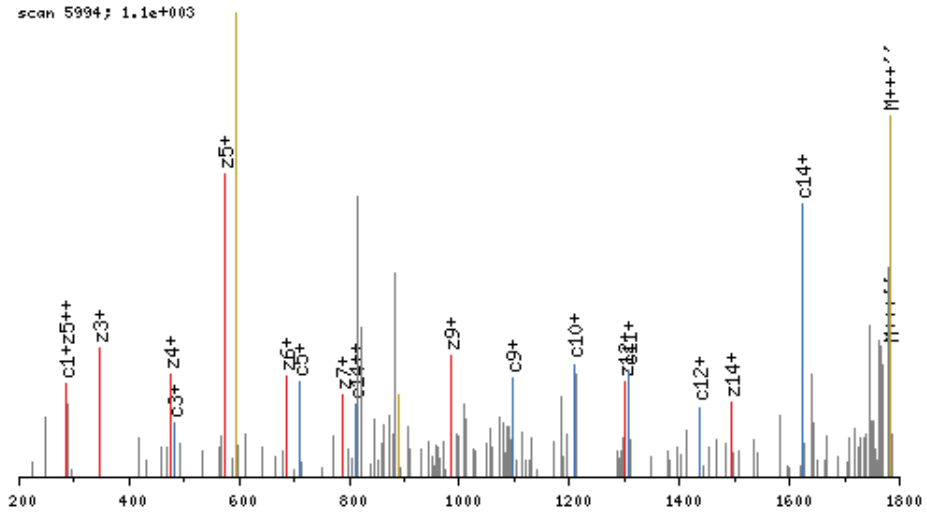
COMET Spectrum View by J.Eng (c) ISB 2001
(TPP v4.4 VUVUZELA rev 1, Build 201010121551 (MinGW))

X-range: 200 - 1800
MassTol: 0.950 Y-zoom: 5.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

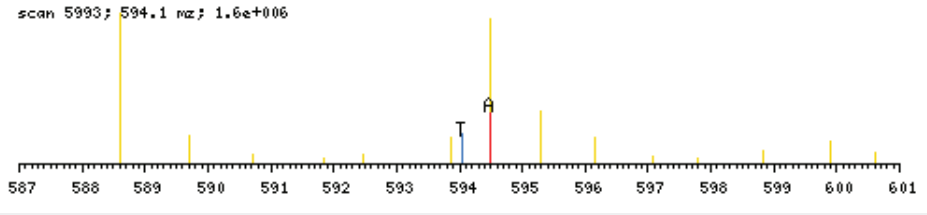
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

KVPQVSTPTLVEVSR, MH+ 1780.1375, m/z 594.0507
10HNE-1HSA-37Trypsin5-LTQ4.5994.5994.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



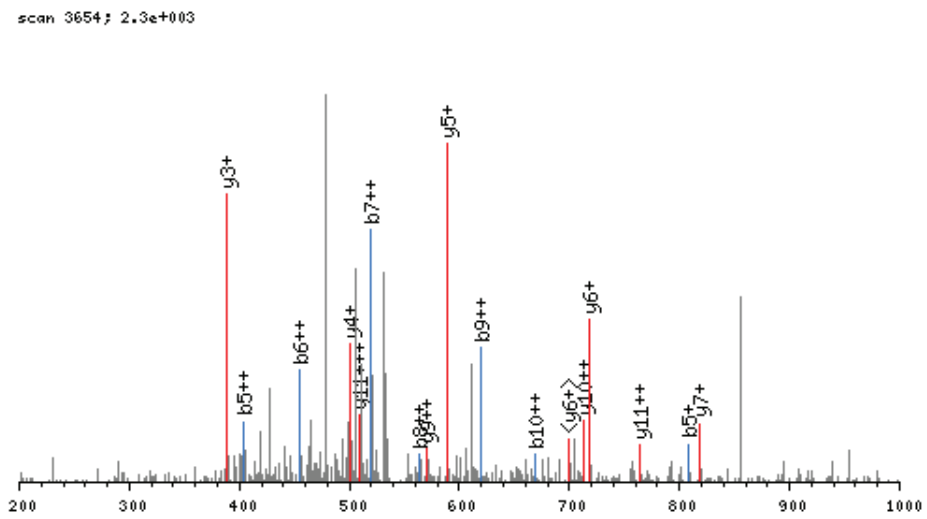
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
286.3286	143.6682	1	K	15			
385.3970	193.2024	2	V	14	1495.8246	748.4162	499.2801
482.4498	241.7288	3	P	13	1396.7562	698.8820	466.2573
610.5083	305.7581	4	Q	12	1299.7034	650.3556	433.9064
709.5768	355.2923	5	V	11	1171.6449	586.3263	391.2202
796.6088	398.8083	6	S	10	1072.5764	536.7921	358.1974
897.6565	449.3321	7	T	9	985.5444	493.2761	329.1867
994.7092	497.8585	8	P	8	884.4967	442.7523	295.5041
1095.7569	548.3824	9	T	7	787.4440	394.2259	263.1532
1208.8410	604.9244	10	L	6	686.3963	343.7021	229.4706
1307.9094	654.4586	11	V	5	573.3122	287.1600	191.7760
1436.9520	718.9799	12	E	4	474.2438	237.6258	158.7532
1536.0204	768.5141	13	V	3	345.2012	173.1045	115.7390
1623.0524	812.0301	14	S	2	246.1328	123.5703	82.7162
		15	R	1	159.1008	80.0543	53.7055

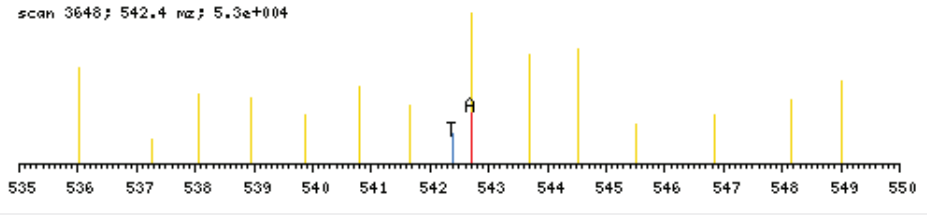
K(1):+268.29

X-range: 200 - 1000
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

VTKCCTESLVNR, MH+ 1625.1787, m/z 542.3977
10HNE-1HSA-37Trypsin2-LTQ3.3654.3654.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



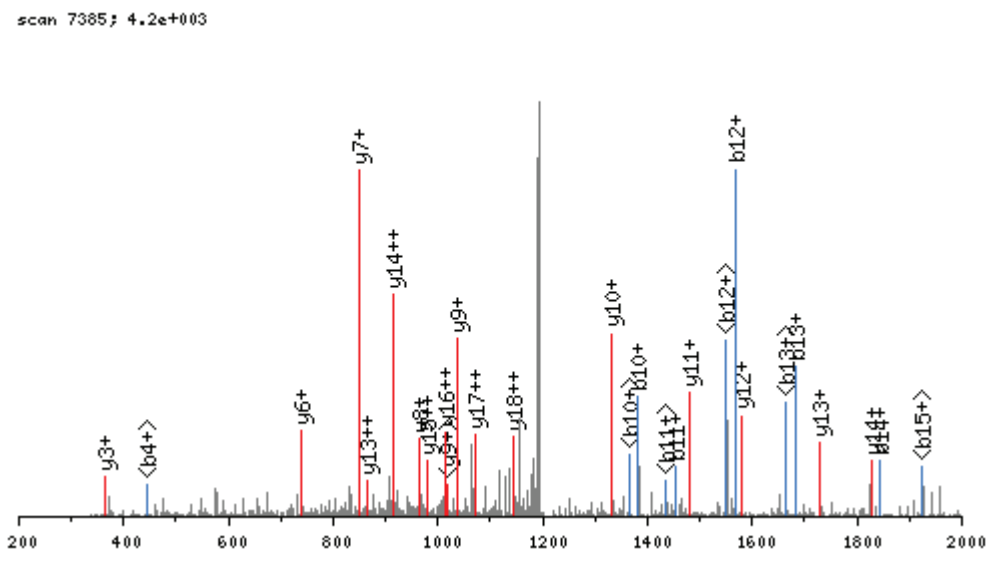
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
100.0762	50.5420	1	V	12			
201.1239	101.0659	2	T	11	1526.1103	763.5590	509.3753
487.4287	244.2183	3	K	10	1425.0626	713.0352	475.6927
647.5890	324.2984	4	C	9	1138.7578	569.8828	380.2578
807.7493	404.3786	5	C	8	978.5975	489.8027	326.8711
908.7970	454.9024	6	T	7	818.4372	409.7225	273.4843
1037.8396	519.4237	7	E	6	717.3895	359.1987	239.8017
1124.8716	562.9397	8	S	5	588.3469	294.6774	196.7875
1237.9557	619.4817	9	L	4	501.3149	251.1614	167.7769
1337.0241	669.0160	10	V	3	388.2308	194.6193	130.0822
1451.0670	726.0374	11	N	2	289.1624	145.0851	97.0594
		12	R	1	175.1195	88.0637	59.0451

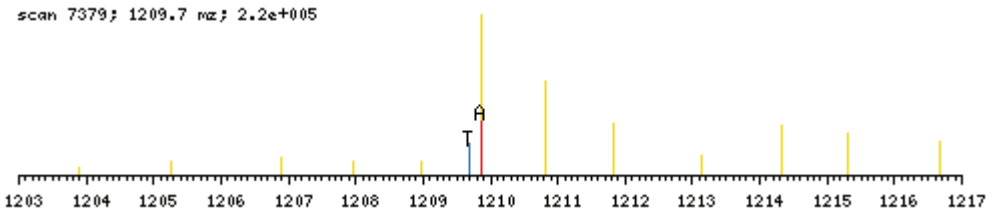
K(3):+286.30 C(4):+160.16 C(5):+160.16

X-range: 200 - 2000
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:
a [ ] + [ ] 2+ [ ] 3+
b [x] + [ ] 2+ [ ] 3+
c [ ] + [ ] 2+ [ ] 3+
x [ ] + [ ] 2+ [ ] 3+
y [x] + [x] 2+ [ ] 3+
z [ ] + [ ] 2+ [ ] 3+
hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

EFNAETFTFHADICTLSEK, MH+ 2418.3657, m/z 1209.6865
10HNE-1HSA-37Trypsin5-LTQ4.7385.7385.2.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	#	AA	#	y^+	y^{2+}
130.0504	1	E	19		
277.1188	2	F	18	2289.3232	1145.1655
391.1618	3	N	17	2142.2547	1071.6313
462.1989	4	A	16	2028.2118	1014.6098
591.2415	5	E	15	1957.1747	979.0913
692.2891	6	T	14	1828.1321	914.5700
839.3576	7	F	13	1727.0844	864.0461
940.4052	8	T	12	1580.0160	790.5119
1087.4737	9	F	11	1478.9683	739.9881
1382.7454	10	H	10	1331.8999	666.4539
1453.7825	11	A	9	1036.6281	518.8180
1568.8095	12	D	8	965.5910	483.2994
1681.8936	13	I	7	850.5641	425.7860
1842.0539	14	C	6	737.4800	369.2439
1943.1015	15	T	5	577.3197	289.1638
2056.1856	16	L	4	476.2720	238.6399
2143.2176	17	S	3	363.1880	182.0979
2272.2602	18	E	2	276.1559	138.5819
	19	K	1	147.1134	74.0606

H(10):+295.27 C(14):+160.16

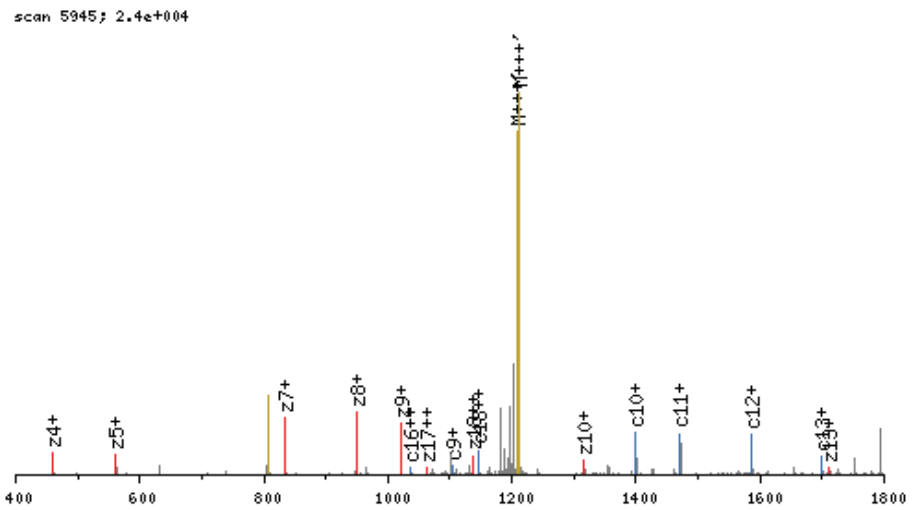
COMET Spectrum View by J.Eng (c) ISB 2001
(TPP v4.4 VUVUZELA rev 1, Build 201010121551 (MinGW))

X-range: 400 - 1800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

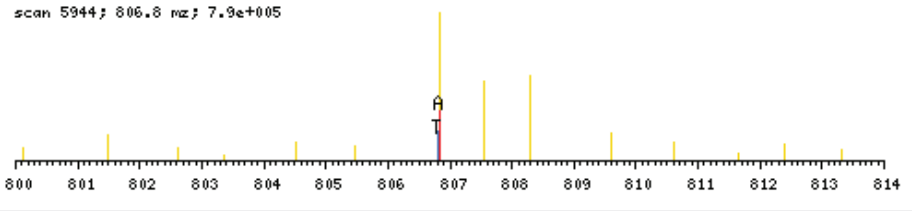
a	☐ +	☐ 2+	☐ 3+
b	☐ +	☐ 2+	☐ 3+
c	☑ +	☑ 2+	☐ 3+
x	☐ +	☐ 2+	☐ 3+
y	☐ +	☐ 2+	☐ 3+
z	☑ +	☑ 2+	☑ 3+

hide H_2O/NH_3 ☐
zoom 112-122 ☐
zoom 124-133 ☐
GO

EFNAETFTFHADICTLSEK, MH+ 2418.3657, m/z 806.7934
10HNE-1HSA-37Trypsin3-LTQ1.5945.5945.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



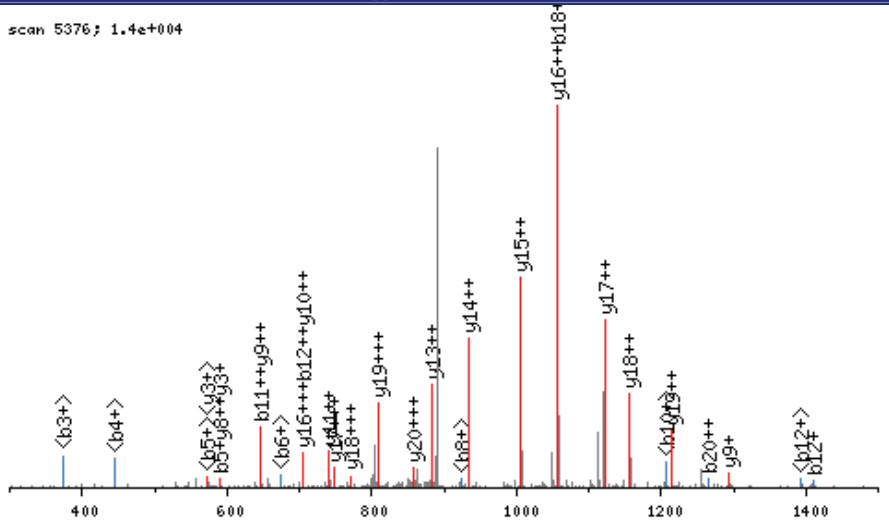
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
147.0770	74.0424	1	E	19			
294.1454	147.5766	2	F	18	2273.3044	**1137.1561**	758.4400
408.1883	204.5981	3	N	17	2126.2360	**1063.6219**	709.4172
479.2254	240.1166	4	A	16	2012.1931	1006.6005	671.4029
608.2680	304.6379	5	E	15	1941.1560	971.0819	647.7239
709.3157	355.1618	6	T	14	1812.1134	906.5606	604.7097
856.3841	428.6960	7	F	13	**1711.0657**	856.0368	571.0271
957.4318	479.2198	8	T	12	1563.9973	782.5026	522.0043
1104.5002	552.7540	9	F	11	1462.9496	731.9787	488.3218
1399.7720	700.3899	10	H	10	**1315.8812**	658.4445	439.2989
1470.8091	735.9085	11	A	9	**1020.6094**	510.8086	340.8750
1585.8360	793.4219	12	D	8	**949.5723**	475.2901	317.1960
1698.9201	849.9640	13	I	7	**834.5454**	417.7766	278.8537
1859.0804	930.0441	14	C	6	721.4613	361.2346	241.1590
1960.1281	980.5680	15	T	5	**561.3010**	281.1544	187.7722
2073.2121	**1037.1100**	16	L	4	**460.2533**	230.6306	154.0897
2160.2442	1080.6260	17	S	3	347.1693	174.0885	116.3950
2289.2868	**1145.1473**	18	E	2	260.1372	130.5725	87.3843
		19	K	1	131.0946	66.0512	44.3701

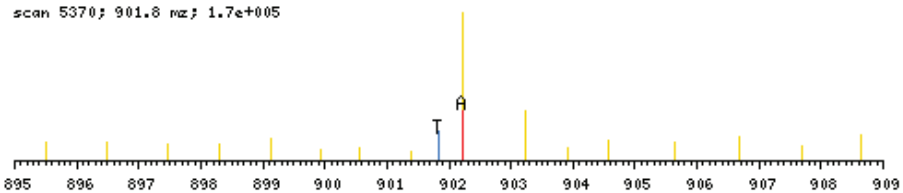
H(10):+295.27 C(14):+160.16

X-range: 300 - 1500
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

EFNAETFTFHADICTLSEKER, MH+ 2703.5064, m/z 901.8403
10HNE-1HSA-37Trypsin5-LTQ1.5376.5376.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
130.0504	65.5291	1	E	21			
277.1188	139.0633	2	F	20	2574.4638	1287.7358	**858.8265**
391.1618	196.0848	3	N	19	2427.3954	**1214.2016**	**809.8037**
462.1989	231.6033	4	A	18	2313.3525	**1157.1801**	**771.7894**
591.2415	296.1246	5	E	17	2242.3153	**1121.6616**	**748.1103**
692.2891	346.6485	6	T	16	2113.2728	**1057.1403**	**705.0961**
839.3576	420.1827	7	F	15	2012.2251	**1006.6165**	671.4136
940.4052	470.7065	8	T	14	1865.1567	**933.0822**	622.3908
1087.4737	544.2407	9	F	13	1764.1090	**882.5584**	588.7082
1224.5326	612.7702	10	H	12	1617.0406	809.0242	539.6854
1295.5697	**648.2888**	11	A	11	1479.9817	**740.4947**	493.9991
1410.5966	**705.8022**	12	D	10	1408.9445	**704.9762**	470.3201
1523.6807	762.3443	13	I	9	**1293.9176**	**647.4627**	431.9778
1683.8410	842.4244	14	C	8	1180.8335	**590.9207**	394.2831
1784.8887	892.9482	15	T	7	1020.6732	510.8405	340.8963
1897.9727	949.4903	16	L	6	919.6256	460.3167	307.2137
1985.0048	993.0063	17	S	5	806.5415	403.7747	269.5190
2114.0473	**1057.5276**	18	E	4	719.5095	360.2586	240.5084
2400.3521	1200.6800	19	K	3	**590.4669**	295.7373	197.4942
2529.3947	**1265.2013**	20	E	2	304.1621	152.5850	102.0592
		21	R	1	175.1195	88.0637	59.0451

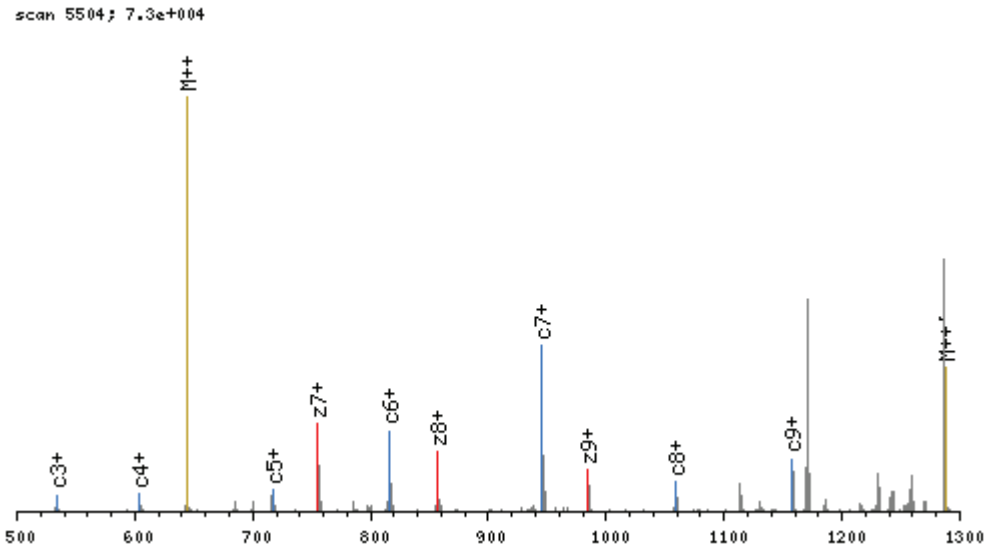
C(14):+160.16 K(19):+286.30

X-range: 500 - 1300
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

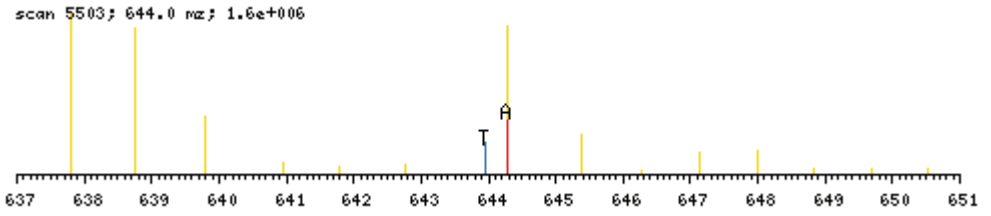
a	☐ +	☐ 2+	☐ 3+
b	☐ +	☐ 2+	☐ 3+
c	☑ +	☐ 2+	☐ 3+
x	☐ +	☐ 2+	☐ 3+
y	☐ +	☐ 2+	☐ 3+
z	☑ +	☑ 2+	☐ 3+

hide H_2O/NH_3 ☐
zoom 112-122 ☐
zoom 124-133 ☐
GO

KQTALVELVK, MH+ 1286.9091, m/z 643.9582
10HNE-1HSA-37Trypsin5-LTQ4.5504.5504.2.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

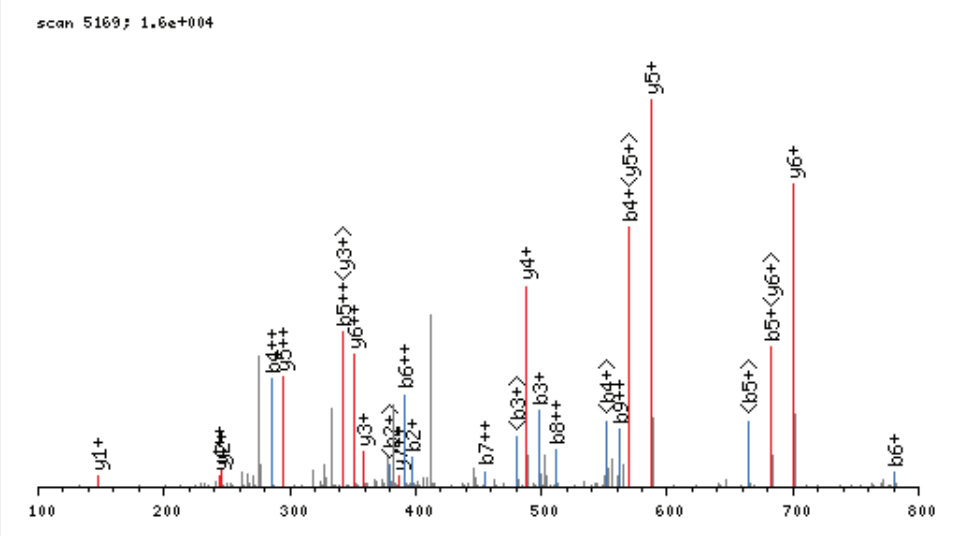
c^+	#	AA	#	z^+	z^{2+}
304.3392	1	K	10		
432.3977	2	Q	9	984.5855	492.7967
533.4454	3	T	8	856.5270	428.7674
604.4825	4	A	7	755.4793	378.2436
717.5666	5	L	6	684.4422	342.7250
816.6350	6	V	5	571.3581	286.1830
945.6776	7	E	4	472.2897	236.6488
1058.7617	8	L	3	343.2471	172.1275
1157.8301	9	V	2	230.1630	115.5854
	10	K	1	131.0946	66.0512

K(1):+286.30

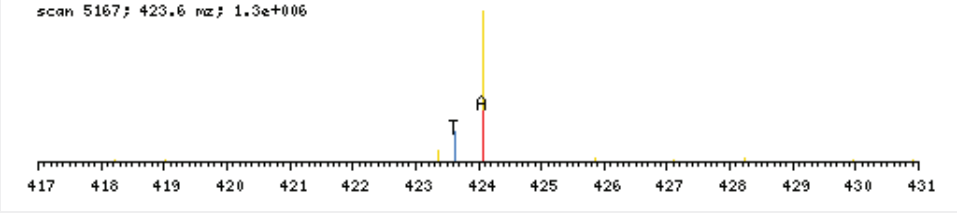
COMET Spectrum View by J.Eng (c) ISB 2001
(TPP v4.4 VUVUZELA rev 1, Build 201010121551 (MinGW))

X-range: 100 - 800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

KQTALVELVK, MH+ 1268.8985, m/z 423.6377
10HNE-1HSA-37Trypsin4-LTQ3.5169.5169.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
269.3020	135.1549	1	K	10			
397.3606	199.1842	2	Q	9	1000.6043	500.8060	334.2066
498.4083	249.7081	3	T	8	872.5457	436.7768	291.5204
569.4454	285.2266	4	A	7	771.4980	386.2529	257.8379
682.5295	341.7686	5	L	6	700.4609	350.7344	234.1589
781.5979	391.3029	6	V	5	587.3768	294.1923	196.4642
910.6405	455.8242	7	E	4	488.3084	244.6581	163.4414
1023.7245	512.3662	8	L	3	359.2658	180.1368	120.4272
1122.7930	561.9004	9	V	2	246.1818	123.5948	82.7325
		10	K	1	147.1134	74.0606	49.7097

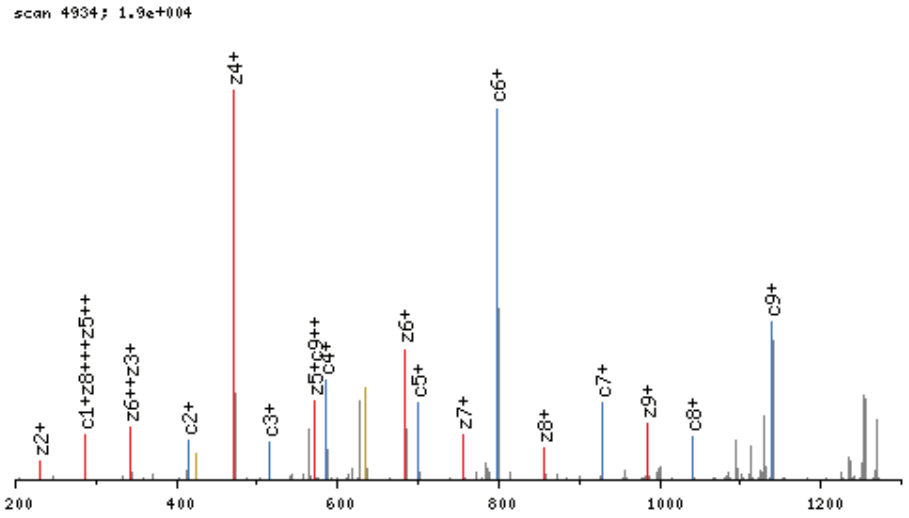
K(1):+268.29

X-range: 200 - 1300
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

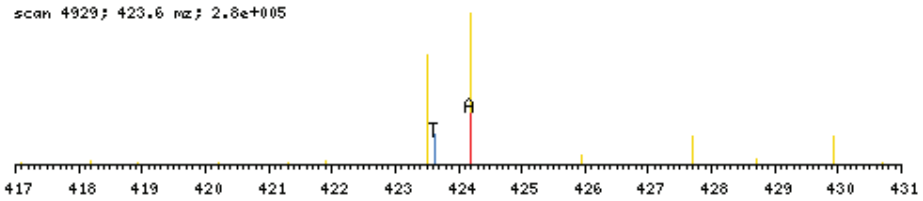
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

KQTALVELVK, MH+ 1268.8985, m/z 423.6377
10HNE-1HSA-37Trypsin3-LTQ3.4934.4934.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



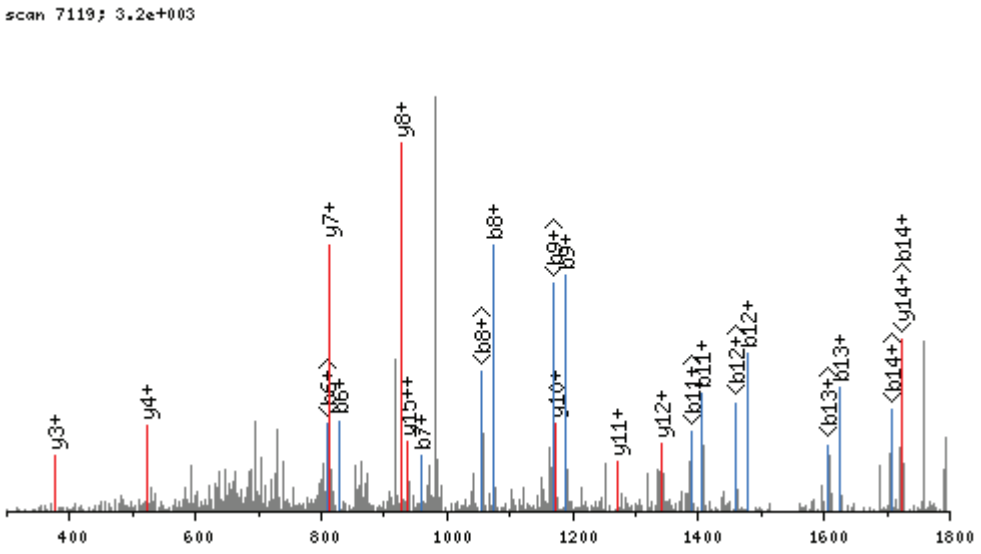
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
286.3286	143.6682	1	K	10			
414.3872	207.6975	2	Q	9	984.5855	492.7967	328.8671
515.4348	258.2213	3	T	8	856.5270	428.7674	286.1809
586.4720	293.7399	4	A	7	755.4793	378.2436	252.4983
699.5560	350.2819	5	L	6	684.4422	342.7250	228.8193
798.6244	399.8161	6	V	5	571.3581	286.1830	191.1246
927.6670	464.3374	7	E	4	472.2897	236.6488	158.1018
1040.7511	520.8795	8	L	3	343.2471	172.1275	115.0876
1139.8195	570.4137	9	V	2	230.1630	115.5854	77.3929
		10	K	1	131.0946	66.0512	44.3701

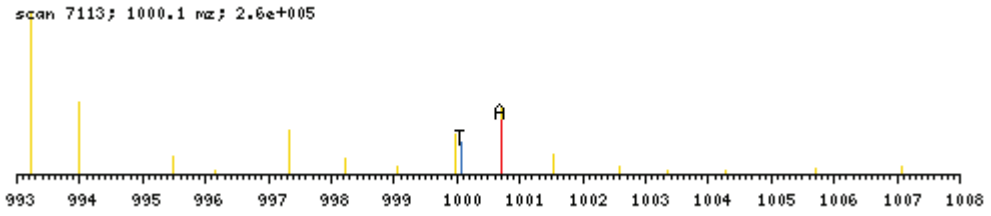
K(1):+268.29

X-range: 300 - 1800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:
a [ ] + [ ] 2+ [ ] 3+
b [x] + [ ] 2+ [ ] 3+
c [ ] + [ ] 2+ [ ] 3+
x [ ] + [ ] 2+ [ ] 3+
y [x] + [x] 2+ [ ] 3+
z [ ] + [ ] 2+ [ ] 3+
hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

EQLKAVMDDFAAFVEK, MH+ 1999.1253, m/z 1000.0663
10HNE-1HSA-37Trypsin3-LTQ1.7119.7119.2.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	#	AA	#	y^+	y^{2+}
130.0504	1	E	16		
258.1090	2	Q	15	1870.0827	**935.5453**
371.1931	3	L	14	1742.0242	871.5160
657.4978	4	K	13	1628.9401	814.9740
728.5350	5	A	12	**1342.6353**	671.8216
827.6034	6	V	11	**1271.5982**	636.3030
958.6439	7	M	10	**1172.5298**	586.7688
1073.6708	8	D	9	1041.4893	521.2486
1188.6977	9	D	8	**926.4624**	463.7351
1335.7662	10	F	7	**811.4354**	406.2216
1406.8033	11	A	6	664.3670	332.6874
1477.8404	12	A	5	593.3299	297.1689
1624.9088	13	F	4	**522.2928**	261.6503
1723.9772	14	V	3	**375.2244**	188.1161
1853.0198	15	E	2	276.1559	138.5819
	16	K	1	147.1134	74.0606

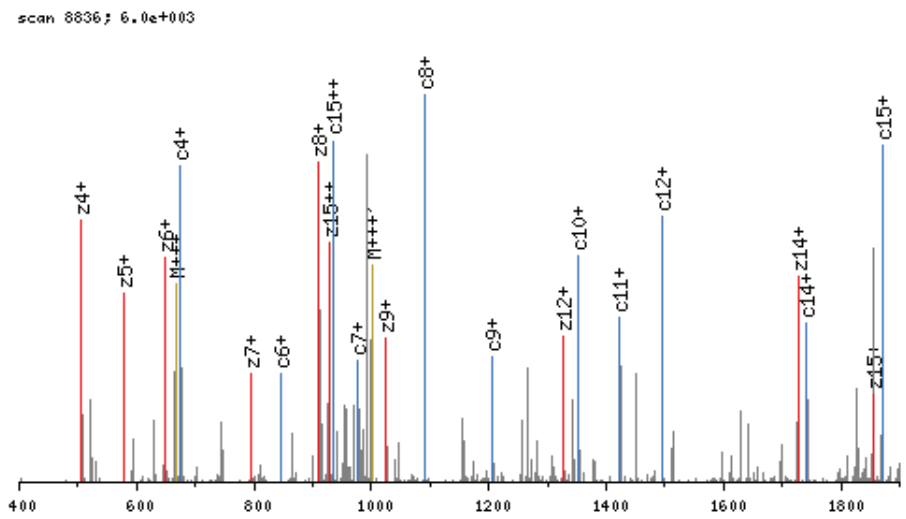
K(4):+286.30

X-range: 400 - 1900
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

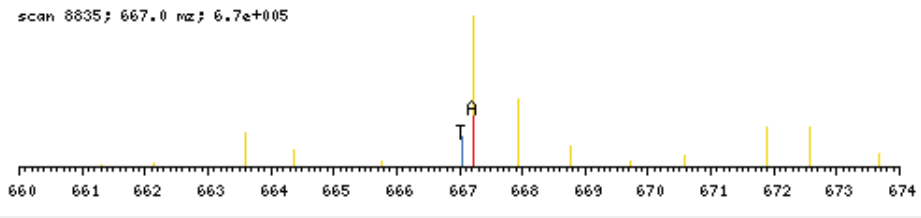
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

EQLKAVMDDFAAFVEK, MH+ 1999.1253, m/z 667.0466
10HNE-1HSA-37Trypsin5-LTQ4.8836.8836.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



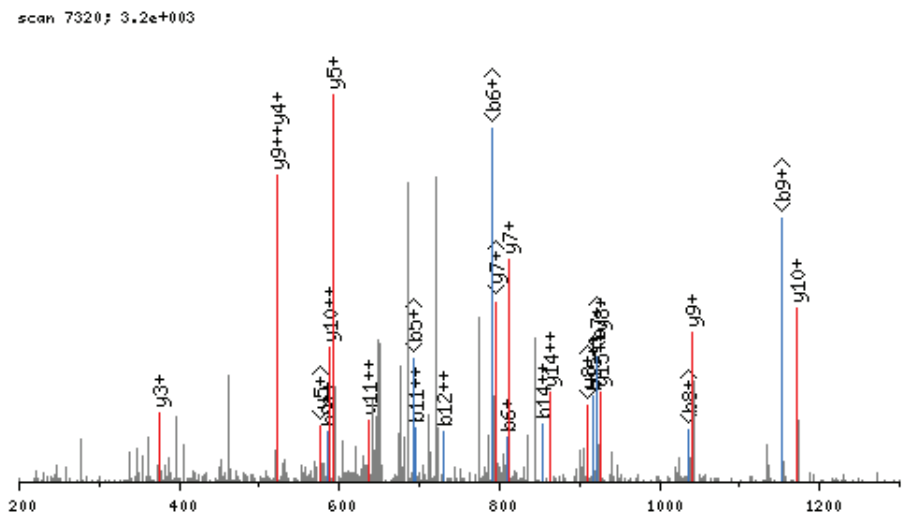
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
147.0770	74.0424	1	E	16			
275.1355	138.0717	2	Q	15	1854.0640	927.5359	618.6932
388.2196	194.6137	3	L	14	1726.0054	863.5066	576.0070
674.5244	337.7661	4	K	13	1612.9214	806.9646	538.3123
745.5615	373.2847	5	A	12	1326.6166	663.8122	442.8774
844.6299	422.8189	6	V	11	1255.5795	628.2937	419.1984
975.6704	488.3391	7	M	10	1156.5111	578.7594	386.1756
1090.6973	545.8526	8	D	9	1025.4706	513.2392	342.4954
1205.7243	603.3661	9	D	8	910.4436	455.7257	304.1531
1352.7927	676.9003	10	F	7	795.4167	398.2123	265.8108
1423.8298	712.4188	11	A	6	648.3483	324.6781	216.7880
1494.8669	747.9374	12	A	5	577.3112	289.1595	193.1089
1641.9353	821.4716	13	F	4	506.2740	253.6409	169.4299
1741.0038	871.0058	14	V	3	359.2056	180.1067	120.4071
1870.0463	935.5271	15	E	2	260.1372	130.5725	87.3843
		16	K	1	131.0946	66.0512	44.3701

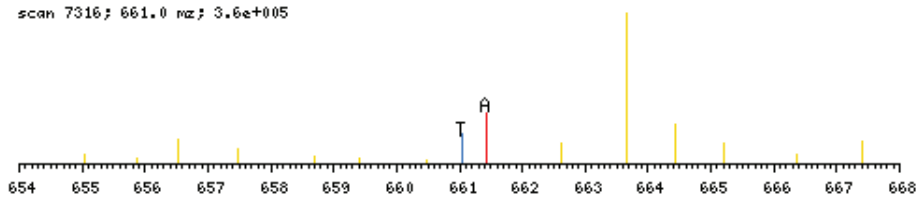
K(4):+286.30

X-range: 200 - 1300
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

EQLKAVMDDFAAFVEK, MH+ 1981.1148, m/z 661.0431
10HNE-1HSA-37Trypsin3-LTQ2.7320.7320.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
130.0504	65.5291	1	E	16			
258.1090	129.5584	2	Q	15	1852.0722	926.5400	618.0293
371.1931	186.1004	3	L	14	1724.0136	862.5107	575.3431
639.4873	320.2475	4	K	13	1610.9295	805.9687	537.6484
710.5244	355.7661	5	A	12	1342.6353	671.8216	448.2170
809.5928	405.3003	6	V	11	1271.5982	636.3030	424.5380
940.6333	470.8206	7	M	10	1172.5298	586.7688	391.5151
1055.6602	528.3340	8	D	9	1041.4893	521.2486	347.8350
1170.6872	585.8475	9	D	8	926.4624	463.7351	309.4927
1317.7556	659.3817	10	F	7	811.4354	406.2216	271.1504
1388.7927	694.9003	11	A	6	664.3670	332.6874	222.1276
1459.8298	730.4188	12	A	5	593.3299	297.1689	198.4485
1606.8982	803.9530	13	F	4	522.2928	261.6503	174.7695
1705.9666	853.4872	14	V	3	375.2244	188.1161	125.7467
1835.0092	918.0085	15	E	2	276.1559	138.5819	92.7239
		16	K	1	147.1134	74.0606	49.7097

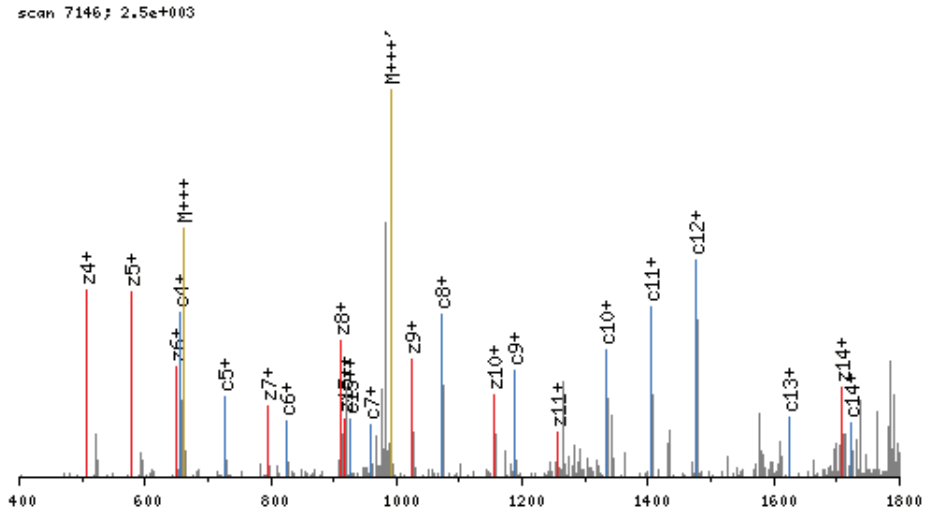
K(4):+268.29

X-range: 400 - 1800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

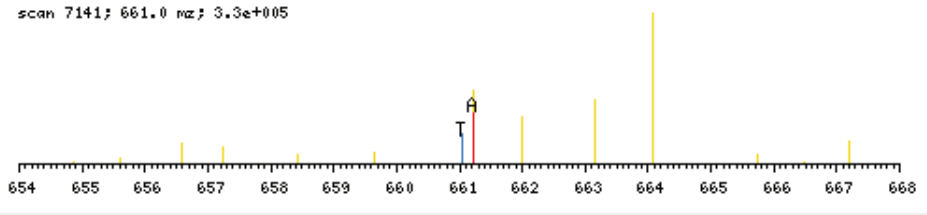
a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

EQLKAVMDDFAAFVEK, MH+ 1981.1148, m/z 661.0431
10HNE-1HSA-37Trypsin2-LTQ1.7146.7146.3.dta



click image to zoom in; click top corners to zoom out [precursor±]



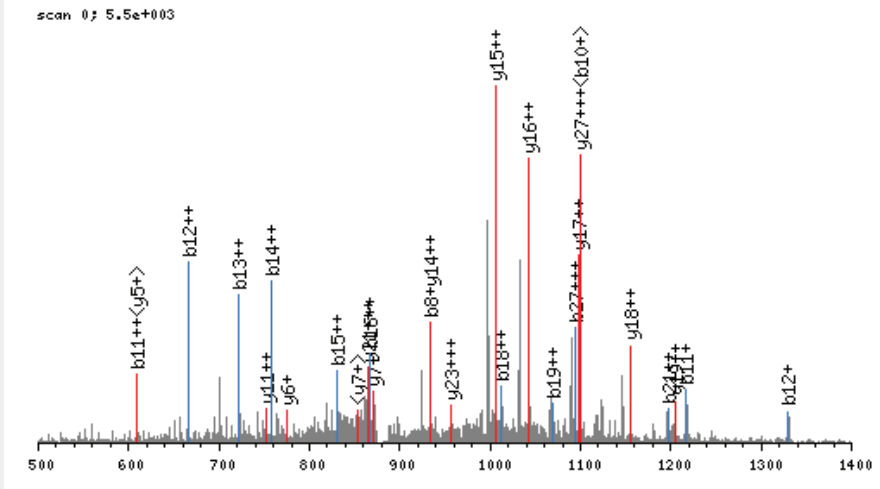
zoomed in precursor plot; T=theoretical m/z, A=acquired m/z

c^+	c^{2+}	#	AA	#	z^+	z^{2+}	z^{3+}
147.0770	74.0424	1	E	16			
275.1355	138.0717	2	Q	15	1836.0534	918.5306	612.6897
388.2196	194.6137	3	L	14	1707.9949	854.5013	570.0035
656.5138	328.7608	4	K	13	1594.9108	797.9593	532.3088
727.5509	364.2794	5	A	12	1326.6166	663.8122	442.8774
826.6194	413.8136	6	V	11	1255.5795	628.2937	419.1984
957.6598	479.3338	7	M	10	1156.5111	578.7594	386.1756
1072.6868	536.8473	8	D	9	1025.4706	513.2392	342.4954
1187.7137	594.3608	9	D	8	910.4436	455.7257	304.1531
1334.7821	667.8950	10	F	7	795.4167	398.2123	265.8108
1405.8193	703.4135	11	A	6	648.3483	324.6781	216.7880
1476.8564	738.9321	12	A	5	577.3112	289.1595	193.1089
1623.9248	812.4663	13	F	4	506.2740	253.6409	169.4299
1722.9932	862.0005	14	V	3	359.2056	180.1067	120.4071
1852.0358	926.5218	15	E	2	260.1372	130.5725	87.3843
		16	K	1	131.0946	66.0512	44.3701

K(4):+268.29

X-range: 500 - 1400
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:
a + 2+ 3+
b + 2+ 3+
c + 2+ 3+
x + 2+ 3+
y + 2+ 3+
z + 2+ 3+
hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

DLGEENFKALVLIAFAQYLQQCPFEDHVK, MH+ 3523.8187, m/z 881.7101
10HNE-1HSA-Trypsin6-Orbit2.04363.04363.4.dta



click image to zoom in; click top corners to zoom out

b^+	b^{2+}	b^{3+}	#	AA	#	y^+	y^{2+}	y^{3+}
116.0348	58.5213	39.3501	1	D	29			
229.1188	115.0633	77.0448	2	L	28	3408.7918	1704.8998	1136.9358
286.1403	143.5741	96.0520	3	G	27	3295.7077	1648.3578	**1099.2411**
415.1829	208.0954	139.0662	4	E	26	3238.6863	1619.8470	1080.2340
544.2255	272.6167	182.0804	5	E	25	3109.6437	1555.3258	1037.2198
658.2684	329.6381	220.0947	6	N	24	2980.6011	1490.8045	994.2056
805.3368	403.1723	269.1175	7	F	23	2866.5582	1433.7830	**956.1913**
933.4318	467.2198	311.8158	8	K	22	2719.4897	1360.2488	907.1685
1004.4689	502.7384	335.4949	9	A	21	2591.3948	1296.2013	**864.4701**
1117.5530	559.2804	373.1895	10	L	20	2520.3577	1260.6827	840.7911
1216.6214	**608.8146**	406.2123	11	V	19	2407.2736	**1204.1407**	803.0964
1329.7054	**665.3566**	443.9070	12	L	18	2308.2052	**1154.6065**	770.0736
1442.7895	**721.8987**	481.6017	13	I	17	2195.1211	**1098.0645**	732.3789
1513.8266	**757.4172**	505.2808	14	A	16	2082.0371	**1041.5224**	694.6842
1660.8950	**830.9514**	554.3036	15	F	15	2010.9999	**1006.0039**	671.0052
1731.9321	**866.4700**	577.9826	16	A	14	1863.9315	**932.4697**	621.9824
1859.9907	930.4993	620.6688	17	Q	13	1792.8944	896.9511	598.3034
2023.0541	**1012.0309**	675.0232	18	Y	12	1664.8358	832.9218	555.6172
2136.1381	**1068.5730**	712.7179	19	L	11	1501.7725	**751.3902**	501.2627
2264.1967	1132.6023	755.4041	20	Q	10	1388.6884	694.8481	463.5680
2392.2553	**1196.6315**	798.0903	21	Q	9	1260.6299	630.8188	420.8818
2653.3952	1327.2015	885.1369	22	C	8	1132.5713	566.7896	378.1956
2750.4479	1375.7279	917.4879	23	P	7	**871.4314**	436.2196	291.1490
2897.5164	1449.2621	966.5107	24	F	6	**774.3786**	387.6932	258.7981
3026.5589	1513.7834	1009.5249	25	E	5	627.3102	314.1590	209.7753
3141.5859	1571.2969	1047.8672	26	D	4	498.2676	249.6377	166.7611
3278.6448	1639.8263	**1093.5535**	27	H	3	383.2407	192.1243	128.4188
3377.7132	1689.3605	1126.5763	28	V	2	246.1818	123.5948	82.7325
			29	K	1	147.1134	74.0606	49.7097

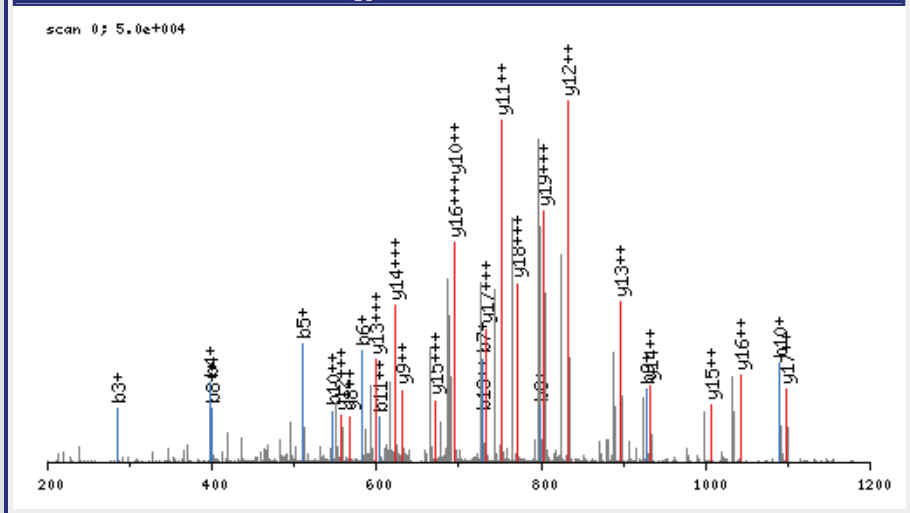
C(22):+261.14

X-range: 200 - 1200
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

a	[ ] +	[ ] 2+	[ ] 3+
b	[x] +	[x] 2+	[x] 3+
c	[ ] +	[ ] 2+	[ ] 3+
x	[ ] +	[ ] 2+	[ ] 3+
y	[x] +	[x] 2+	[x] 3+
z	[ ] +	[ ] 2+	[ ] 3+

hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

ALVLIAFAQYLQQCPFEDHVK, MH+ 2591.3948, m/z 648.6042
10HNE-1HSA-Trypsin6-Orbit2.04329.04329.4.dta



click image to zoom in; click top corners to zoom out

b^+	b^{2+}	b^{3+}	#	AA	#	y^+	y^{2+}	y^{3+}
72.0449	36.5264	24.6869	1	A	21			
185.1290	93.0684	62.3816	2	L	20	2520.3577	1260.6827	840.7911
284.1974	142.6026	95.4044	3	V	19	2407.2736	1204.1407	**803.0964**
397.2815	199.1447	133.0990	4	L	18	2308.2052	1154.6065	**770.0736**
510.3655	255.6867	170.7937	5	I	17	2195.1211	**1098.0645**	**732.3789**
581.4027	291.2052	194.4728	6	A	16	2082.0371	**1041.5224**	**694.6842**
728.4711	364.7394	243.4956	7	F	15	2010.9999	**1006.0039**	**671.0052**
799.5082	**400.2580**	267.1746	8	A	14	1863.9315	**932.4697**	**621.9824**
927.5668	464.2873	309.8608	9	Q	13	1792.8944	**896.9511**	**598.3034**
1090.6301	**545.8190**	364.2152	10	Y	12	1664.8358	**832.9218**	**555.6172**
1203.7142	**602.3610**	401.9099	11	L	11	1501.7725	**751.3902**	501.2627
1331.7727	666.3903	444.5961	12	Q	10	1388.6884	**694.8481**	463.5680
1459.8313	**730.4196**	487.2823	13	Q	9	1260.6299	**630.8188**	420.8818
1720.9712	860.9895	574.3290	14	C	8	1132.5713	**566.7896**	378.1956
1818.0240	909.5159	606.6799	15	P	7	871.4314	436.2196	291.1490
1965.0924	983.0501	655.7027	16	F	6	774.3786	387.6932	258.7981
2094.1350	1047.5714	698.7169	17	E	5	627.3102	314.1590	209.7753
2209.1619	1105.0849	737.0592	18	D	4	498.2676	249.6377	166.7611
2346.2208	1173.6143	782.7455	19	H	3	383.2407	192.1243	128.4188
2445.2893	1223.1485	815.7683	20	V	2	246.1818	123.5948	82.7325
			21	K	1	147.1134	74.0606	49.7097

C(14):+261.14

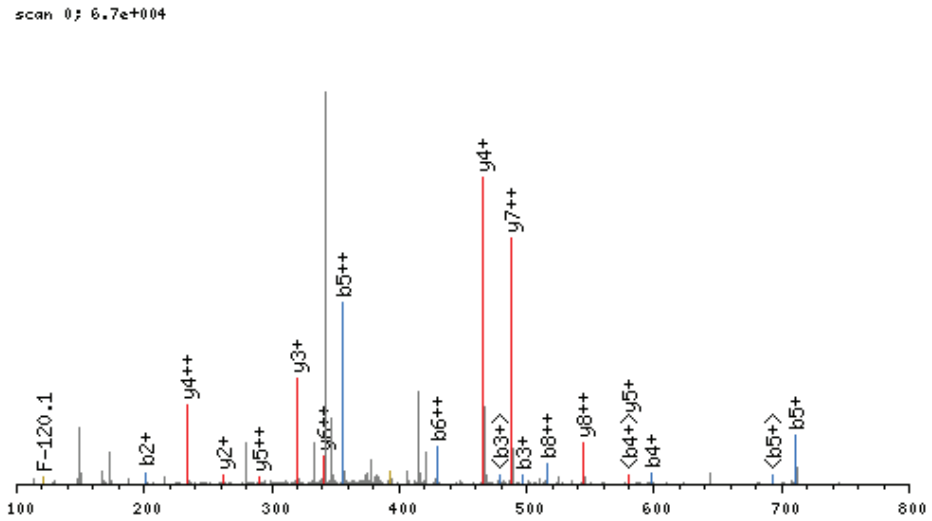
COMET Spectrum View by J.Eng (c) ISB 2001
(TPP v4.4 VUVUZELA rev 1, Build 201010121551 (MinGW))

X-range: 100 - 800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

a	☐ +	☐ 2+	☐ 3+
b	☑ +	☑ 2+	☐ 3+
c	☐ +	☐ 2+	☐ 3+
x	☐ +	☐ 2+	☐ 3+
y	☑ +	☑ 2+	☑ 3+
z	☐ +	☐ 2+	☐ 3+

hide H_2O/NH_3 ☐
zoom 112-122 ☐
zoom 124-133 ☐
GO

SLHTLFGDK, MH+ 1175.6676, m/z 392.5607
10HNE-1HSA-Trypsin6-Orbit3.03026.03026.3.dta



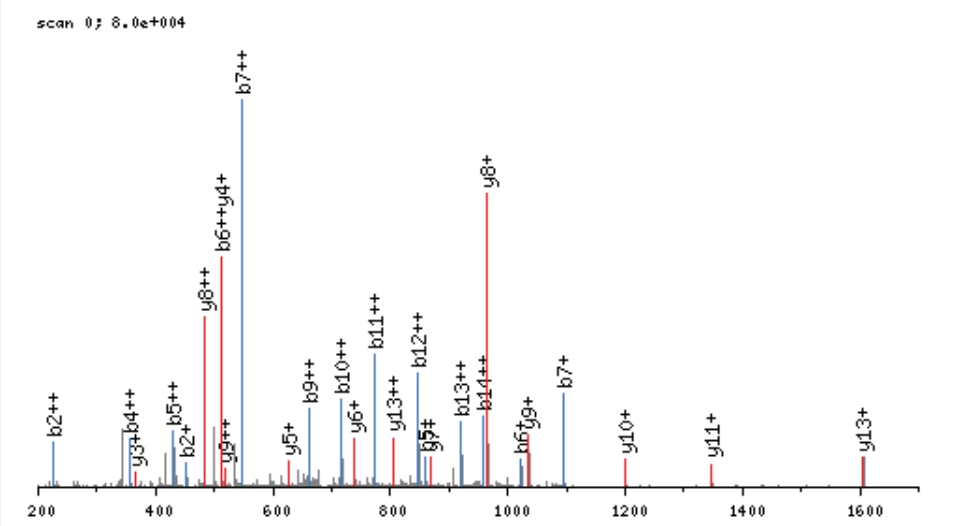
click image to zoom in; click top corners to zoom out

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
88.0399	44.5238	1	S	9			
201.1239	101.0659	2	L	8	1088.6356	**544.8217**	363.5504
496.3135	248.6607	3	H	7	975.5515	**488.2797**	325.8557
597.3612	299.1845	4	T	6	680.3619	**340.6849**	227.4592
710.4453	**355.7265**	5	L	5	**579.3142**	**290.1610**	193.7766
857.5137	**429.2607**	6	F	4	**466.2302**	**233.6190**	156.0819
914.5351	457.7715	7	G	3	**319.1618**	160.0848	107.0591
1029.5621	**515.2849**	8	D	2	**262.1403**	131.5741	88.0520
		9	K	1	147.1134	74.0606	49.7097

H(3):+295.19

X-range: 200 - 1700
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:
a [ ] + [ ] 2+ [ ] 3+
b [x] + [x] 2+ [ ] 3+
c [ ] + [ ] 2+ [ ] 3+
x [ ] + [ ] 2+ [ ] 3+
y [x] + [x] 2+ [x] 3+
z [ ] + [ ] 2+ [ ] 3+
hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

RHPYFYAPELLFFAK, MH+ 2057.1264, m/z 686.3803
10HNE-1HSA-Trypsin6-Orbit2.03830.03830.3.dta



click image to zoom in; click top corners to zoom out

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
157.1089	79.0584	1	R	15			
452.2985	226.6532	2	H	14	1901.0253	951.0166	634.3470
549.3513	275.1796	3	P	13	1605.8357	803.4218	535.9505
712.4146	356.7112	4	Y	12	1508.7830	754.8954	503.5995
859.4830	430.2454	5	F	11	1345.7196	673.3637	449.2451
1022.5464	511.7771	6	Y	10	1198.6512	599.8295	400.2223
1093.5835	547.2957	7	A	9	1035.5879	518.2979	345.8678
1190.6362	595.8220	8	P	8	964.5508	482.7793	322.1888
1319.6788	660.3433	9	E	7	867.4980	434.2529	289.8379
1432.7629	716.8854	10	L	6	738.4554	369.7316	246.8237
1545.8470	773.4274	11	L	5	625.3714	313.1896	209.1290
1692.9154	846.9616	12	F	4	512.2873	256.6476	171.4343
1839.9838	920.4958	13	F	3	365.2189	183.1134	122.4115
1911.0209	956.0144	14	A	2	218.1505	109.5791	73.3887
		15	K	1	147.1134	74.0606	49.7097

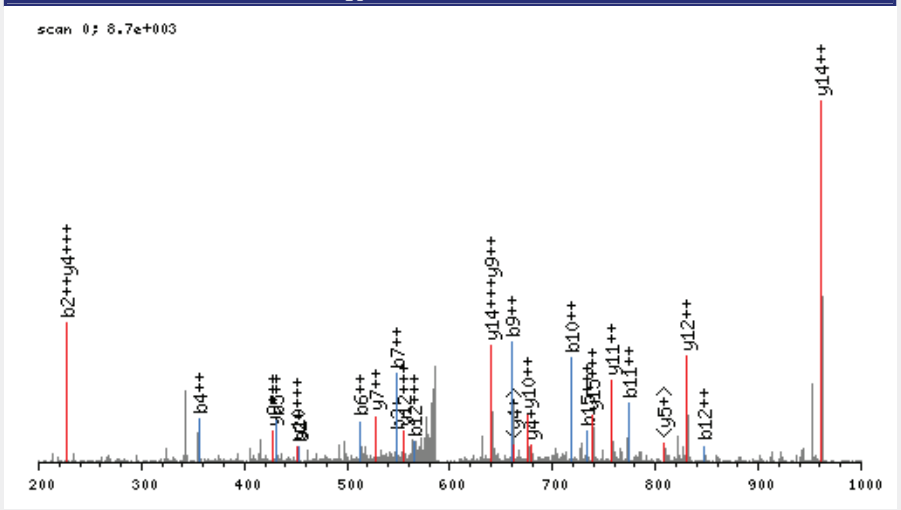
H(2):+295.19

X-range: 200 - 1000
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

RHPYFYAPELLFFAKR, MH+ 2371.3582, m/z 593.5950
10HNE-1HSA-Trypsin6-Orbit2.04047.04047.4.dta



click image to zoom in; click top corners to zoom out

b^+	b^{2+}	b^{3+}	#	AA	#	y^+	y^{2+}	y^{3+}
157.1089	79.0584	53.0415	1	R	16			
452.2985	**226.6532**	151.4381	2	H	15	2215.2571	1108.1325	**739.0909**
549.3513	275.1796	183.7890	3	P	14	1920.0675	**960.5377**	**640.6944**
712.4146	**356.7112**	238.1434	4	Y	13	1823.0148	912.0113	608.3435
859.4830	**430.2454**	287.1662	5	F	12	1659.9514	**830.4796**	**553.9890**
1022.5464	**511.7771**	341.5207	6	Y	11	1512.8830	**756.9454**	504.9662
1093.5835	**547.2957**	365.1997	7	A	10	1349.8197	**675.4138**	**450.6118**
1190.6362	595.8220	397.5506	8	P	9	1278.7826	**639.8952**	**426.9327**
1319.6788	**660.3433**	440.5648	9	E	8	1181.7298	591.3688	394.5818
1432.7629	**716.8854**	478.2595	10	L	7	1052.6872	**526.8475**	351.5676
1545.8470	**773.4274**	515.9542	11	L	6	939.6031	470.3055	313.8729
1692.9154	**846.9616**	**564.9770**	12	F	5	826.5191	413.7635	276.1782
1839.9838	920.4958	613.9998	13	F	4	**679.4507**	340.2292	**227.1554**
1911.0209	956.0144	637.6789	14	A	3	532.3823	266.6950	178.1326
2197.2465	1099.1272	**733.0874**	15	K	2	461.3451	231.1765	154.4536
			16	R	1	175.1195	88.0637	59.0451

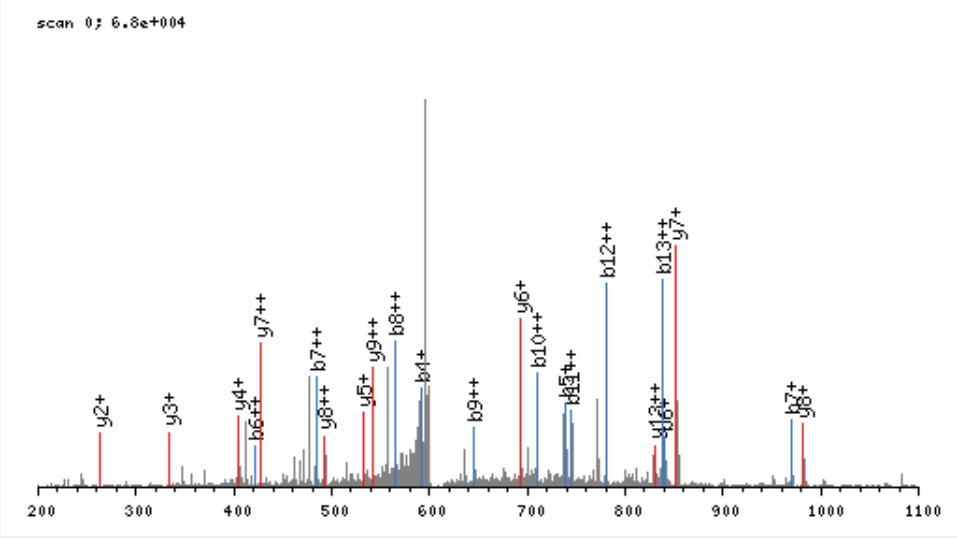
H(2):+295.19 K(15):+286.23

X-range: 200 - 1100
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

a	[ ] +	[ ] 2+	[ ] 3+
b	[x] +	[x] 2+	[ ] 3+
c	[ ] +	[ ] 2+	[ ] 3+
x	[ ] +	[ ] 2+	[ ] 3+
y	[x] +	[x] 2+	[x] 3+
z	[ ] +	[ ] 2+	[ ] 3+

hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

YKAAFTECCQAADK, MH+ 1820.8564, m/z 607.6236
10HNE-1HSA-Trypsin6-Orbit1.02272.02272.3.dta



click image to zoom in; click top corners to zoom out

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
164.0712	82.5395	1	Y	14			
450.2968	225.6523	2	K	13	1657.7930	**829.4004**	553.2696
521.3339	261.1709	3	A	12	1371.5674	686.2876	457.8610
592.3710	296.6894	4	A	11	1300.5303	650.7690	434.1820
739.4394	370.2236	5	F	10	1229.4932	615.2505	410.5029
840.4871	**420.7475**	6	T	9	1082.4247	**541.7163**	361.4801
969.5297	**485.2688**	7	E	8	**981.3771**	**491.1924**	327.7976
1129.5604	**565.2841**	8	C	7	**852.3345**	**426.6711**	284.7834
1289.5911	**645.2995**	9	C	6	**692.3038**	346.6558	231.4398
1417.6497	**709.3287**	10	Q	5	**532.2731**	266.6405	178.0963
1488.6868	**744.8473**	11	A	4	**404.2145**	202.6112	135.4101
1559.7239	**780.3659**	12	A	3	**333.1774**	167.0926	111.7310
1674.7508	**837.8793**	13	D	2	**262.1403**	131.5741	88.0520
		14	K	1	147.1134	74.0606	49.7097

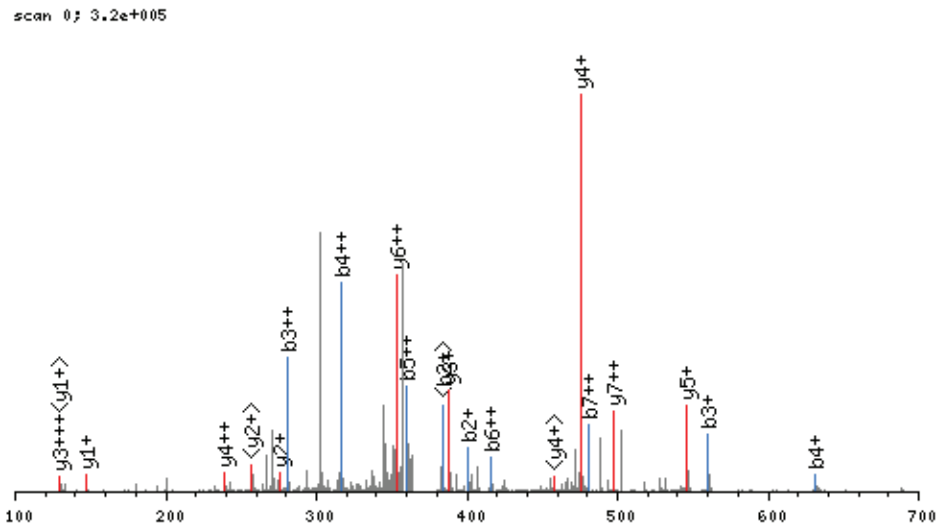
K(2):+286.23 C(8):+160.03 C(9):+160.03

X-range: 100 - 700
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

a	☐ +	☐ 2+	☐ 3+
b	☑ +	☑ 2+	☐ 3+
c	☐ +	☐ 2+	☐ 3+
x	☐ +	☐ 2+	☐ 3+
y	☑ +	☑ 2+	☑ 3+
z	☐ +	☐ 2+	☐ 3+

hide H_2O/NH_3 ☐
zoom 112-122 ☐
zoom 124-133 ☐
GO

LKCASLQK, MH+ 1105.6655, m/z 369.2267
10HNE-1HSA-Trypsin6-Orbit2.01837.01837.3.dta



click image to zoom in; click top corners to zoom out

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
114.0919	57.5499	1	L	8			
400.3175	200.6627	2	K	7	992.5815	496.7946	331.5324
560.3482	280.6780	3	C	6	706.3558	353.6818	236.1238
631.3853	316.1966	4	A	5	546.3251	273.6665	182.7803
718.4174	359.7126	5	S	4	475.2880	238.1479	159.1012
831.5014	416.2546	6	L	3	388.2560	194.6319	130.0905
959.5600	480.2839	7	Q	2	275.1719	138.0899	92.3959
		8	K	1	147.1134	74.0606	49.7097

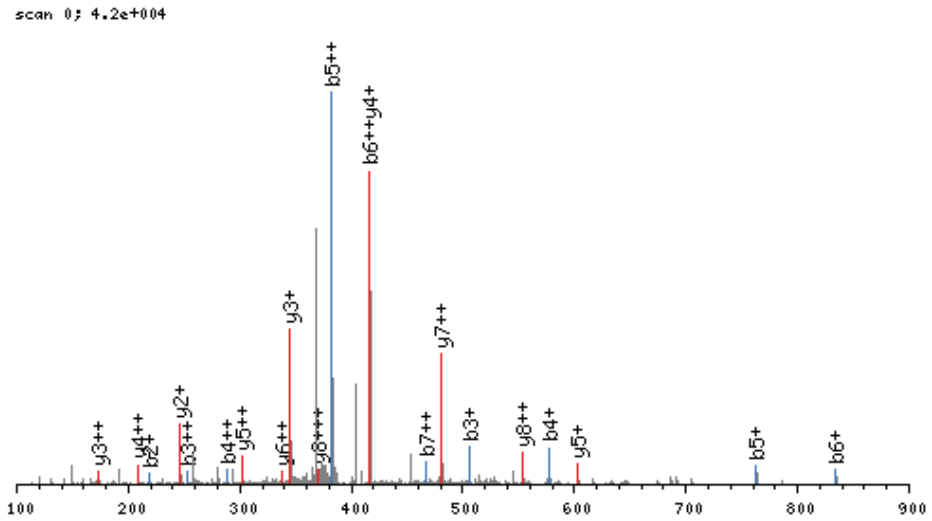
K(2):+286.23 C(3):+160.03

X-range: 100 - 900
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

a	[ ] +	[ ] 2+	[ ] 3+
b	[x] +	[x] 2+	[ ] 3+
c	[ ] +	[ ] 2+	[ ] 3+
x	[ ] +	[ ] 2+	[ ] 3+
y	[x] +	[x] 2+	[x] 3+
z	[ ] +	[ ] 2+	[ ] 3+

hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

AFKAWAVAR, MH+ 1177.7097, m/z 393.2414
10HNE-1HSA-Trypsin6-Orbit2.02804.02804.3.dta



click image to zoom in; click top corners to zoom out

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
72.0449	36.5264	1	A	9			
219.1134	110.0606	2	F	8	1106.6726	**553.8402**	**369.5628**
505.3390	**253.1734**	3	K	7	959.6042	**480.3060**	320.5400
576.3761	**288.6920**	4	A	6	673.3786	**337.1932**	225.1314
762.4554	**381.7316**	5	W	5	**602.3415**	**301.6746**	201.4524
833.4925	**417.2502**	6	A	4	**416.2621**	**208.6350**	139.4259
932.5610	**466.7844**	7	V	3	**345.2250**	**173.1164**	115.7469
1003.5981	502.3029	8	A	2	**246.1566**	123.5822	82.7241
		9	R	1	175.1195	88.0637	59.0451

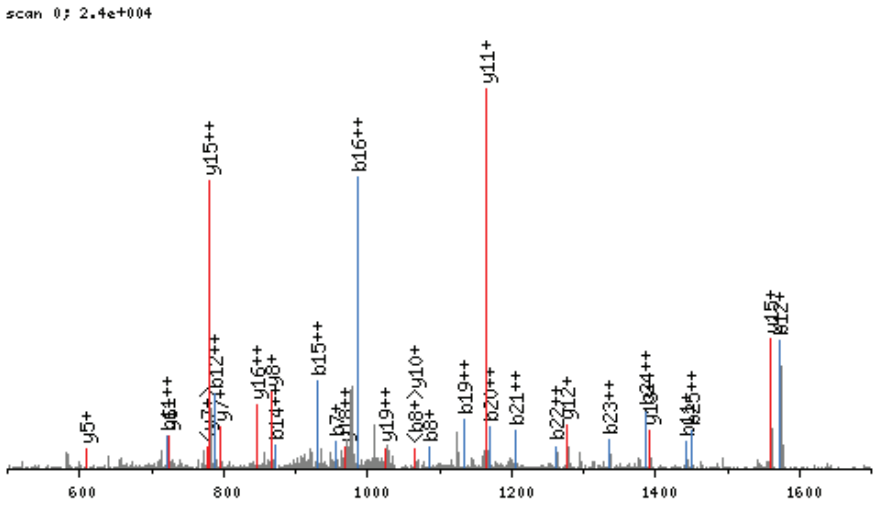
K(3):+286.23

X-range: 500 - 1700
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

SHCIAEVENDEMPADLPSLAADFVESK, MH+ 3132.4757, m/z 1044.8301
10HNE-1HSA-Trypsin6-Orbit2.03858.03858.3.dta



click image to zoom in; click top corners to zoom out

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
88.0399	44.5238	1	S	27			
383.2294	192.1186	2	H	26	3045.4437	1523.2258	1015.8198
543.2601	272.1340	3	C	25	2750.2541	1375.6310	917.4233
656.3442	328.6760	4	I	24	2590.2234	1295.6156	864.0797
727.3813	364.1946	5	A	23	2477.1394	1239.0736	826.3850
856.4239	428.7159	6	E	22	2406.1023	1203.5550	802.7060
955.4923	478.2501	7	V	21	2277.0597	1139.0337	759.6918
1084.5349	542.7714	8	E	20	2177.9913	1089.4995	726.6690
1198.5778	599.7928	9	N	19	2048.9487	**1024.9782**	683.6548
1313.6048	657.3063	10	D	18	1934.9057	**967.9568**	645.6405
1442.6474	**721.8276**	11	E	17	1819.8788	910.4433	607.2981
1573.6879	**787.3478**	12	M	16	1690.8362	**845.9220**	564.2839
1670.7406	835.8742	13	P	15	**1559.7957**	**780.4018**	520.6038
1741.7777	**871.3928**	14	A	14	1462.7430	731.8754	488.2529
1856.8047	**928.9063**	15	D	13	**1391.7058**	696.3568	464.5738
1969.8887	**985.4483**	16	L	12	**1276.6789**	638.8434	426.2315
2066.9415	1033.9747	17	P	11	**1163.5948**	582.3013	388.5368
2153.9735	1077.4907	18	S	10	**1066.5421**	533.7749	356.1859
2267.0576	**1134.0327**	19	L	9	979.5100	490.2589	327.1752
2338.0947	**1169.5513**	20	A	8	**866.4260**	433.7169	289.4805
2409.1318	**1205.0698**	21	A	7	**795.3889**	398.1983	265.8015
2524.1588	**1262.5833**	22	D	6	**724.3517**	362.6798	242.1225
2671.2272	**1336.1175**	23	F	5	**609.3248**	305.1663	203.7802
2770.2956	**1385.6517**	24	V	4	462.2564	231.6321	154.7573
2899.3382	**1450.1730**	25	E	3	363.1880	182.0979	121.7345
2986.3702	1493.6890	26	S	2	234.1454	117.5766	78.7203
		27	K	1	147.1134	74.0606	49.7097

H(2):+295.19 C(3):+160.03

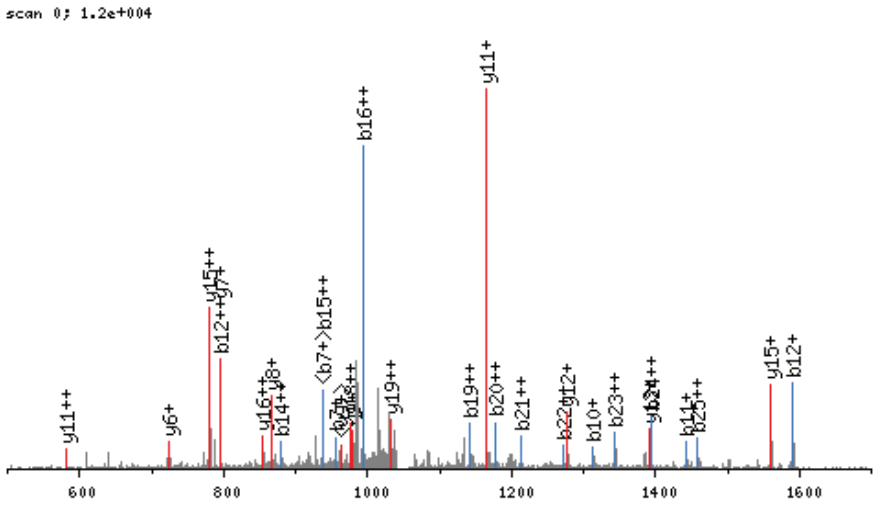
COMET Spectrum View by J.Eng (c) ISB 2001
(TPP v4.4 VUVUZELA rev 1, Build 201010121551 (MinGW))

X-range: 500 - 1700
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

SHCIAEVENDEMPADLPSLAADFVESK, MH+ 3148.4707, m/z 1050.1617
10HNE-1HSA-Trypsin6-Orbit1.03632.03632.3.dta



click image to zoom in; click top corners to zoom out

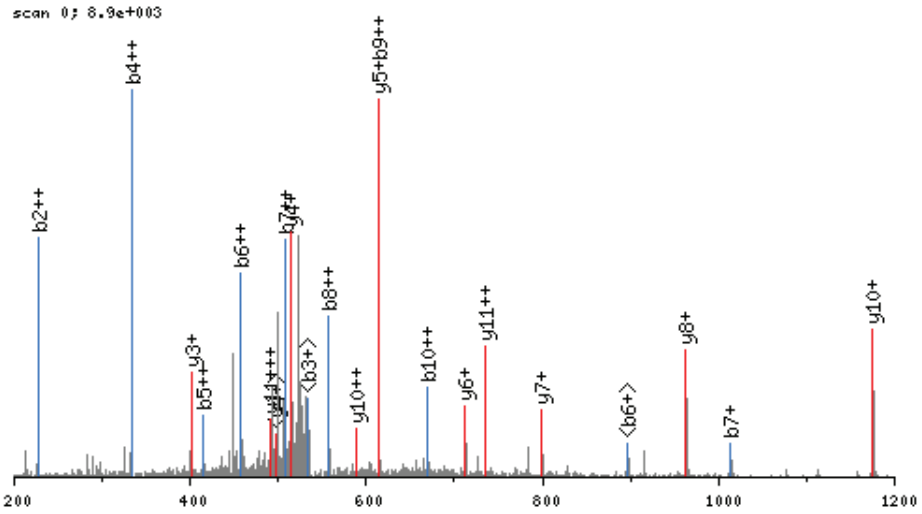
b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
88.0399	44.5238	1	S	27			
383.2294	192.1186	2	H	26	3061.4386	1531.2232	1021.1514
543.2601	272.1340	3	C	25	2766.2490	1383.6284	922.7549
656.3442	328.6760	4	I	24	2606.2184	1303.6131	869.4113
727.3813	364.1946	5	A	23	2493.1343	1247.0711	831.7166
856.4239	428.7159	6	E	22	2422.0972	1211.5525	808.0376
955.4923	478.2501	7	V	21	2293.0546	1147.0312	765.0234
1084.5349	542.7714	8	E	20	2193.9862	1097.4970	732.0006
1198.5778	599.7928	9	N	19	2064.9436	**1032.9757**	688.9864
1313.6048	657.3063	10	D	18	1950.9007	**975.9542**	650.9721
1442.6474	721.8276	11	E	17	1835.8737	918.4408	612.6298
1589.6828	**795.3453**	12	M	16	1706.8311	**853.9195**	569.6156
1686.7355	843.8717	13	P	15	**1559.7957**	**780.4018**	520.6038
1757.7726	**879.3902**	14	A	14	1462.7430	731.8754	488.2529
1872.7996	**936.9037**	15	D	13	**1391.7058**	696.3568	464.5738
1985.8837	**993.4457**	16	L	12	**1276.6789**	638.8434	426.2315
2082.9364	1041.9721	17	P	11	**1163.5948**	**582.3013**	388.5368
2169.9684	1085.4881	18	S	10	1066.5421	533.7749	356.1859
2283.0525	**1142.0302**	19	L	9	**979.5100**	490.2589	327.1752
2354.0896	**1177.5487**	20	A	8	**866.4260**	433.7169	289.4805
2425.1267	**1213.0673**	21	A	7	**795.3889**	398.1983	265.8015
2540.1537	**1270.5808**	22	D	6	**724.3517**	362.6798	242.1225
2687.2221	**1344.1150**	23	F	5	609.3248	305.1663	203.7802
2786.2905	**1393.6492**	24	V	4	462.2564	231.6321	154.7573
2915.3331	**1458.1705**	25	E	3	363.1880	182.0979	121.7345
3002.3651	1501.6865	26	S	2	234.1454	117.5766	78.7203
		27	K	1	147.1134	74.0606	49.7097

H(2):+295.19 C(3):+160.03 M(12):+147.04

COMET Spectrum View by J.Eng (c) ISB 2001
(TPP v4.4 VUVUZELA rev 1, Build 201010121551 (MinGW))

X-range: 200 - 1200
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:
a [ ] + [ ] 2+ [ ] 3+
b [x] + [x] 2+ [ ] 3+
c [ ] + [ ] 2+ [ ] 3+
x [ ] + [ ] 2+ [ ] 3+
y [x] + [x] 2+ [x] 3+
z [ ] + [ ] 2+ [ ] 3+
hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

RHPDYSVVLLLR, MH+ 1625.9743, m/z 542.6629
10HNE-1HSA-Trypsin6-Orbit3.03322.03322.3.dta



click image to zoom in; click top corners to zoom out

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
157.1089	79.0584	1	R	12			
452.2985	226.6532	2	H	11	1469.8732	735.4405	490.6296
549.3513	275.1796	3	P	10	1174.6836	587.8457	392.2331
664.3782	332.6930	4	D	9	1077.6308	539.3193	359.8822
827.4416	414.2247	5	Y	8	962.6039	481.8059	321.5398
914.4736	457.7407	6	S	7	799.5405	400.2742	267.1854
1013.5420	507.2749	7	V	6	712.5085	356.7582	238.1747
1112.6104	556.8091	8	V	5	613.4401	307.2240	205.1519
1225.6945	613.3512	9	L	4	514.3717	257.6898	172.1291
1338.7785	669.8932	10	L	3	401.2876	201.1477	134.4344
1451.8626	726.4352	11	L	2	288.2036	144.6057	96.7397
		12	R	1	175.1195	88.0637	59.0451

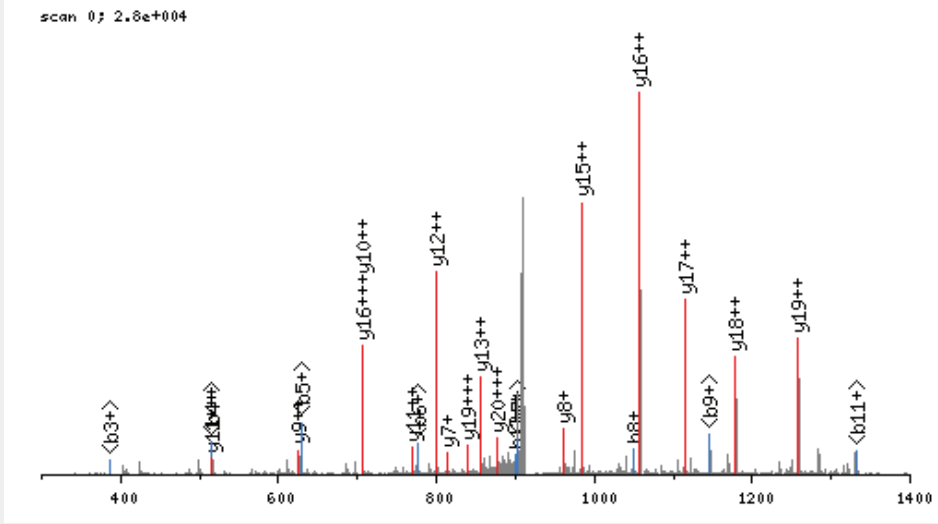
H(2):+295.19

X-range: 300 - 1400
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

QNCELFEQLGEYKFQNALLVR, MH+ 2757.4286, m/z 919.8144
10HNE-1HSA-Trypsin6-Orbit2.03895.03895.3.dta



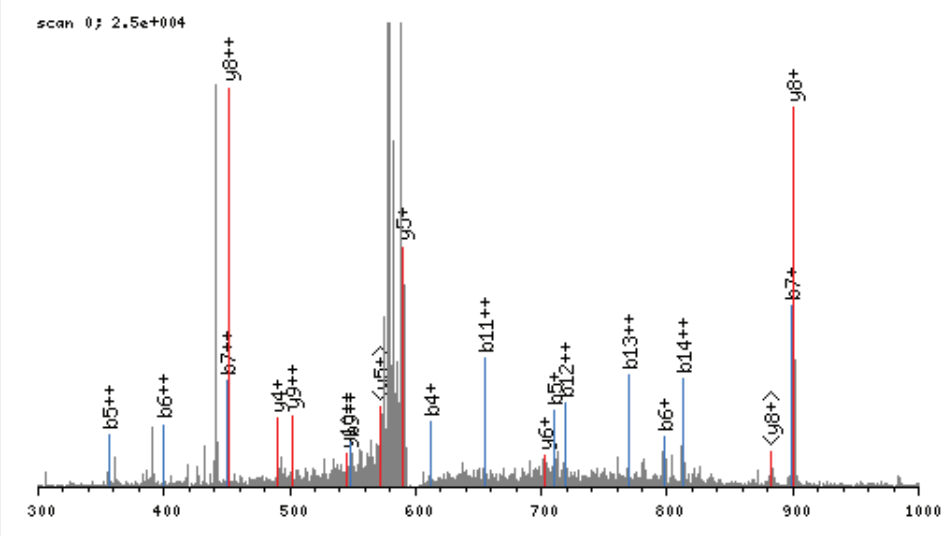
click image to zoom in; click top corners to zoom out

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
129.0664	65.0371	1	Q	21			
243.1093	122.0586	2	N	20	2629.3700	1315.1889	**877.1286**
403.1400	202.0739	3	C	19	2515.3271	**1258.1675**	**839.1142**
532.1826	266.5952	4	E	18	2355.2964	**1178.1521**	785.7707
645.2667	323.1372	5	L	17	2226.2538	**1113.6308**	742.7565
792.3351	396.6715	6	F	16	2113.1698	**1057.0888**	**705.0618**
921.3777	461.1928	7	E	15	1966.1013	**983.5546**	656.0390
1049.4363	525.2220	8	Q	14	1837.0587	919.0333	613.0248
1162.5203	581.7641	9	L	13	1709.0002	**855.0040**	570.3386
1219.5418	610.2748	10	G	12	1595.9161	**798.4620**	532.6439
1348.5844	674.7961	11	E	11	1538.8946	**769.9512**	**513.6368**
1511.6477	756.3278	12	Y	10	1409.8520	**705.4299**	470.6226
1797.8733	**899.4406**	13	K	9	1246.7887	**623.8983**	416.2681
1944.9418	972.9748	14	F	8	**960.5631**	480.7855	320.8596
2073.0003	1037.0041	15	Q	7	**813.4947**	407.2512	271.8368
2187.0433	1094.0255	16	N	6	685.4361	343.2220	229.1506
2258.0804	1129.5441	17	A	5	571.3932	286.2005	191.1363
2371.1644	1186.0861	18	L	4	500.3560	250.6819	167.4572
2484.2485	1242.6282	19	L	3	387.2720	194.1399	129.7625
2583.3169	1292.1624	20	V	2	274.1879	137.5979	92.0679
		21	R	1	175.1195	88.0637	59.0451

C(3):+160.03 K(13):+286.23

X-range: 300 - 1000
MassTol: 0.950 Y-zoom: 7.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:
a [ ] + [ ] 2+ [ ] 3+
b [x] + [x] 2+ [ ] 3+
c [ ] + [ ] 2+ [ ] 3+
x [ ] + [ ] 2+ [ ] 3+
y [x] + [x] 2+ [x] 3+
z [ ] + [ ] 2+ [ ] 3+
hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

KVPQVSTPTLVEVSR, MH+ 1798.0690, m/z 600.0278
10HNE-1HSA-Trypsin6-Orbit2.02814.02814.3.dta



click image to zoom in; click top corners to zoom out

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
287.2335	144.1206	1	K	15			
386.3019	193.6549	2	V	14	1511.8433	756.4256	504.6197
483.3546	242.1812	3	P	13	1412.7749	706.8914	471.5969
611.4132	306.2105	4	Q	12	1315.7222	658.3650	439.2459
710.4816	**355.7447**	5	V	11	1187.6636	594.3357	396.5597
797.5137	**399.2607**	6	S	10	1088.5952	**544.8015**	363.5369
898.5613	**449.7846**	7	T	9	1001.5631	**501.2855**	334.5263
995.6141	498.3110	8	P	8	**900.5155**	**450.7616**	300.8437
1096.6618	**548.8348**	9	T	7	803.4627	402.2353	268.4928
1209.7459	605.3768	10	L	6	**702.4150**	351.7114	234.8102
1308.8143	**654.9110**	11	V	5	**589.3310**	295.1694	197.1155
1437.8569	**719.4323**	12	E	4	**490.2625**	245.6352	164.0927
1536.9253	**768.9665**	13	V	3	361.2199	181.1139	121.0785
1623.9573	**812.4826**	14	S	2	262.1515	131.5797	88.0557
		15	R	1	175.1195	88.0637	59.0451

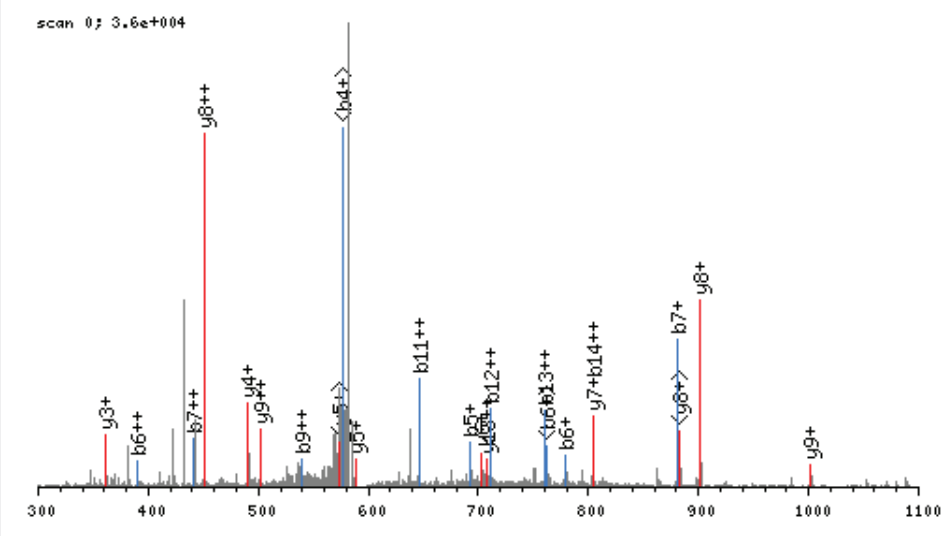
K(1):+286.23

X-range: 300 - 1100
MassTol: 0.950 Y-zoom: 3.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

KVPQVSTPTLVEVSR, MH+ 1780.0584, m/z 594.0243
10HNE-1HSA-Trypsin6-Orbit1.02940.02940.3.dta



click image to zoom in; click top corners to zoom out

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
269.2229	135.1154	1	K	15			
368.2913	184.6496	2	V	14	1511.8433	756.4256	504.6197
465.3441	233.1760	3	P	13	1412.7749	706.8914	471.5969
593.4027	297.2052	4	Q	12	1315.7222	658.3650	439.2459
692.4711	346.7394	5	V	11	1187.6636	594.3357	396.5597
779.5031	390.2555	6	S	10	1088.5952	544.8015	363.5369
880.5508	440.7793	7	T	9	1001.5631	501.2855	334.5263
977.6035	489.3057	8	P	8	900.5155	450.7616	300.8437
1078.6512	539.8295	9	T	7	803.4627	402.2353	268.4928
1191.7353	596.3716	10	L	6	702.4150	351.7114	234.8102
1290.8037	645.9058	11	V	5	589.3310	295.1694	197.1155
1419.8463	710.4271	12	E	4	490.2625	245.6352	164.0927
1518.9147	759.9613	13	V	3	361.2199	181.1139	121.0785
1605.9467	803.4773	14	S	2	262.1515	131.5797	88.0557
		15	R	1	175.1195	88.0637	59.0451

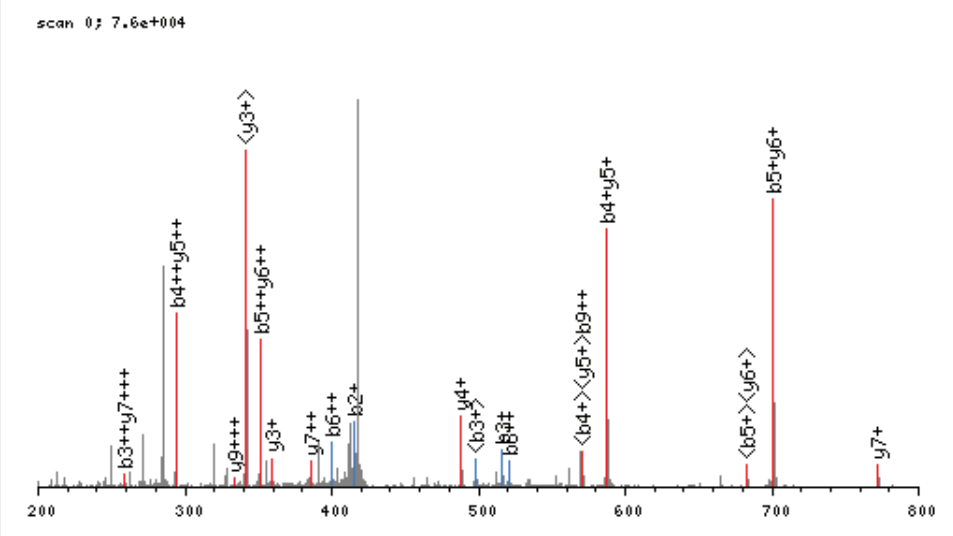
K(1):+268.22

X-range: 200 - 800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: Sm Lg
MassType: AVG MONO
Axis: 1 2
Label: I M -
Ions:

a	+	2+	3+
b	+	2+	3+
c	+	2+	3+
x	+	2+	3+
y	+	2+	3+
z	+	2+	3+

hide H_2O/NH_3
zoom 112-122
zoom 124-133
GO

KQTALVELVK, MH+ 1286.8299, m/z 429.6148
10HNE-1HSA-Trypsin6-Orbit1.02905.02905.3.dta



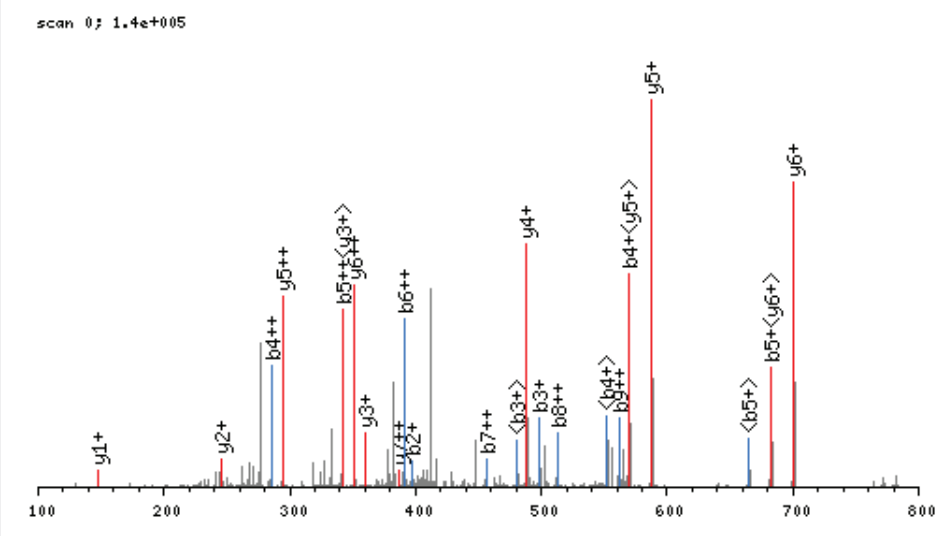
click image to zoom in; click top corners to zoom out

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
287.2335	144.1206	1	K	10			
415.2920	208.1499	2	Q	9	1000.6043	500.8060	334.2066
516.3397	258.6738	3	T	8	872.5457	436.7768	291.5204
587.3768	294.1923	4	A	7	771.4980	386.2529	257.8379
700.4609	350.7344	5	L	6	700.4609	350.7344	234.1589
799.5293	400.2686	6	V	5	587.3768	294.1923	196.4642
928.5719	464.7899	7	E	4	488.3084	244.6581	163.4414
1041.6560	521.3319	8	L	3	359.2658	180.1368	120.4272
1140.7244	570.8661	9	V	2	246.1818	123.5948	82.7325
		10	K	1	147.1134	74.0606	49.7097

K(1):+286.23

X-range: 100 - 800
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:
a [ ] + [ ] 2+ [ ] 3+
b [x] + [x] 2+ [ ] 3+
c [ ] + [ ] 2+ [ ] 3+
x [ ] + [ ] 2+ [ ] 3+
y [x] + [x] 2+ [x] 3+
z [ ] + [ ] 2+ [ ] 3+
hide H_2O/NH_3 [ ]
zoom 112-122 [ ]
zoom 124-133 [ ]
GO

KQTALVELVK, MH+ 1268.8193, m/z 423.6113
10HNE-1HSA-Trypsin6-Orbit3.02993.02993.3.dta



click image to zoom in; click top corners to zoom out

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
269.2229	135.1154	1	K	10			
397.2815	199.1447	2	Q	9	1000.6043	500.8060	334.2066
498.3292	249.6685	3	T	8	872.5457	436.7768	291.5204
569.3663	285.1870	4	A	7	771.4980	386.2529	257.8379
682.4503	341.7291	5	L	6	700.4609	350.7344	234.1589
781.5188	391.2633	6	V	5	587.3768	294.1923	196.4642
910.5613	455.7846	7	E	4	488.3084	244.6581	163.4414
1023.6454	512.3266	8	L	3	359.2658	180.1368	120.4272
1122.7138	561.8608	9	V	2	246.1818	123.5948	82.7325
		10	K	1	147.1134	74.0606	49.7097

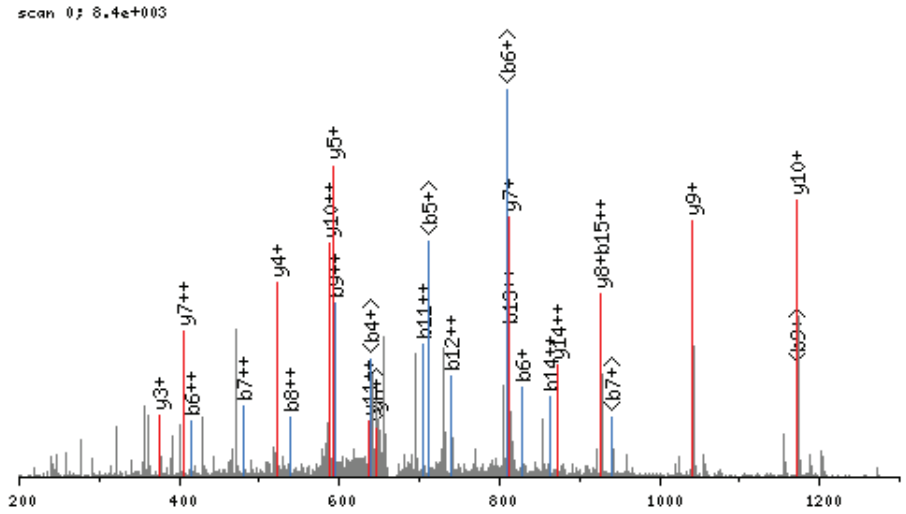
K(1):+268.22

X-range: 200 - 1300
MassTol: 0.950 Y-zoom: 1.00
ImageSize: (•) Sm ( ) Lg
MassType: ( ) AVG (•) MONO
Axis: (•) 1 ( ) 2
Label: (•) I ( ) M ( ) -
Ions:

a	☐ +	☐ 2+	☐ 3+
b	☑ +	☑ 2+	☐ 3+
c	☐ +	☐ 2+	☐ 3+
x	☐ +	☐ 2+	☐ 3+
y	☑ +	☑ 2+	☑ 3+
z	☐ +	☐ 2+	☐ 3+

hide H_2O/NH_3 ☐
zoom 112-122 ☐
zoom 124-133 ☐
GO

EQLKAVMDDFAAFVEK, MH+ 1999.0462, m/z 667.0202
10HNE-1HSA-Trypsin6-Orbit1.03946.03946.3.dta



click image to zoom in; click top corners to zoom out

b^+	b^{2+}	#	AA	#	y^+	y^{2+}	y^{3+}
130.0504	65.5291	1	E	16			
258.1090	129.5584	2	Q	15	1870.0036	935.5057	624.0064
371.1931	186.1004	3	L	14	1741.9450	**871.4764**	581.3202
657.4187	329.2133	4	K	13	1628.8610	814.9344	543.6255
728.4558	364.7318	5	A	12	1342.6353	671.8216	448.2170
827.5242	**414.2660**	6	V	11	1271.5982	**636.3030**	424.5380
958.5647	**479.7863**	7	M	10	**1172.5298**	**586.7688**	391.5151
1073.5917	**537.2997**	8	D	9	**1041.4893**	521.2486	347.8350
1188.6186	**594.8132**	9	D	8	**926.4624**	463.7351	309.4927
1335.6870	668.3474	10	F	7	**811.4354**	**406.2216**	271.1504
1406.7241	**703.8660**	11	A	6	664.3670	332.6874	222.1276
1477.7612	**739.3845**	12	A	5	**593.3299**	297.1689	198.4485
1624.8297	**812.9187**	13	F	4	**522.2928**	261.6503	174.7695
1723.8981	**862.4529**	14	V	3	**375.2244**	188.1161	125.7467
1852.9407	**926.9742**	15	E	2	276.1559	138.5819	92.7239
		16	K	1	147.1134	74.0606	49.7097

K(4):+286.23