Araujo et al.,

A novel intracellular peptide derived from G1/S cyclin D2 induces cell death

Supplementary data from MS and MS/MS analyses

All Mascot results shown here were manually checked, and this was necessary for several reasons, as previously described (Castro, L. M., Berti, D. A., et al. (2010). *AAPS Journal* **12**, 608-616; Fricker, L. D., Gelman, J. S., et al. (2012). *J Proteome Res* **11**, 1981-1990; Gelman, J. S., Wardman, et al. (2012). *Methods Mol Biol* **829**, 487-503; Lyons, P. J., and Fricker, L. D. (2011) *Curr Protoc Protein Sci* **Chapter 18**, Unit18 13).

The peptides being analyzed represent endogenous peptides and not tryptic fragments; therefore a larger number of false positives are possible without the constraints of Lys/Arg residues of the tryptic cleavage site. Secondly, the isotopic tags present several features that are not considered by Mascot, and which therefore are not listed as “matched” ions. For example, neutral loss of trimethylamine from the parent ion is not considered by Mascot, but often represents one of the major peaks in the MS/MS spectra. In contrast, neutral loss is very common for the fragment ions, and this is considered by the Mascot program. However, neutral loss does not always occur for the fragment ions and this is not considered by Mascot. Therefore, fragment ions that contain the intact TMAB label are not assigned by Mascot. Finally, some a ions are abundant for most peptides, especially the a2 ion. Although a ions could be considered by Mascot, we found it was optimal to run the initial Mascot analysis without consideration of a-ions in order to decrease the rate of false positives.

Because of these issues, there are often several major peaks in the MS/MS spectra that are not assigned by Mascot, and so manual interpretation is necessary to assign these peaks. In general, the peptides assigned to the spectra corresponded to the top score of the Mascot search results. However, in some cases two or more peptides were equally likely, differing only in Leu/Ile. When a longer fragment of the same peptide was also found and unambiguously identified by Mascot and the manual interpretation, then the shorter peptide corresponding to this fragment was considered to also be correct. The following MS/MS spectra are arranged in alphabetical order of the peptide sequence and animal tissue sample. The indicated parent mass in the spectra do not match that in the supplemental tables. The mass in these tables represents the theoretical monoisotopic mass of the peptide without isotopic tags or protons, while that in the Mascot results is parent mass with isotopic tags. To convert the observed m/z into the unmodified mass M, multiply m/z and z, and then subtract 128.12 for each D0-TMAB, 131.14 for each D3-TMAB, or 137.17 for each D9-TMAB. Also subtract the number of protons; unlike most proteomic studies, the number of protons is not the same as the charge state because the TMAB labels impart one + charge per label. The number of protons is therefore z-T (where z is charge and T is number of TMAB labels). As described above, the TMAB labels are stable in MS mode, but usually decompose in MS/MS mode, losing the trimethylamine group from each of the tags corresponding to loss of 59 Da, 62 Da, or 68 Da from the D0-, D3- and D9-TMAB, respectively; this represents neutral loss of trimethylamine, with retention of the + charge on the tag remaining on the peptide. To generate a theoretical fragmentation pattern, Protein Prospector (or a comparable program) can be used. The N-terminus should contain the addition of C4 H4 O1 to reflect the mass of the TMAB group minus neutral loss of trimethylamine and also minus 1H so that the automatic addition of an H+ by the program will lead to the correct final mass of +69 (note that this +69 is the same for D0-, D3- and D9-TMAB labels because the isotopic tag is lost upon MS/MS CID). Likewise, internal Lys should be replaced by the user-designated C10 H16 O2 N2 to reflect the mass of Lys with the TMAB group with the same modification as the N-term described above.

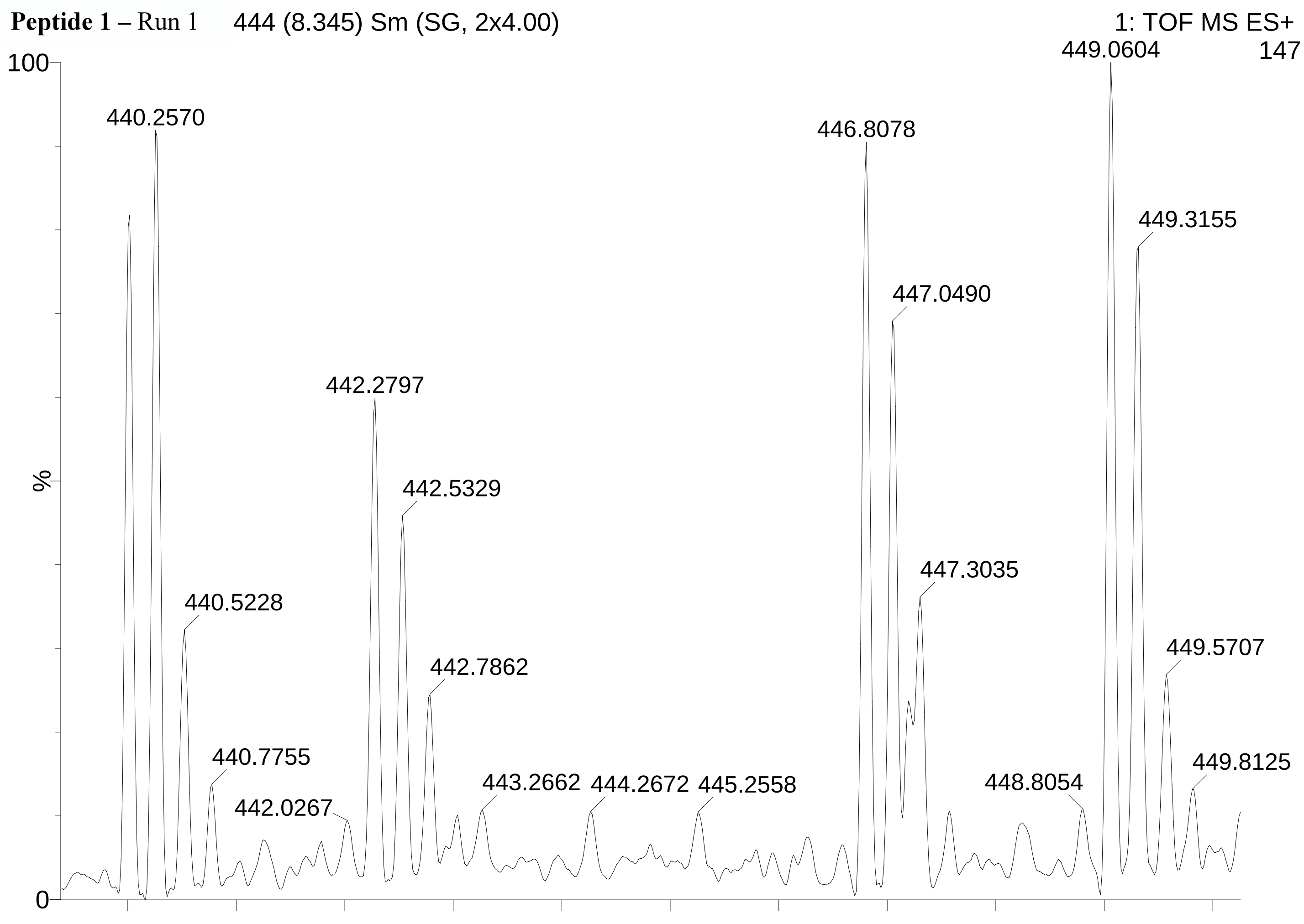
Accordingly, the supplemental data shown both the MS spectra and the Mascot search results for the peptides identified in HeLa cells synchronized or not in G1, S and G2/M phases. The MS and the MS/MS spectra for the 19 peptides were organized in the same order they were described in Table 1.

Run 1: Peptides isolated from asynchronous cells were labeled with D0-TMAB; peptides isolated from S phase were labeled with D3- TMAB; peptides isolated from the

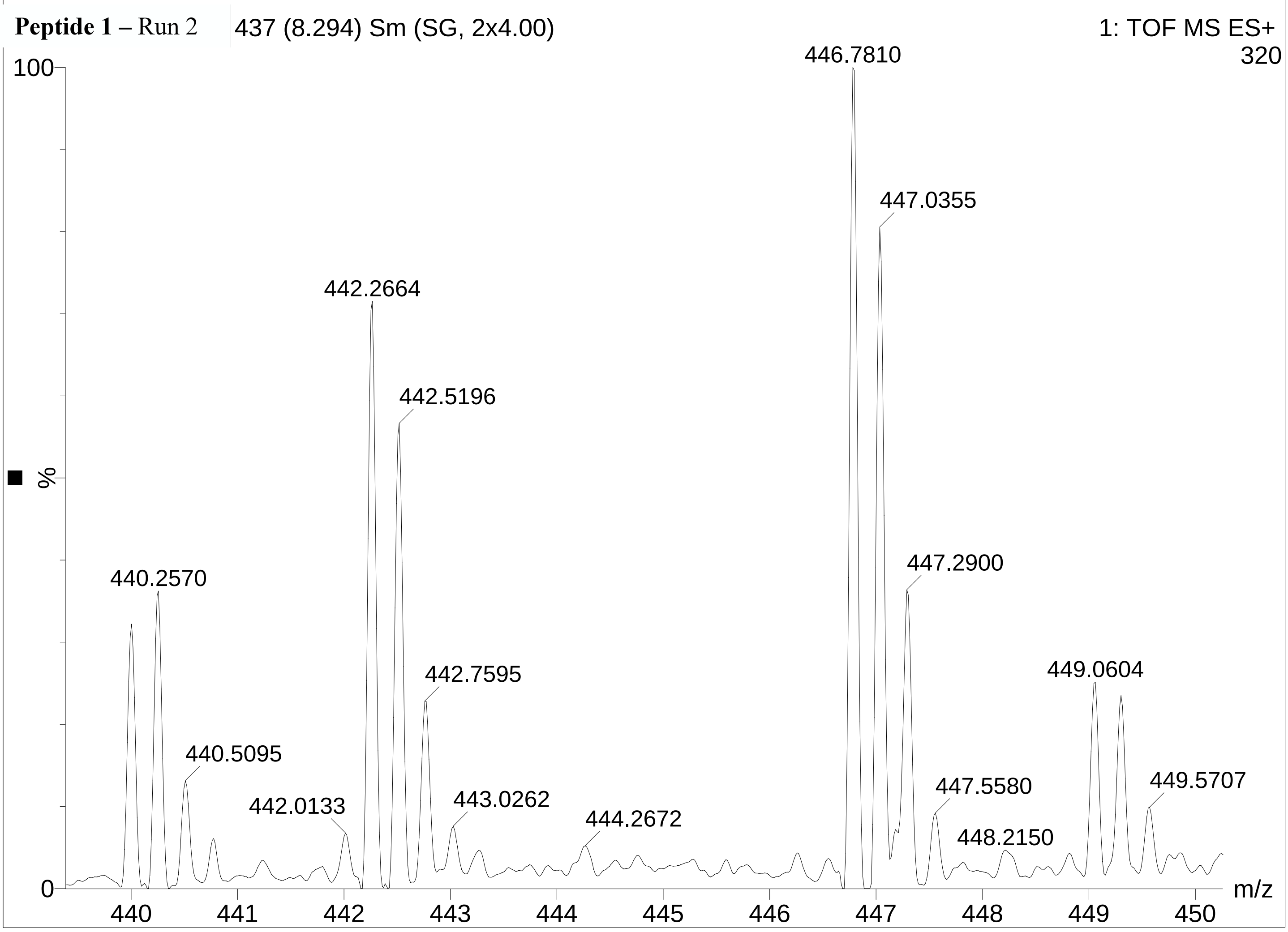
G2/M were labeled with D9-TMAB and peptides isolated from the G1 were labeled with D12-TMAB.

Run 2: Reverse labeling: Peptides isolated from cells in G1 phase of cell cycle were labeled with D0-TMAB; peptides isolated from cells in G2/M phase of the cell cycle with D3-TMAB; peptides isolated from cells in the S phase of the cell cycle were labeled with D9-TMAB; and peptides isolated from asynchronous cells were labeled with D12-TMAB.

Peptide 1 – Run 1



Peptide 1 – Run 2



MATRIX SCIENCE Mascot Search Results

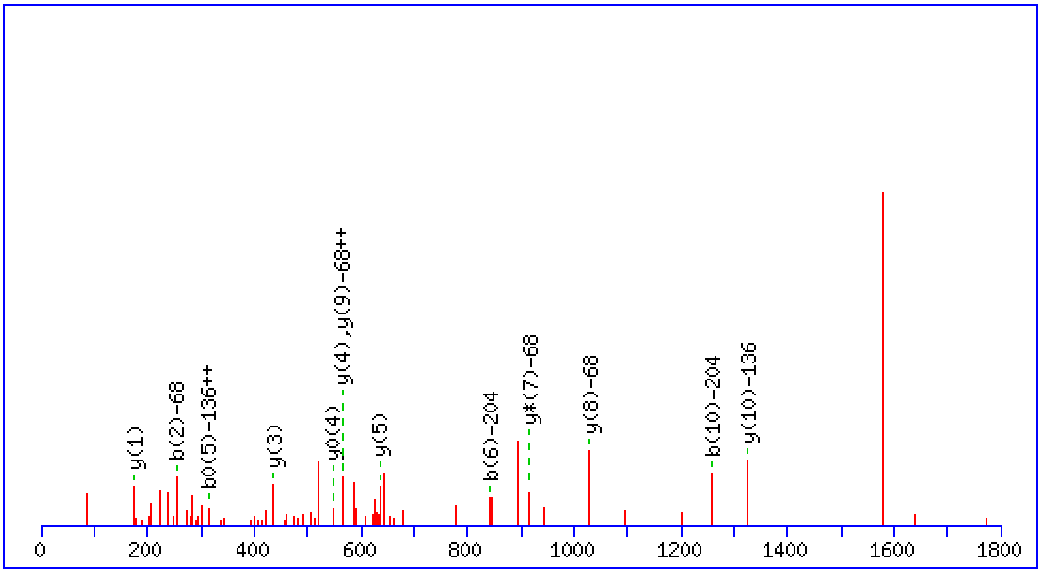
Peptide View

Peptide 1

MS/MS Fragmentation of **ADKVPKTAENFR**
Found in **PPIA_HUMAN**, Peptidyl-prolyl cis-trans isomerase A OS=Homo sapiens GN=PPIA PE=1 SV=2

Match to Query 461: 1783.216976 from(446.811520,4+) intensity(4876.0000)
Title: 28: Sum of 2 scans in range 517 (rt=533.639, f=2, i=19) to 521 (rt=537.737, f=2, i=20) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

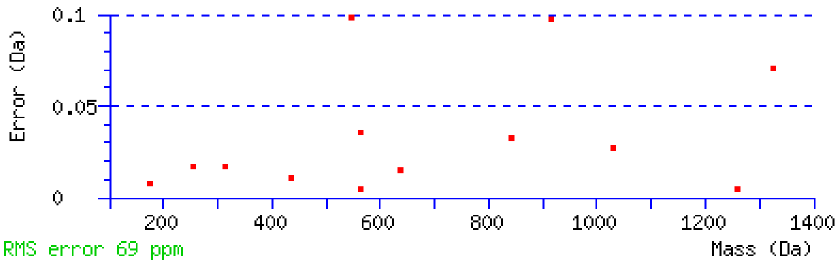
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 0 to 1800 Da Full range
Label all possible matches ○ Label matches used for scoring ●

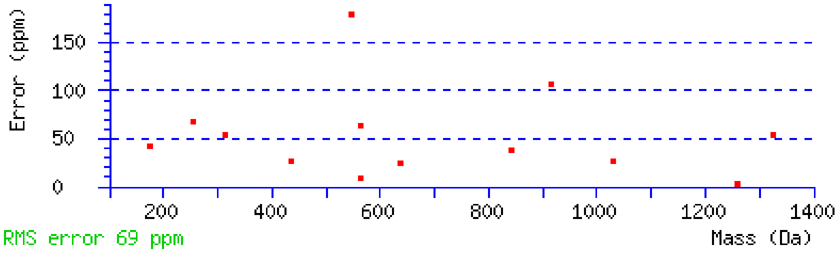


Monoisotopic mass of neutral peptide Mr(calc): 1783.1942
Variable modifications:
N-term : GIST-Quat:2H(9) (N-term), with neutral loss 68.1300
K3 : GIST-Quat:2H(9) (K), with neutral loss 68.1300
K6 : GIST-Quat:2H(9) (K), with neutral loss 68.1300
Ions Score: 17 **Expect:** 7.5e+002
Matches : 13/120 fragment ions using 34 most intense peaks (help)

#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	140.0706	70.5389					A							12
2	***255.0975***	128.0524			237.0870	119.0471	D	1440.7482	720.8777	1423.7216	712.3644	1422.7376	711.8724	11
3	451.2187	226.1130	434.1922	217.5997	433.2082	217.1077	K	***1325.7212***	663.3642	1308.6947	654.8510	1307.7106	654.3590	10
4	550.2871	275.6472	533.2606	267.1339	532.2766	266.6419	V	1129.6000	565.3037	1112.5735	556.7904	1111.5895	556.2984	9
5	647.3399	324.1736	630.3134	315.6603	629.3293	315.1683	P	***1030.5316***	515.7694	1013.5051	507.2562	1012.5211	506.7642	8
6	***843.4611***	422.2342	826.4345	413.7209	825.4505	413.2289	K	933.4789	467.2431	916.4523	458.7298	915.4683	458.2378	7
7	944.5088	472.7580	927.4822	464.2447	926.4982	463.7527	T	737.3577	369.1825	720.3311	360.6692	719.3471	360.1772	6
8	1015.5459	508.2766	998.5193	499.7633	997.5353	499.2713	A	***636.3100***	318.6586	619.2835	310.1454	618.2994	309.6534	5
9	1144.5885	572.7979	1127.5619	564.2846	1126.5779	563.7926	E	***565.2729***	283.1401	548.2463	274.6268	547.2623	274.1348	4

10	***1258.6314***	629.8193	1241.6048	621.3061	1240.6208	620.8141	**N**	***436.2303***	218.6188	419.2037	210.1055			**3**
11	1405.6998	703.3535	1388.6733	694.8403	1387.6892	694.3483	**F**	322.1874	161.5973	305.1608	153.0840			**2**
12							**R**	***175.1190***	88.0631	158.0924	79.5498			**1**



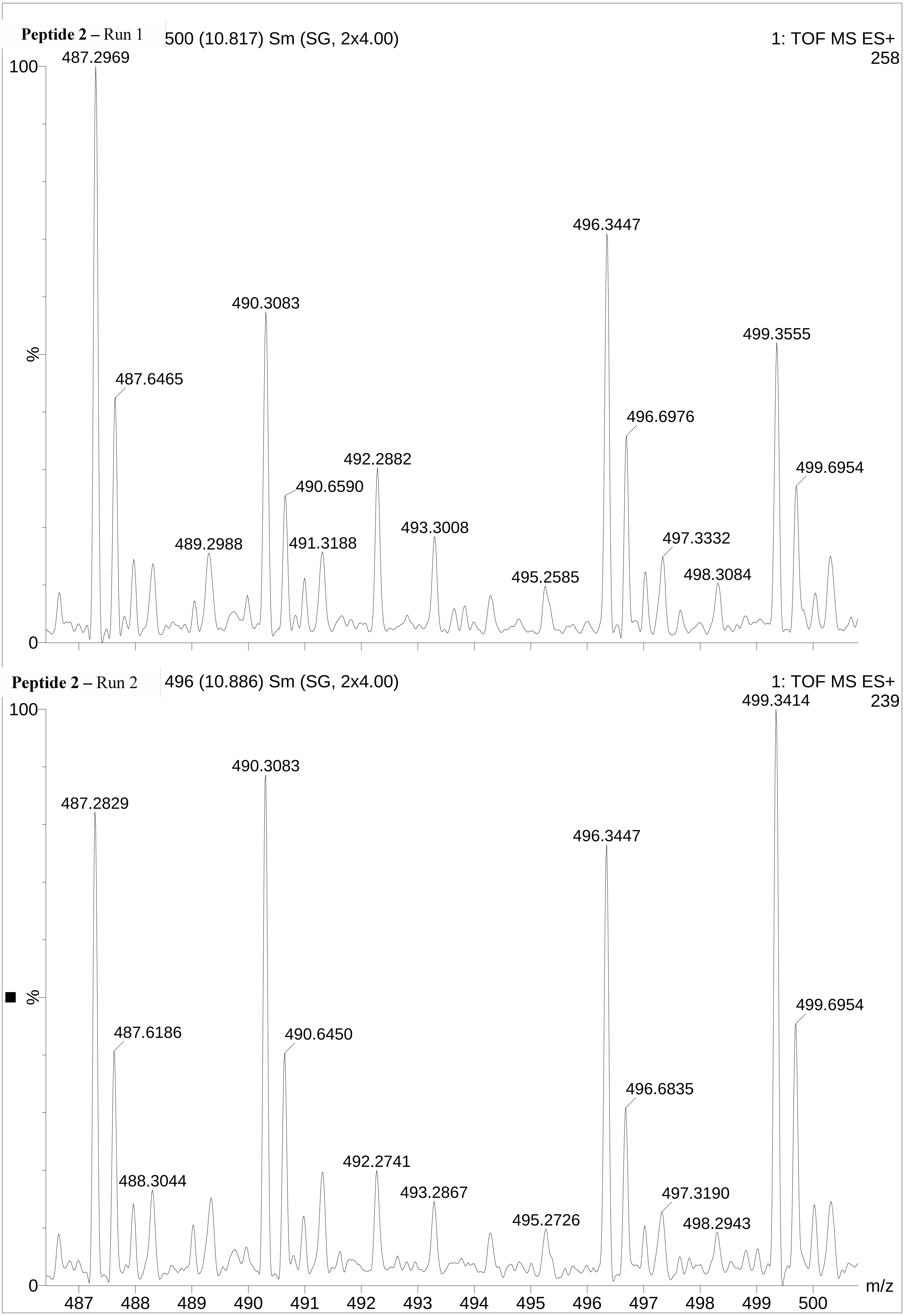


NCBI **BLAST** search of ADKVPKTAENFR
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc):	Delta	Sequence
17.1	1783.1942	0.0228	ADKVPKTAENFR
5.8	1783.0911	0.1259	WEIPRESIKLVKR
4.2	1783.0509	0.1661	PGLTFHIKAAIQHP
4.0	1783.1367	0.0803	ILRGQTRHQVRKGV
3.8	1783.0567	0.1603	SVEAKIEDKKVQR
3.7	1783.0641	0.1529	IIIGASTAAKIMGVAGG
3.1	1783.0567	0.1603	KLEENGIEVSKKR
2.7	1783.1335	0.0835	ILIDLTKQGLLFR
2.4	1783.0945	0.1225	GTFKVRVVTRNPR
2.3	1783.0567	0.1603	QLLNVDLTKDSKR

Mascot: http://www.matrixscience.com/



Peptide 2 – Run 1

Peptide 2 – Run 2

MATRIX SCIENCE

Mascot Search Results

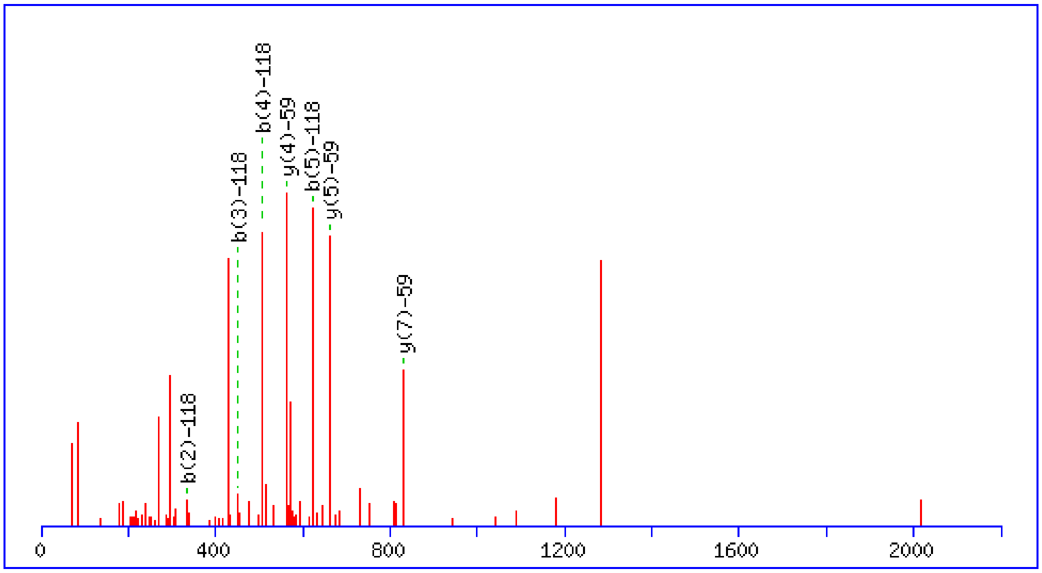
Peptide View

Peptide 2

MS/MS Fragmentation of **KADGIVSKNF**
Found in **RS21_HUMAN**, 40S ribosomal protein S21 OS=Homo sapiens GN=RPS21 PE=1 SV=1

Match to Query 360: 1458.897732 from(487.306520,3+) intensity(6268.0000)
Title: 170: Sum of 2 scans in range 663 (rt=684.036, f=2, i=53) to 665 (rt=686.088, f=4, i=24) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

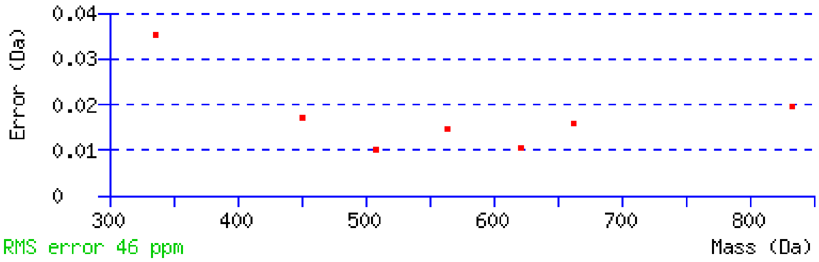
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 0 to 2200 Da Full range
Label all possible matches ○ Label matches used for scoring ○



Monoisotopic mass of neutral peptide Mr(calc): 1458.8810
Variable modifications:
N-term : GIST-Quat (N-term), with neutral loss 59.0735
K1 : GIST-Quat (K), with neutral loss 59.0735
K8 : GIST-Quat (K), with neutral loss 59.0735
Ions Score: 12 **Expect:** 3.4e+003
Matches : 7/96 fragment ions using 22 most intense peaks (help)

#	b	b^{++}	b*	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y^{*++}	y^{0}	y^{0++}	#
1	265.1547	133.0810	248.1281	124.5677			K							10
2	***336.1918***	168.5995	319.1652	160.0863			A	1018.5204	509.7638	1001.4938	501.2506	1000.5098	500.7585	9
3	***451.2187***	226.1130	434.1922	217.5997	433.2082	217.1077	D	947.4833	474.2453	930.4567	465.7320	929.4727	465.2400	8
4	***508.2402***	254.6237	491.2136	246.1105	490.2296	245.6185	G	***832.4563***	416.7318	815.4298	408.2185	814.4458	407.7265	7
5	***621.3243***	311.1658	604.2977	302.6525	603.3137	302.1605	I	775.4349	388.2211	758.4083	379.7078	757.4243	379.2158	6
6	720.3927	360.7000	703.3661	352.1867	702.3821	351.6947	V	***662.3508***	331.6790	645.3243	323.1658	644.3402	322.6738	5
7	807.4247	404.2160	790.3981	395.7027	789.4141	395.2107	S	***563.2824***	282.1448	546.2558	273.6316	545.2718	273.1395	4
8	1003.5459	502.2766	986.5193	493.7633	985.5353	493.2713	K	476.2504	238.6288	459.2238	230.1155			3
9	1117.5888	559.2980	1100.5623	550.7848	1099.5782	550.2928	N	280.1292	140.5682	263.1026	132.0550			2

10							**F**	166.0863	83.5468					**1**



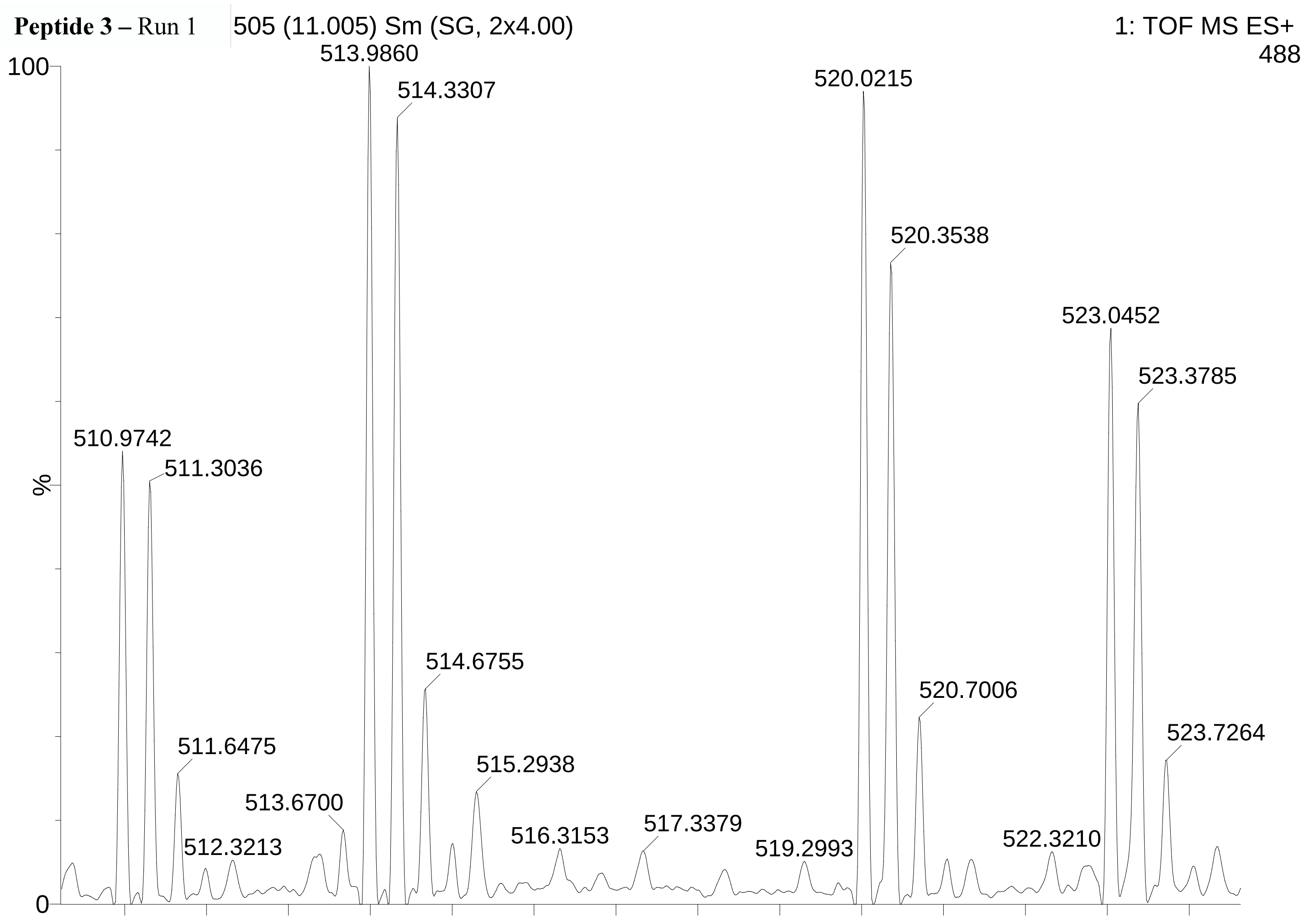
Error Distribution (ppm)

NCBI **BLAST** search of KADGIVSKNF
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

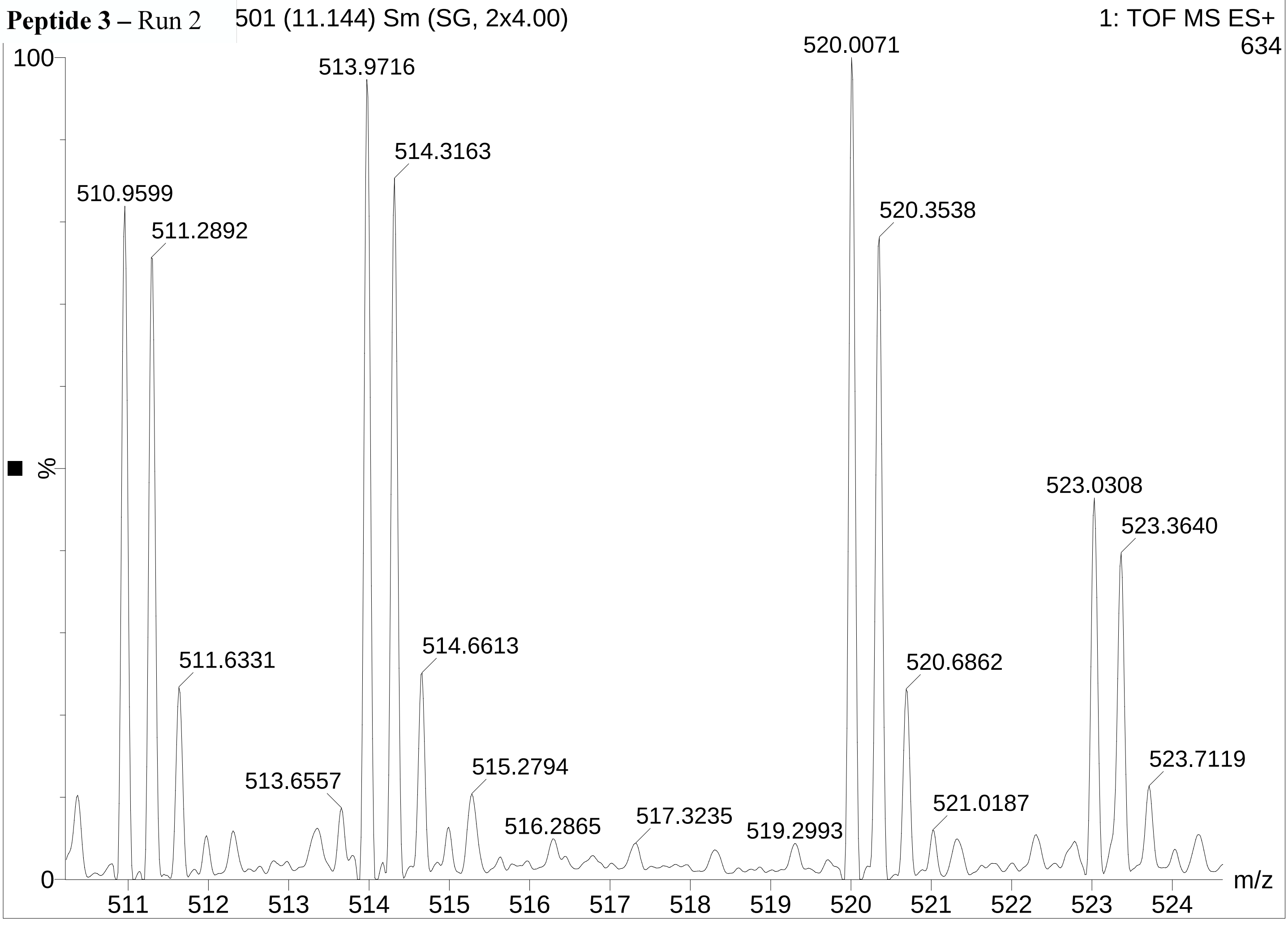
All matches to this query

Score	Mr(calc):	Delta	Sequence
12.4	1458.8678	0.0299	WTLPYKIGVVGP
12.0	1458.8810	0.0167	KADGIVSKNF
10.9	1458.8025	0.0953	FVLTLSCVGFFP
9.9	1458.8176	0.0801	DLMKEFPLLSM
9.3	1458.7599	0.1378	NNCHPTPGLSGIN
9.2	1458.8392	0.0585	PGLDGAKGEAGAPG
9.2	1458.8392	0.0585	PGLDGAKGEAGAPG
6.3	1458.9901	-0.0924	GIPLNVLPKK
5.9	1458.8433	0.0545	LDKEFQLFQGV
5.8	1458.7943	0.1034	AQHILSSAHPSGK

Mascot: http://www.matrixscience.com/



Peptide 3 – Run 1



Peptide 3 – Run 2

Mascot Search Results

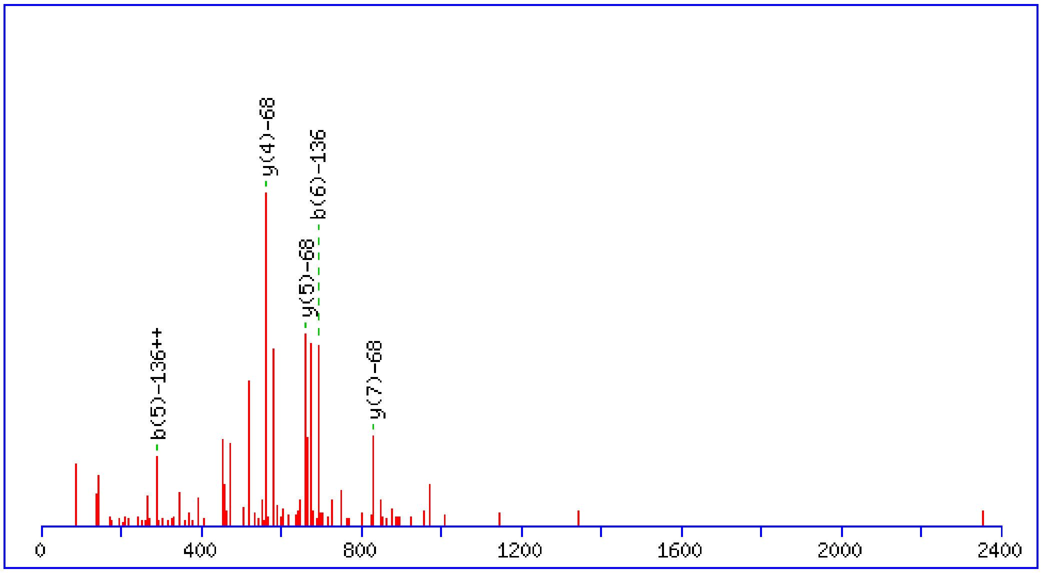
Peptide View

Peptide 3

MS/MS Fragmentation of **AKADGIVSKNF**
Found in **RS21_HUMAN**, 40S ribosomal protein S21 OS=Homo sapiens GN=RPS21 PE=1 SV=1

Match to Query 415: 1557.075012 from(520.032280,3+) intensity(2453.0000)
Title: 194: Scan 691 (rt=712.887, f=4, i=29) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

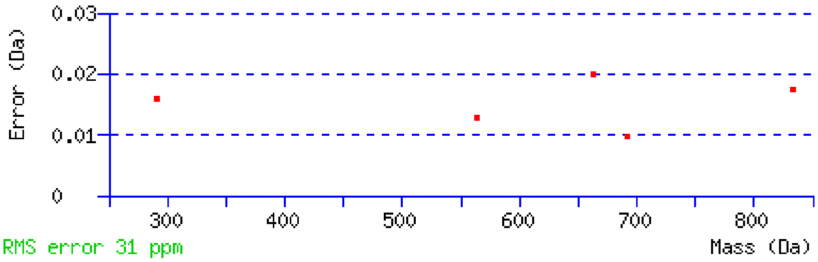
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 0 to 2400 Da Full range
Label all possible matches ○ Label matches used for scoring ○

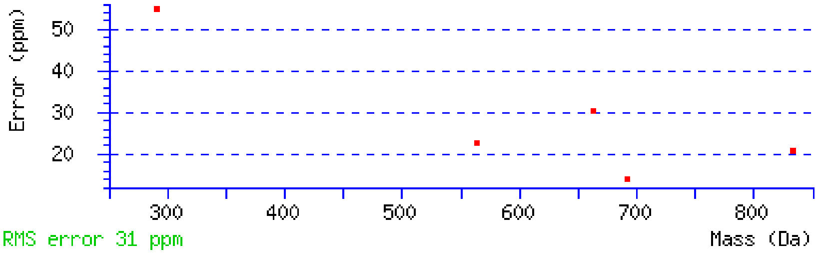


Monoisotopic mass of neutral peptide Mr(calc): 1557.0876
Variable modifications:
N-term : GIST-Quat:2H(9) (N-term), with neutral loss 68.1300
K2 : GIST-Quat:2H(9) (K), with neutral loss 68.1300
K9 : GIST-Quat:2H(9) (K), with neutral loss 68.1300
Ions Score: 9 **Expect:** 4.7e+003
Matches : 5/104 fragment ions using 12 most intense peaks (help)

#	b	b^{++}	b*	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y^{*++}	y^{0}	y^{0++}	#
1	140.0706	70.5389					**A**							11
2	336.1918	168.5995	319.1652	160.0863			**K**	1214.6416	607.8244	1197.6150	599.3111	1196.6310	598.8191	10
3	407.2289	204.1181	390.2023	195.6048			**A**	1018.5204	509.7638	1001.4938	501.2506	1000.5098	500.7585	9
4	522.2558	261.6316	505.2293	253.1183	504.2453	252.6263	**D**	947.4833	474.2453	930.4567	465.7320	929.4727	465.2400	8
5	579.2773	**290.1423**	562.2508	281.6290	561.2667	281.1370	**G**	***832.4563***	416.7318	815.4298	408.2185	814.4458	407.7265	7
6	**692.3614**	346.6843	675.3348	338.1710	674.3508	337.6790	**I**	775.4349	388.2211	758.4083	379.7078	757.4243	379.2158	6
7	791.4298	396.2185	774.4032	387.7053	773.4192	387.2132	**V**	***662.3508***	331.6790	645.3243	323.1658	644.3402	322.6738	5
8	878.4618	439.7345	861.4353	431.2213	860.4512	430.7293	**S**	***563.2824***	282.1448	546.2558	273.6316	545.2718	273.1395	4
9	1074.5830	537.7951	1057.5564	529.2819	1056.5724	528.7898	**K**	476.2504	238.6288	459.2238	230.1155			3
10	1188.6259	594.8166	1171.5994	586.3033	1170.6153	585.8113	**N**	280.1292	140.5682	263.1026	132.0550			2

11							**F**	166.0863	83.5468					**1**



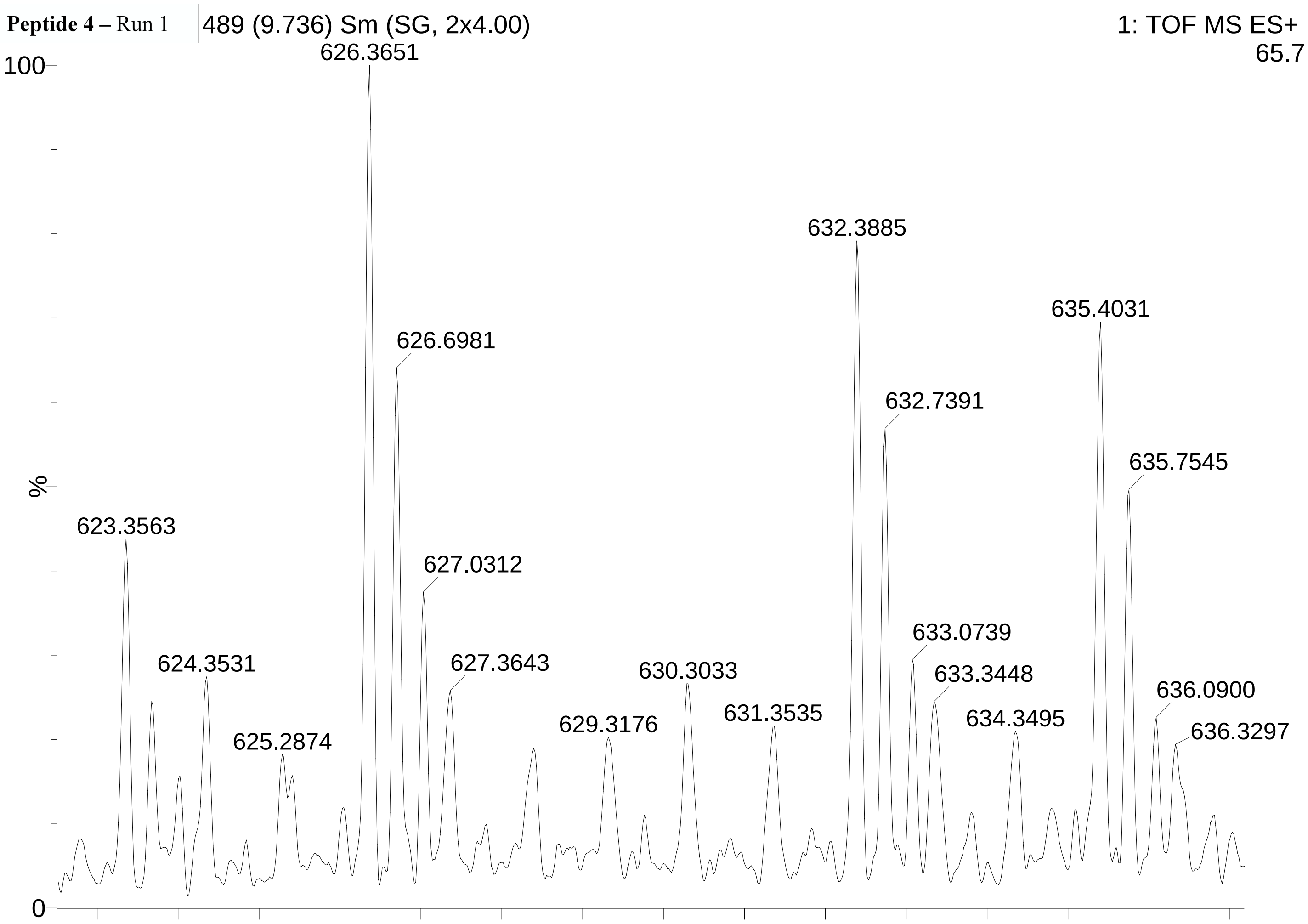


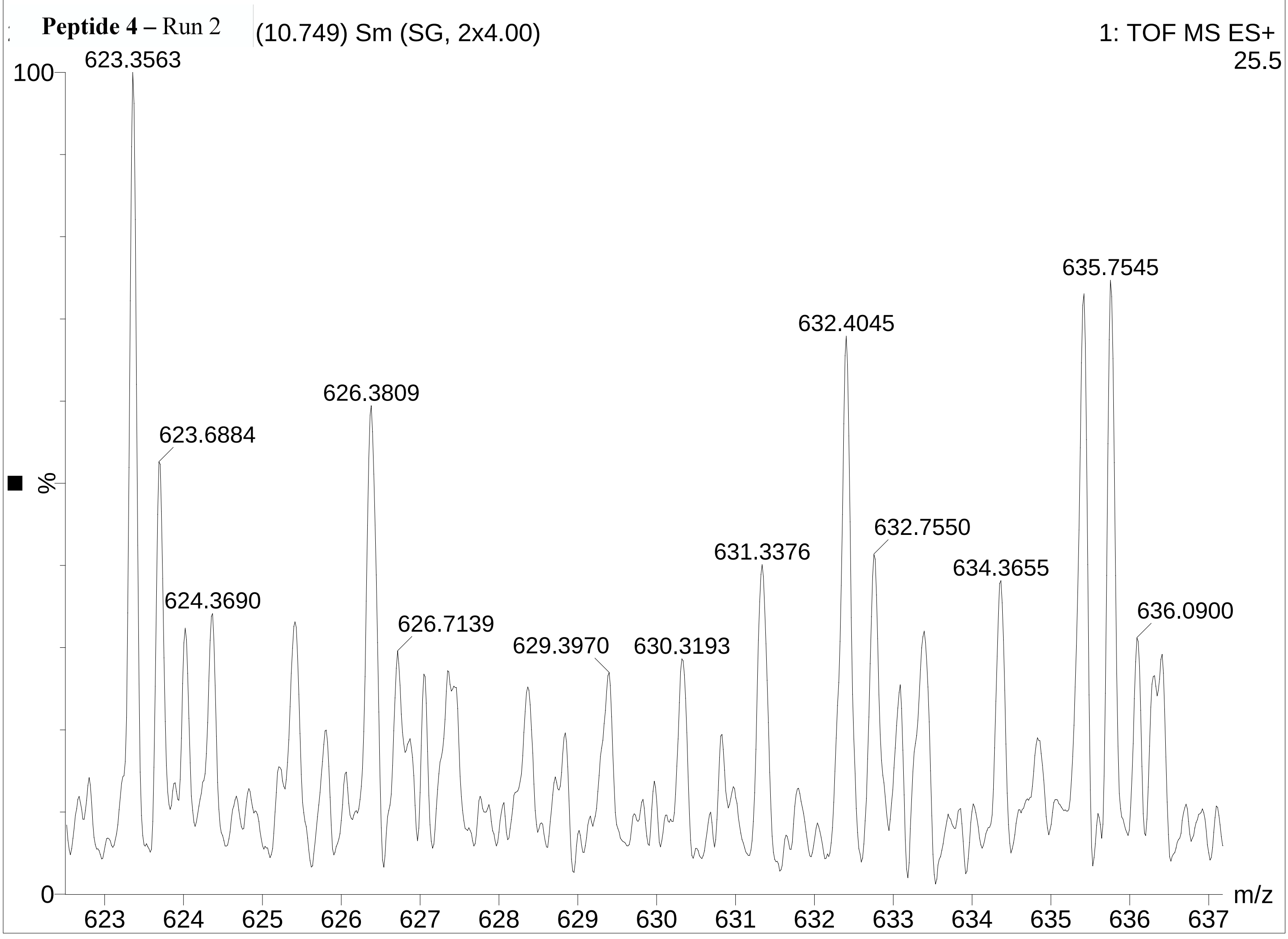
NCBI **BLAST** search of AKADGIVSKNF
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc):	Delta	Sequence
8.9	1557.0876	-0.0126	AKADGIVSKNF
7.5	1557.2331	-0.1581	KGLKVLPKGIP
7.5	1556.9522	0.1228	LGLVKLPLHQFY
6.9	1556.9079	0.1672	IGNKNPALWKY
6.7	1557.0268	0.0482	HEGRKGAIAKKP
6.7	1557.0268	0.0482	HEGRKGAIAKKP
6.7	1557.0268	0.0482	HEGRKGALAKKP
6.7	1557.0268	0.0482	HEGRKGALAKKP
5.8	1556.9613	0.1137	KKRAKLSGSTLD
4.8	1556.9488	0.1262	GDLQPLPIQKGE

Mascot: http://www.matrixscience.com/


Peptide 4 – Run 1
489 (9.736) Sm (SG, 2x4.00)
1: TOF MS ES+
65.7
100
%
0
626.3651
632.3885
635.4031
626.6981
632.7391
635.7545
623.3563
627.0312
633.0739
624.3531
627.3643
630.3033
633.3448
636.0900
625.2874
629.3176
631.3535
634.3495
636.3297


Peptide 4 – Run 2
(10.749) Sm (SG, 2x4.00)
1: TOF MS ES+
25.5
100
%
0
623.3563
635.7545
632.4045
626.3809
623.6884
632.7550
631.3376
634.3655
624.3690
636.0900
626.7139
629.3970
630.3193
m/z
623
624
625
626
627
628
629
630
631
632
633
634
635
636
637

Mascot Search Results

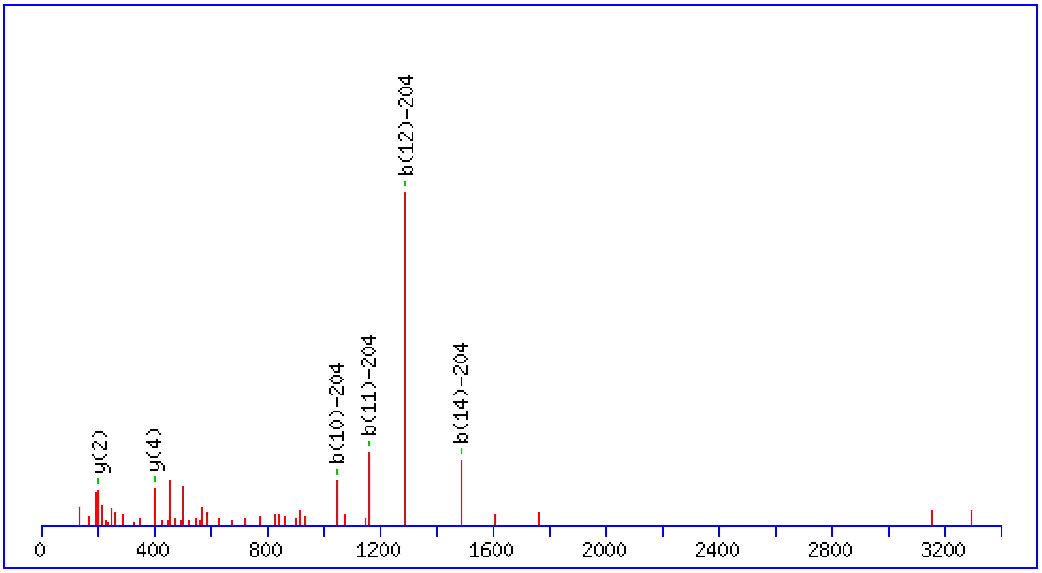
Peptide View

Peptide 4

MS/MS Fragmentation of **GSGSKGKGGEIQPVSV**
Found in **CH10_HUMAN**, 10 kDa heat shock protein, mitochondrial OS=Homo sapiens GN=HSPE1 PE=1 SV=2

Match to Query 489: 1894.253022 from(632.424950,3+) intensity(2786.0000)
Title: 56: Sum of 2 scans in range 568 (rt=586.216, f=3, i=17) to 569 (rt=587.237, f=4, i=10) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

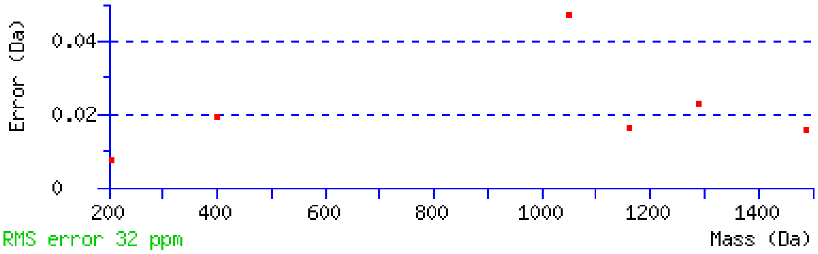
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 0 to 3400 Da Full range
Label all possible matches ○ Label matches used for scoring ○

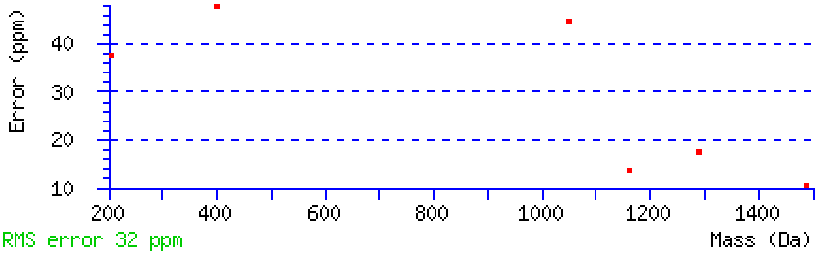


Monoisotopic mass of neutral peptide Mr(calc): 1894.2473
Variable modifications:
N-term : GIST-Quat:2H(9) (N-term), with neutral loss 68.1300
K5 : GIST-Quat:2H(9) (K), with neutral loss 68.1300
K7 : GIST-Quat:2H(9) (K), with neutral loss 68.1300
Ions Score: 16 **Expect:** 1.2e+003
Matches : 6/160 fragment ions using 14 most intense peaks (help)

#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	126.0550	63.5311					G							16
2	213.0870	107.0471			195.0764	98.0418	S	1565.8170	783.4121	1548.7904	774.8988	1547.8064	774.4068	15
3	270.1084	135.5579			252.0979	126.5526	G	1478.7849	739.8961	1461.7584	731.3828	1460.7744	730.8908	14
4	357.1405	179.0739			339.1299	170.0686	S	1421.7635	711.3854	1404.7369	702.8721	1403.7529	702.3801	13
5	553.2617	277.1345	536.2351	268.6212	535.2511	268.1292	K	1334.7314	667.8694	1317.7049	659.3561	1316.7209	658.8641	12
6	610.2831	305.6452	593.2566	297.1319	592.2726	296.6399	G	1138.6103	569.8088	1121.5837	561.2955	1120.5997	560.8035	11
7	806.4043	403.7058	789.3777	395.1925	788.3937	394.7005	K	1081.5888	541.2980	1064.5623	532.7848	1063.5782	532.2928	10
8	863.4258	432.2165	846.3992	423.7032	845.4152	423.2112	G	885.4676	443.2375	868.4411	434.7242	867.4571	434.2322	9
9	920.4472	460.7272	903.4207	452.2140	902.4367	451.7220	G	828.4462	414.7267	811.4196	406.2134	810.4356	405.7214	8

10	*1049.4898*	525.2485	1032.4633	516.7353	1031.4793	516.2433	**E**	771.4247	386.2160	754.3981	377.7027	753.4141	377.2107	**7**
11	*1162.5739*	581.7906	1145.5473	573.2773	1144.5633	572.7853	**I**	642.3821	321.6947	625.3556	313.1814	624.3715	312.6894	**6**
12	*1290.6325*	645.8199	1273.6059	637.3066	1272.6219	636.8146	**Q**	529.2980	265.1527	512.2715	256.6394	511.2875	256.1474	**5**
13	1387.6852	694.3462	1370.6587	685.8330	1369.6747	685.3410	**P**	**401.2395**	201.1234			383.2289	192.1181	**4**
14	*1486.7536*	743.8805	1469.7271	735.3672	1468.7431	734.8752	**V**	304.1867	152.5970			286.1761	143.5917	**3**
15	1573.7857	787.3965	1556.7591	778.8832	1555.7751	778.3912	**S**	**205.1183**	103.0628			187.1077	94.0575	**2**
16							**V**	118.0863	59.5468					**1**





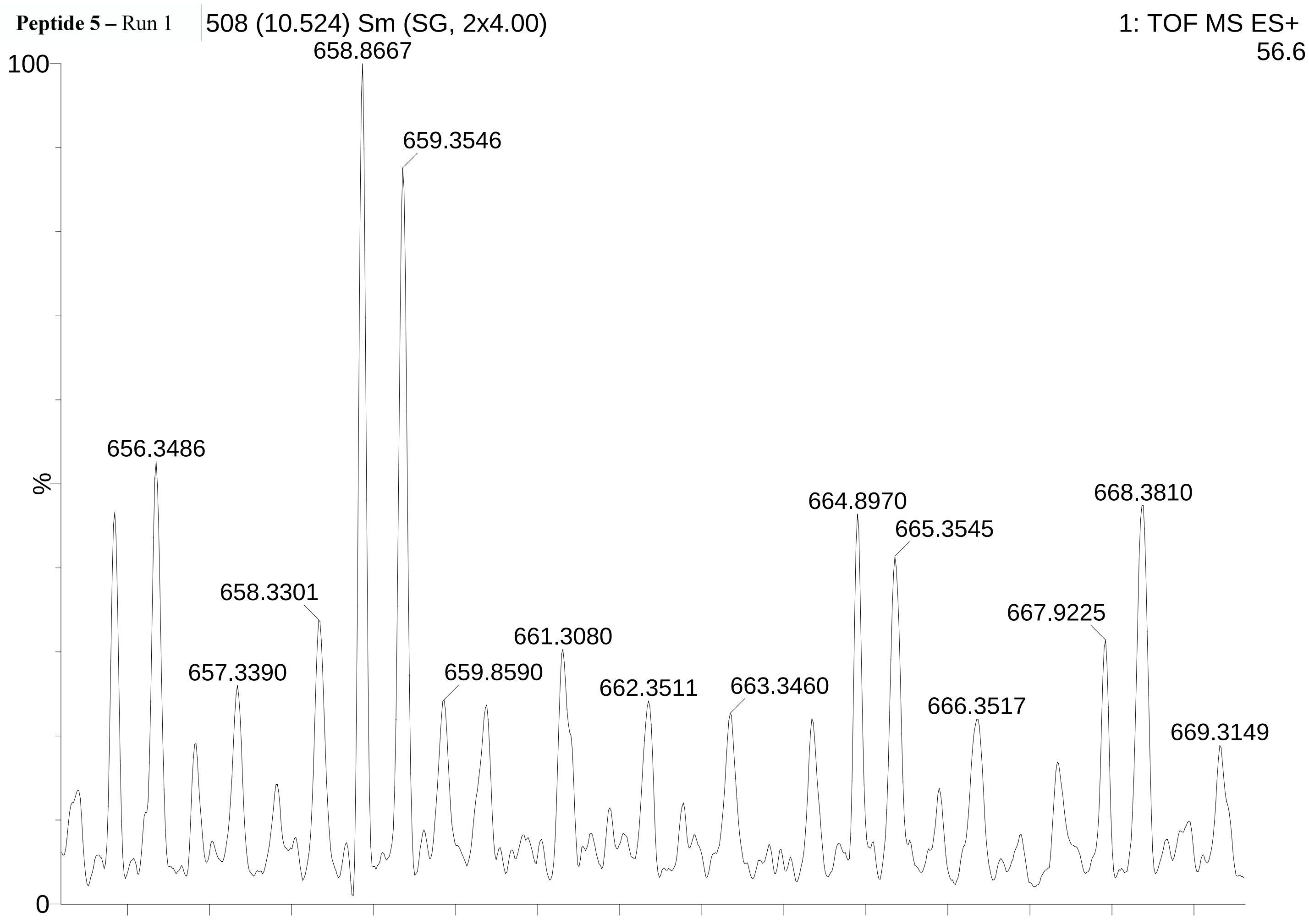
NCBI **BLAST** search of GSGSKGKGGEIQPVSV
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

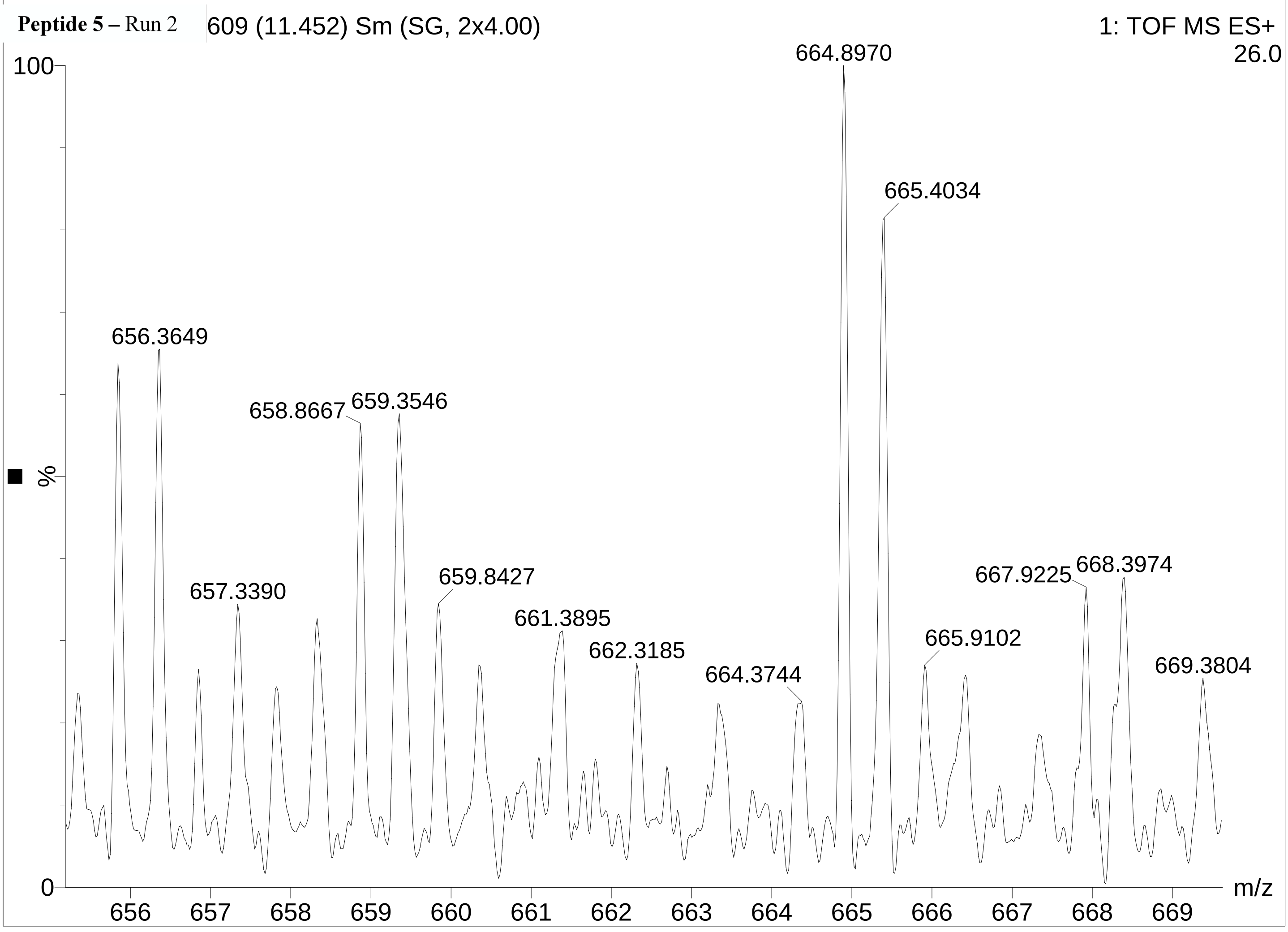
Score	Mr(calc):	Delta	Sequence
22.2	1894.2462	0.0069	GKSKKFTLKRLMAD
20.1	1894.1503	0.1028	RGKKLPNNPAFGFVS
20.1	1894.1503	0.1028	RGKKLPNNPAFGFVS
20.1	1894.0927	0.1603	YKKYALQSAAGKDA
15.9	1894.1006	0.1525	ESKKVSASTLKRDAD
15.9	1894.2473	0.0057	GSGSKGKGGEIQPVSV
15.9	1894.3717	-0.1187	RLTGFKIPLKKDA
15.9	1894.2989	-0.0459	TPEERTKALKKW
14.2	1894.1000	0.1531	DSKKKKHELKITQQG
14.2	1894.1000	0.1531	DSKKKKHELKITQQG

Mascot: http://www.matrixscience.com/

Peptide 5 – Run 1



Peptide 5 – Run 2



Mascot Search Results

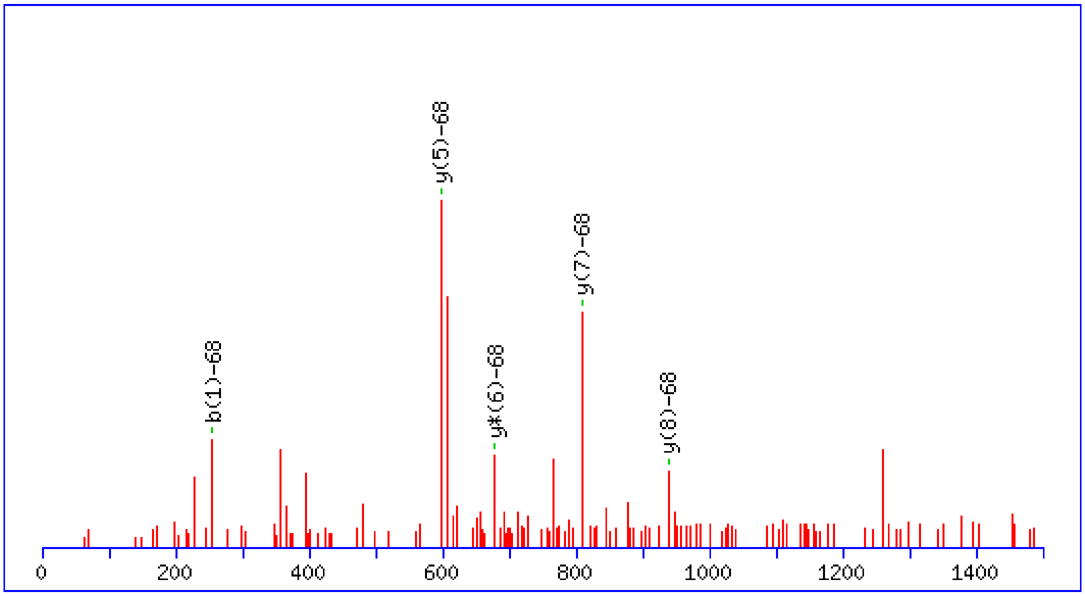
Peptide View

Peptide 5

MS/MS Fragmentation of **WELVVLGKL**
Found in **CCND2_HUMAN**, G1/S-specific cyclin-D2 OS=Homo sapiens GN=CCND2 PE=1 SV=1

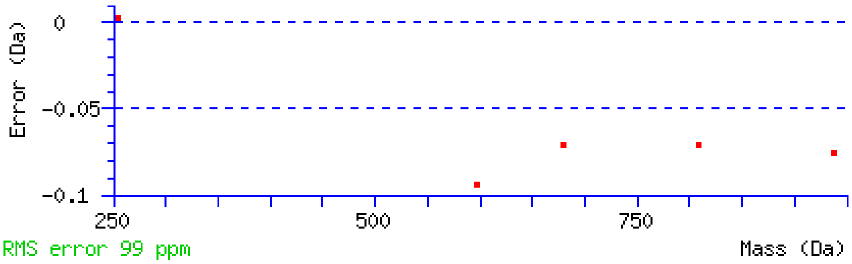
Match to Query 299: 1327.812108 from(664.913330,2+) intensity(1067.0000)
Title: 110: Scan 616 (rt=635.716, f=4, i=16) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

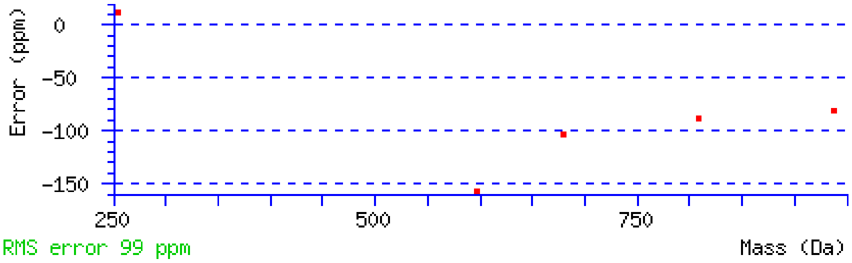
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 0 to 1500 Da Full range
Label all possible matches ○ Label matches used for scoring ○



Monoisotopic mass of neutral peptide Mr(calc): 1327.9503
Variable modifications:
N-term : GIST-Quat:2H(9) (N-term), with neutral loss 68.1300
K8 : GIST-Quat:2H(9) (K), with neutral loss 68.1300
Ions Score: 7 **Expect:** 2
Matches : 5/64 fragment ions using 13 most intense peaks (help)

#	b	b^{++}	b^*	b^{*++}	b^0	b^{0++}	Seq.	y	y^{++}	y^*	y^{*++}	y^0	y^{0++}	#
1	**255.1128**	128.0600					W							9
2	384.1554	192.5813			366.1448	183.5761	E	***938.5921***	469.7997	921.5655	461.2864	920.5815	460.7944	8
3	497.2395	249.1234			479.2289	240.1181	L	***809.5495***	405.2784	792.5230	396.7651			7
4	596.3079	298.6576			578.2973	289.6523	V	696.4654	348.7364	679.4389	340.2231			6
5	695.3763	348.1918			677.3657	339.1865	V	***597.3970***	299.2022	580.3705	290.6889			5
6	808.4604	404.7338			790.4498	395.7285	L	498.3286	249.6679	481.3021	241.1547			4
7	865.4818	433.2445			847.4713	424.2393	G	385.2445	193.1259	368.2180	184.6126			3
8	1061.6030	531.3051	1044.5764	522.7919	1043.5924	522.2999	K	328.2231	164.6152	311.1965	156.1019			2
9							L	132.1019	66.5546					1



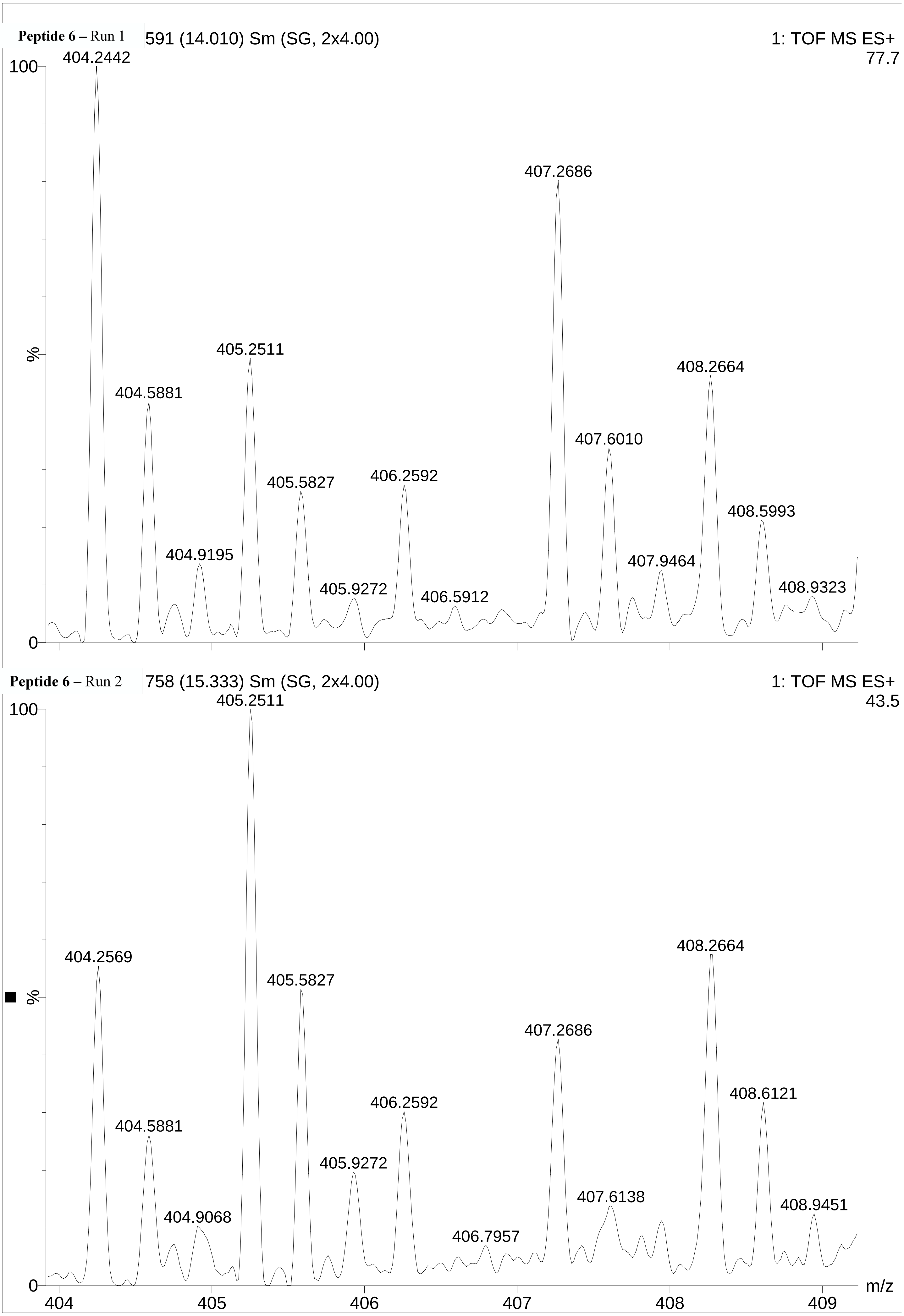


NCBI **BLAST** search of WELVVLGKL
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc):	Delta	Sequence
11.5	1327.6983	0.1138	ADRDAIVEALE
9.8	1327.7525	0.0596	WTEQKENQ
9.8	1327.7525	0.0596	WTEQKENQ
8.9	1327.8266	-0.0145	VGKGLAAVLENK
7.5	1327.9503	-0.1382	WELVVLGKL
7.0	1327.6442	0.1679	EHKDSVMAVLEA
7.0	1327.6792	0.1329	GPGDGIVMAFDN
6.4	1327.7004	0.1117	DATQLVCTDLN
6.4	1327.8518	-0.0397	ELLLQVLSVGK
6.3	1327.8847	-0.0726	EGTLQPQKR

Mascot: http://www.matrixscience.com/


Peptide 6 – Run 1
591 (14.010) Sm (SG, 2x4.00)
1: TOF MS ES+
77.7
100
%
0
404.2442
404.5881
404.9195
405.2511
405.5827
405.9272
406.2592
406.5912
407.2686
407.6010
407.9464
408.2664
408.5993
408.9323
Peptide 6 – Run 2
758 (15.333) Sm (SG, 2x4.00)
1: TOF MS ES+
43.5
100
%
0
405.2511
404.2569
405.5827
404.5881
404.9068
405.9272
406.2592
406.7957
407.2686
407.6138
408.2664
408.6121
408.9451
404
405
406
407
408
409
m/z

Mascot Search Results

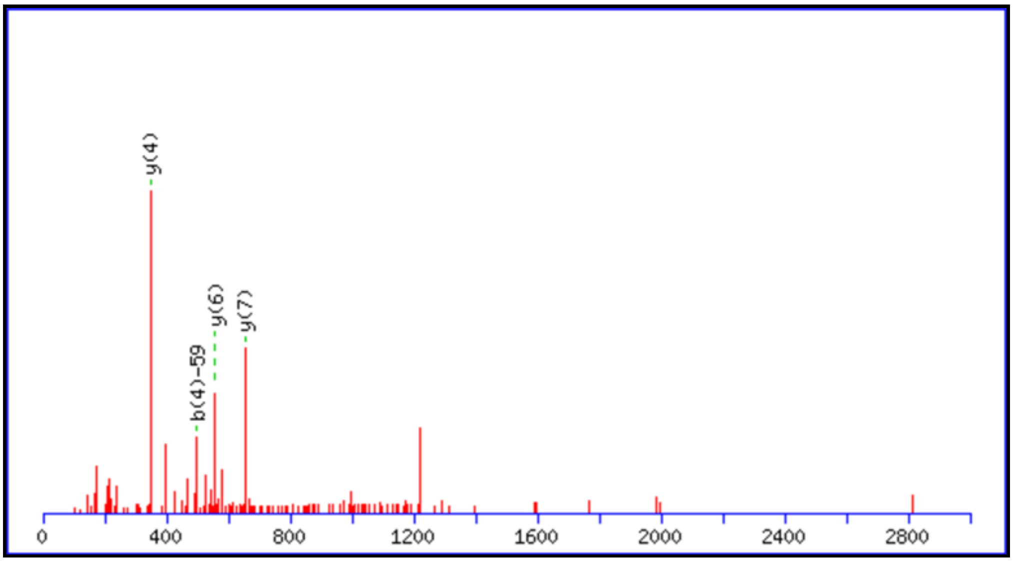
Peptide View

Peptide 6

MS/MS Fragmentation of **QITSPIPAIGS**
Found in **TOX3_HUMAN**, TOX high mobility group box family member 3 OS=Homo sapiens GN=TOX3 PE=2 SV=2

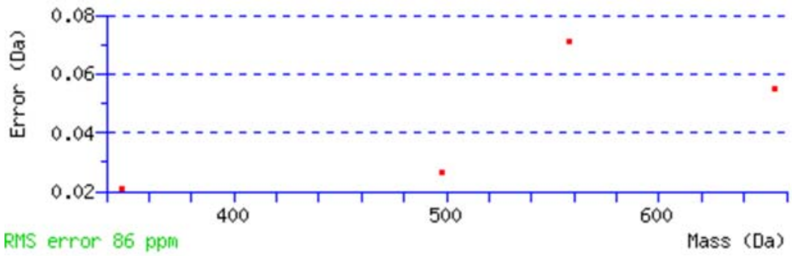
Match to Query 238: 1209.781272 from(404.267700,3+) intensity(1687.0000)
Title: 312: Scan 808 (rt=833.413, f=2, i=87) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

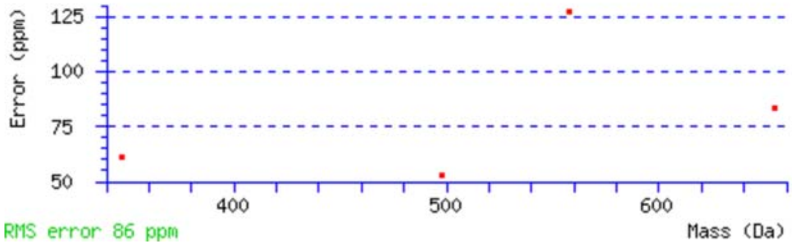
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 0 to 3000 Da Full range
Label all possible matches ○ Label matches used for scoring ●



Monoisotopic mass of neutral peptide Mr(calc): 1209.6969
Variable modifications:
N-term : GIST-Quat (N-term), with neutral loss 59.0735
Ions Score: 10 **Expect:** 1.8
Matches : 4/96 fragment ions using 11 most intense peaks (help)

#	b	b^{++}	b*	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{0}	y^{0++}	#
1	197.0921	99.0497	180.0655	90.5364			Q					11
2	310.1761	155.5917	293.1496	147.0784			I	955.5459	478.2766	937.5353	469.2713	10
3	411.2238	206.1155	394.1973	197.6023	393.2132	197.1103	T	842.4618	421.7345	824.4512	412.7293	9
4	**498.2558**	249.6316	481.2293	241.1183	480.2453	240.6263	S	741.4141	371.2107	723.4036	362.2054	8
5	595.3086	298.1579	578.2821	289.6447	577.2980	289.1527	P	***654.3821***	327.6947	636.3715	318.6894	7
6	708.3927	354.7000	691.3661	346.1867	690.3821	345.6947	I	***557.3293***	279.1683	539.3188	270.1630	6
7	805.4454	403.2264	788.4189	394.7131	787.4349	394.2211	P	444.2453	222.6263	426.2347	213.6210	5
8	876.4825	438.7449	859.4560	430.2316	858.4720	429.7396	A	***347.1925***	174.0999	329.1819	165.0946	4
9	989.5666	495.2869	972.5401	486.7737	971.5560	486.2817	I	276.1554	138.5813	258.1448	129.5761	3
10	1046.5881	523.7977	1029.5615	515.2844	1028.5775	514.7924	G	163.0713	82.0393	145.0608	73.0340	2
11							S	106.0499	53.5286	88.0393	44.5233	1



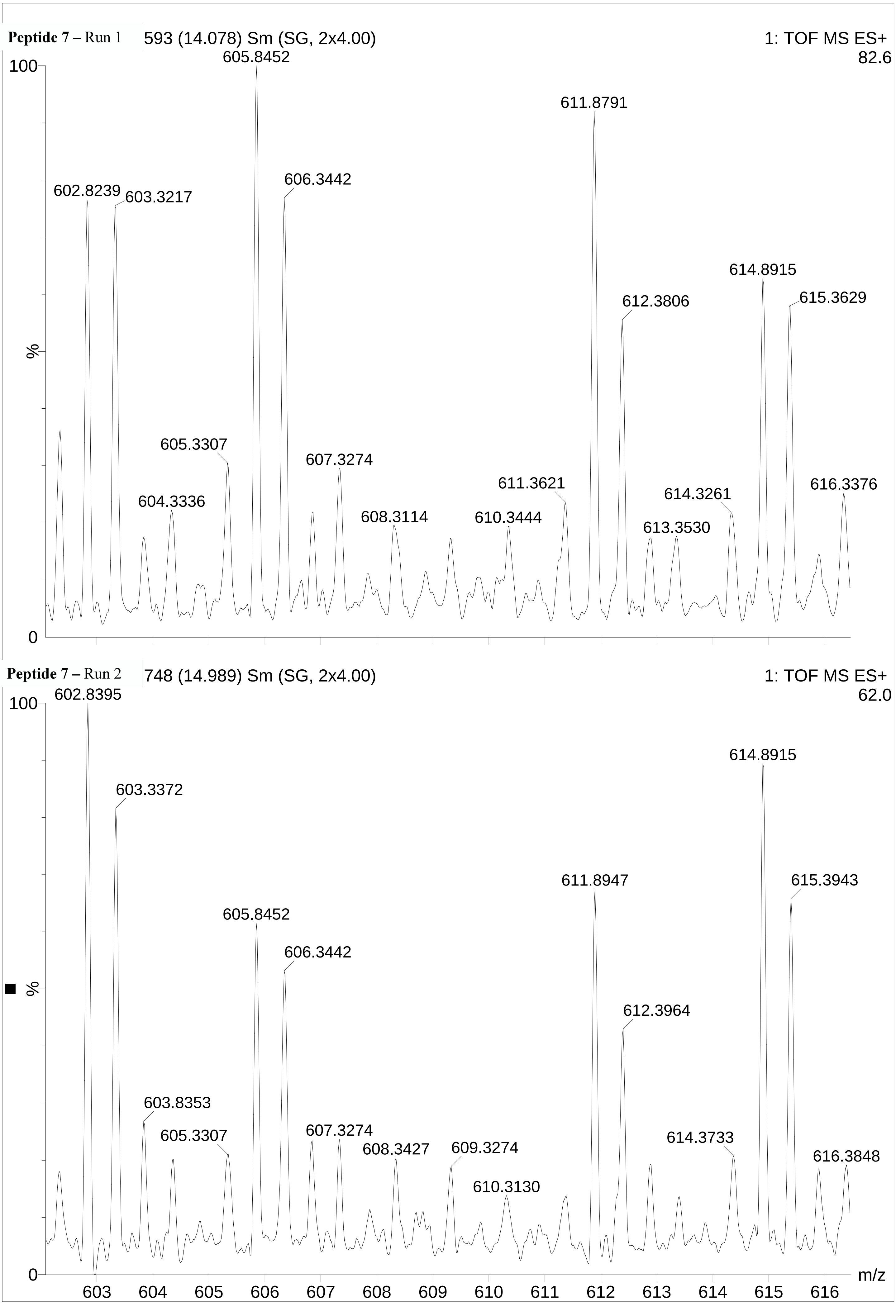


NCBI **BLAST** search of QITSPIPAIGS
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc):	Delta	Sequence
13.4	1209.7524	0.0288	GLKQPTPVQL
13.3	1209.7445	0.0368	KAKTKPPLQVT
12.0	1209.6466	0.1347	QSRNAPLPSLQ
10.2	1209.6580	0.1233	PGFQPIPCKP
10.2	1209.6969	0.0844	QITSPIPAIGS
10.2	1209.6717	0.1095	SRSVPLPAEQ
10.1	1209.7160	0.0652	VNNVPLPNTL
9.9	1209.7048	0.0765	ELSPPLPLSQ
9.9	1209.8410	-0.0598	IPIPPLPSKL
9.9	1209.7524	0.0288	KNGPLPLQS

Mascot: http://www.matrixscience.com/


Peptide 7 – Run 1
593 (14.078) Sm (SG, 2x4.00)
1: TOF MS ES+
82.6
100
%
0
605.8452
611.8791
602.8239
603.3217
606.3442
614.8915
612.3806
615.3629
605.3307
607.3274
604.3336
611.3621
614.3261
616.3376
608.3114
610.3444
613.3530
Peptide 7 – Run 2
748 (14.989) Sm (SG, 2x4.00)
1: TOF MS ES+
62.0
100
%
0
602.8395
614.8915
603.3372
611.8947
615.3943
605.8452
606.3442
612.3964
603.8353
605.3307
607.3274
608.3427
609.3274
614.3733
616.3848
610.3130
m/z
603
604
605
606
607
608
609
610
611
612
613
614
615
616

Mascot Search Results

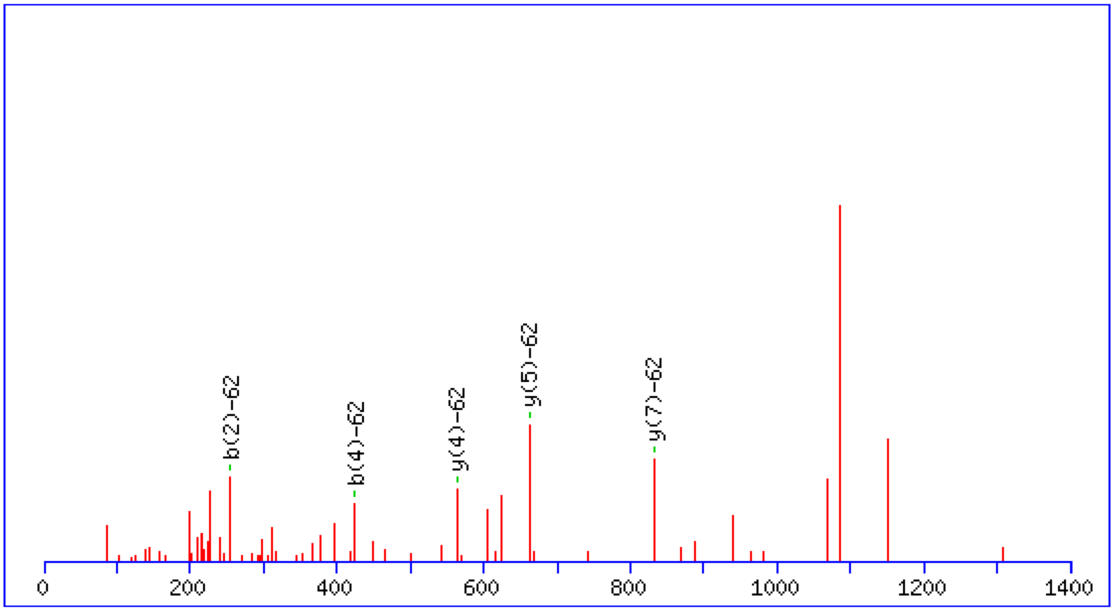
Peptide View

Peptide 7

MS/MS Fragmentation of **ADGIVSKNF**
Found in **RS21_HUMAN**, 40S ribosomal protein S21 OS=Homo sapiens GN=RPS21 PE=1 SV=1

Match to Query 237: 1209.732728 from(605.873640,2+) intensity(3452.0000)
Title: 318: Sum of 2 scans in range 813 (rt=838.537, f=3, i=64) to 814 (rt=839.563, f=4, i=44) [C:\Users\synapt\Desktop\28062011 raw \290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

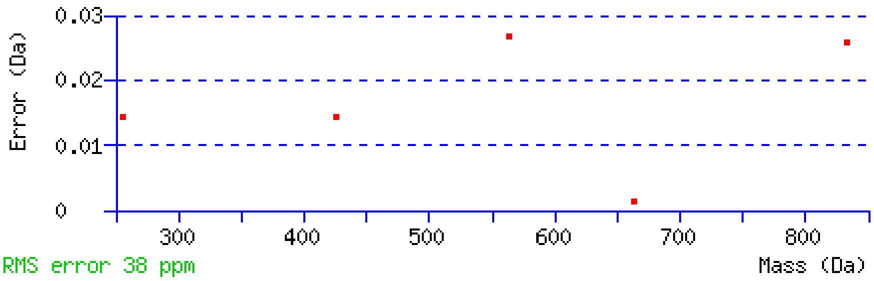
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 0 to 1400 Da Full range
Label all possible matches ○ Label matches used for scoring ○

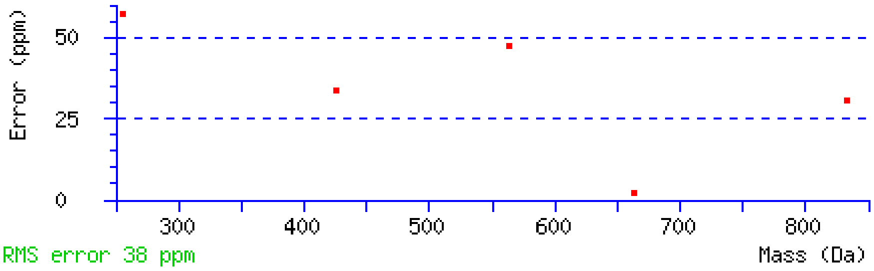


Monoisotopic mass of neutral peptide Mr(calc): 1209.7240
Variable modifications:
N-term : GIST-Quat:2H(3) (N-term), with neutral loss 62.0923
K7 : GIST-Quat:2H(3) (K), with neutral loss 62.0923
Ions Score: 10 **Expect:** 4.9e+003
Matches : 5/74 fragment ions using 11 most intense peaks (help)

#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	140.0706	70.5389					A							9
2	**255.0975**	128.0524			237.0870	119.0471	D	947.4833	474.2453	930.4567	465.7320	929.4727	465.2400	8
3	312.1190	156.5631			294.1084	147.5579	G	***832.4563***	416.7318	815.4298	408.2185	814.4458	407.7265	7
4	**425.2031**	213.1052			407.1925	204.0999	I	775.4349	388.2211	758.4083	379.7078	757.4243	379.2158	6
5	524.2715	262.6394			506.2609	253.6341	V	***662.3508***	331.6790	645.3243	323.1658	644.3402	322.6738	5
6	611.3035	306.1554			593.2930	297.1501	S	***563.2824***	282.1448	546.2558	273.6316	545.2718	273.1395	4
7	807.4247	404.2160	790.3981	395.7027	789.4141	395.2107	K	476.2504	238.6288	459.2238	230.1155			3

8	921.4676	461.2374	904.4411	452.7242	903.4571	452.2322	**N**	280.1292	140.5682	263.1026	132.0550			**2**
9							**F**	166.0863	83.5468					**1**



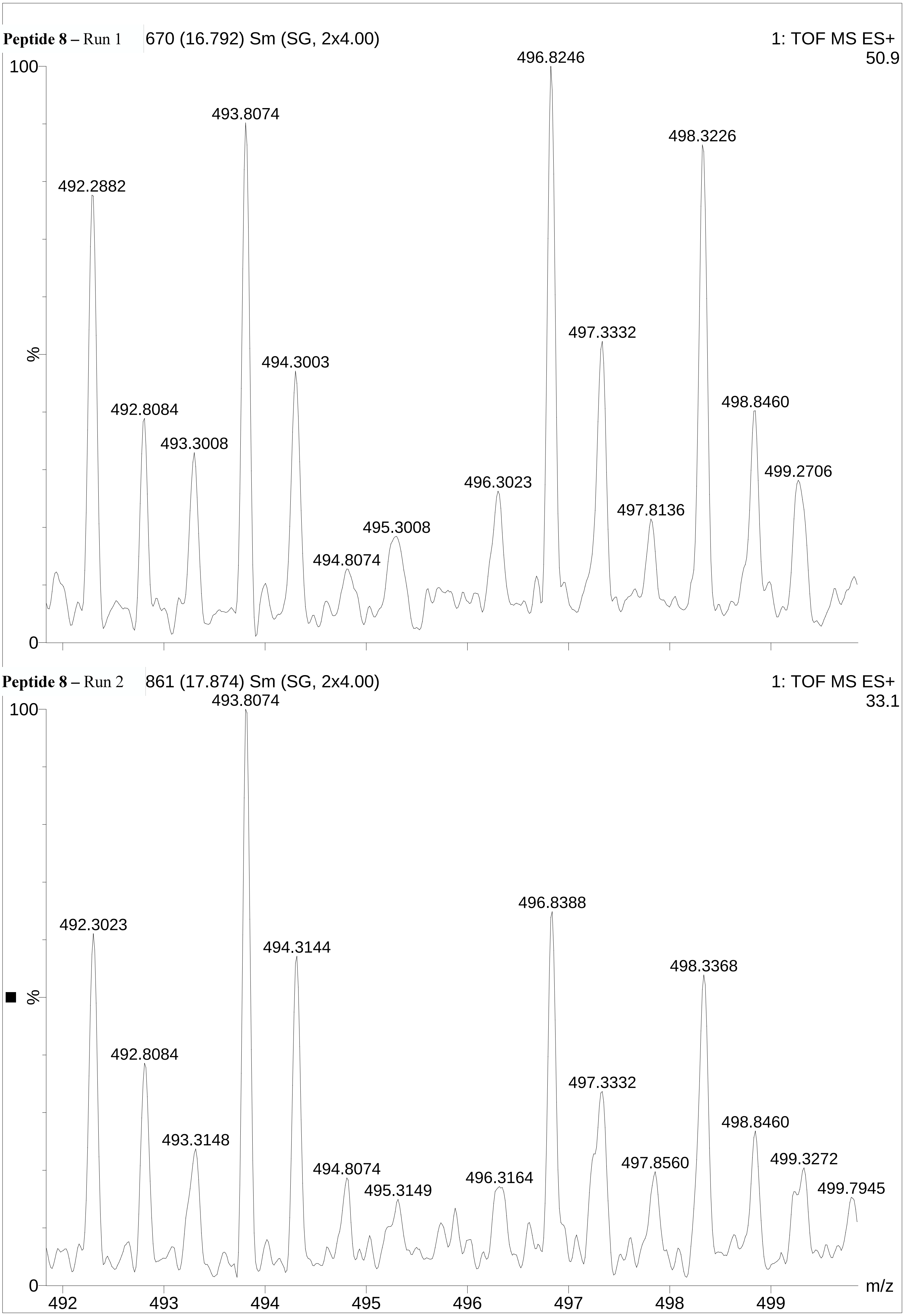


NCBI **BLAST** search of ADGIVSKNF
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc):	Delta	Sequence
16.0	1209.8444	-0.1116	AKVKVIGVH
9.8	1209.7240	0.0087	ADGIVSKNF
9.8	1209.8444	-0.1116	AKVKVIGVH
9.8	1209.8444	-0.1116	AKVKVIGVH
9.8	1209.7240	0.0087	EGGIVSKNF
9.3	1209.7279	0.0048	NQVAVSSLSAV
8.9	1209.6909	0.0418	KNSECLKE
8.7	1209.7273	0.0054	NKMTSLKE
8.2	1209.6663	0.0664	NKNQEEAGGK
8.1	1209.7623	-0.0296	EGPPRGKGF

Mascot: http://www.matrixscience.com/


Peptide 8 – Run 1
670 (16.792) Sm (SG, 2x4.00)
1: TOF MS ES+
50.9
100
%
0
492.2882
492.8084
493.3008
493.8074
494.3003
494.8074
495.3008
496.3023
496.8246
497.3332
497.8136
498.3226
498.8460
499.2706
Peptide 8 – Run 2
861 (17.874) Sm (SG, 2x4.00)
1: TOF MS ES+
33.1
100
%
0
492.3023
492.8084
493.3148
493.8074
494.3144
494.8074
495.3149
496.3164
496.8388
497.3332
497.8560
498.3368
498.8460
499.3272
499.7945
m/z
492
493
494
495
496
497
498
499

Mascot Search Results

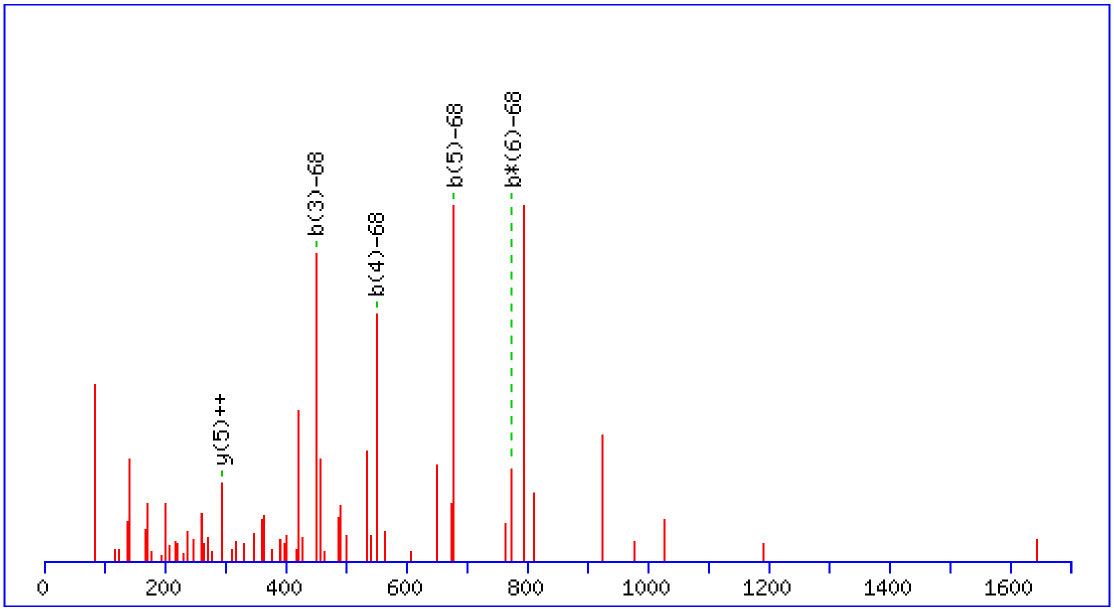
Peptide View

Peptide 8

MS/MS Fragmentation of **RIIVENL**
Found in **PTBP1_HUMAN**, Polypyrimidine tract-binding protein 1 OS=Homo sapiens GN=PTBP1 PE=1 SV=1

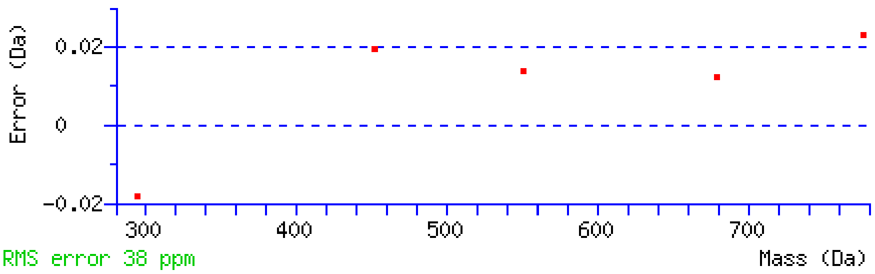
Match to Query 81: 991.683668 from(496.849110,2+) intensity(4349.0000)
Title: 433: Sum of 3 scans in range 970 (rt=1000.36, f=2, i=125) to 974 (rt=1004.46, f=2, i=127) [C:\Users\synapt\Desktop\28062011 raw \290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

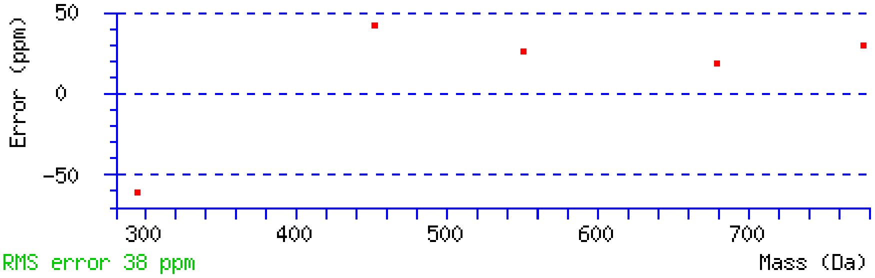
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 0 to 1700 Da Full range
Label all possible matches ○ Label matches used for scoring ○



Monoisotopic mass of neutral peptide Mr(calc): 991.6740
Variable modifications:
N-term : GIST-Quat:2H(9) (N-term), with neutral loss 68.1300
Ions Score: 15 **Expect:** 1.2e+003
Matches : 5/58 fragment ions using 9 most intense peaks (help)

#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	225.1346	113.0709	208.1081	104.5577			R							7
2	338.2187	169.6130	321.1921	161.0997			I	700.4240	350.7156	683.3974	342.2023	682.4134	341.7103	6
3	***451.3027***	226.1550	434.2762	217.6417			I	587.3399	294.1736	570.3134	285.6603	569.3293	285.1683	5
4	***550.3711***	275.6892	533.3446	267.1759			V	474.2558	237.6316	457.2293	229.1183	456.2453	228.6263	4
5	***679.4137***	340.2105	662.3872	331.6972	661.4032	331.2052	E	375.1874	188.0974	358.1609	179.5841	357.1769	179.0921	3
6	793.4567	397.2320	776.4301	388.7187	775.4461	388.2267	N	246.1448	123.5761	229.1183	115.0628			2
7							L	132.1019	66.5546					1





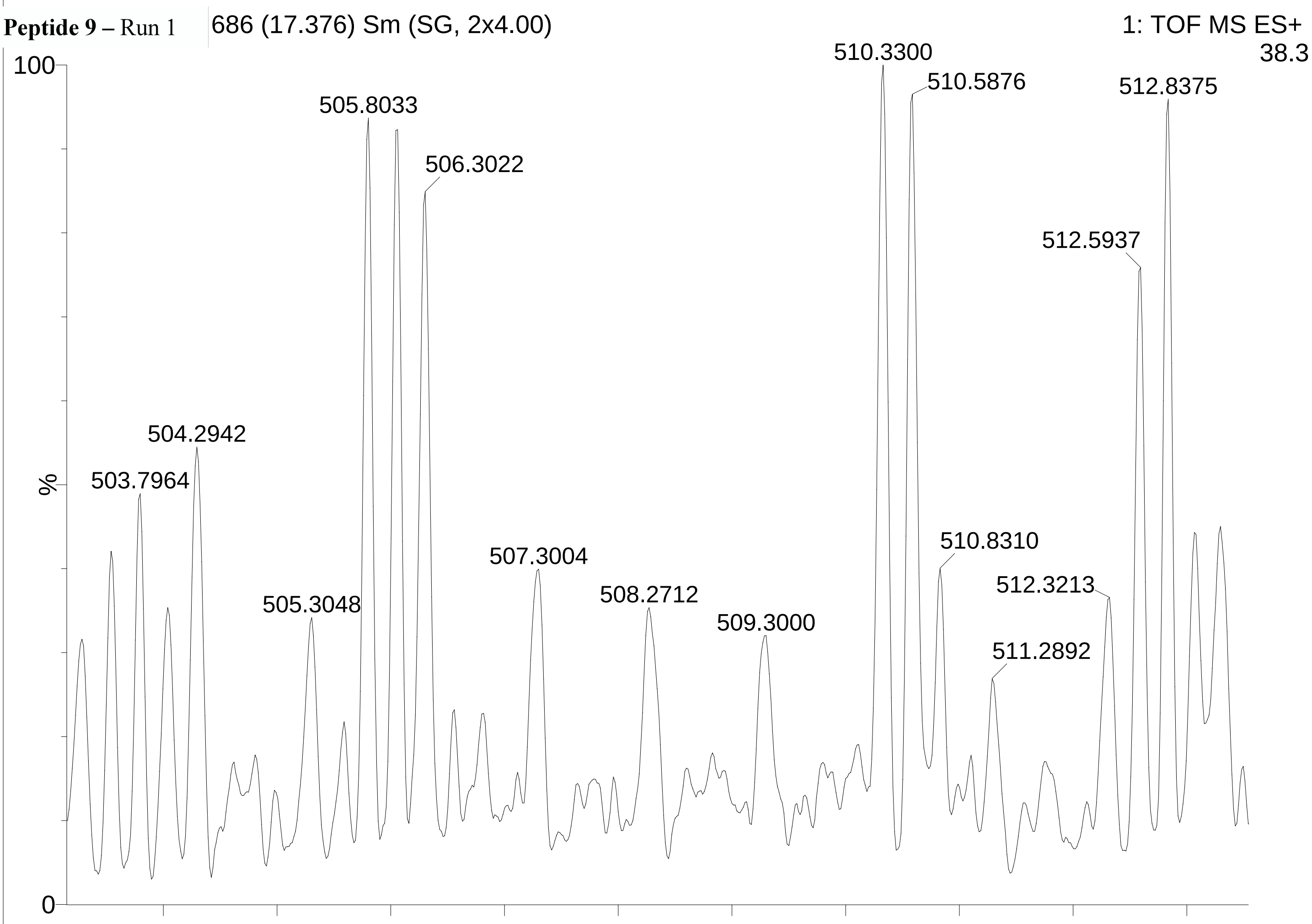
NCBI **BLAST** search of RIIVENL
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

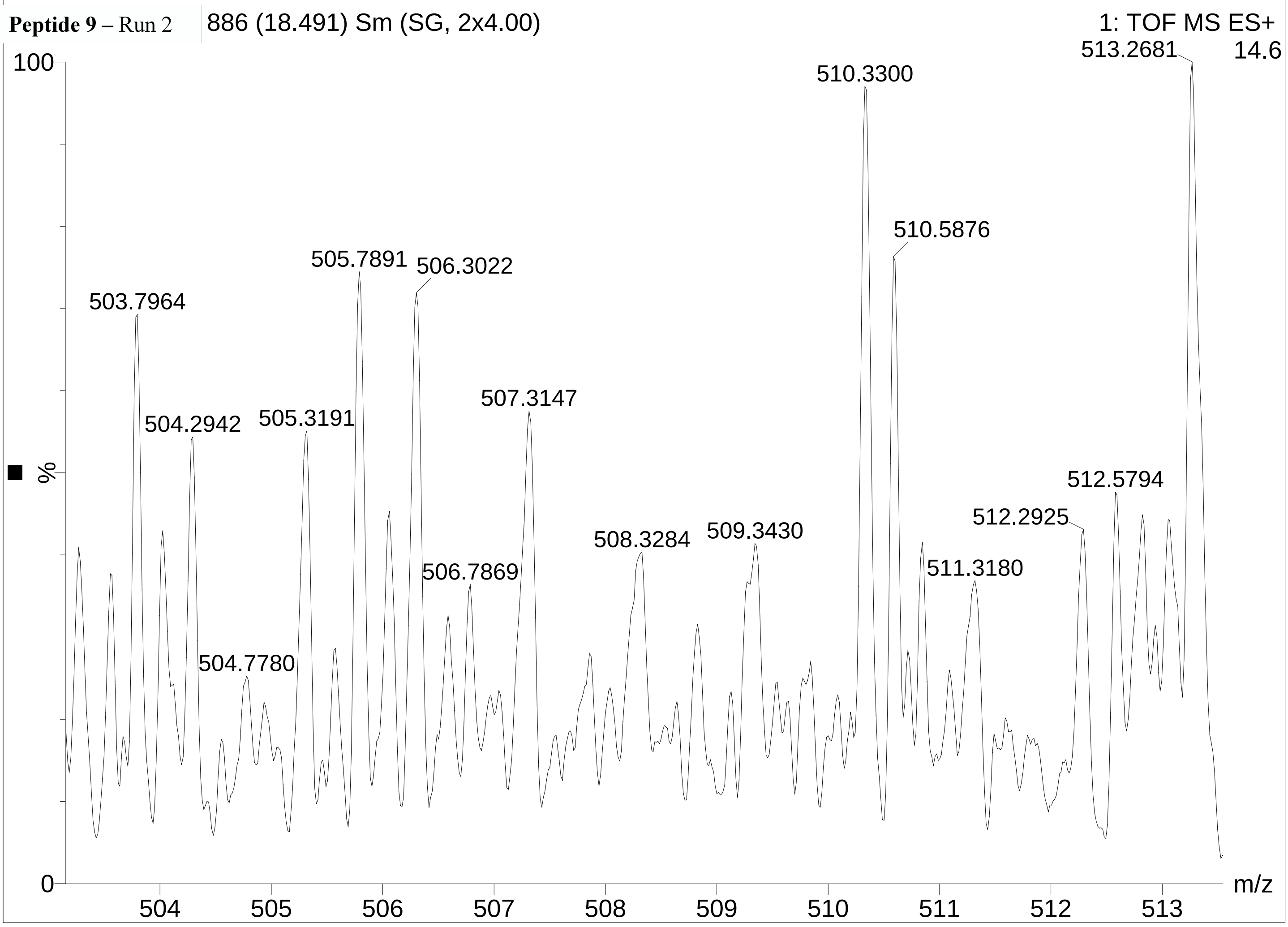
Score	Mr(calc):	Delta	Sequence
26.9	991.5338	0.1498	ADEKKFQ
23.8	991.5226	0.1611	ADELYAAL
15.8	991.5702	0.1135	ADKKEFK
14.5	991.6740	0.0097	RIIVENL
14.5	991.6740	0.0097	RLIVENL
14.5	991.6740	0.0097	RLLVENL
14.0	991.6740	0.0097	KPKKENI
14.0	991.6740	0.0097	KPKKENL
13.5	991.6740	0.0097	PKAGKEKV
13.4	991.6740	0.0097	KPKKENI

Mascot: http://www.matrixscience.com/

Peptide 9 – Run 1



Peptide 9 – Run 2



Mascot Search Results

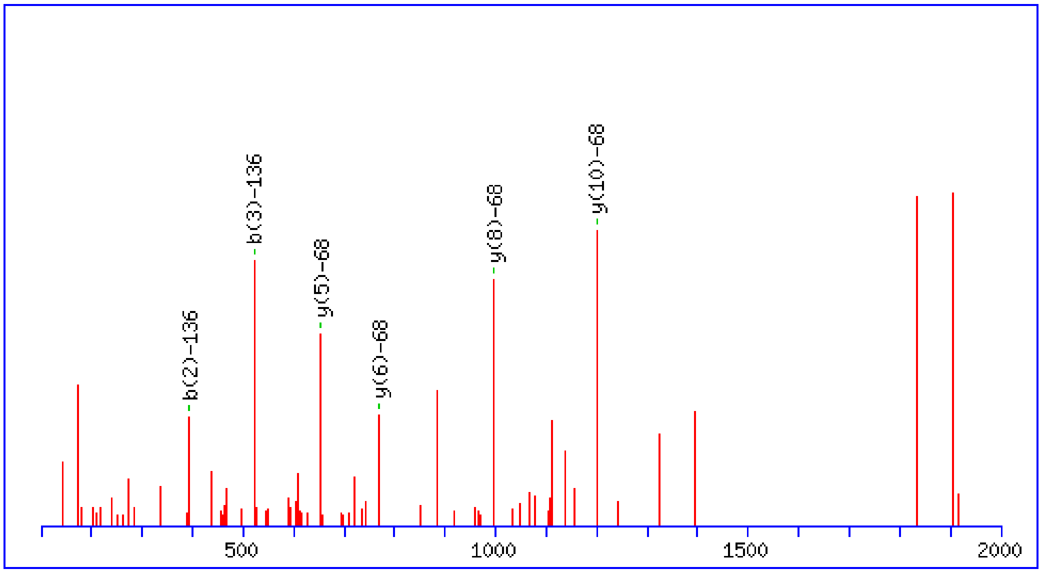
Peptide View

Peptide 9

MS/MS Fragmentation of **KEQISDIDDAVRKL**
Found in **TCP4_HUMAN**, Activated RNA polymerase II transcriptional coactivator p15 OS=Homo sapiens GN=SUB1 PE=1 SV=3

Match to Query 519: 2037.385616 from(510.353680,4+) intensity(3594.0000)
Title: 453: Sum of 2 scans in range 1008 (rt=1039.47, f=2, i=136) to 1009 (rt=1040.49, f=3, i=94) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

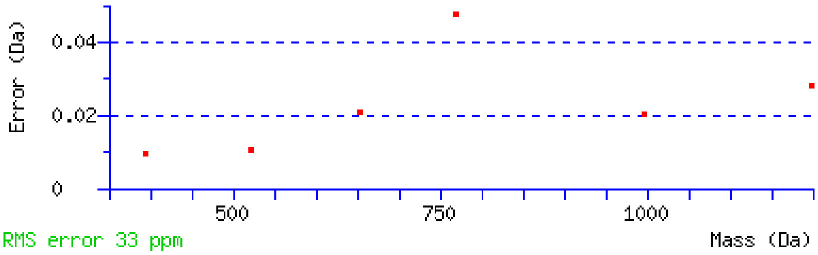
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 100 to 2000 Da Full range
Label all possible matches ○ Label matches used for scoring ○

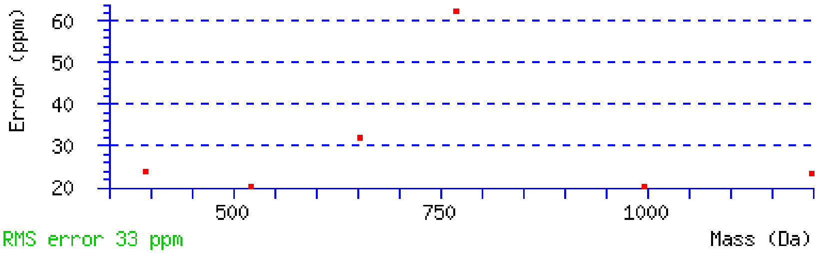


Monoisotopic mass of neutral peptide Mr(calc): 2037.3419
Variable modifications:
N-term : GIST-Quat:2H(9) (N-term), with neutral loss 68.1300
K1 : GIST-Quat:2H(9) (K), with neutral loss 68.1300
K13 : GIST-Quat:2H(9) (K), with neutral loss 68.1300
Ions Score: 13 **Expect:** 1.9e+003
Matches : 6/142 fragment ions using 15 most intense peaks (help)

#	b	b^{++}	b*	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y^{*++}	y^{0}	y^{0++}	#
1	265.1547	133.0810	248.1281	124.5677			K							14
2	***394.1973***	197.6023	377.1707	189.0890	376.1867	188.5970	E	1569.8119	785.4096	1552.7853	776.8963	1551.8013	776.4043	13
3	***522.2558***	261.6316	505.2293	253.1183	504.2453	252.6263	Q	1440.7693	720.8883	1423.7427	712.3750	1422.7587	711.8830	12
4	635.3399	318.1736	618.3134	309.6603	617.3293	309.1683	I	1312.7107	656.8590	1295.6842	648.3457	1294.7001	647.8537	11
5	722.3719	361.6896	705.3454	353.1763	704.3614	352.6843	S	***1199.6266***	600.3170	1182.6001	591.8037	1181.6161	591.3117	10
6	837.3989	419.2031	820.3723	410.6898	819.3883	410.1978	D	1112.5946	556.8009	1095.5681	548.2877	1094.5841	547.7957	9
7	950.4829	475.7451	933.4564	467.2318	932.4724	466.7398	I	***997.5677***	499.2875	980.5411	490.7742	979.5571	490.2822	8
8	1065.5099	533.2586	1048.4833	524.7453	1047.4993	524.2533	D	884.4836	442.7454	867.4571	434.2322	866.4730	433.7402	7
9	1180.5368	590.7721	1163.5103	582.2588	1162.5263	581.7668	D	***769.4567***	385.2320	752.4301	376.7187	751.4461	376.2267	6

10	1251.5739	626.2906	1234.5474	617.7773	1233.5634	617.2853	**A**	***654.4297***	327.7185	637.4032	319.2052			**5**
11	1350.6424	675.8248	1333.6158	667.3115	1332.6318	666.8195	**V**	583.3926	292.1999	566.3661	283.6867			**4**
12	1506.7435	753.8754	1489.7169	745.3621	1488.7329	744.8701	**R**	484.3242	242.6657	467.2976	234.1525			**3**
13	1702.8646	851.9360	1685.8381	843.4227	1684.8541	842.9307	**K**	328.2231	164.6152	311.1965	156.1019			**2**
14							**L**	132.1019	66.5546					**1**



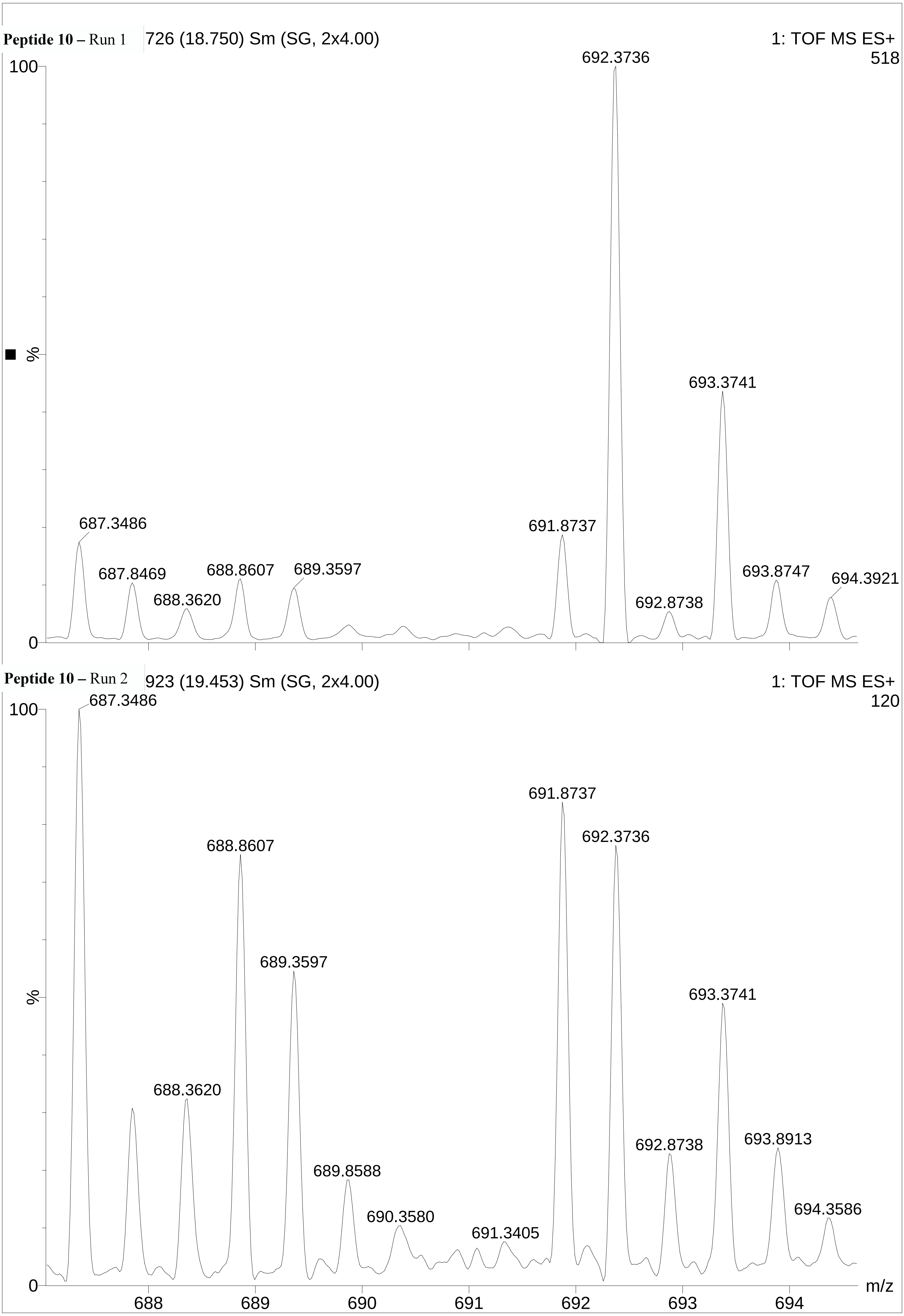


NCBI **BLAST** search of KEQISDIDDAVRKL
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc):	Delta	Sequence
13.0	2037.3419	0.0437	KEQISDIDDAVRKL
11.7	2037.2415	0.1442	GNATKNDDLNKPINK
11.7	2037.2415	0.1442	GNATKNDDLNKPINK
11.7	2037.2415	0.1442	GNATKNDDLNKPINK
9.9	2037.2415	0.1442	GNATKNDDLNKPINK
9.9	2037.2415	0.1442	GNATKNDDLNKPINK
9.9	2037.2415	0.1442	GNATKNDDLNKPINK
9.5	2037.2548	0.1308	IVIFLDTLARLKAVDNT
8.5	2037.3837	0.0019	IVLKGVVQVEKIKSPE
8.5	2037.3837	0.0019	IVLKGVVQVEKIKSPE

Mascot: http://www.matrixscience.com/


Peptide 10 – Run 1
726 (18.750) Sm (SG, 2x4.00)
1: TOF MS ES+
518
100
%
0
692.3736
693.3741
687.3486
691.8737
687.8469
688.8607
689.3597
688.3620
692.8738
693.8747
694.3921
Peptide 10 – Run 2
923 (19.453) Sm (SG, 2x4.00)
1: TOF MS ES+
120
100
%
0
687.3486
691.8737
692.3736
688.8607
689.3597
693.3741
688.3620
692.8738
693.8913
689.8588
690.3580
691.3405
694.3586
m/z
688
689
690
691
692
693
694

Mascot Search Results

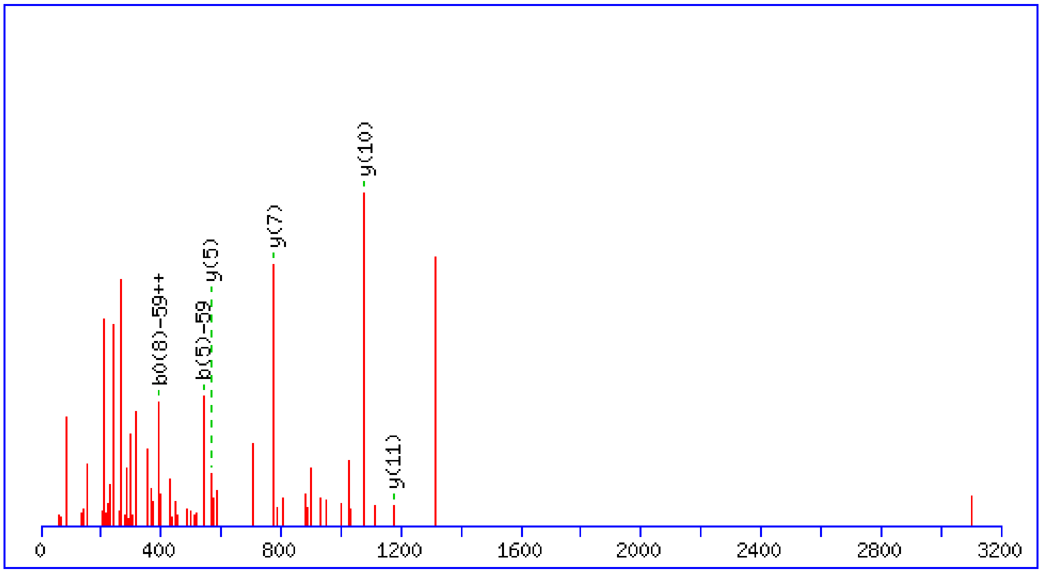
Peptide View

Peptide 10

MS/MS Fragmentation of **AVDGEPLGRVSF**
Found in **PPIA_HUMAN**, Peptidyl-prolyl cis-trans isomerase A OS=Homo sapiens GN=PPIA PE=1 SV=2

Match to Query 322: 1372.760388 from(687.387470,2+) intensity(3331.0000)
Title: 511: Sum of 2 scans in range 1113 (rt=1147.54, f=2, i=166) to 1114 (rt=1148.56, f=2, i=167) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

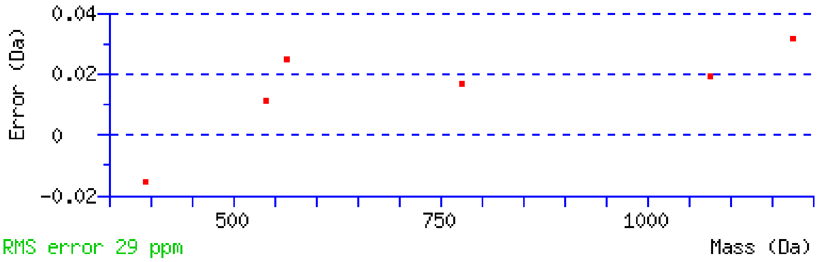
Click mouse within plot area to zoom in by factor of two about that point
Or, [Plot from] [0] to [3200] Da [Full range]
Label all possible matches ○ Label matches used for scoring ○

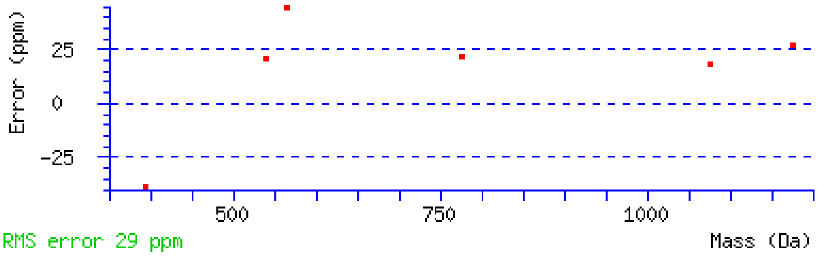


Monoisotopic mass of neutral peptide Mr(calc): 1372.7351
Variable modifications:
N-term : GIST-Quat (N-term), with neutral loss 59.0735
Ions Score: 16 **Expect:** 1.3e+003
Matches : 6/104 fragment ions using 13 most intense peaks (help)

#	b	b++	b*	b*++	b0	b0++	Seq.	y	y++	y*	y*++	y0	y0++	#
1	140.0706	70.5389					A							12
2	239.1390	120.0731					V	***1175.6055***	588.3064	1158.5790	579.7931	1157.5949	579.3011	11
3	354.1660	177.5866			336.1554	168.5813	D	***1076.5371***	538.7722	1059.5106	530.2589	1058.5265	529.7669	10
4	411.1874	206.0974			393.1769	197.0921	G	961.5102	481.2587	944.4836	472.7454	943.4996	472.2534	9
5	540.2300	270.6186			522.2195	261.6134	E	904.4887	452.7480	887.4621	444.2347	886.4781	443.7427	8
6	637.2828	319.1450			619.2722	310.1397	P	***775.4461***	388.2267	758.4196	379.7134	757.4355	379.2214	7
7	750.3668	375.6871			732.3563	366.6818	L	678.3933	339.7003	661.3668	331.1870	660.3828	330.6950	6
8	807.3883	404.1978			789.3777	395.1925	G	***565.3093***	283.1583	548.2827	274.6450	547.2987	274.1530	5
9	963.4894	482.2483	946.4629	473.7351	945.4789	473.2431	R	508.2878	254.6475	491.2613	246.1343	490.2772	245.6423	4
10	1062.5578	531.7826	1045.5313	523.2693	1044.5473	522.7773	V	352.1867	176.5970			334.1761	167.5917	3
11	1149.5899	575.2986	1132.5633	566.7853	1131.5793	566.2933	S	253.1183	127.0628			235.1077	118.0575	2

12							**F**	166.0863	83.5468					**1**





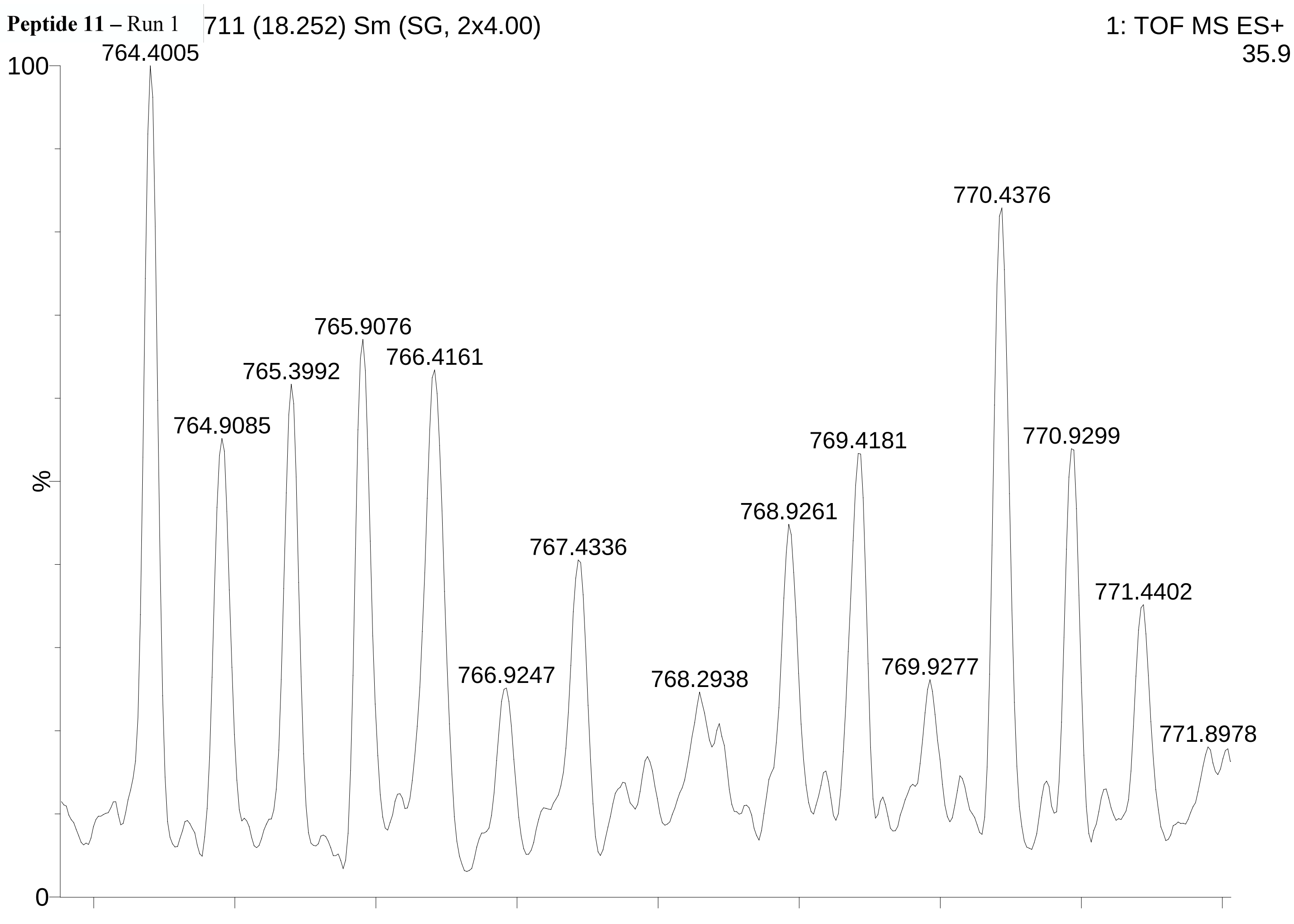
NCBI **BLAST** search of AVDGEPLGRVSF
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

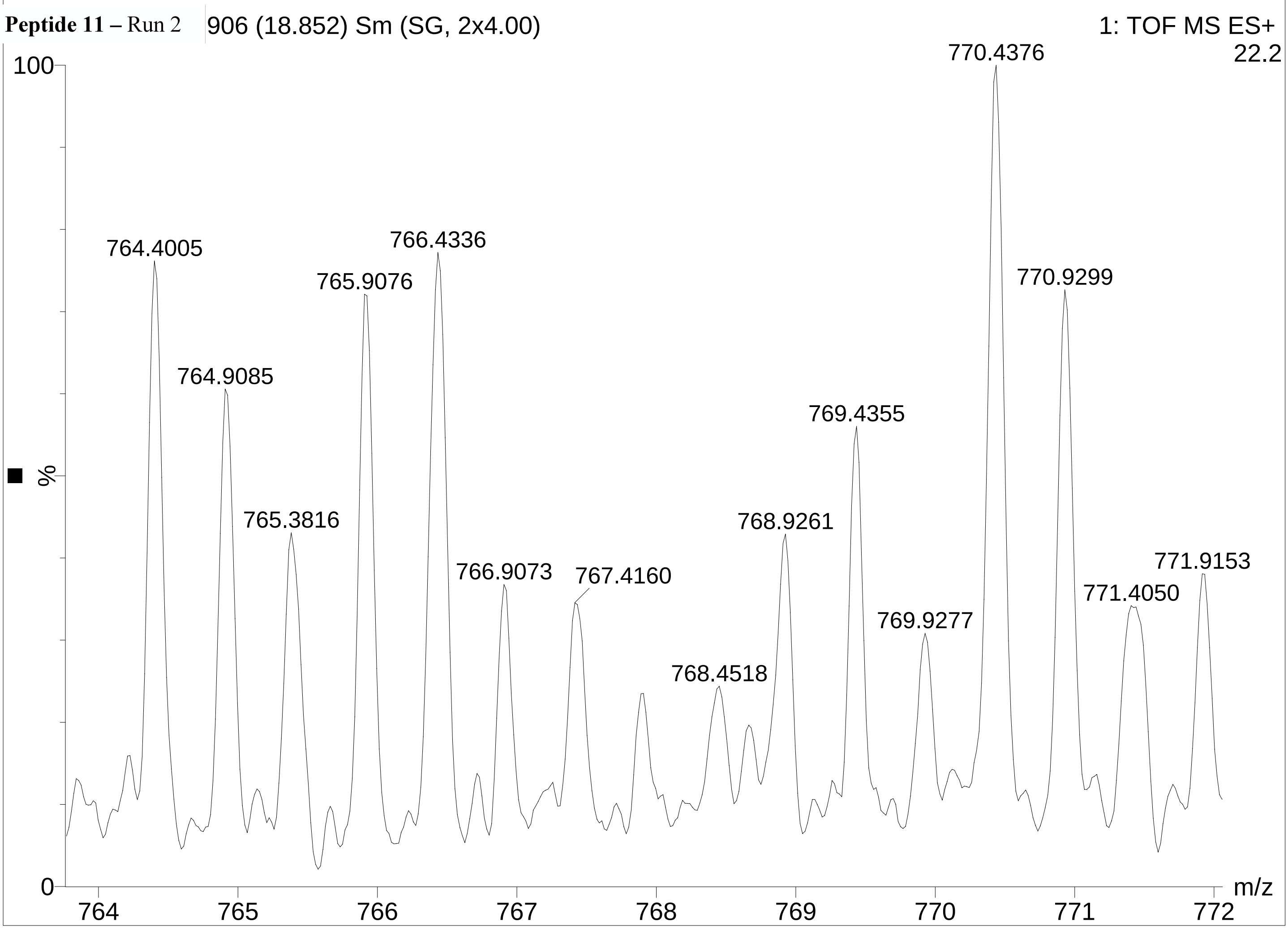
Score	Mr(calc):	Delta	Sequence
15.9	1372.7351	0.0253	AVDGEPLGRVSF
10.7	1372.8152	-0.0548	LPLCLLKNLGY
8.7	1372.7173	0.0431	PLAIIGGNCALQGF
8.2	1372.7602	0.0002	AALESQPLLGFT
7.9	1372.8177	-0.0573	AVSITITTITNI
7.6	1372.8330	-0.0726	AAPSVLAPTLPLP
7.3	1372.8191	-0.0587	SLIKHQIIHTG
7.2	1372.7674	-0.0070	AASNKKGGEKEK
7.2	1372.8415	-0.0811	AVRRGRKTGVF
7.2	1372.6987	0.0617	AADTLEDLRGW

Mascot: http://www.matrixscience.com/

Peptide 11 – Run 1



Peptide 11 – Run 2



Mascot Search Results

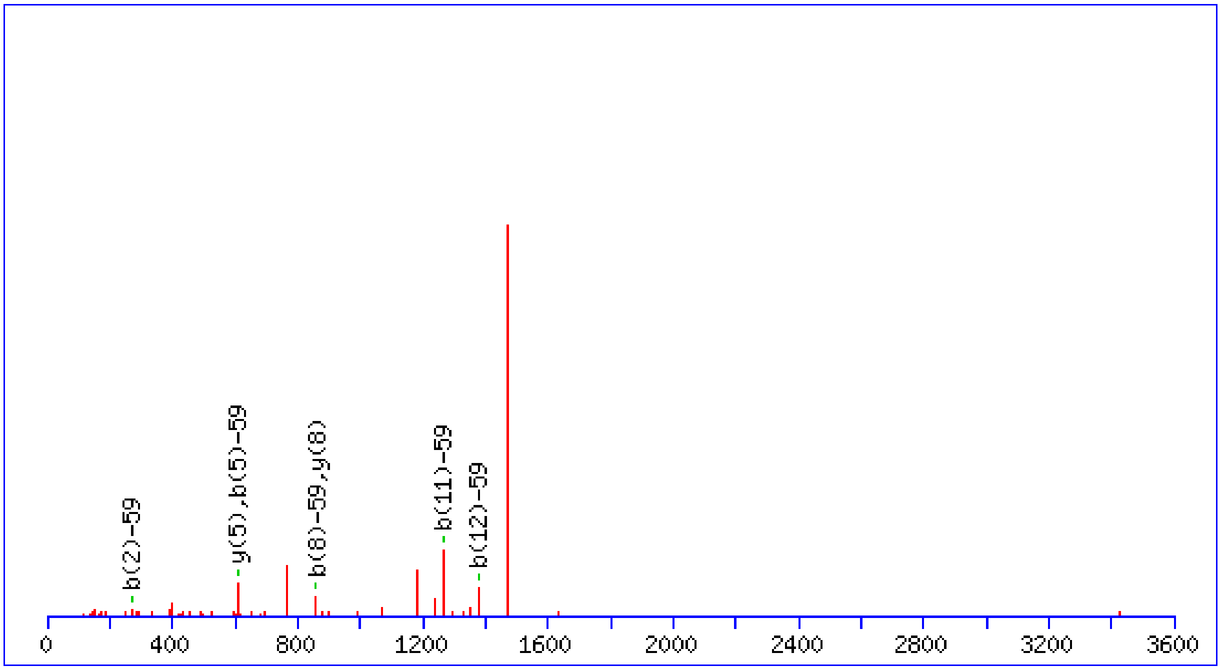
Peptide View

Peptide 11

MS/MS Fragmentation of **SILLNPGPRHILA**
Found in **KCNT1_HUMAN**, Potassium channel subfamily T member 1 OS=Homo sapiens GN=KCNT1 PE=2 SV=2

Match to Query 403: 1526.868628 from(764.441590,2+) intensity(3249.0000)
Title: 483: Sum of 2 scans in range 1059 (rt=1092.04, f=2, i=154) to 1060 (rt=1093.06, f=3, i=98) [C:\Users\synapt\Desktop \28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

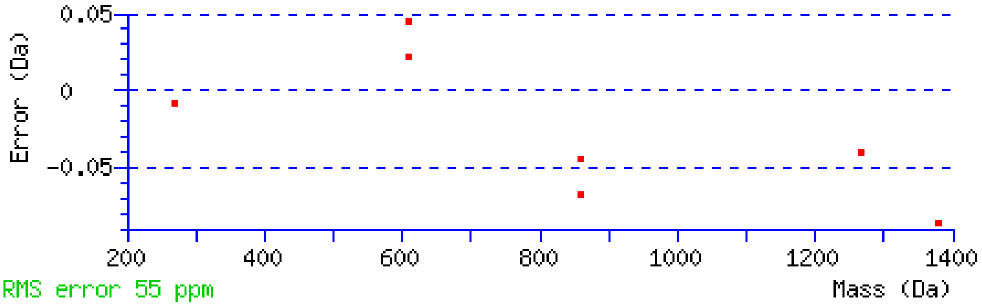
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 0 to 3600 Da Full range
Label all possible matches ○ Label matches used for scoring ○

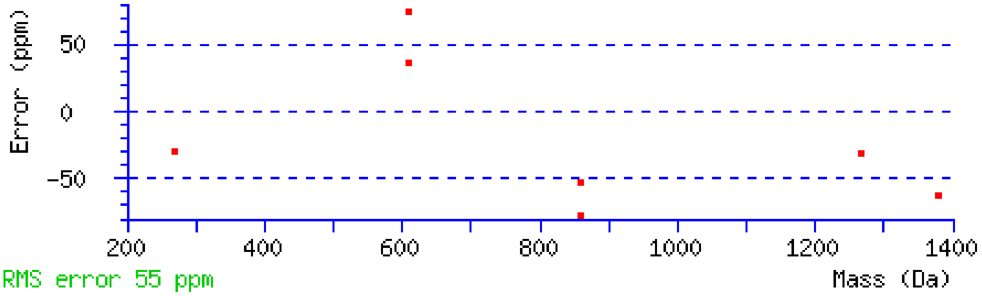


Monoisotopic mass of neutral peptide Mr(calc): 1526.9297
Variable modifications:
N-term : GIST-Quat (N-term), with neutral loss 59.0735
Ions Score: 18 **Expect:** 9.8e+002
Matches : 7/104 fragment ions using 14 most intense peaks (help)

#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	#
1	156.0655	78.5364			138.0550	69.5311	S					13
2	*269.1496*	135.0784			251.1390	126.0731	I	1313.8052	657.4062	1296.7787	648.8930	12
3	382.2336	191.6205			364.2231	182.6152	L	1200.7212	600.8642	1183.6946	592.3509	11
4	495.3177	248.1625			477.3071	239.1572	L	1087.6371	544.3222	1070.6105	535.8089	10

5	***609.3606***	305.1840	592.3341	296.6707	591.3501	296.1787	**N**	974.5530	487.7802	957.5265	479.2669	**9**
6	706.4134	353.7103	689.3869	345.1971	688.4028	344.7051	**P**	**860.5101**	430.7587	843.4835	422.2454	**8**
7	763.4349	382.2211	746.4083	373.7078	745.4243	373.2158	**G**	763.4573	382.2323	746.4308	373.7190	**7**
8	***860.4876***	430.7475	843.4611	422.2342	842.4771	421.7422	**P**	706.4359	353.7216	689.4093	345.2083	**6**
9	1016.5887	508.7980	999.5622	500.2847	998.5782	499.7927	**R**	**609.3831**	305.1952	592.3566	296.6819	**5**
10	1153.6477	577.3275	1136.6211	568.8142	1135.6371	568.3222	**H**	453.2820	227.1446			**4**
11	***1266.7317***	633.8695	1249.7052	625.3562	1248.7212	624.8642	**I**	316.2231	158.6152			**3**
12	***1379.8158***	690.4115	1362.7892	681.8983	1361.8052	681.4062	**L**	203.1390	102.0731			**2**
13							**A**	90.0550	45.5311			**1**





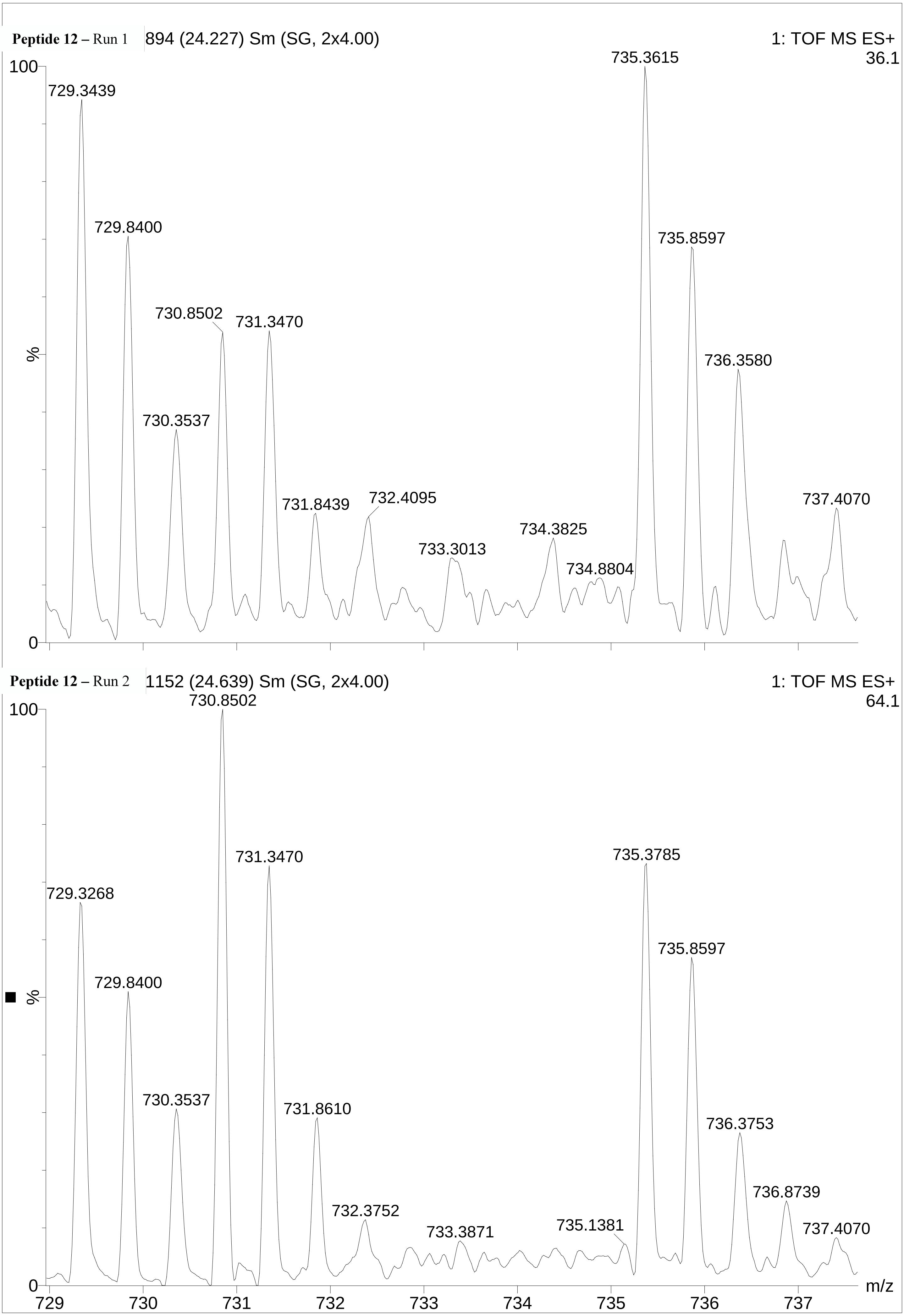
NCBI **BLAST** search of SILLNPGPRHILA
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc):	Delta	Sequence
17.6	1526.9297	-0.0610	SILLNPGPRHILA
15.6	1526.8854	-0.0168	SLALRCAQELLLA
14.8	1526.8529	0.0158	LKGDRGATGERGLA
14.4	1526.8820	-0.0134	ALFEGKGAAPQIAK
13.9	1526.8894	-0.0208	GAIGCTPLFIPKLA
12.9	1526.8933	-0.0246	EAIRAIFPSRGLA
11.1	1526.8742	-0.0056	TVPPDTSKMLKLA
11.0	1526.9495	-0.0809	EAMVKASPKTSL

11.0	1526.9495	-0.0809	EAMVKASPKTSL
10.9	1526.8055	0.0632	LSFLDLCFTASIA

Mascot: http://www.matrixscience.com/


Peptide 12 – Run 1
894 (24.227) Sm (SG, 2x4.00)
1: TOF MS ES+
36.1
100
%
0
735.3615
729.3439
729.8400
735.8597
730.8502
731.3470
736.3580
730.3537
732.4095
731.8439
737.4070
734.3825
733.3013
734.8804
Peptide 12 – Run 2
1152 (24.639) Sm (SG, 2x4.00)
1: TOF MS ES+
64.1
100
%
0
730.8502
731.3470
735.3785
729.3268
735.8597
729.8400
730.3537
731.8610
736.3753
736.8739
732.3752
737.4070
733.3871
735.1381
m/z
729
730
731
732
733
734
735
736
737

MATRIX SCIENCE Mascot Search Results

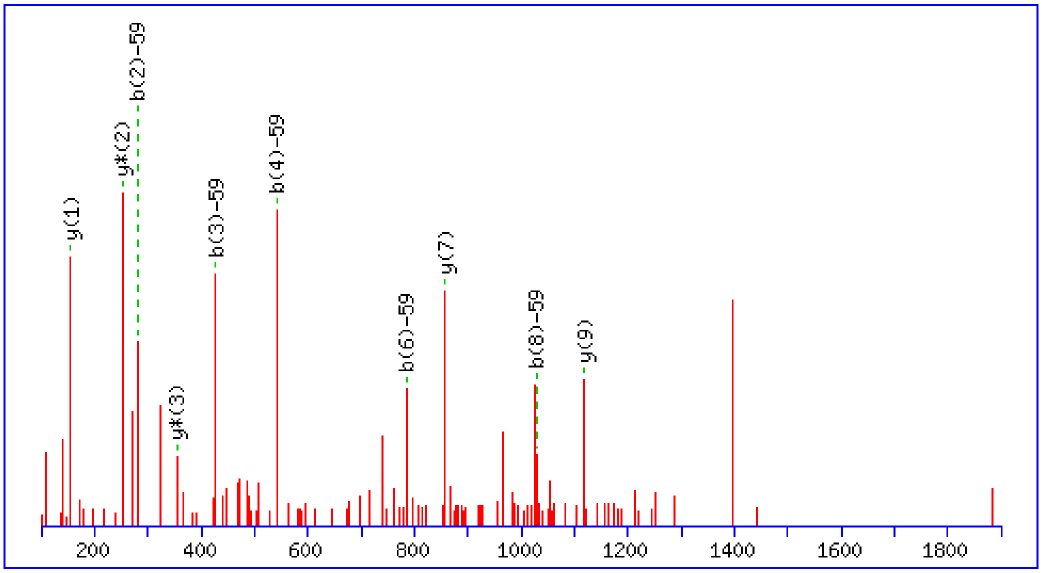
Peptide View

Peptide 12

MS/MS Fragmentation of **DPFNPFELTNH**
Found in **CATC_HUMAN**, Dipeptidyl peptidase 1 OS=Homo sapiens GN=CTSC PE=1 SV=1

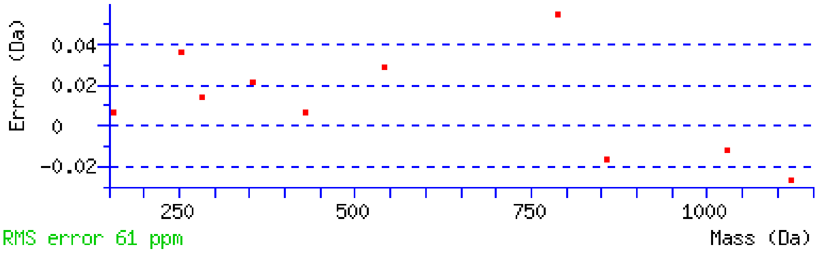
Match to Query 356: 1456.728968 from(729.371760,2+) intensity(1411.0000)
Title: 629: Scan 1409 (rt=1452.59, f=4, i=85) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

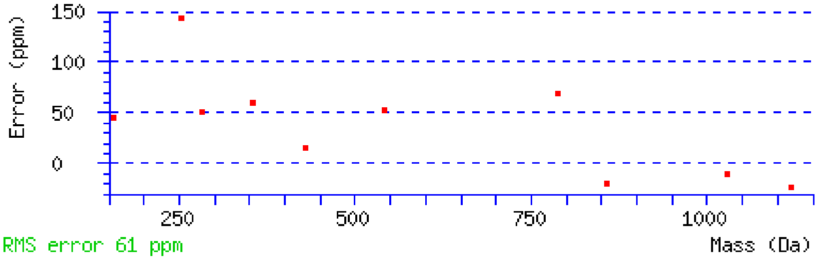
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 100 to 1900 Da Full range
Label all possible matches ○ Label matches used for scoring ○



Monoisotopic mass of neutral peptide Mr(calc): 1456.6987
Variable modifications:
N-term : GIST-Quat (N-term), with neutral loss 59.0735
Ions Score: 17 **Expect:** 7.6e+002
Matches : 10/108 fragment ions using 26 most intense peaks (help)

#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	184.0604	92.5339			166.0499	83.5286	D							11
2	***281.1132***	141.0602			263.1026	132.0550	P	1215.5793	608.2933	1198.5527	599.7800	1197.5687	599.2880	10
3	***428.1816***	214.5944			410.1710	205.5892	F	**1118.5265**	559.7669	1101.5000	551.2536	1100.5160	550.7616	9
4	***542.2245***	271.6159	525.1980	263.1026	524.2140	262.6106	N	971.4581	486.2327	954.4316	477.7194	953.4476	477.2274	8
5	639.2773	320.1423	622.2508	311.6290	621.2667	311.1370	P	**857.4152**	429.2112	840.3886	420.6980	839.4046	420.2060	7
6	***786.3457***	393.6765	769.3192	385.1632	768.3352	384.6712	F	760.3624	380.6849	743.3359	372.1716	742.3519	371.6796	6
7	915.3883	458.1978	898.3618	449.6845	897.3777	449.1925	E	613.2940	307.1506	596.2675	298.6374	595.2835	298.1454	5
8	***1028.4724***	514.7398	1011.4458	506.2266	1010.4618	505.7345	L	484.2514	242.6293	467.2249	234.1161	466.2409	233.6241	4
9	1129.5201	565.2637	1112.4935	556.7504	1111.5095	556.2584	T	371.1674	186.0873	354.1408	177.5740	353.1568	177.0820	3
10	1243.5630	622.2851	1226.5364	613.7719	1225.5524	613.2798	N	270.1197	135.5635	253.0931	127.0502			2
11							H	**156.0768**	78.5420					1



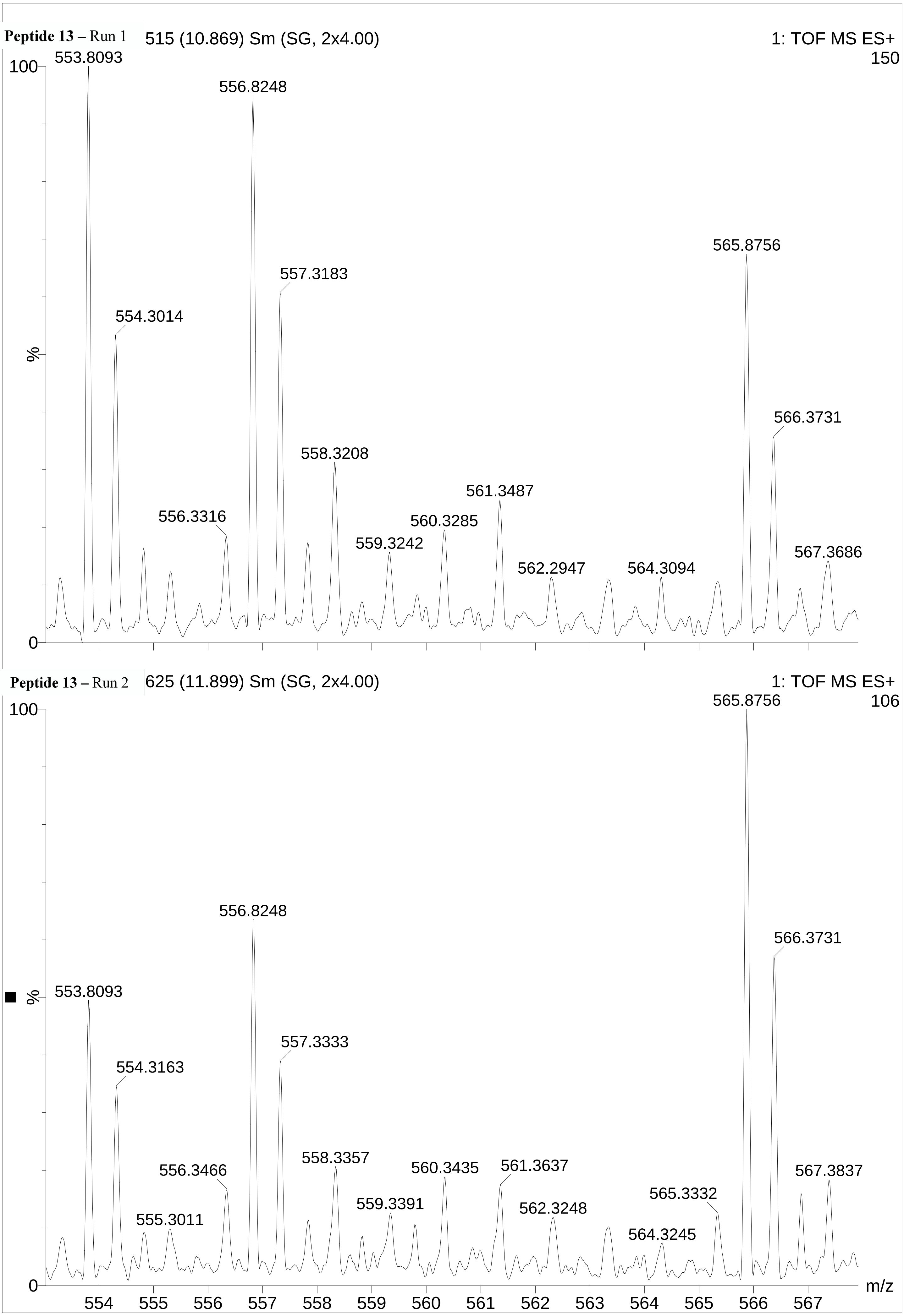


NCBI **BLAST** search of DPFNPFELTNH
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc):	Delta	Sequence
18.4	1456.8594	-0.1304	SPGKGPPPAVAPRP
17.3	1456.6987	0.0303	DPFNPFELTNH
11.3	1456.8348	-0.1059	SPLHTPRASPTGT
11.2	1456.7866	-0.0576	GTALKANPFGGASH
11.1	1456.7926	-0.0636	KNPPPSPAPEPTV
10.9	1456.8110	-0.0820	SSALDRIRERQ
10.9	1456.7946	-0.0656	LVFNPMSQDLSA
10.8	1456.7926	-0.0636	KPFTAITVTTDH
10.2	1456.7404	-0.0115	SPAFAMSPVPGSAC
9.8	1456.8514	-0.1224	IITYIRRNPQAL

Mascot: http://www.matrixscience.com/


Peptide 13 – Run 1
515 (10.869) Sm (SG, 2x4.00)
1: TOF MS ES+
150
100
%
0
553.8093
554.3014
556.3316
556.8248
557.3183
558.3208
559.3242
560.3285
561.3487
562.2947
564.3094
565.8756
566.3731
567.3686
Peptide 13 – Run 2
625 (11.899) Sm (SG, 2x4.00)
1: TOF MS ES+
106
100
%
0
553.8093
554.3163
555.3011
556.3466
556.8248
557.3333
558.3357
559.3391
560.3435
561.3637
562.3248
564.3245
565.3332
565.8756
566.3731
567.3837
554
555
556
557
558
559
560
561
562
563
564
565
566
567
m/z

Mascot Search Results

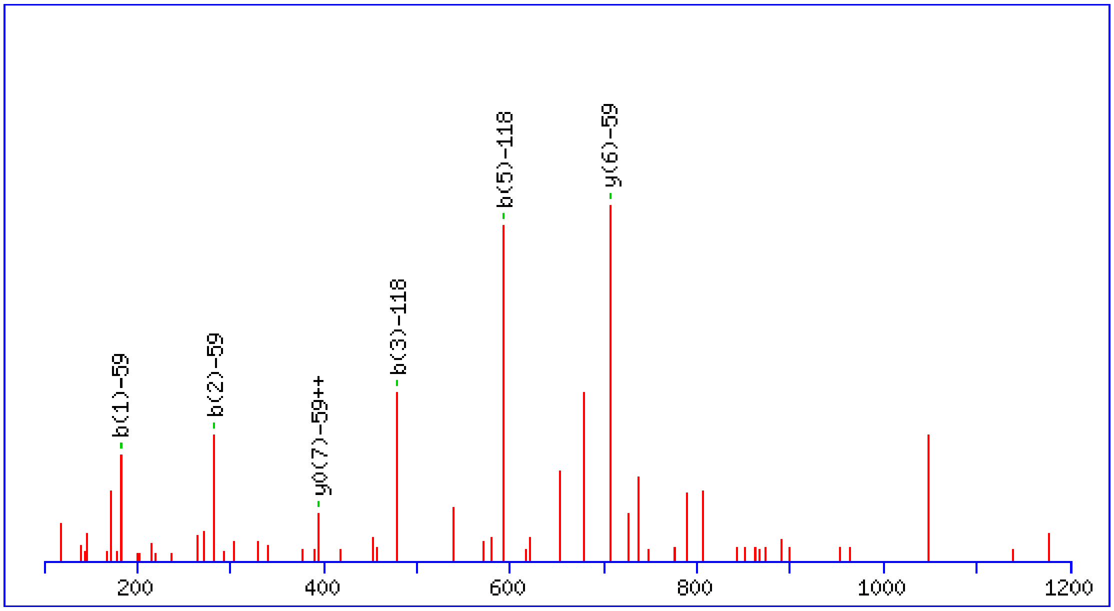
Peptide View

Peptide 13

MS/MS Fragmentation of **LTKGGYTL**
Found in **HEMO_HUMAN**, Hemopexin OS=Homo sapiens GN=HPX PE=1 SV=2

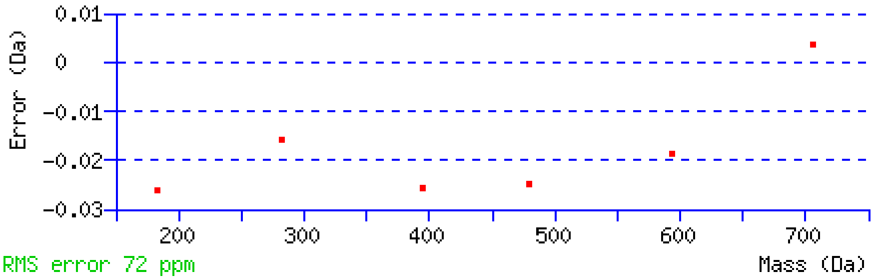
Match to Query 159: 1105.652068 from(553.833310,2+) intensity(2083.0000)
Title: 135: Scan 629 (rt=649.041, f=2, i=46) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

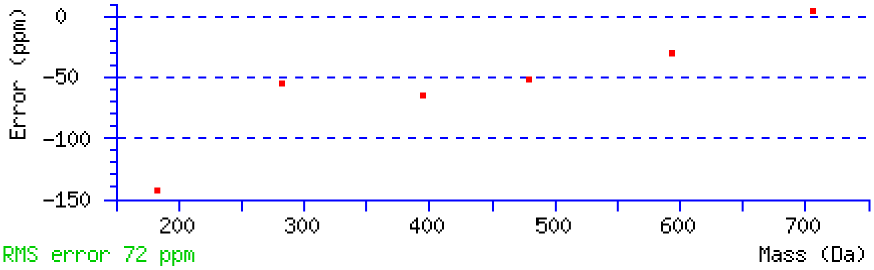
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 100 to 1200 Da Full range
Label all possible matches ○ Label matches used for scoring ○



Monoisotopic mass of neutral peptide Mr(calc): 1105.6747
Variable modifications:
N-term : GIST-Quat (N-term), with neutral loss 59.0735
K3 : GIST-Quat (K), with neutral loss 59.0735
Ions Score: 25 **Expect:** 1.4e+002
Matches : 6/66 fragment ions using 10 most intense peaks (help)

#	b	b^{++}	b*	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y^{*++}	y^{0}	y^{0++}	#
1	***182.1176***	91.5624					L							8
2	***283.1652***	142.0863			265.1547	133.0810	T	807.4247	404.2160	790.3981	395.7027	789.4141	395.2107	7
3	***479.2864***	240.1468	462.2599	231.6336	461.2758	231.1416	K	**706.3770**	353.6921	689.3505	345.1789	688.3665	344.6869	6
4	536.3079	268.6576	519.2813	260.1443	518.2973	259.6523	G	510.2558	255.6316			492.2453	246.6263	5
5	***593.3293***	297.1683	576.3028	288.6550	575.3188	288.1630	G	453.2344	227.1208			435.2238	218.1155	4
6	756.3927	378.7000	739.3661	370.1867	738.3821	369.6947	Y	396.2129	198.6101			378.2023	189.6048	3
7	857.4403	429.2238	840.4138	420.7105	839.4298	420.2185	T	233.1496	117.0784			215.1390	108.0731	2
8							L	132.1019	66.5546					1





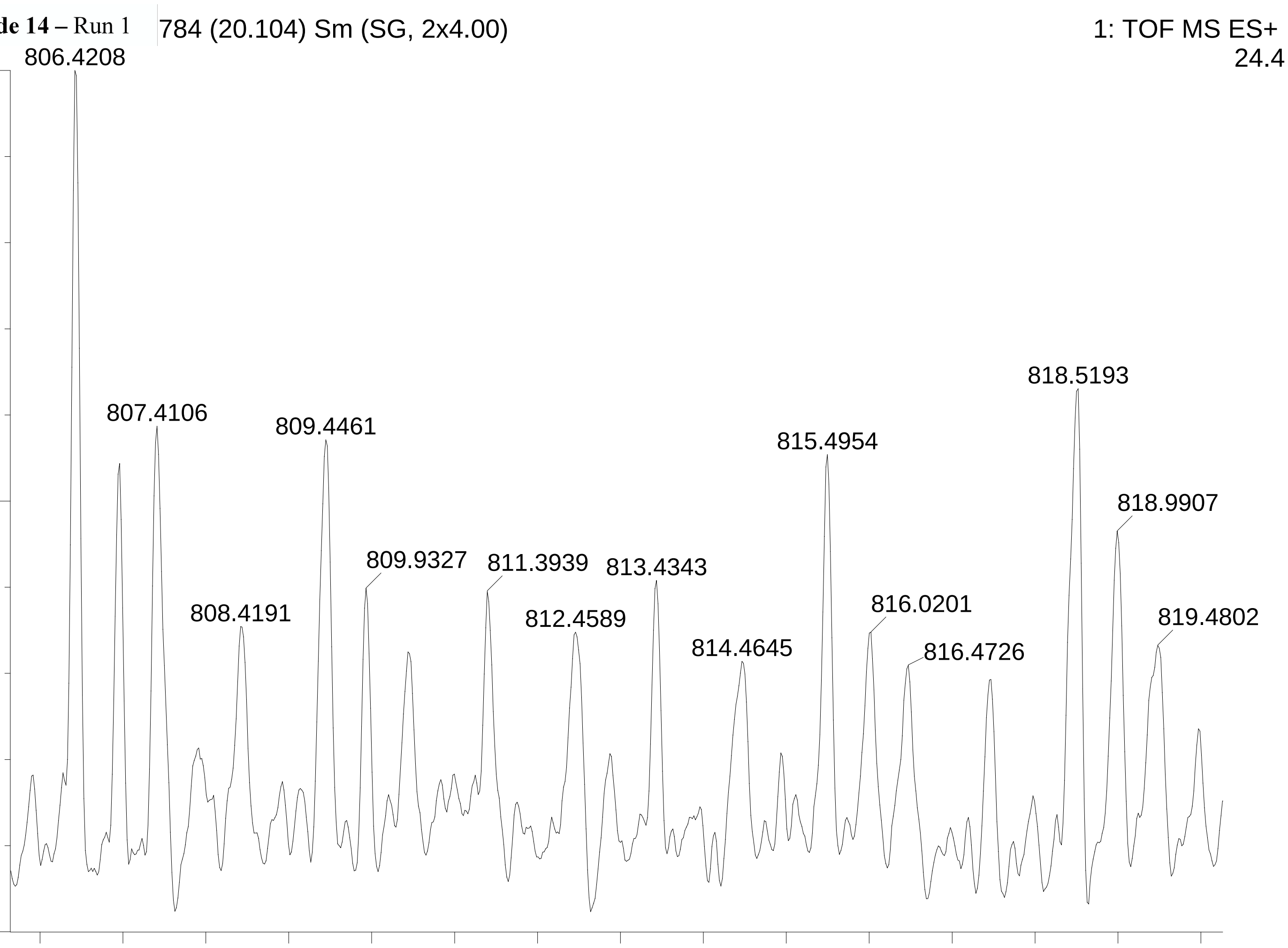
NCBI **BLAST** search of LTKGGYTL
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

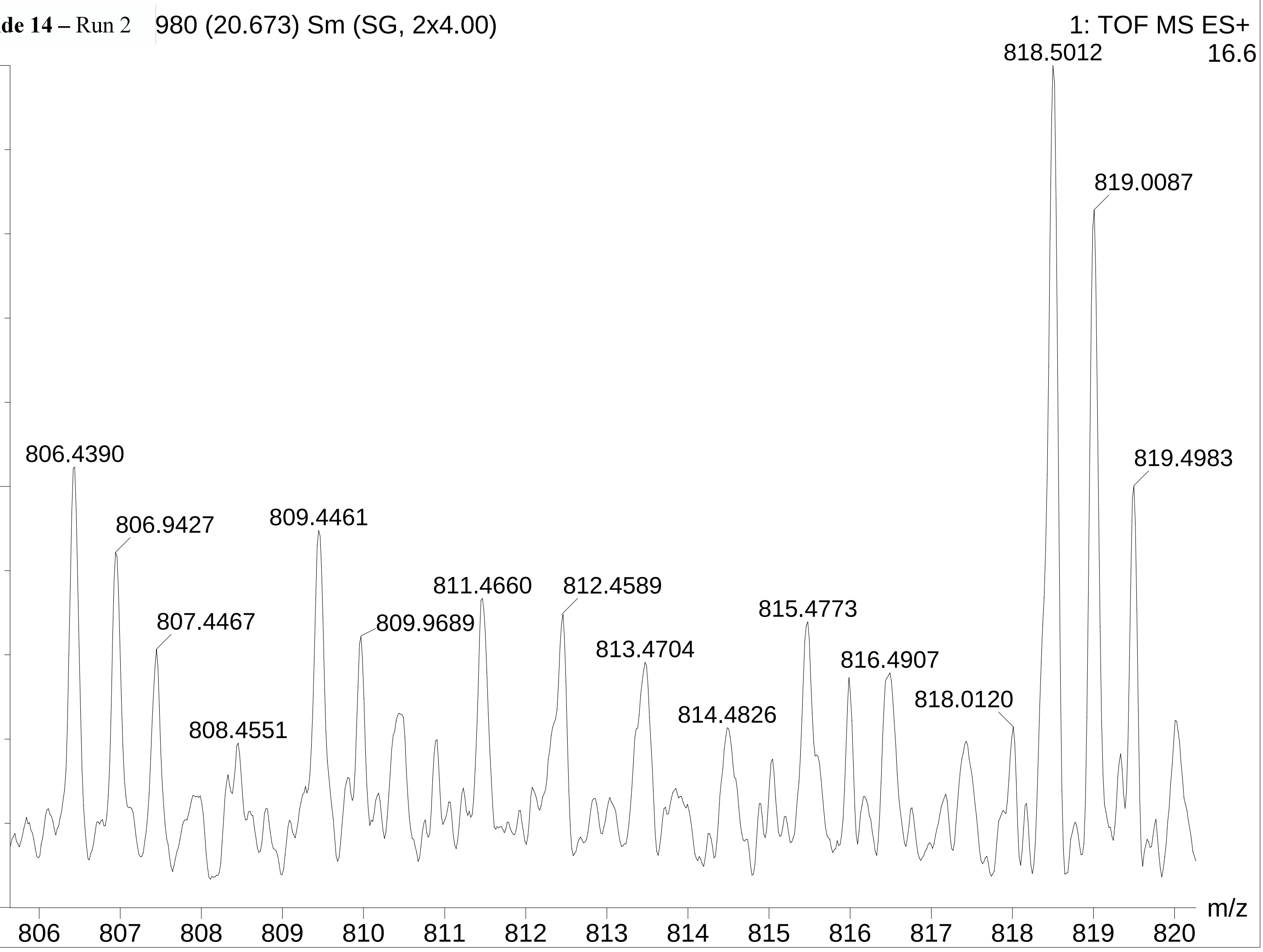
Score	Mr(calc):	Delta	Sequence
31.6	1105.6938	-0.0418	IKPLNKTY
31.6	1105.8148	-0.1628	ITKNIK
31.6	1105.8148	-0.1628	ITKNIK
31.6	1105.8148	-0.1628	ITKNIK
31.6	1105.8148	-0.1628	ITKNIK
31.6	1105.6939	-0.0418	ITKNLGFG
31.6	1105.6939	-0.0418	ITKNLGFG
24.9	1105.6747	-0.0226	LTKGGYTL
23.5	1105.6383	0.0138	PDTKKTY
23.5	1105.7136	-0.0616	TTNLKTY

Mascot: http://www.matrixscience.com/

Peptide 14 – Run 1



Peptide 14 – Run 2



MATRIX SCIENCE Mascot Search Results

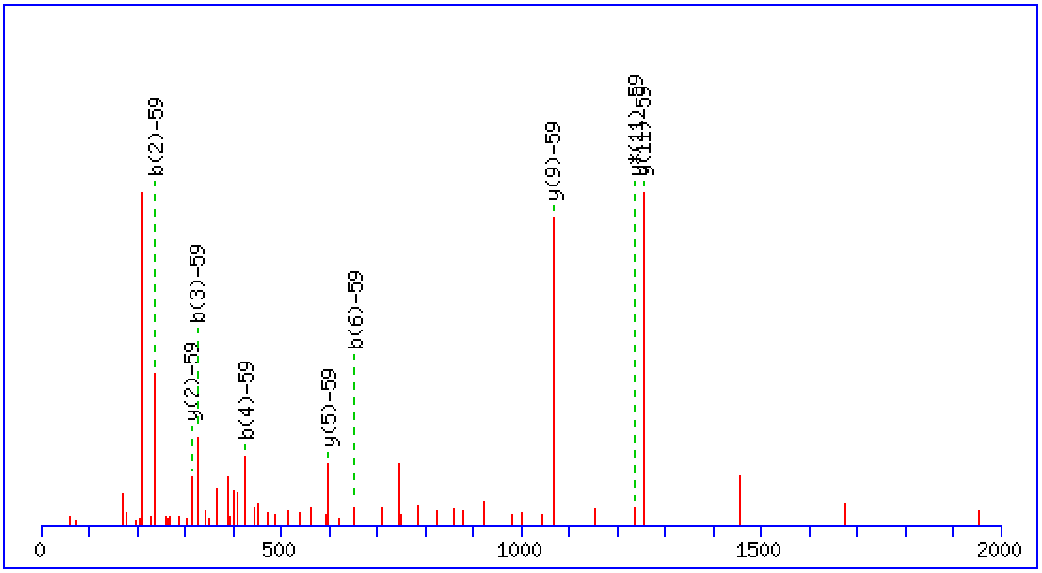
Peptide View

Peptide 14

MS/MS Fragmentation of **GISTPEELGLDKV**
Found in **COX5A_HUMAN**, Cytochrome c oxidase subunit 5A, mitochondrial OS=Homo sapiens GN=COX5A PE=1 SV=2

Match to Query 430: 1610.922688 from(806.468620,2+) intensity(2100.0000)
Title: 527: Sum of 2 scans in range 1171 (rt=1207.29, f=2, i=177) to 1172 (rt=1208.31, f=2, i=178) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

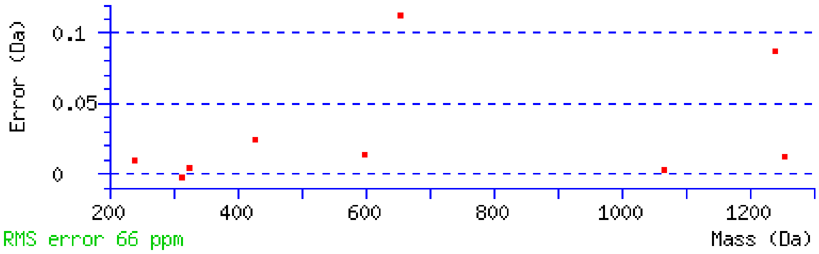
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 0 to 2000 Da Full range
Label all possible matches ○ Label matches used for scoring ○

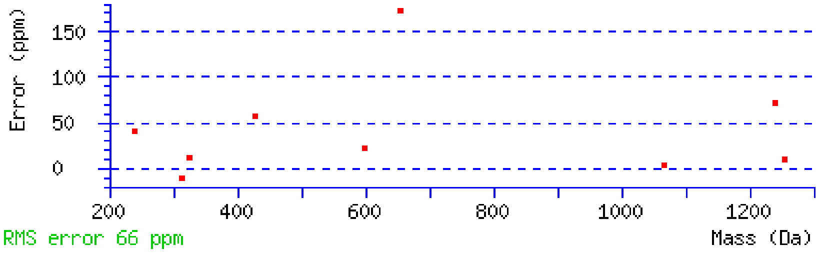


Monoisotopic mass of neutral peptide Mr(calc): 1610.9131
Variable modifications:
N-term : GIST-Quat (N-term), with neutral loss 59.0735
K12 : GIST-Quat (K), with neutral loss 59.0735
Ions Score: 18 **Expect:** 1e+003
Matches : 9/112 fragment ions using 25 most intense peaks (help)

#	b	b^{++}	b*	b*$^{++}$	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y*$^{++}$	y^{0}	y^{0++}	#
1	126.0550	63.5311					G							13
2	*239.1390*	120.0731					I	1368.7257	684.8665	1351.6991	676.3532	1350.7151	675.8612	12
3	*326.1710*	163.5892			308.1605	154.5839	S	*1255.6416*	628.3245	1238.6151	619.8112	1237.6311	619.3192	11
4	*427.2187*	214.1130			409.2082	205.1077	T	1168.6096	584.8084	1151.5830	576.2952	1150.5990	575.8032	10
5	524.2715	262.6394			506.2609	253.6341	P	*1067.5619*	534.2846	1050.5354	525.7713	1049.5514	525.2793	9
6	*653.3141*	327.1607			635.3035	318.1554	E	970.5092	485.7582	953.4826	477.2449	952.4986	476.7529	8
7	782.3567	391.6820			764.3461	382.6767	E	841.4666	421.2369	824.4400	412.7236	823.4560	412.2316	7
8	895.4407	448.2240			877.4302	439.2187	L	712.4240	356.7156	695.3974	348.2023	694.4134	347.7103	6
9	952.4622	476.7347			934.4516	467.7295	G	*599.3399*	300.1736	582.3134	291.6603	581.3293	291.1683	5
10	1065.5463	533.2768			1047.5357	524.2715	L	542.3184	271.6629	525.2919	263.1496	524.3079	262.6576	4

11	1180.5732	590.7902			1162.5626	581.7850	**D**	429.2344	215.1208	412.2078	206.6076	411.2238	206.1155	**3**
12	1376.6944	688.8508	1359.6678	680.3376	1358.6838	679.8456	**K**	***314.2074***	157.6074	297.1809	149.0941			**2**
13							**V**	118.0863	59.5468					**1**





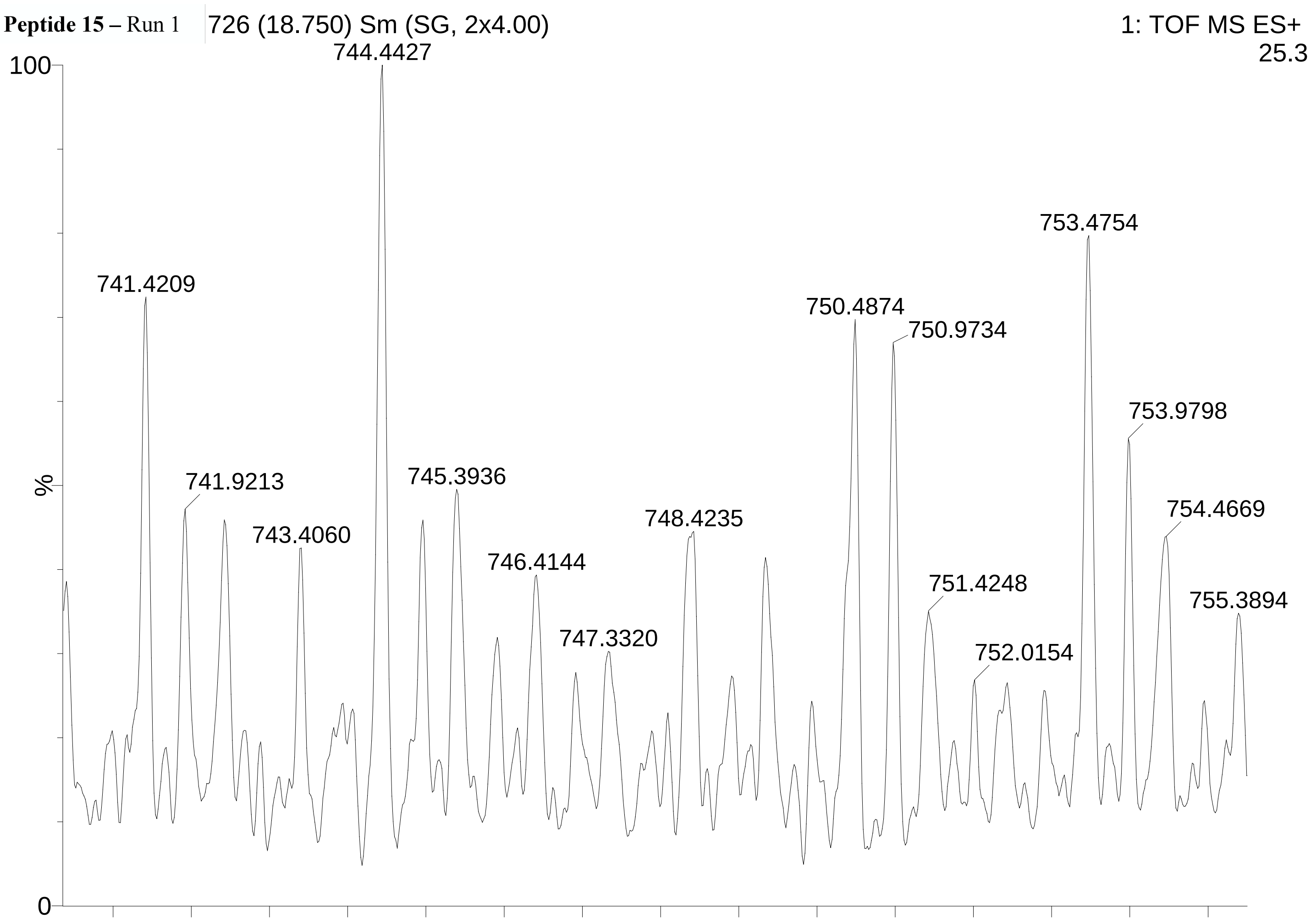
NCBI **BLAST** search of GISTPEELGLDKV
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

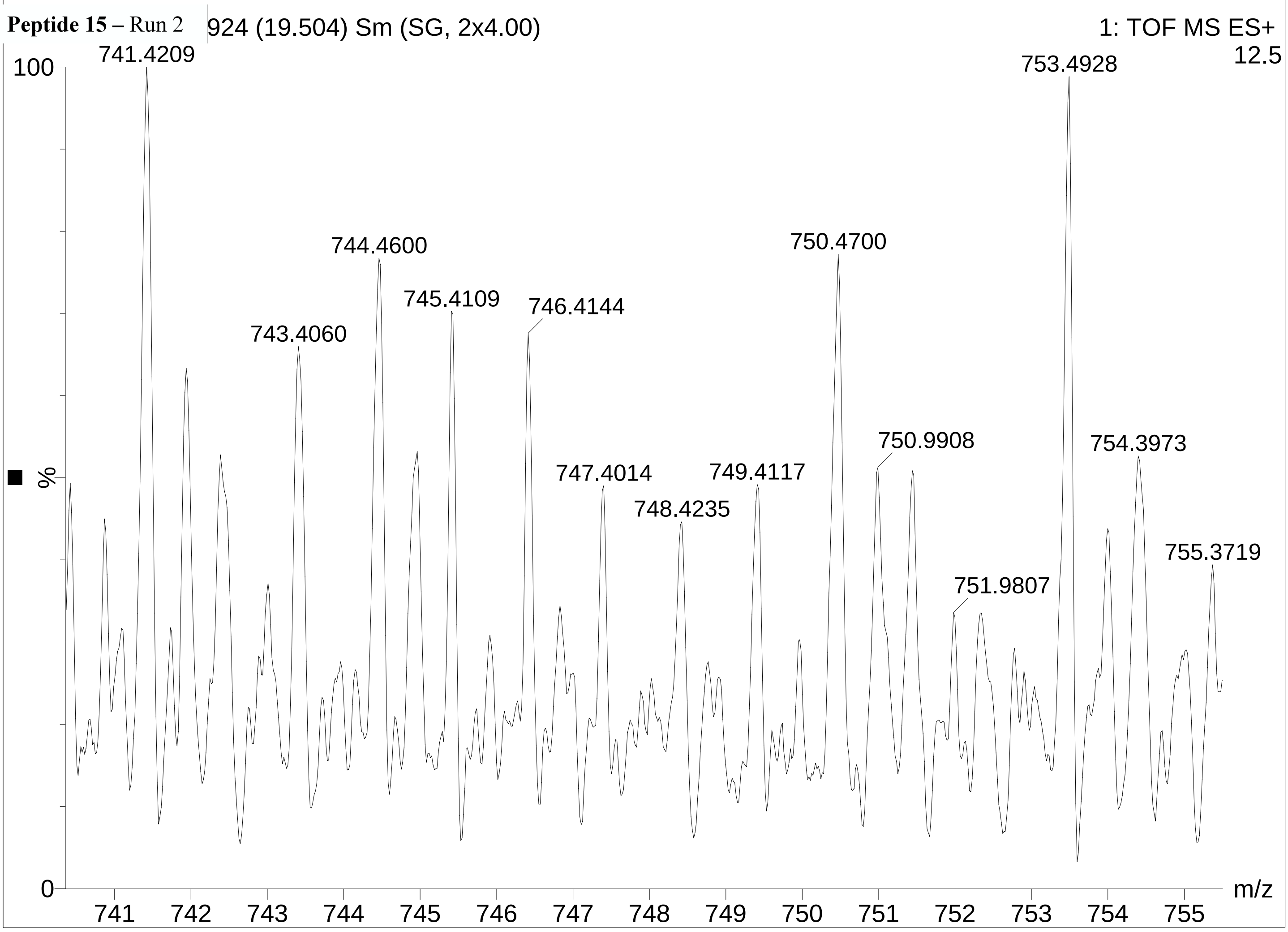
Score	Mr(calc):	Delta	Sequence
17.7	1610.9131	0.0096	GISTPEELGLDKV
12.6	1610.9494	-0.0268	LPESTVKVWFRN
11.2	1610.8574	0.0653	AADTDGRLRSGDEL
10.9	1610.7665	0.1562	PLDTPCGHTFCYK
10.1	1610.8628	0.0599	AADTKKQNADPQA
9.1	1611.0739	-0.1512	GLAASLLFLLLVK
8.9	1610.8628	0.0599	AADTKKQNADPQA
8.9	1610.8338	0.0889	AADTPGKPSASPMAG
8.5	1610.9548	-0.0321	VAWFHEKTKIV
8.4	1611.0011	-0.0784	ISPLGILYTPALKV

Mascot: http://www.matrixscience.com/

Peptide 15 – Run 1



Peptide 15 – Run 2



Mascot Search Results

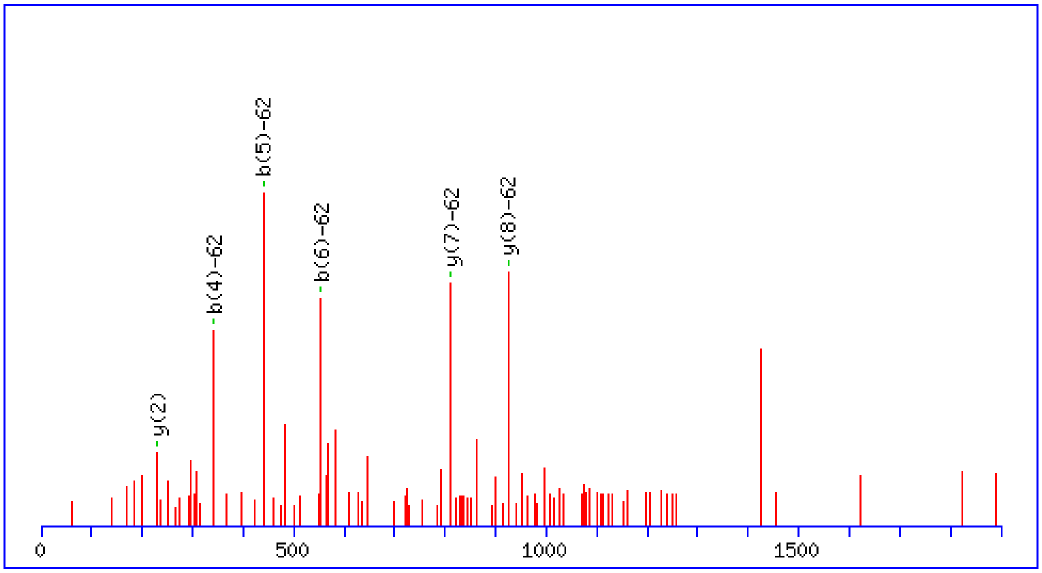
Peptide View

Peptide 15

MS/MS Fragmentation of **GGSAVISLEGKPL**
Found in **COF1_HUMAN**, Cofilin-1 OS=Homo sapiens GN=CFL1 PE=1 SV=3

Match to Query 383: 1486.899428 from(744.456990,2+) intensity(1205.0000)
Title: 503: Scan 1090 (rt=1123.96, f=4, i=65) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

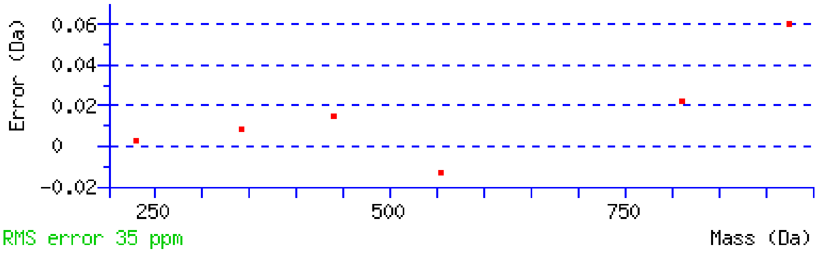
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 0 to 1900 Da Full range
Label all possible matches ○ Label matches used for scoring ○

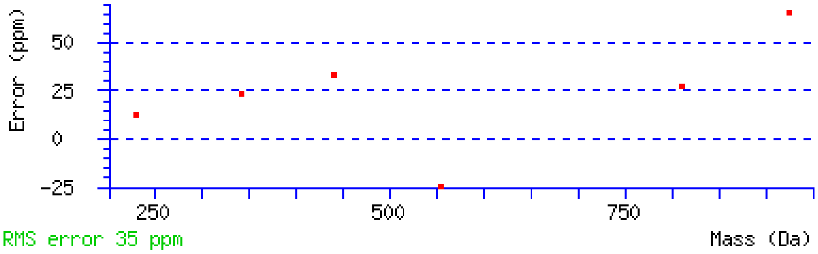


Monoisotopic mass of neutral peptide Mr(calc): 1486.9241
Variable modifications:
N-term : GIST-Quat:2H(3) (N-term), with neutral loss 62.0923
K11 : GIST-Quat:2H(3) (K), with neutral loss 62.0923
Ions Score: 13 **Expect:** 3.1e+003
Matches : 6/108 fragment ions using 13 most intense peaks (help)

#	b	b^{++}	b*	b*$^{++}$	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y*$^{++}$	y^{0}	y^{0++}	#
1	126.0550	63.5311					**G**							**13**
2	183.0764	92.0418					**G**	1238.6991	619.8532	1221.6725	611.3399	1220.6885	610.8479	**12**
3	270.1084	135.5579			252.0979	126.5526	**S**	1181.6776	591.3424	1164.6511	582.8292	1163.6671	582.3372	**11**
4	***341.1456***	171.0764			323.1350	162.0711	**A**	1094.6456	547.8264	1077.6190	539.3132	1076.6350	538.8211	**10**
5	***440.2140***	220.6106			422.2034	211.6053	**V**	1023.6085	512.3079	1006.5819	503.7946	1005.5979	503.3026	**9**
6	***553.2980***	277.1527			535.2875	268.1474	**I**	***924.5401***	462.7737	907.5135	454.2604	906.5295	453.7684	**8**
7	640.3301	320.6687			622.3195	311.6634	**S**	***811.4560***	406.2316	794.4294	397.7184	793.4454	397.2264	**7**
8	753.4141	377.2107			735.4036	368.2054	**L**	724.4240	362.7156	707.3974	354.2023	706.4134	353.7103	**6**
9	882.4567	441.7320			864.4462	432.7267	**E**	611.3399	306.1736	594.3134	297.6603	593.3293	297.1683	**5**
10	939.4782	470.2427			921.4676	461.2374	**G**	482.2973	241.6523	465.2708	233.1390			**4**
11	1135.5994	568.3033	1118.5728	559.7900	1117.5888	559.2980	**K**	425.2758	213.1416	408.2493	204.6283			**3**

12	1232.6521	616.8297	1215.6256	608.3164	1214.6416	607.8244	**P**	***229.1547***	115.0810					**2**
13							**L**	132.1019	66.5546					**1**



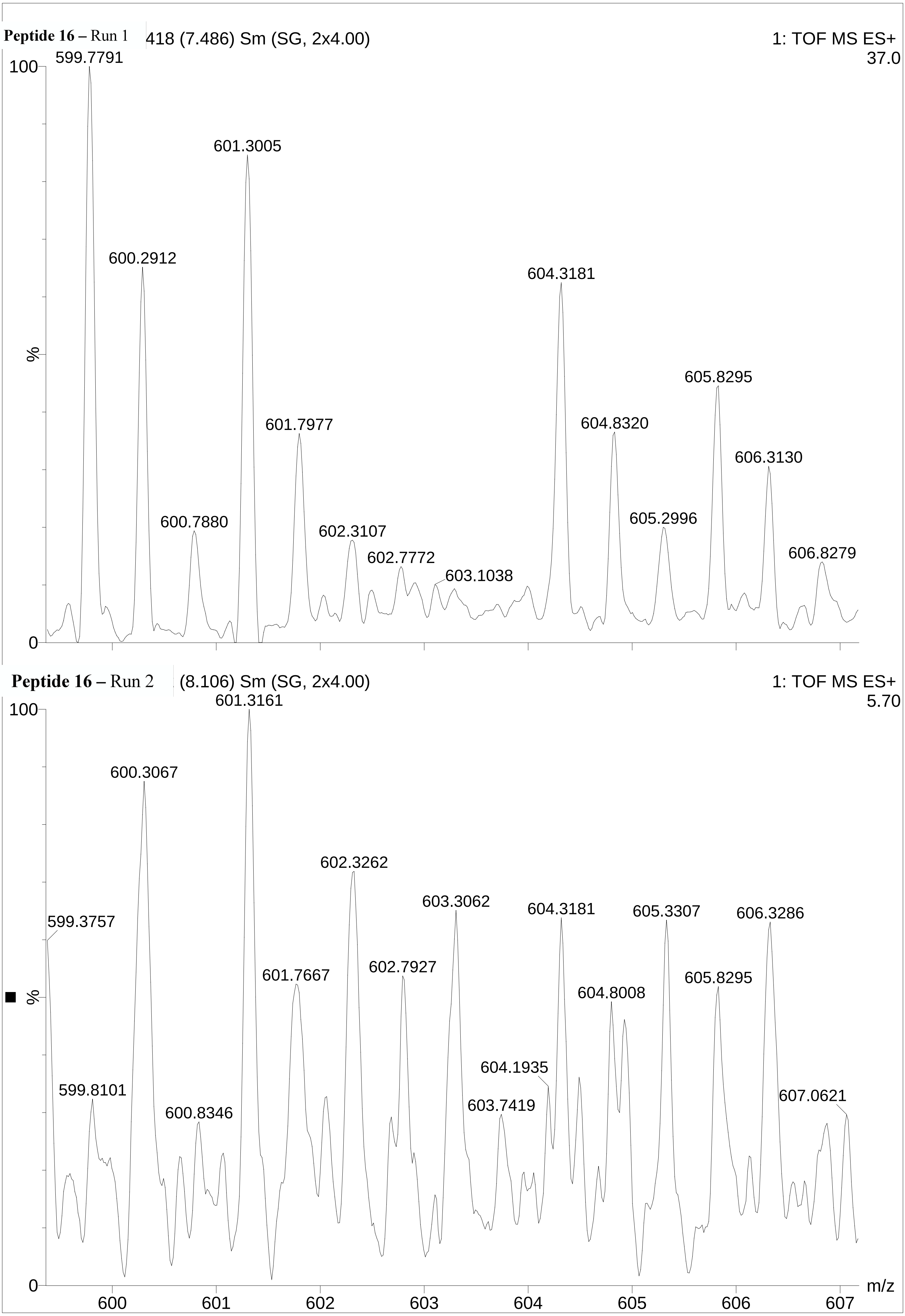


NCBI **BLAST** search of GGSAVISLEGKPL
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc):	Delta	Sequence
17.6	1486.8454	0.0541	EVGNDLDIAHLR
15.8	1486.9354	-0.0359	ASNVLNTKVKGP
14.8	1486.8965	0.0029	DIICGKLLAKMF
13.2	1486.7402	0.1592	LEELEEIDLSGN
13.1	1486.9770	-0.0775	KSGVKSRIHALR
13.1	1486.9770	-0.0775	KSGVKSRIHALR
12.6	1486.9241	-0.0247	GGSAVISLEGKPL
12.6	1486.8566	0.0428	EVQARDRGNPPL
12.4	1486.8872	0.0122	MPVLKSSLALGLE
12.1	1486.8930	0.0065	ATADRDILARLH

Mascot: http://www.matrixscience.com/



Peptide 16 – Run 1
418 (7.486) Sm (SG, 2x4.00)
1: TOF MS ES+
37.0
100
%
0
599.7791
600.2912
600.7880
601.3005
601.7977
602.3107
602.7772
603.1038
604.3181
604.8320
605.2996
605.8295
606.3130
606.8279
Peptide 16 – Run 2
(8.106) Sm (SG, 2x4.00)
1: TOF MS ES+
5.70
100
%
0
599.3757
599.8101
600.3067
600.8346
601.3161
601.7667
602.3262
602.7927
603.3062
603.7419
604.1935
604.3181
604.8008
605.3307
605.8295
606.3286
607.0621
600
601
602
603
604
605
606
607
m/z

MATRIX SCIENCE Mascot Search Results

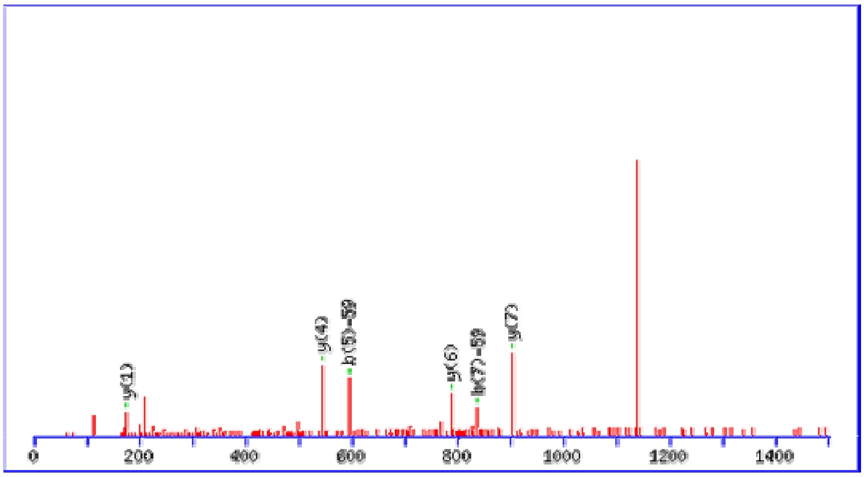
Peptide View

Peptide 16

MS/MS Fragmentation of **APDQDEIQR**
Found in **PPGB_HUMAN**, Lysosomal protective protein OS=Homo sapiens GN=CTSA PE=1 SV=2

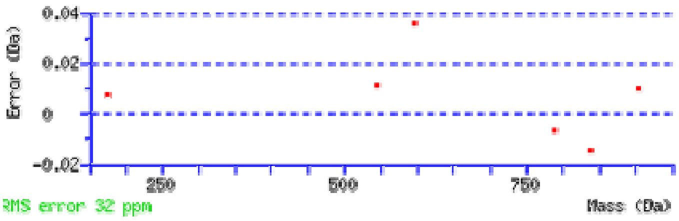
Match to Query 228: 1197.613788 from(599.814170,2+) intensity(879.0000)
Title: 3: Scan 437 (rt=451.339, f=2, i=2) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

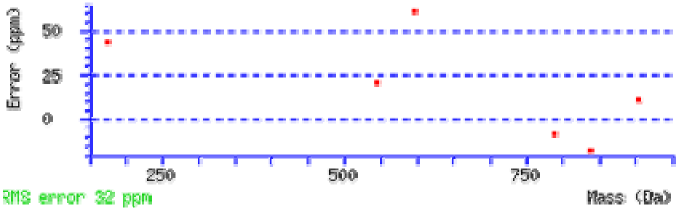
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 0 to 1500 Da Full range
Label all possible matches ○ Label matches used for scoring ●



Monoisotopic mass of neutral peptide Mr(calc): 1197.5990
Fixed modifications: GIST-Quat (K),GIST-Quat (N-term) (apply to specified residues or termini only)
Ions Score: 8 **Expect:** 9.3e+002
Matches : 6/80 fragment ions using 24 most intense peaks (help)

#	b	b^{++}	b*	b^{*++}	b^0	b^{0++}	Seq.	y	y^{++}	y*	y^{*++}	y^0	y^{0++}	#
1	140.0706	70.5389					A							9
2	237.1234	119.0653					P	1000.4694	500.7383	983.4429	492.2251	982.4589	491.7331	8
3	352.1503	176.5788			334.1397	167.5735	D	***903.4167***	452.2120	886.3901	443.6987	885.4061	443.2067	7
4	480.2089	240.6081	463.1823	232.0948	462.1983	231.6028	Q	***788.3897***	394.6985	771.3632	386.1852	770.3791	385.6932	6
5	**595.2358**	298.1216	578.2093	289.6083	577.2253	289.1163	D	660.3311	330.6692	643.3046	322.1559	642.3206	321.6639	5
6	724.2784	362.6429	707.2519	354.1296	706.2679	353.6376	E	***545.3042***	273.1557	528.2776	264.6425	527.2936	264.1504	4
7	**837.3625**	419.1849	820.3359	410.6716	819.3519	410.1796	I	416.2616	208.6344	399.2350	200.1212			3
8	965.4211	483.2142	948.3945	474.7009	947.4105	474.2089	Q	303.1775	152.0924	286.1510	143.5791			2
9							R	***175.1190***	88.0631	158.0924	79.5498			1





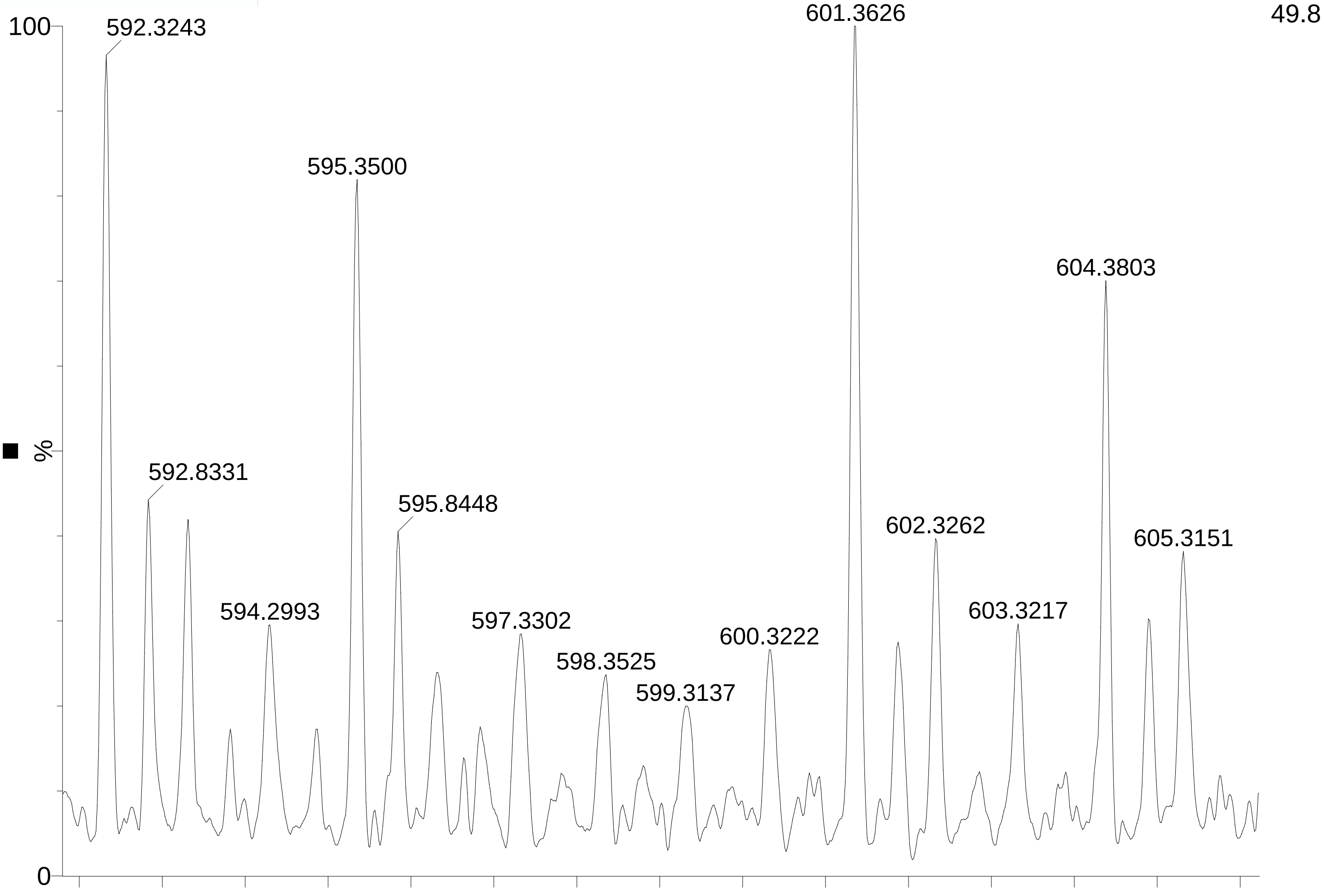
NCBI **BLAST** search of APDQDEIQR
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

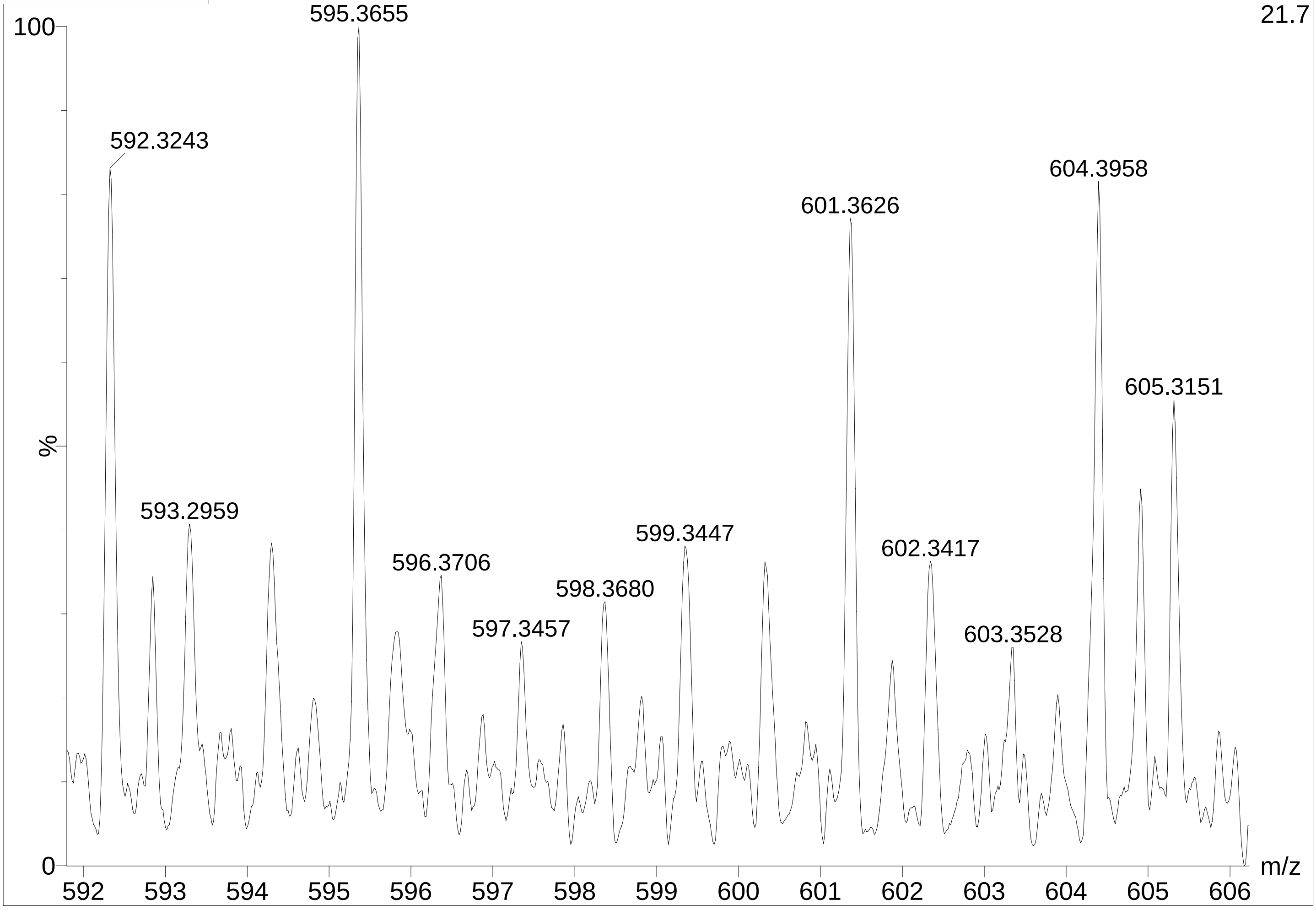
Score	Mr(calc):	Delta	Sequence
7.5	1197.5990	0.0148	APDQDEIQR
2.9	1197.4166	0.1972	DDDMDENSM
2.6	1197.6353	-0.0215	TEAGAPELQR
2.1	1197.5554	0.0584	PADQDSLYY
2.0	1197.5666	0.0472	YPTDSRGEF
2.0	1197.6717	-0.0579	LLGALGEGDAR
1.4	1197.5990	0.0148	NESVPDSPAR

Mascot: http://www.matrixscience.com/

Peptide 17 – Run 1



Peptide 17 – Run 2



Mascot Search Results

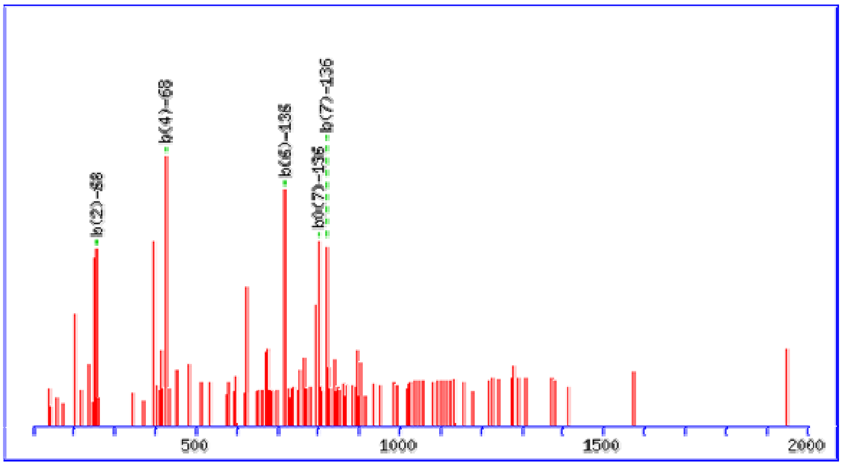
Peptide View

Peptide 17

MS/MS Fragmentation of **GEGLPKTDL**
Found in **PCDA3_HUMAN**, Protocadherin alpha-3 OS=Homo sapiens GN=PCDHA3 PE=1 SV=1

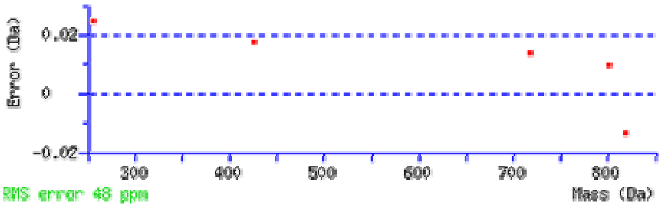
Match to Query 231: 1200.710668 from(601.362610,2+) intensity(1202.0000)
Title: 37: Scan 538 (rt=555.314, f=4, i=7) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

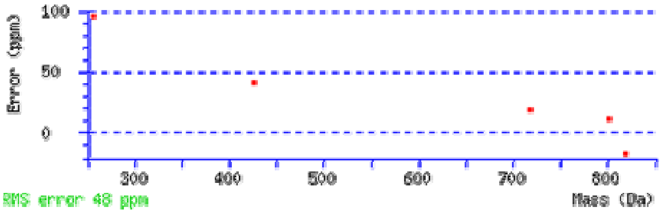
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 100 to 2000 Da Full range
Label all possible matches ○ Label matches used for scoring ●



Monoisotopic mass of neutral peptide Mr(calc): 1200.7990
Fixed modifications: GIST-Quat:2H(9) (K),GIST-Quat:2H(9) (N-term) (apply to specified residues or termini only)
Ions Score: 8 **Expect:** 7e+002
Matches : 5/76 fragment ions using 22 most intense peaks (help)

#	b	b^{++}	b*	b^{*++}	b^0	b^{0++}	Seq.	y	y^{++}	y*	y^{*++}	y^0	y^{0++}	#
1	126.0550	63.5311					G							9
2	*255.0975*	128.0524			237.0870	119.0471	E	940.4986	470.7529	923.4720	462.2397	922.4880	461.7477	8
3	312.1190	156.5631			294.1084	147.5579	G	811.4560	406.2316	794.4294	397.7184	793.4454	397.2264	7
4	*425.2031*	213.1052			407.1925	204.0999	L	754.4345	377.7209	737.4080	369.2076	736.4240	368.7156	6
5	522.2558	261.6316			504.2453	252.6263	P	641.3505	321.1789	624.3239	312.6656	623.3399	312.1736	5
6	*718.3770*	359.6921	701.3505	351.1789	700.3665	350.6869	K	544.2977	272.6525	527.2712	264.1392	526.2871	263.6472	4
7	*819.4247*	410.2160	802.3981	401.7027	801.4141	401.2107	T	348.1765	174.5919			330.1660	165.5866	3
8	934.4516	467.7295	917.4251	459.2162	916.4411	458.7242	D	247.1288	124.0681			229.1183	115.0628	2
9							L	132.1019	66.5546					1



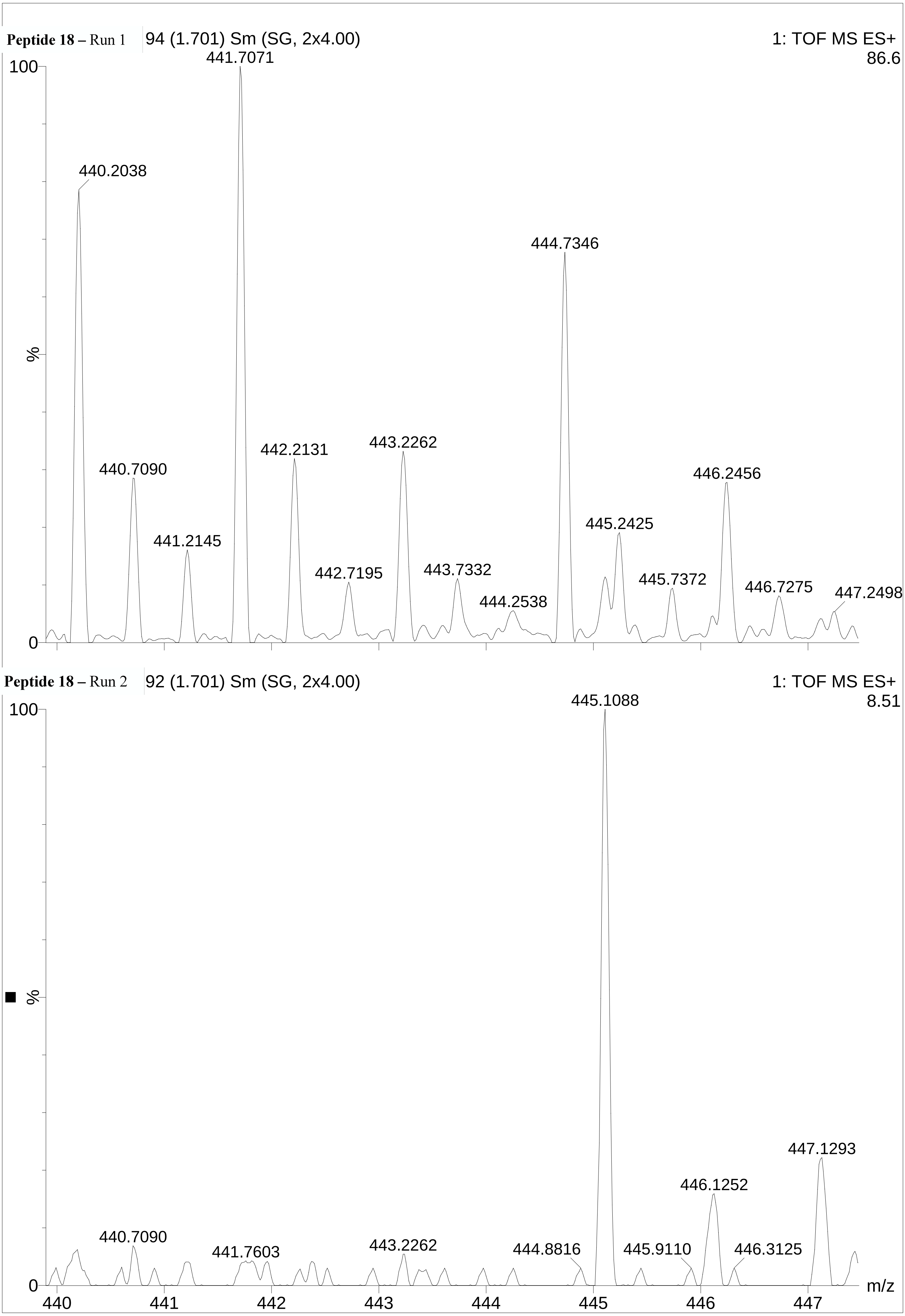


NCBI **BLAST** search of GEGLPKTDL
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc):	Delta	Sequence
8.2	1200.7990	-0.0883	GEGLPKTDL
3.3	1200.7990	-0.0883	STPAKPTVE
0.9	1200.8354	-0.1247	SVGIKPSLE
0.8	1200.7289	-0.0182	VAQAAEALRH
0.3	1200.8353	-0.1247	ADAVAELKL
0.3	1200.8717	-0.1611	DAIGISLLK
0.3	1200.6548	0.0559	EGGLISSSTQS
0.3	1200.6597	0.0510	WGLTVMDLM
0.3	1200.6563	0.0544	WLGPCDIVY

Mascot: http://www.matrixscience.com/


Peptide 18 – Run 1
94 (1.701) Sm (SG, 2x4.00)
1: TOF MS ES+
86.6
100
%
0
441.7071
440.2038
444.7346
440.7090
442.2131
443.2262
446.2456
441.2145
445.2425
442.7195
443.7332
445.7372
446.7275
444.2538
447.2498
Peptide 18 – Run 2
92 (1.701) Sm (SG, 2x4.00)
1: TOF MS ES+
8.51
100
%
0
445.1088
447.1293
446.1252
440.7090
441.7603
443.2262
444.8816
445.9110
446.3125
440
441
442
443
444
445
446
447
m/z

Mascot Search Results

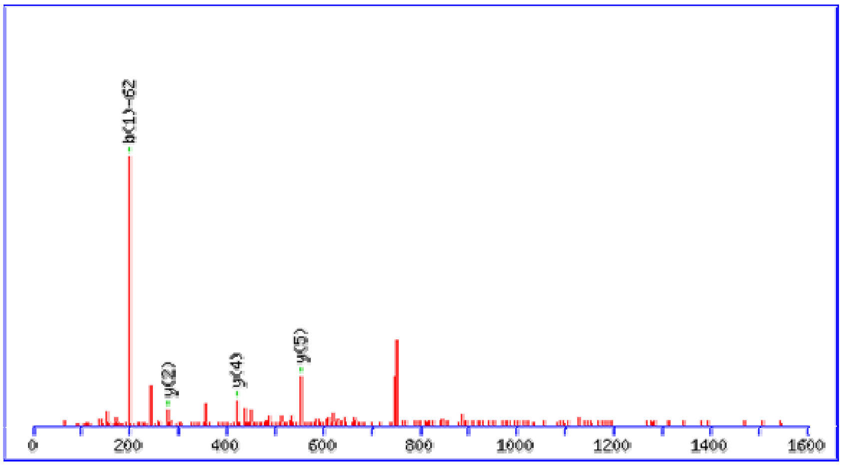
Peptide View

Peptide 18

MS/MS Fragmentation of **EAMAAIF**
Found in **M3K2_HUMAN**, Mitogen-activated protein kinase kinase kinase 2 OS=Homo sapiens GN=MAP3K2 PE=1 SV=2

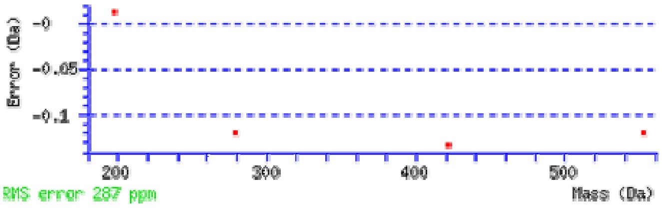
Match to Query 23: 881.453108 from(441.733830,2+) intensity(1104.0000)
Title: 1: Scan 99 (rt=103.091, f=3, i=1) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

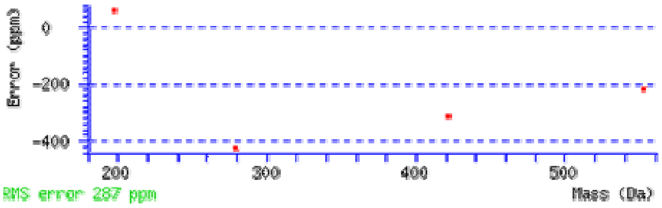
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 0 to 1600 Da Full range
Label all possible matches ○ Label matches used for scoring ●



```
Monoisotopic mass of neutral peptide Mr(calc): 881.4760
Fixed modifications: GIST-Quat:2H(3) (K),GIST-Quat:2H(3) (N-term) (apply to specified residues or termini only)
Ions Score: 3  Expect: 2e+003
Matches : 4/36 fragment ions using 17 most intense peaks   (help)
```

#	b	b^{++}	b^0	b^{0++}	Seq.	y	y^{++}	#
1	198.0761	99.5417	180.0655	90.5364	**E**			**7**
2	269.1132	135.0602	251.1026	126.0550	**A**	623.3221	312.1647	**6**
3	400.1537	200.5805	382.1431	191.5752	**M**	***552.2850***	276.6462	**5**
4	471.1908	236.0990	453.1802	227.0938	**A**	***421.2445***	211.1259	**4**
5	542.2279	271.6176	524.2173	262.6123	**A**	350.2074	175.6074	**3**
6	655.3120	328.1596	637.3014	319.1543	**I**	***279.1703***	140.0888	**2**
7					**F**	166.0863	83.5468	**1**





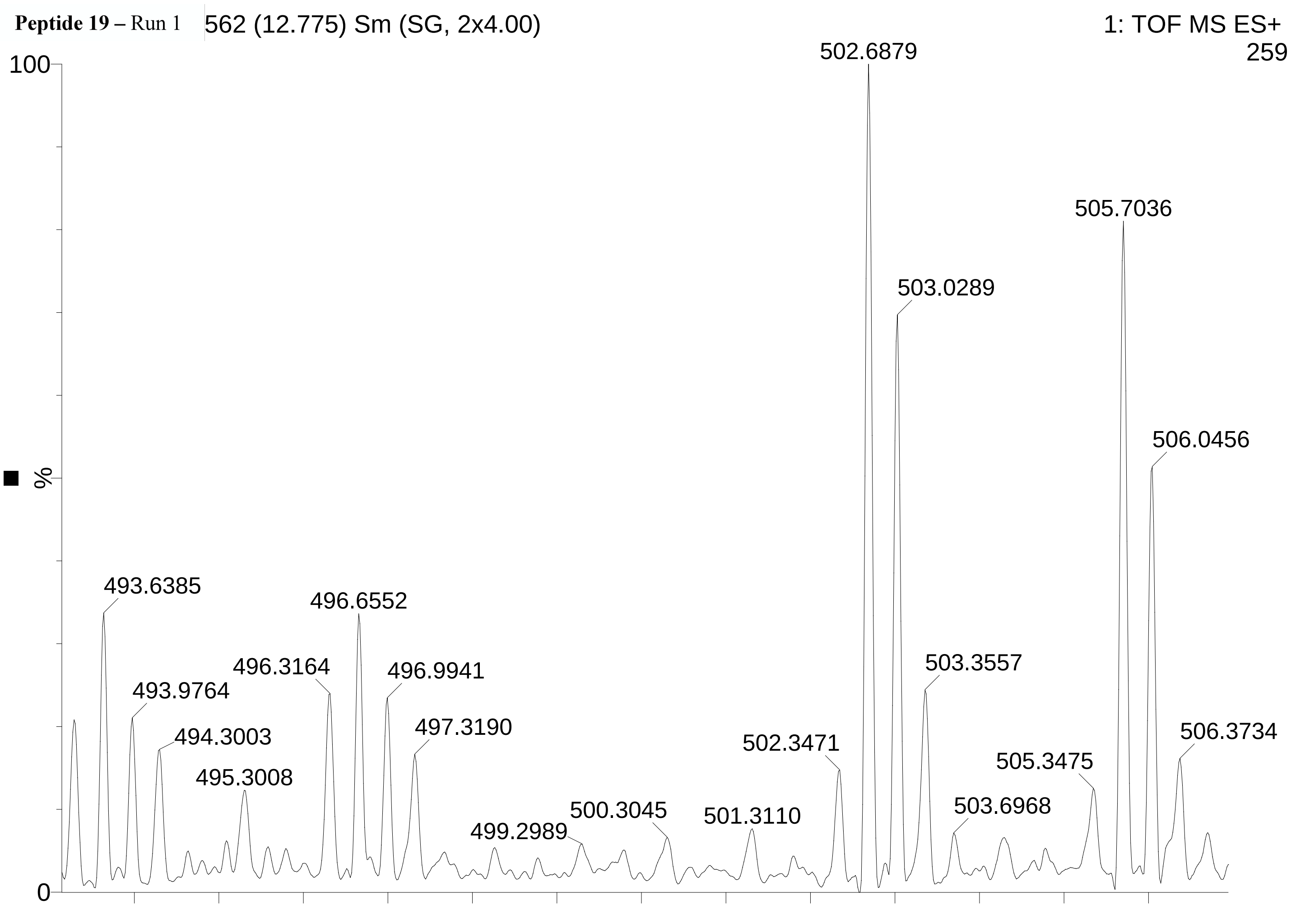
NCBI **BLAST** search of EAMAAIF
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

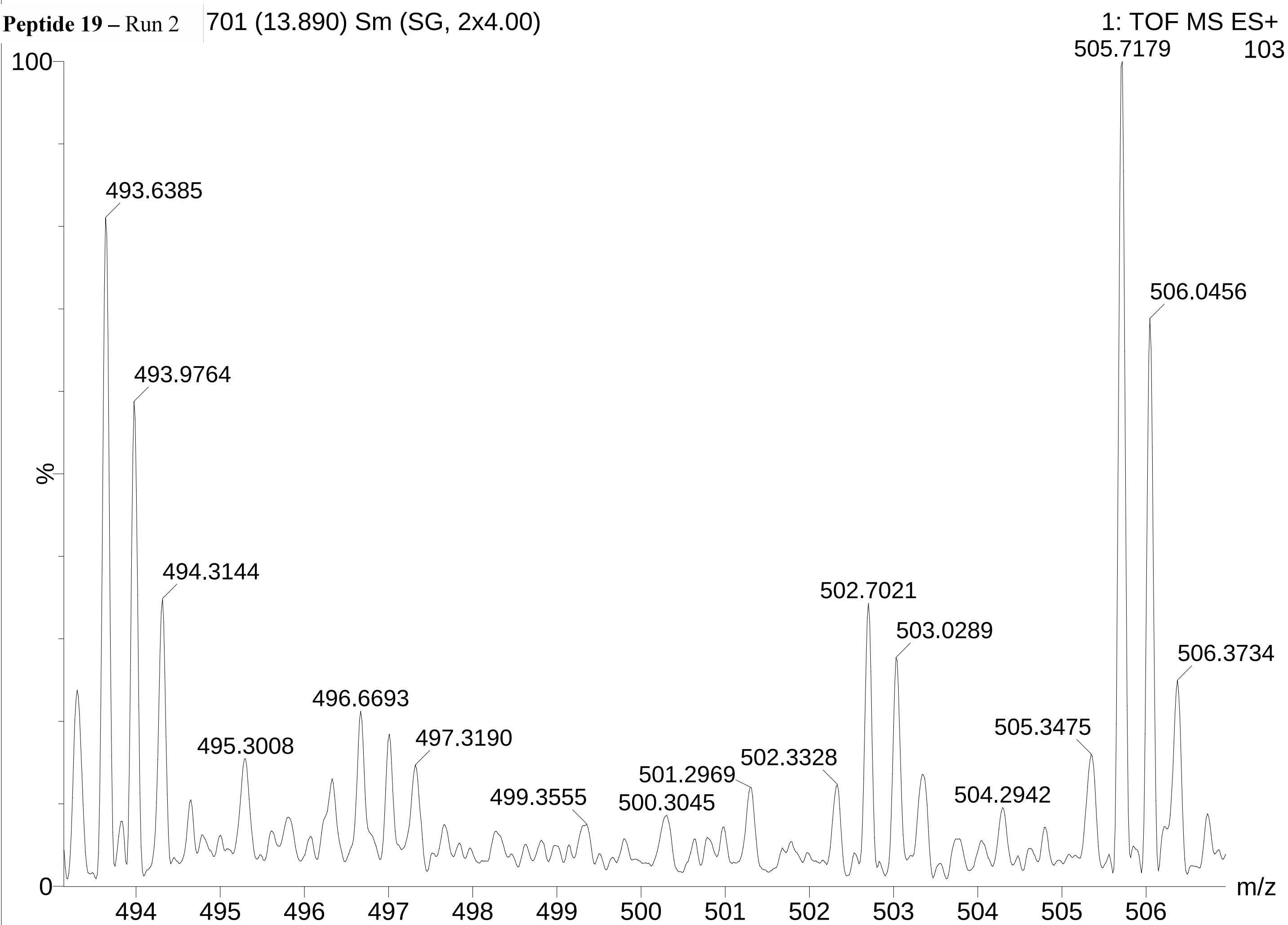
All matches to this query

Score	Mr(calc):	Delta	Sequence

7.4	881.4574	-0.0043	ESFGEIA
5.0	881.4057	0.0474	ESEATSE
5.0	881.4607	-0.0076	ESLSTLC
4.9	881.5050	-0.0519	ESPVAIH
3.2	881.4760	-0.0229	EAMAAIF
2.5	881.5414	-0.0883	EAGLLLH
2.5	881.5414	-0.0883	EALGLHL
2.5	881.4937	-0.0406	EALVASY
2.5	881.3880	0.0652	EAMASDE
2.5	881.3880	0.0652	EAMEDAS

Mascot: http://www.matrixscience.com/


Peptide 19 – Run 1
562 (12.775) Sm (SG, 2x4.00)
1: TOF MS ES+
259
100
%
0
502.6879
505.7036
503.0289
506.0456
493.6385
496.6552
496.3164
496.9941
493.9764
503.3557
494.3003
497.3190
506.3734
502.3471
495.3008
505.3475
503.6968
500.3045
501.3110
499.2989


Peptide 19 – Run 2
701 (13.890) Sm (SG, 2x4.00)
1: TOF MS ES+
103
100
%
0
505.7179
493.6385
506.0456
493.9764
494.3144
502.7021
503.0289
506.3734
496.6693
505.3475
495.3008
497.3190
502.3328
501.2969
504.2942
499.3555
500.3045
m/z
494
495
496
497
498
499
500
501
502
503
504
505
506

Mascot Search Results

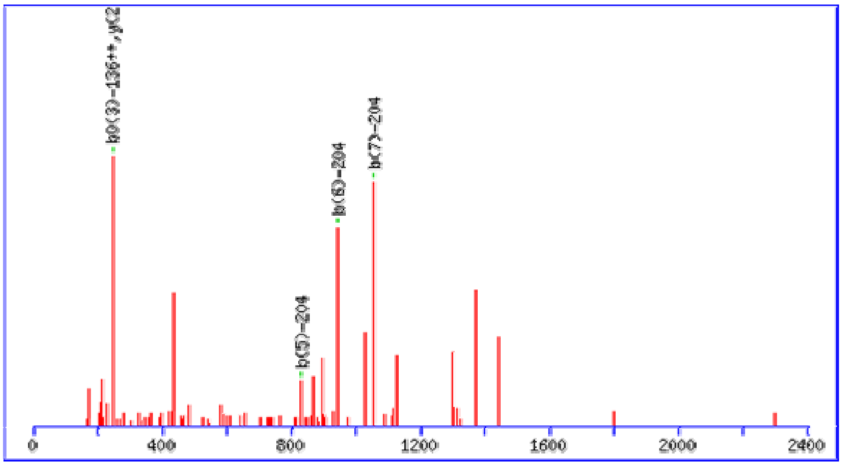
Peptide View

Peptide 19

MS/MS Fragmentation of **EIKKQLLLI**
Found in **CDC23_HUMAN**, Cell division cycle protein 23 homolog OS=Homo sapiens GN=CDC23 PE=1 SV=3

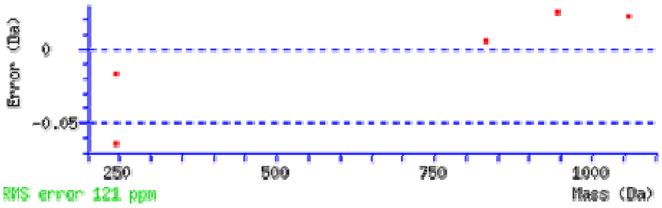
Match to Query 394: 1505.114262 from(502.712030,3+) intensity(2341.0000)
Title: 234: Scan 737 (rt=760.34, f=3, i=50) [C:\Users\synapt\Desktop\28062011 raw\290611 Leandro E1.raw]
Data file 290611 Chris E1.mgf

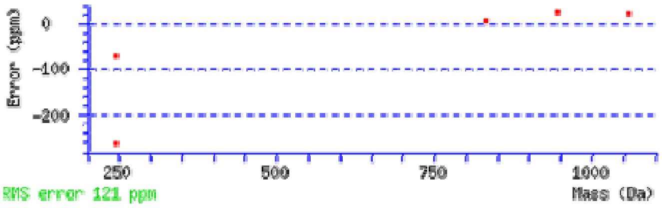
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 0 to 2400 Da Full range
Label all possible matches ○ Label matches used for scoring ●



```
Monoisotopic mass of neutral peptide Mr(calc): 1505.1906
Fixed modifications: GIST-Quat:2H(9) (K),GIST-Quat:2H(9) (N-term) (apply to specified residues or termini only)
Ions Score: 5  Expect: 1.1e+003
Matches : 5/68 fragment ions using 12 most intense peaks   (help)
```

#	b	b^{++}	b*	b*$^{++}$	b^{0}	b^{0++}	Seq.	y	y^{++}	y*	y*$^{++}$	#
1	198.0761	99.5417			180.0655	90.5364	E					9
2	311.1601	156.0837			293.1496	147.0784	I	1104.7391	552.8732	1087.7125	544.3599	8
3	507.2813	254.1443	490.2548	245.6310	489.2708	245.1390	K	991.6550	496.3312	974.6285	487.8179	7
4	703.4025	352.2049	686.3760	343.6916	685.3919	343.1996	K	795.5339	398.2706	778.5073	389.7573	6
5	***831.4611***	416.2342	814.4345	407.7209	813.4505	407.2289	Q	599.4127	300.2100	582.3861	291.6967	5
6	***944.5451***	472.7762	927.5186	464.2629	926.5346	463.7709	L	471.3541	236.1807			4
7	***1057.6292***	529.3182	1040.6027	520.8050	1039.6186	520.3130	L	358.2700	179.6387			3
8	1170.7133	585.8603	1153.6867	577.3470	1152.7027	576.8550	L	245.1860	123.0966			2
9							I	132.1019	66.5546			1





NCBI **BLAST** search of EIKKQLLLI
(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)
Other BLAST web gateways

All matches to this query

Score	Mr(calc):	Delta	Sequence
23.8	1504.9062	0.2081	LAGALLEEAEQLL
14.8	1504.9440	0.1703	AVAALLWAAVTRAG
12.9	1504.9287	0.1856	LQIAIDNSRNIL
12.9	1504.8811	0.2332	SGPSPLEETRALL
12.7	1504.9790	0.1352	GSPALLLLTTLLGT
12.7	1504.9976	0.1166	LQALLMIIGALTL
12.2	1504.9579	0.1564	VVNLINEPLVIF
10.0	1504.9633	0.1510	MLLLLEKMQD
5.0	1505.1178	-0.0036	KIKQEILPE
5.0	1505.1906	-0.0763	EIKKQLLLI

Mascot: http://www.matrixscience.com/