Selenoproteome Identification in Inflamed Murine Primary Bone Marrow-derived Macrophages by nano-LC Orbitrap Fusion Tribrid Mass Spectrometry

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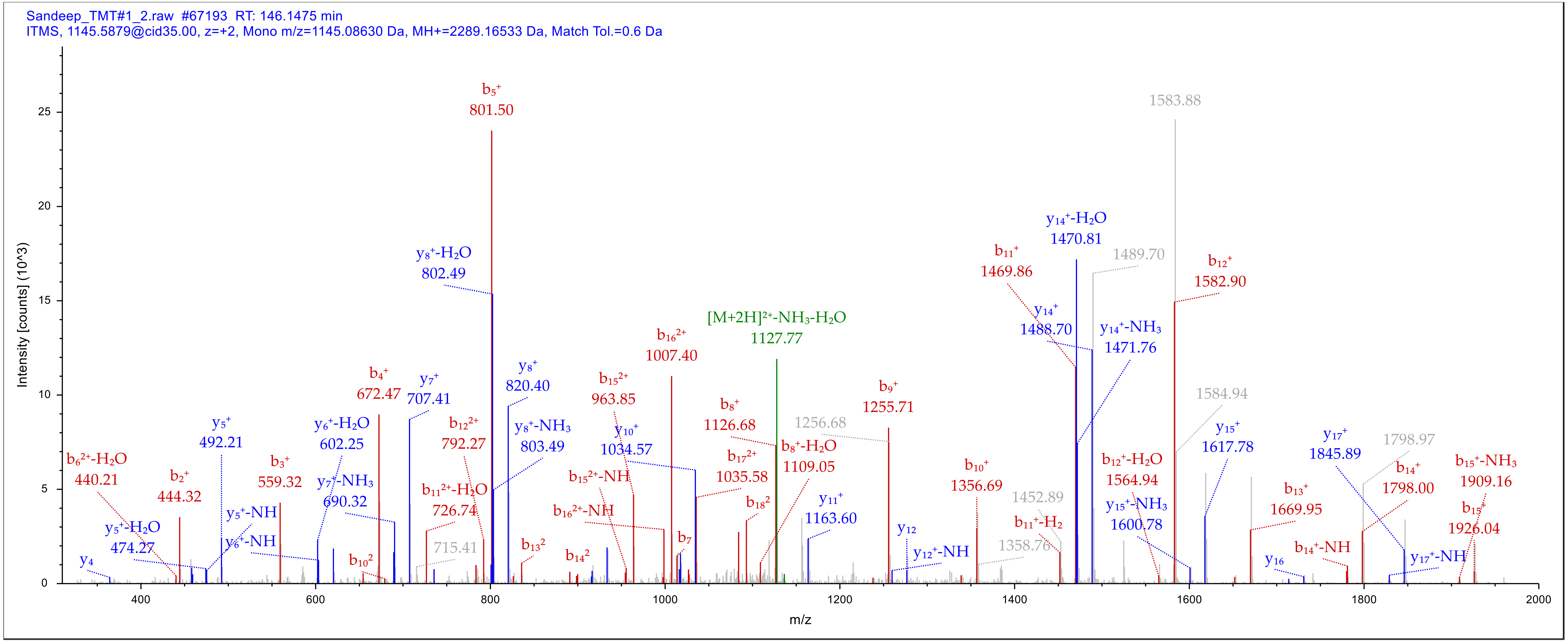
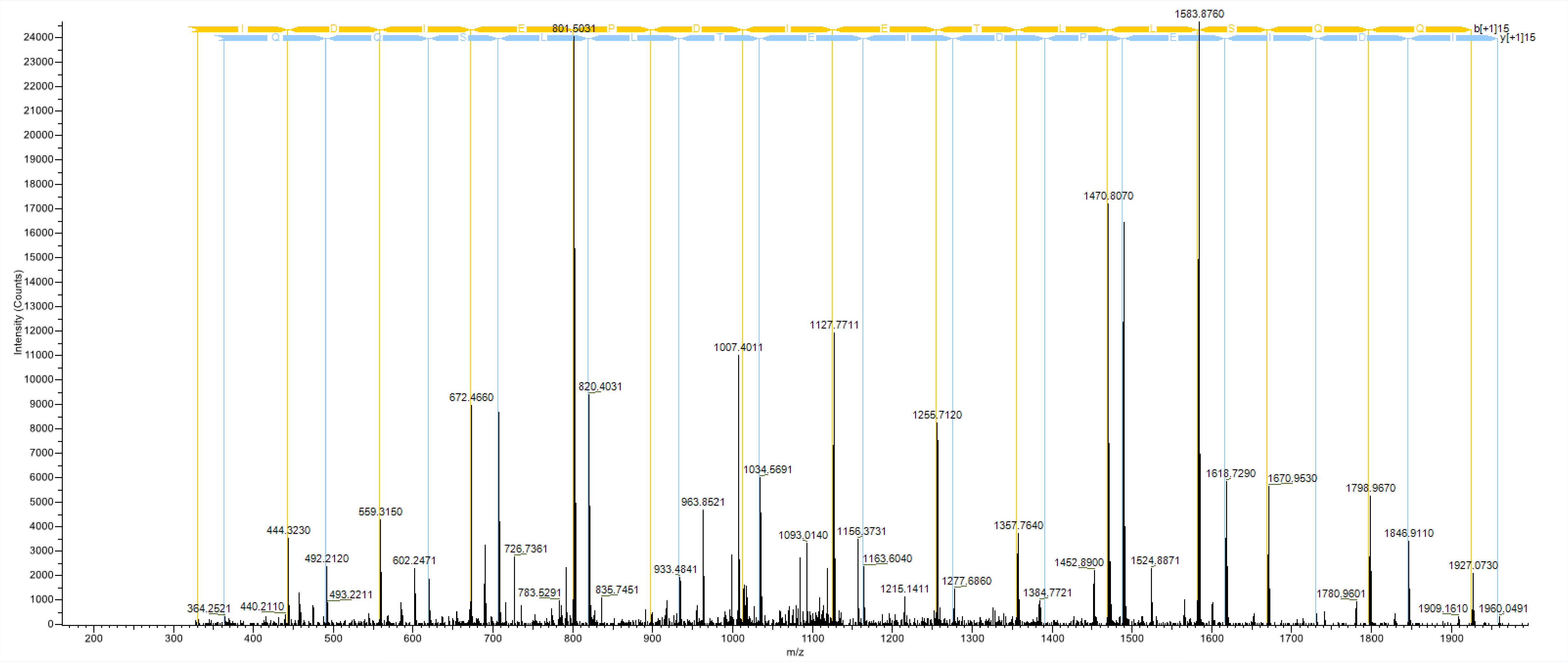
Figure S1. MS/MS spectra of representative selenoprotein peptides found in TMT data-set acquired on high resolution accurate mass spectrometry (HR/AM) Orbitrap Fusion MS

Sl	Uniprot Accession	Gene name
1	P11352	Gpx1
2	O70325	Gpx4
3	Q9JMH6	Txnrd1
4	Q9JLT4	Txnrd2
5	Q9JLC3	Msrb1
6	Q9ERR7	Selenof
7	Q80TA1	Selenoi
8	Q9JLJ1	Selenok
9	Q8VHC3	Selenom
10	D3Z2R5	Selenon
11	Q9BCZ4	Selenos
12	P62342	Selenot
13	P63300	Selenow

Sequence: TIDIEPDIETLLSQQSGNS, T1-TMT6plex (229.16293 Da)
Charge: +2, Monoisotopic m/z: 1145.08630 Da (-0.29 mmu/-0.26 ppm), MH+: 2289.16533 Da, RT: 146.1475 min,
Identified with: Sequest HT (v1.17); XCorr:6.18, Percolator q-Value:0.0e0, Percolator PEP:1.3e-5, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): - Glutathione peroxidase 1 OS=Mus musculus OX=10090 GN=**Gpx1** PE=1 SV=2

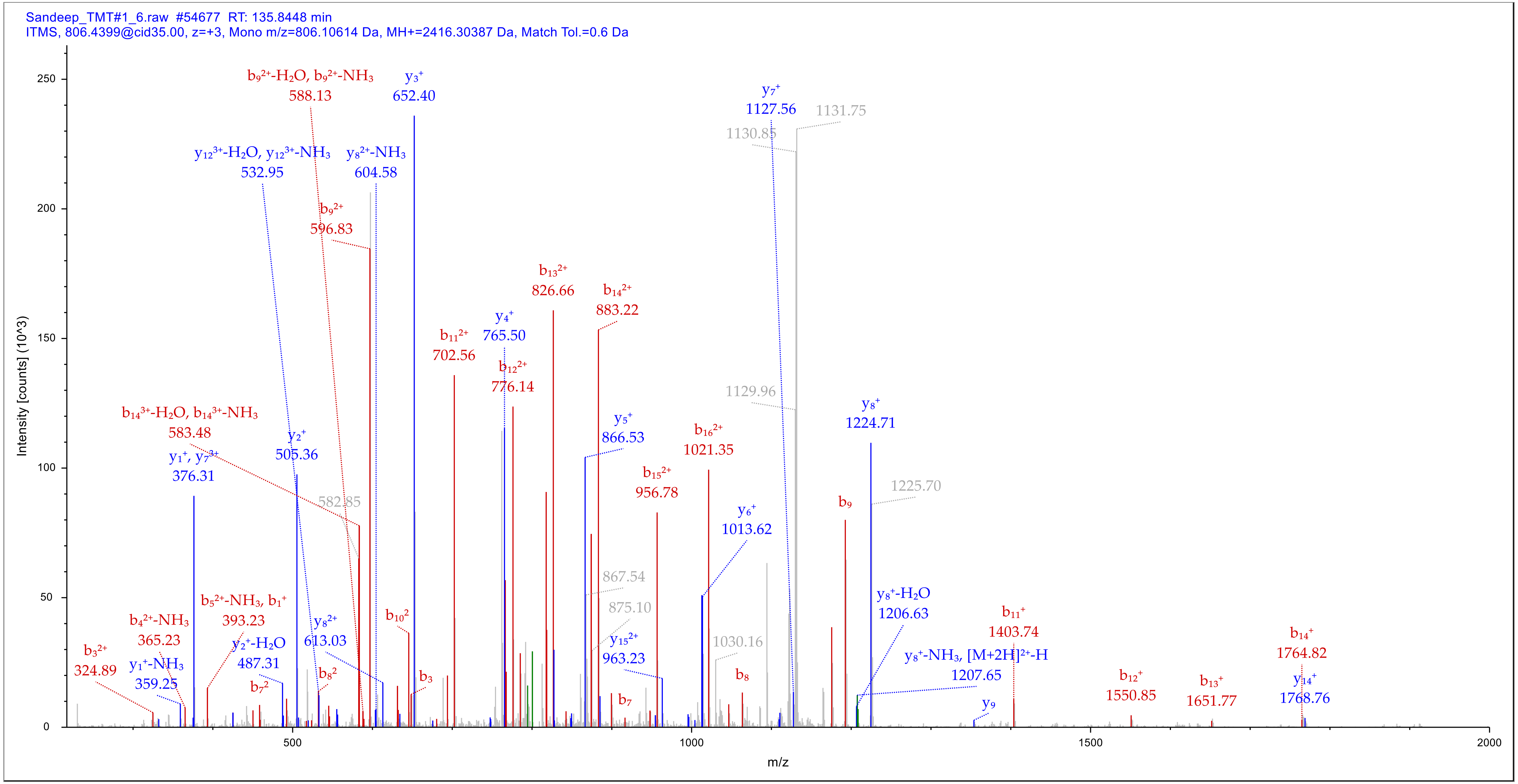


Peptide consensus view

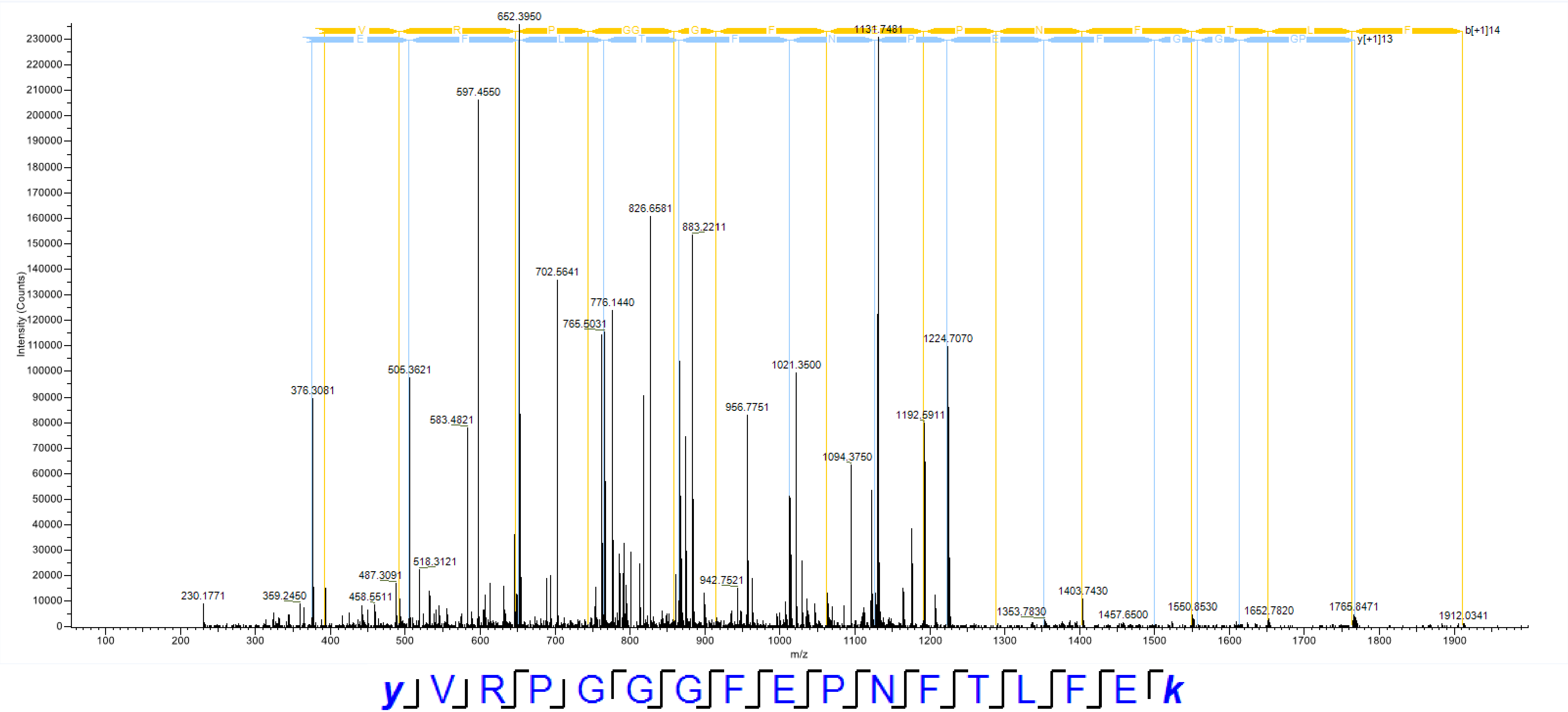


t I D I E P D I E T L L S Q Q S G N S

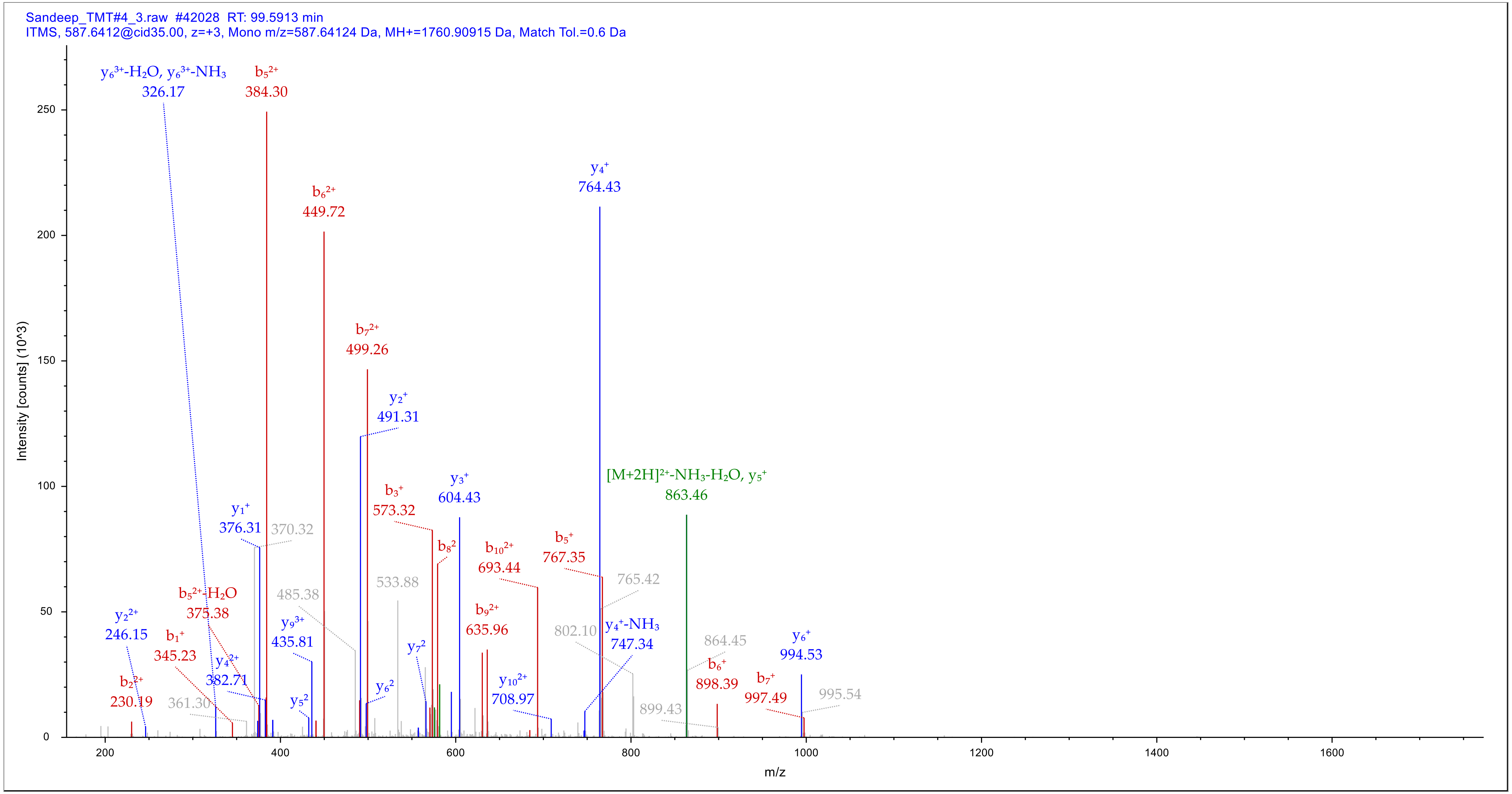
Sequence: YVRPGGGFEPNFTLFEK, K17-TMT6plex (229.16293 Da), Y1-TMT6plex (229.16293 Da)
Charge: +3, Monoisotopic m/z: 806.10614 Da (-0.89 mmu/-1.11 ppm), MH+: 2416.30387 Da, RT: 135.8448 min,
Identified with: Sequest HT (v1.17); XCorr:5.73, Percolator q-Value:0.0e0, Percolator PEP:3.2e-5, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): - Glutathione peroxidase 1 OS=Mus musculus OX=10090 GN=**Gpx1** PE=1 SV=2



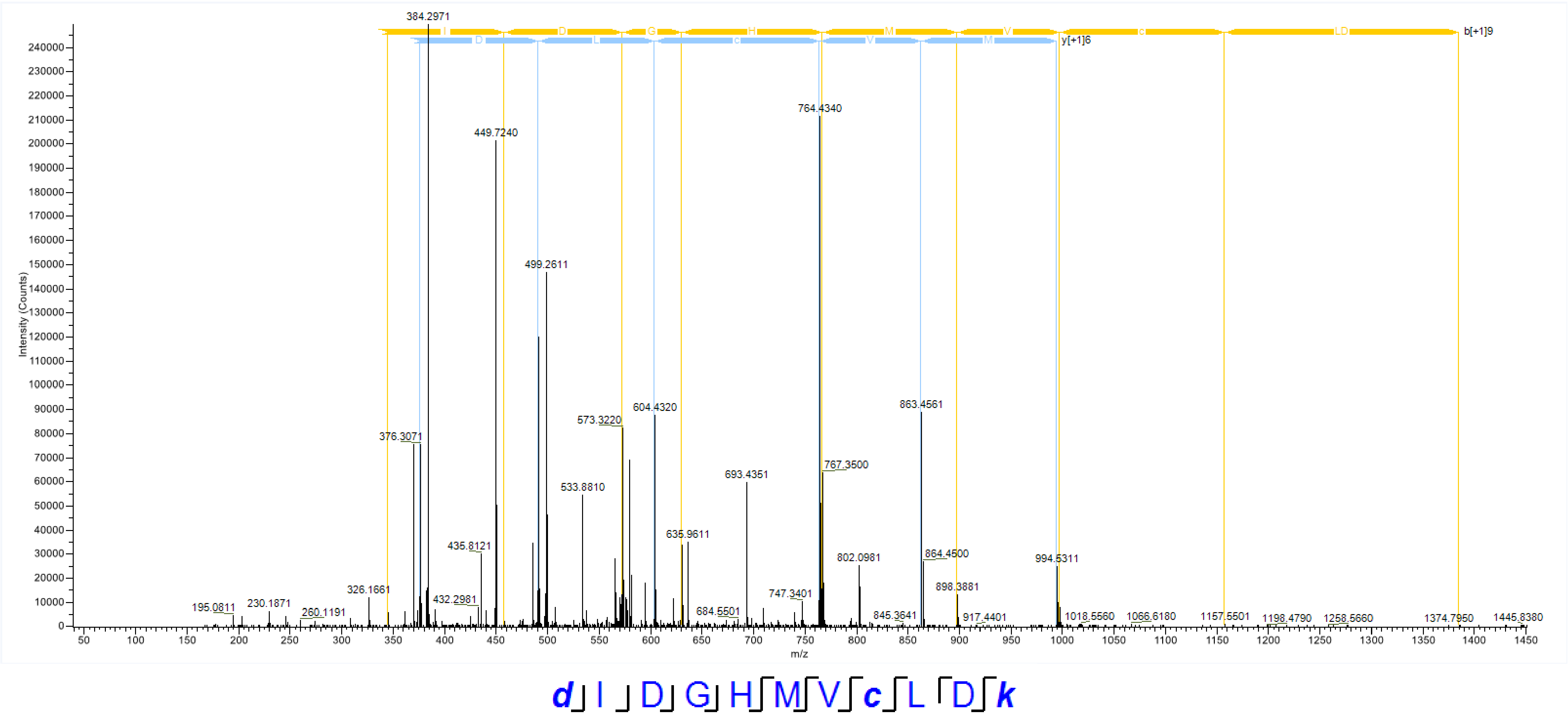
Peptide consensus view



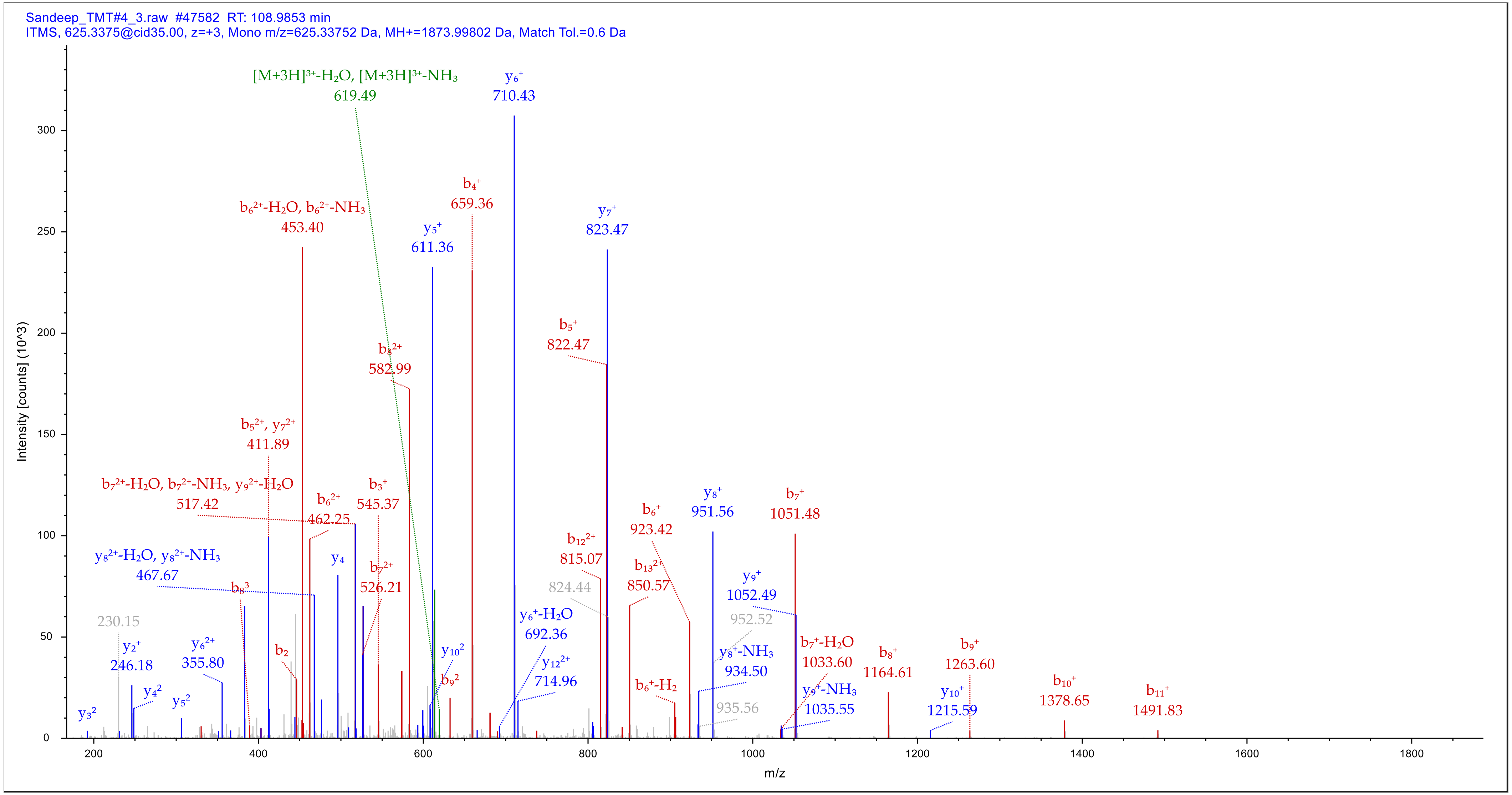
Sequence: DIDGHMVCLDK, C8-Carbamidomethyl (57.02146 Da), K11-TMT6plex (229.16293 Da), D1-TMT6plex (229.16293 Da)
Charge: +3, Monoisotopic m/z: 587.64124 Da (+0.54 mmu/+0.91 ppm), MH+: 1760.90915 Da, RT: 99.5913 min,
Identified with: Sequest HT (v1.17); XCorr:4.99, Percolator q-Value:0.0e0, Percolator PEP:9.4e-5, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; y; y-H_2O; y-NH_3
Protein references (1): Phospholipid hydroperoxide glutathione peroxidase OS=Mus musculus OX=10090 GN=**Gpx4** PE=1 SV=4



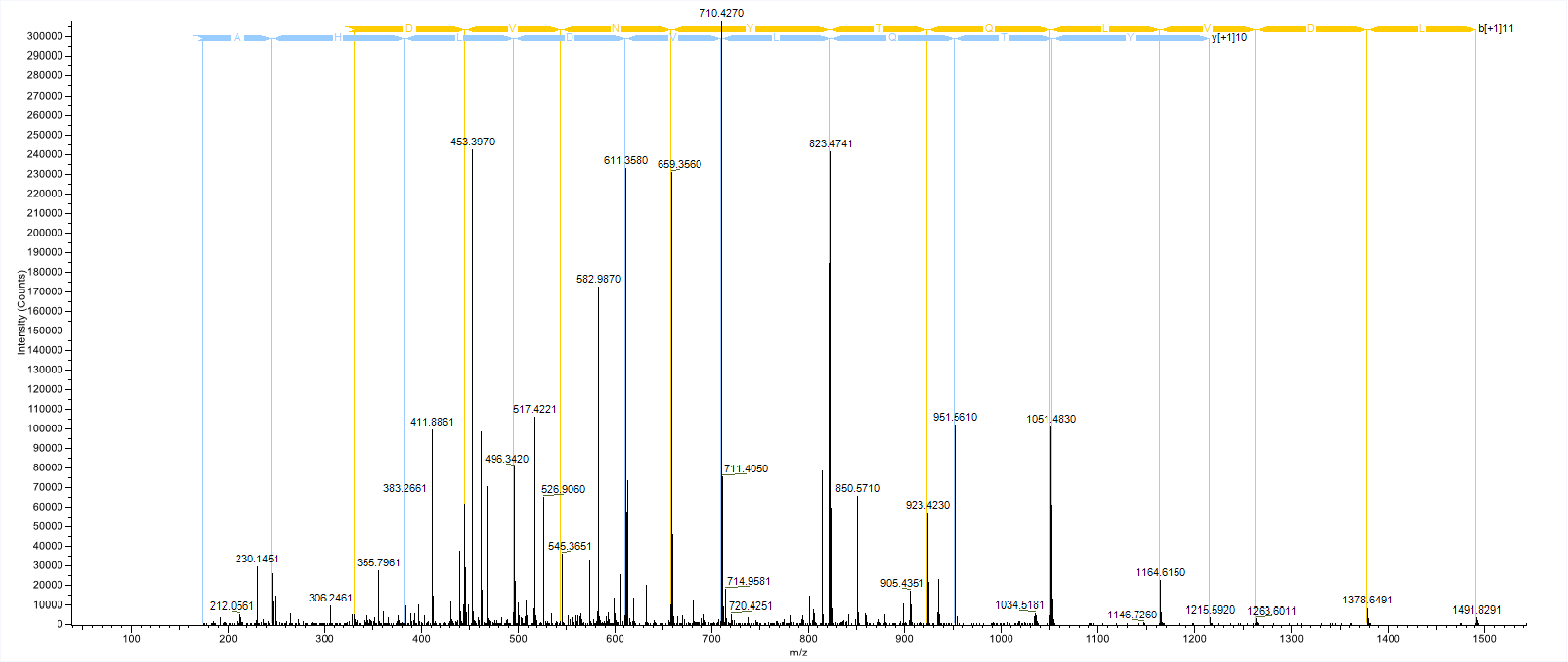
Peptide consensus view



Sequence: TDVNYTQLVDLHAR, T1-TMT6plex (229.16293 Da)
Charge: +3,   Monoisotopic m/z: 625.33752 Da (+0.36 mmu/+0.58 ppm),   MH+: 1873.99802 Da,   RT: 108.9853 min,
Identified with: Sequest HT (v1.17); XCorr:6.13, Percolator q-Value:0.0e0, Percolator PEP:5.3e-8, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): Phospholipid hydroperoxide glutathione peroxidase OS=Mus musculus OX=10090 GN=**Gpx4** PE=1 SV=4

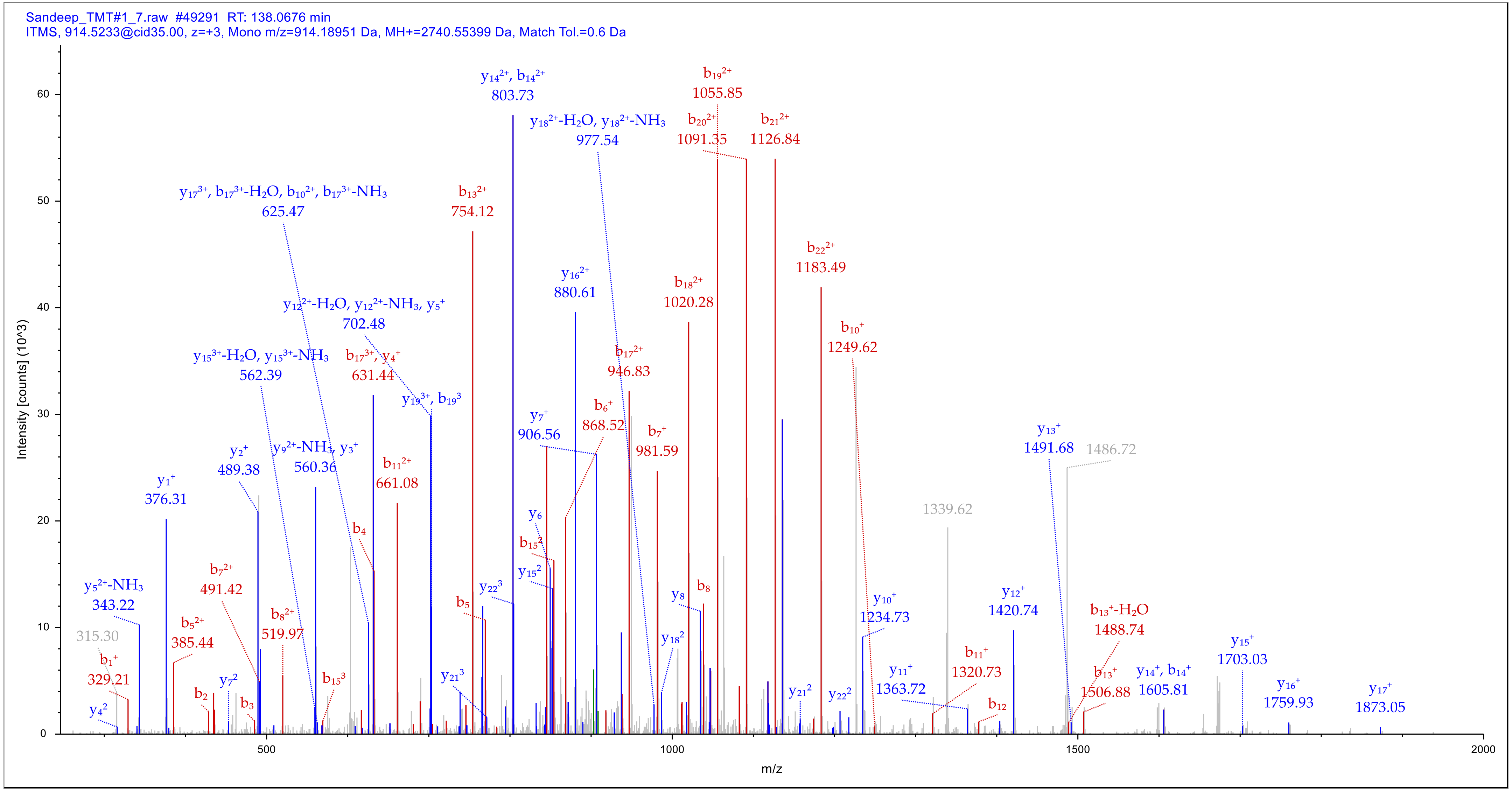


Peptide consensus view

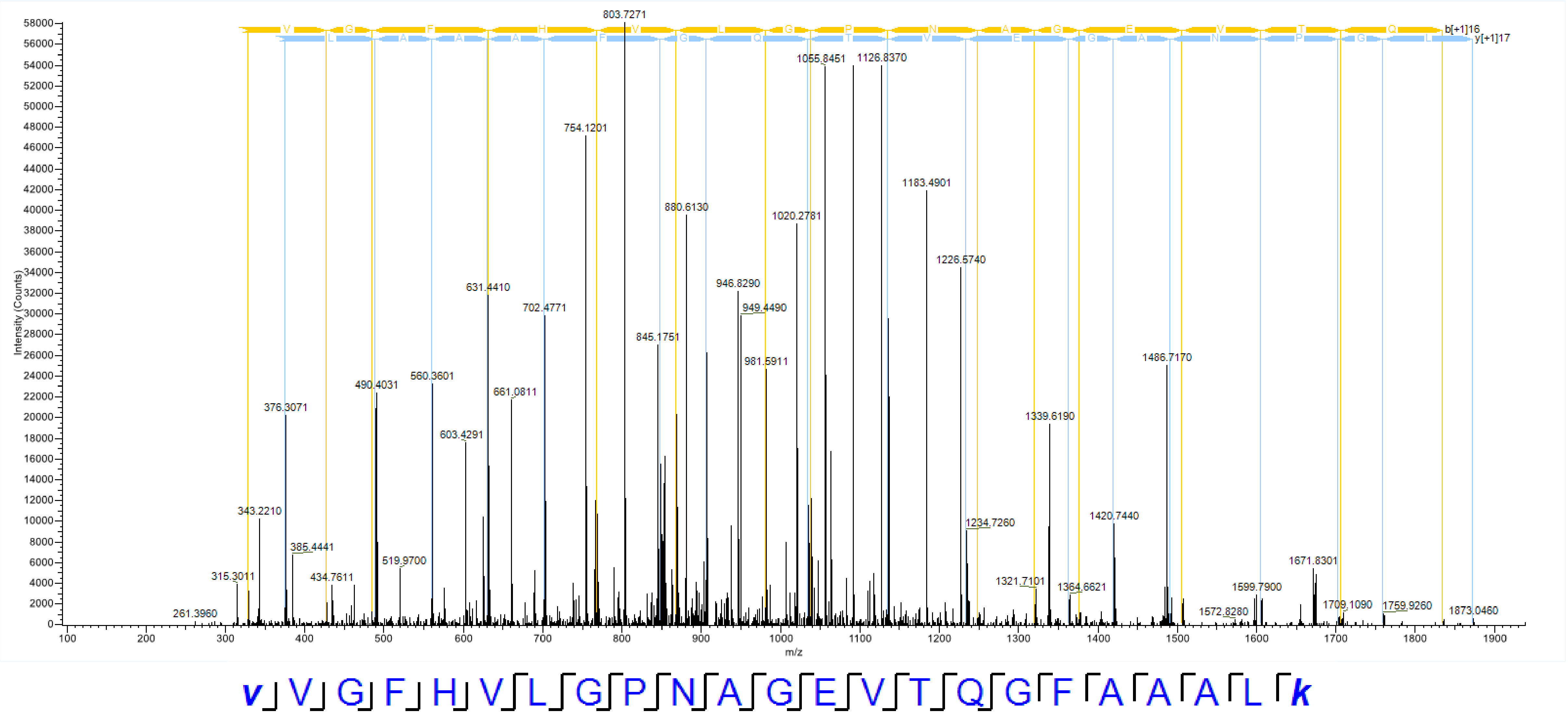


t ⌋D⌋V⌋N⌠Y⌠T⌠Q⌠L⌠V⌠D⌠L⌠H⌈A⌈R

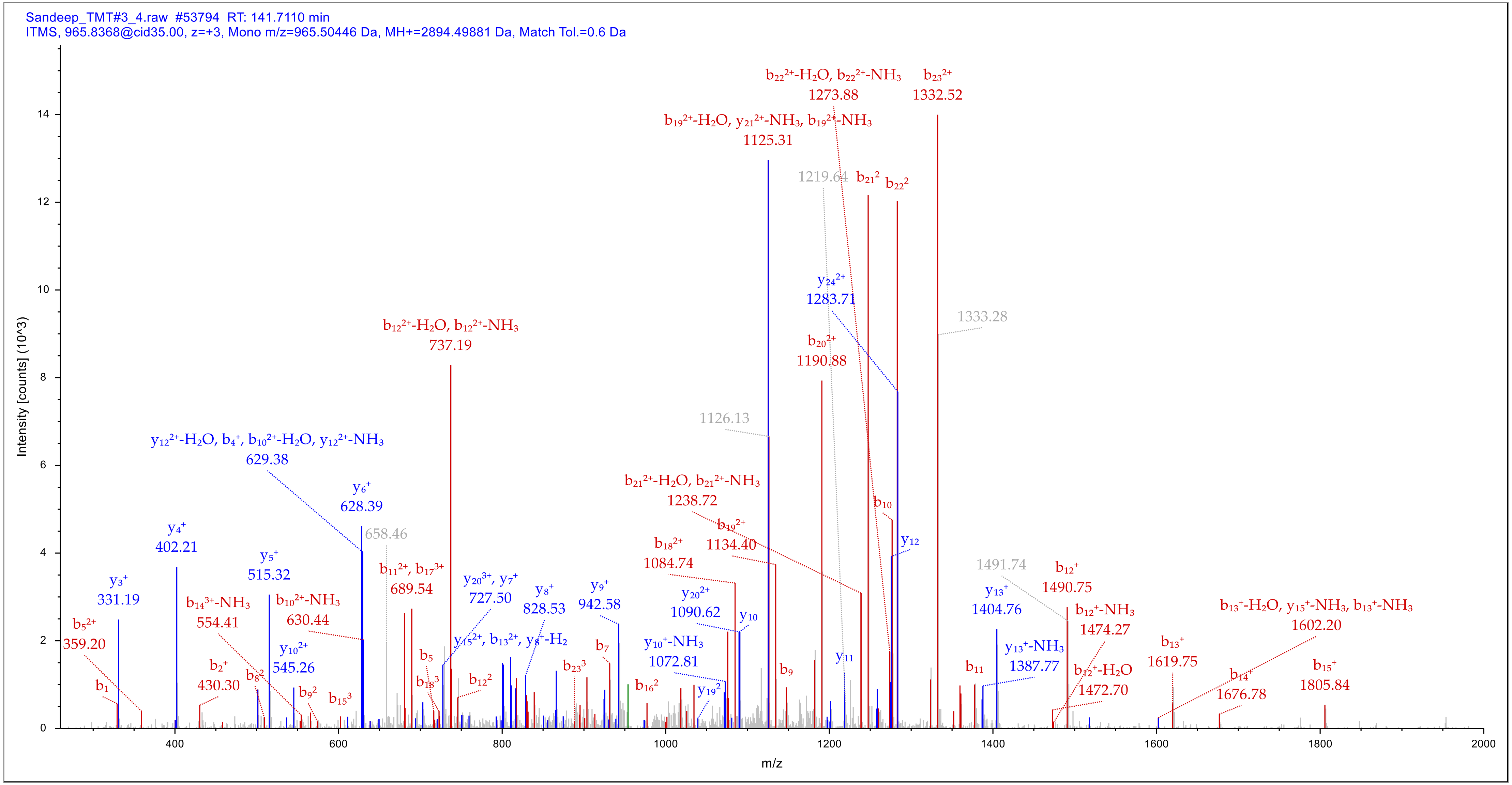
Sequence: VVGFHVLGPNAGEVTQGFAAALK, K23-TMT6plex (229.16293 Da), V1-TMT6plex (229.16293 Da)
Charge: +3, Monoisotopic m/z: 914.18951 Da (-0.35 mmu/-0.38 ppm), MH+: 2740.55399 Da, RT: 138.0676 min,
Identified with: Sequest HT (v1.17); XCorr:7.40, Percolator q-Value:0.0e0, Percolator PEP:6.2e-9, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): Thioredoxin reductase 1, cytoplasmic OS=Mus musculus OX=10090 GN=Txnrd1 PE=1 SV=3



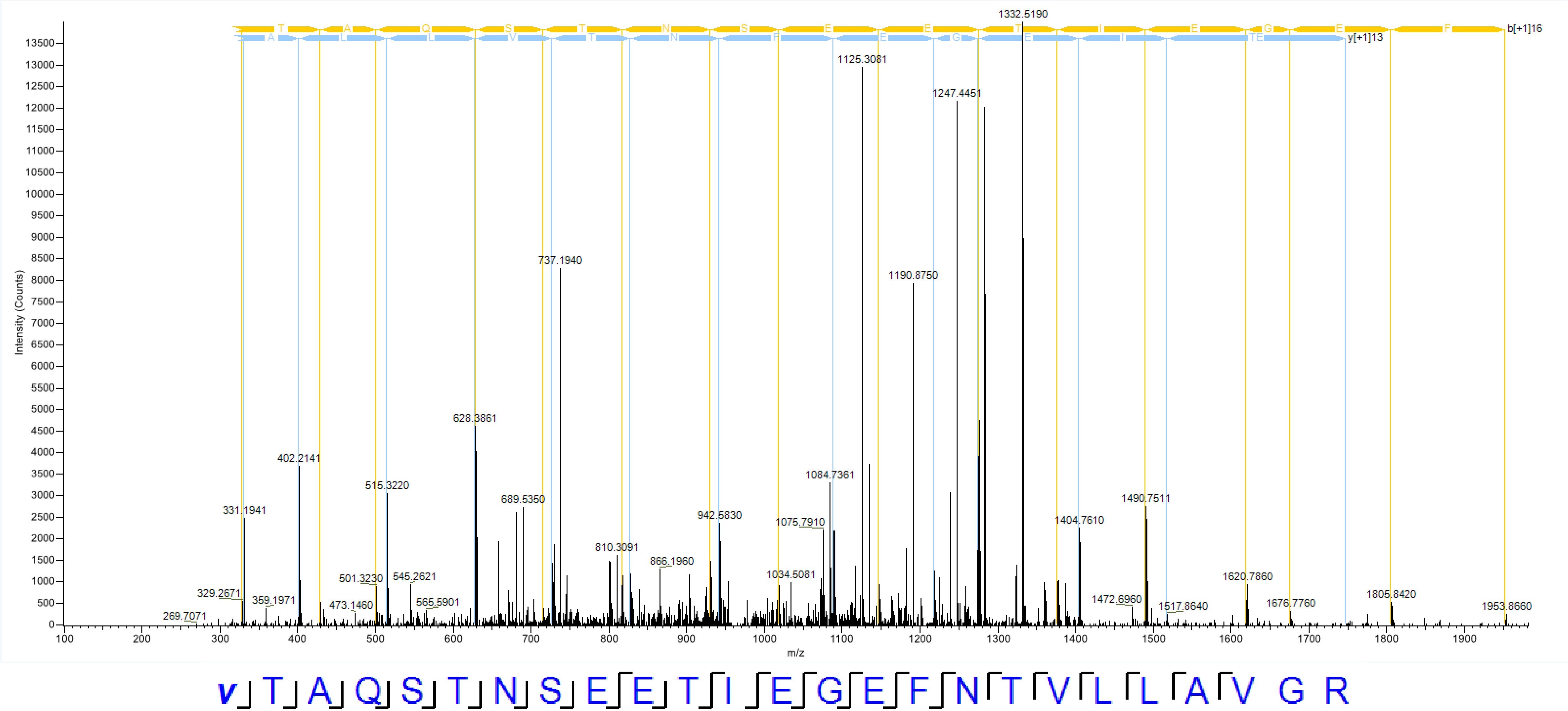
Peptide consensus view



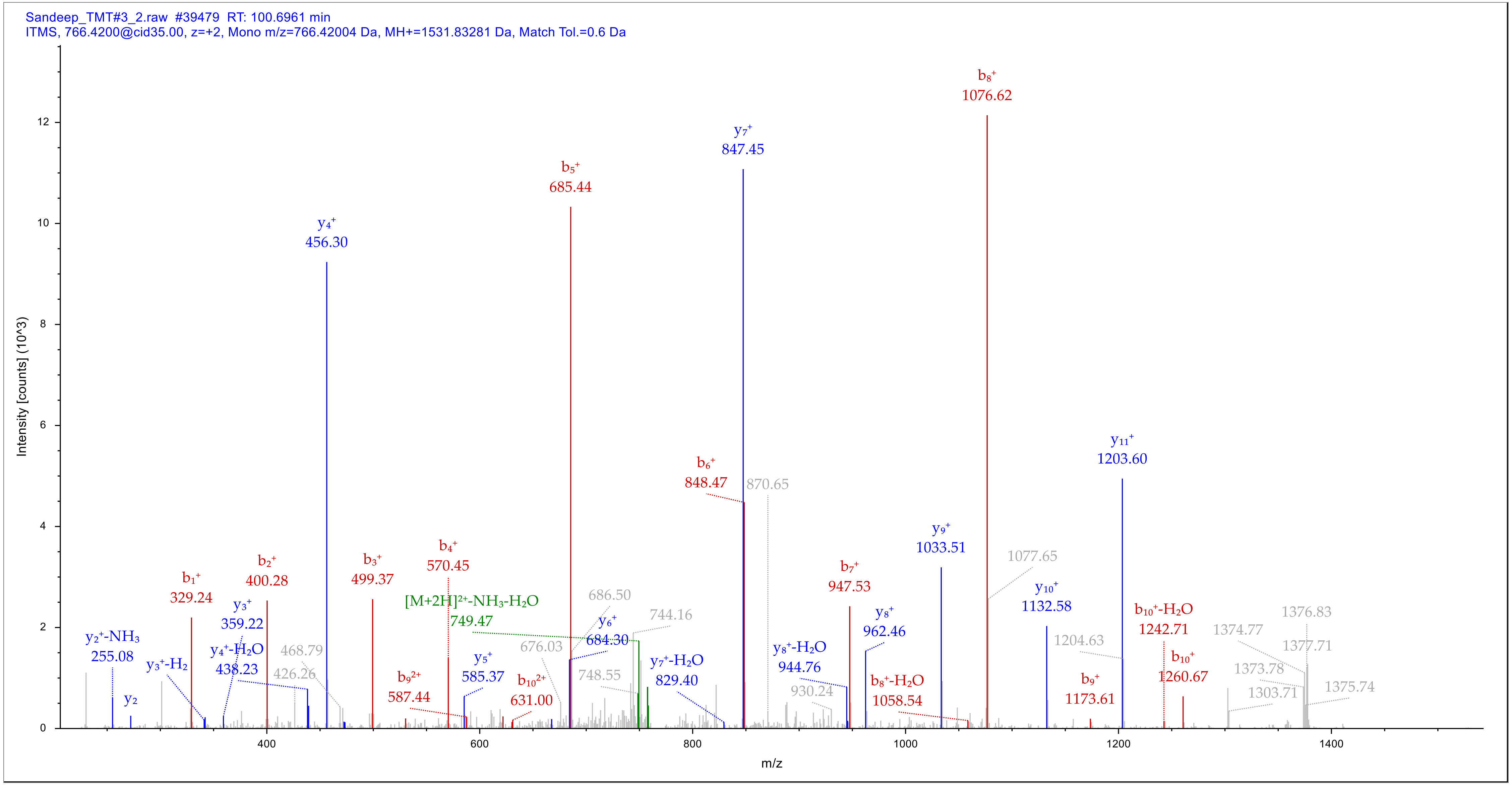
Sequence: VTAQSTNSEETIEGEFNTVLLAVGR, V1-TMT6plex (229.16293 Da)
Charge: +3, Monoisotopic m/z: 965.50446 Da (+1.45 mmu/+1.5 ppm), MH+: 2894.49881 Da, RT: 141.7110 min,
Identified with: Sequest HT (v1.17); XCorr:6.68, Percolator q-Value:0.0e0, Percolator PEP:8.8e-7, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): Thioredoxin reductase 1, cytoplasmic OS=Mus musculus OX=10090 GN=Txnrd1 PE=1 SV=3



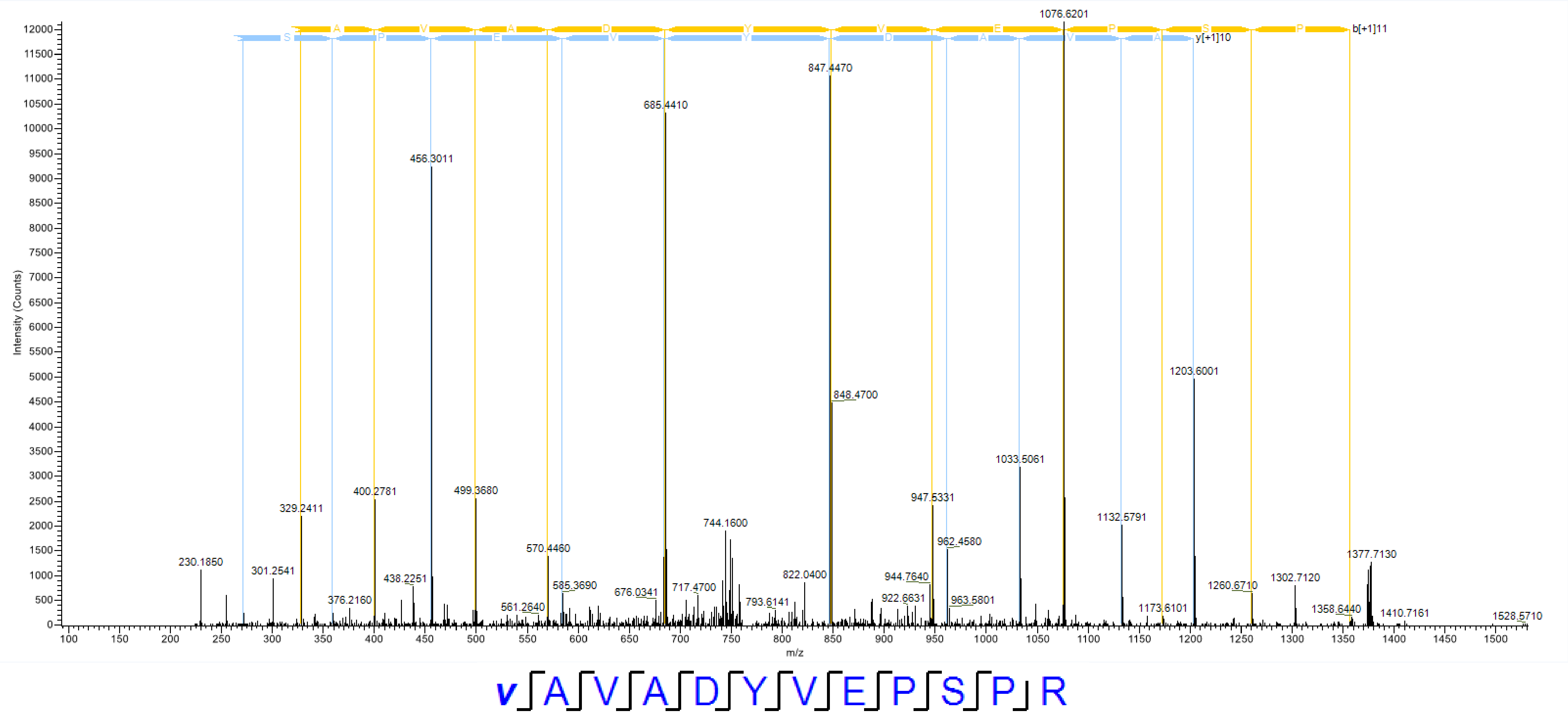
Peptide consensus view



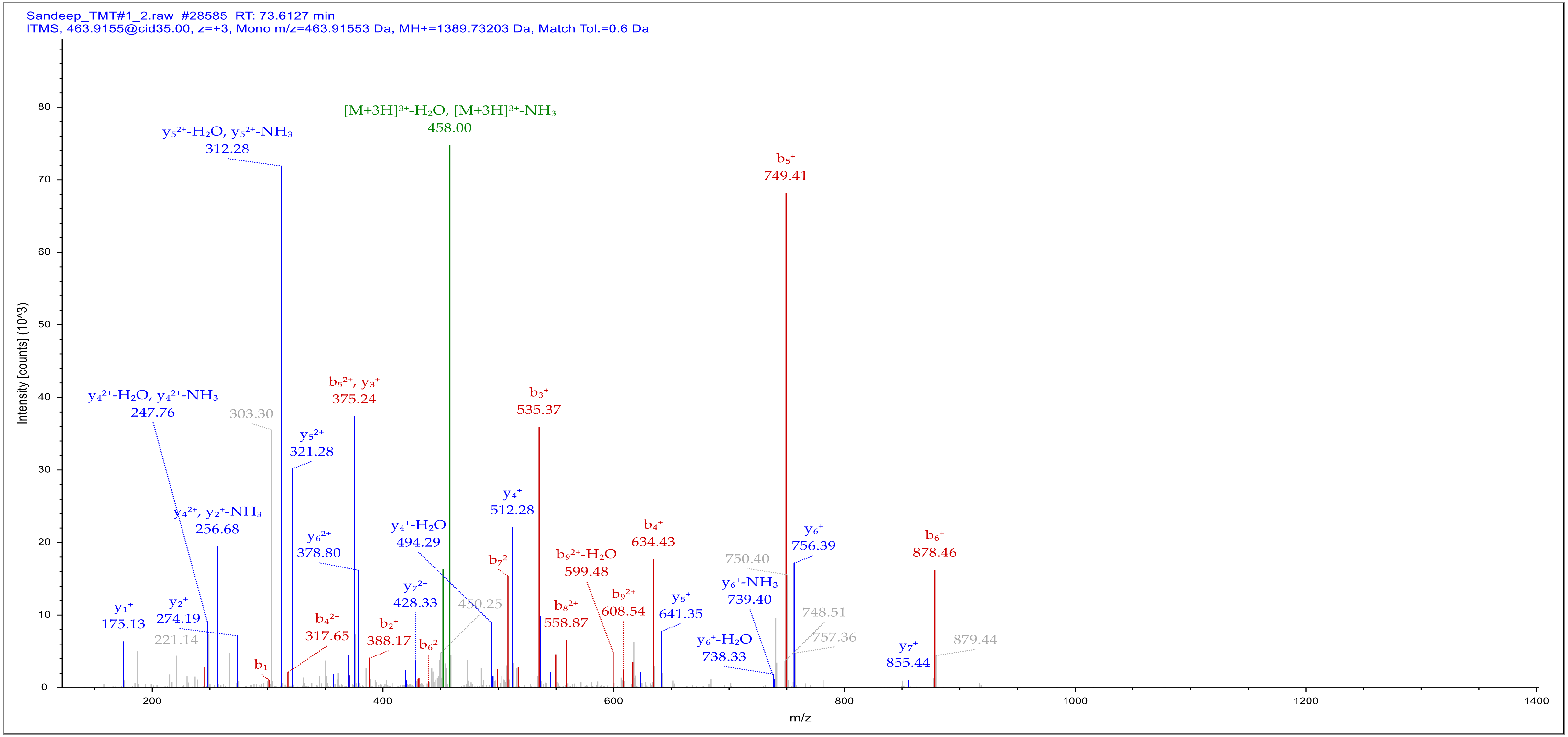
Sequence: VAVADYVEPSPR, V1-TMT6plex (229.16293 Da)
Charge: +2, Monoisotopic m/z: 766.42004 Da (+0.52 mmu/+0.68 ppm), MH+: 1531.83281 Da, RT: 100.6961 min,
Identified with: Sequest HT (v1.17); XCorr:3.99, Percolator q-Value:5.9e-5, Percolator PEP:8.9e-5, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; y; y-H_2O; y-NH_3
Protein references (1): Thioredoxin reductase 2, mitochondrial OS=Mus musculus OX=10090 GN=Txnrd2 PE=1 SV=4

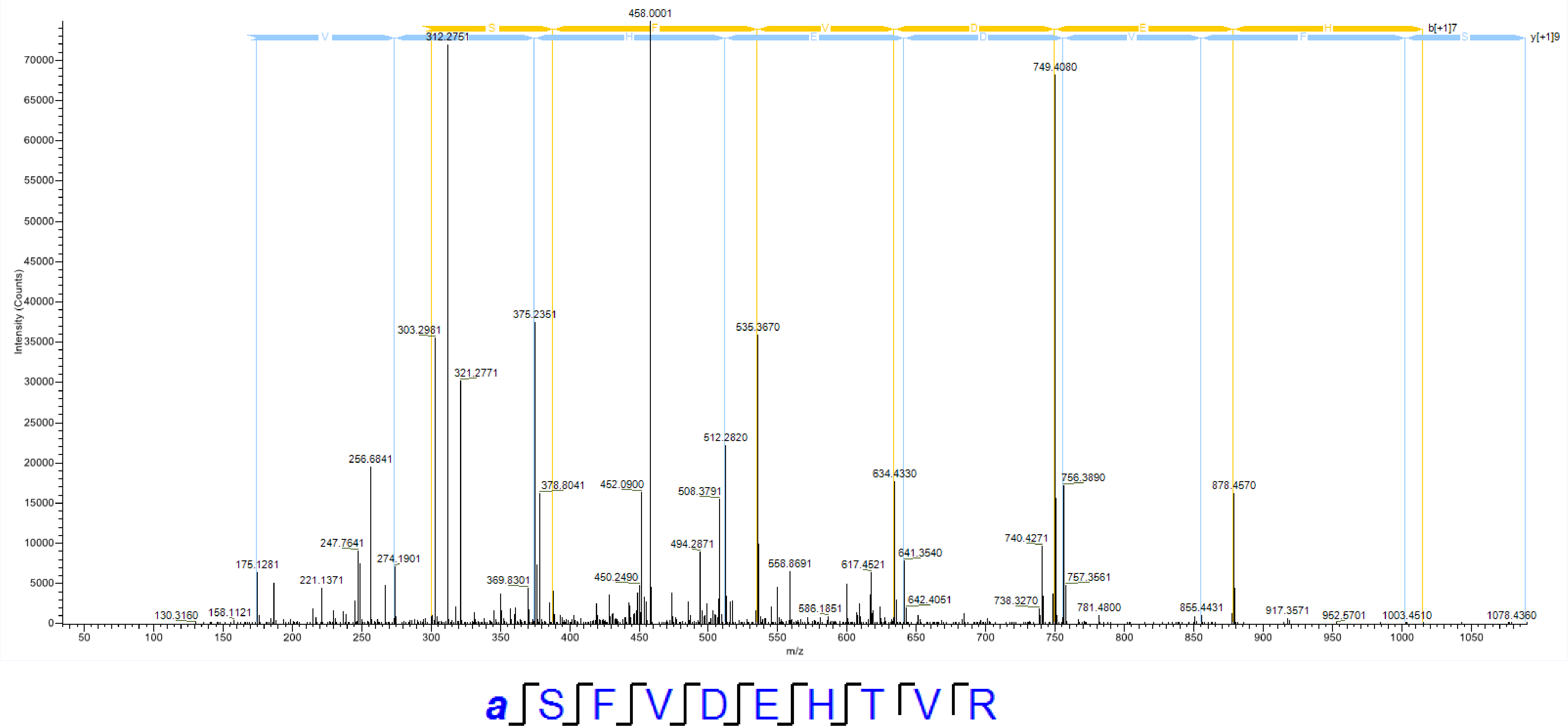


Peptide consensus view



Sequence: ASFVDEHTVR, A1-TMT6plex (229.16293 Da)
Charge: +3, Monoisotopic m/z: 463.91553 Da (-0.12 mmu/-0.26 ppm), MH+: 1389.73203 Da, RT: 73.6127 min,
Identified with: Sequest HT (v1.17); XCorr:3.74, Percolator q-Value:4.7e-5, Percolator PEP:1.7e-4, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; y; y-H_2O; y-NH_3
Protein references (1): - Thioredoxin reductase 2, mitochondrial OS=Mus musculus OX=10090 GN=Txnrd2 PE=1 SV=4

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y[+1]9
S
F
V
D
E
H
V
H
E
D
V
F
S
Intensity (Counts)
m/z
0
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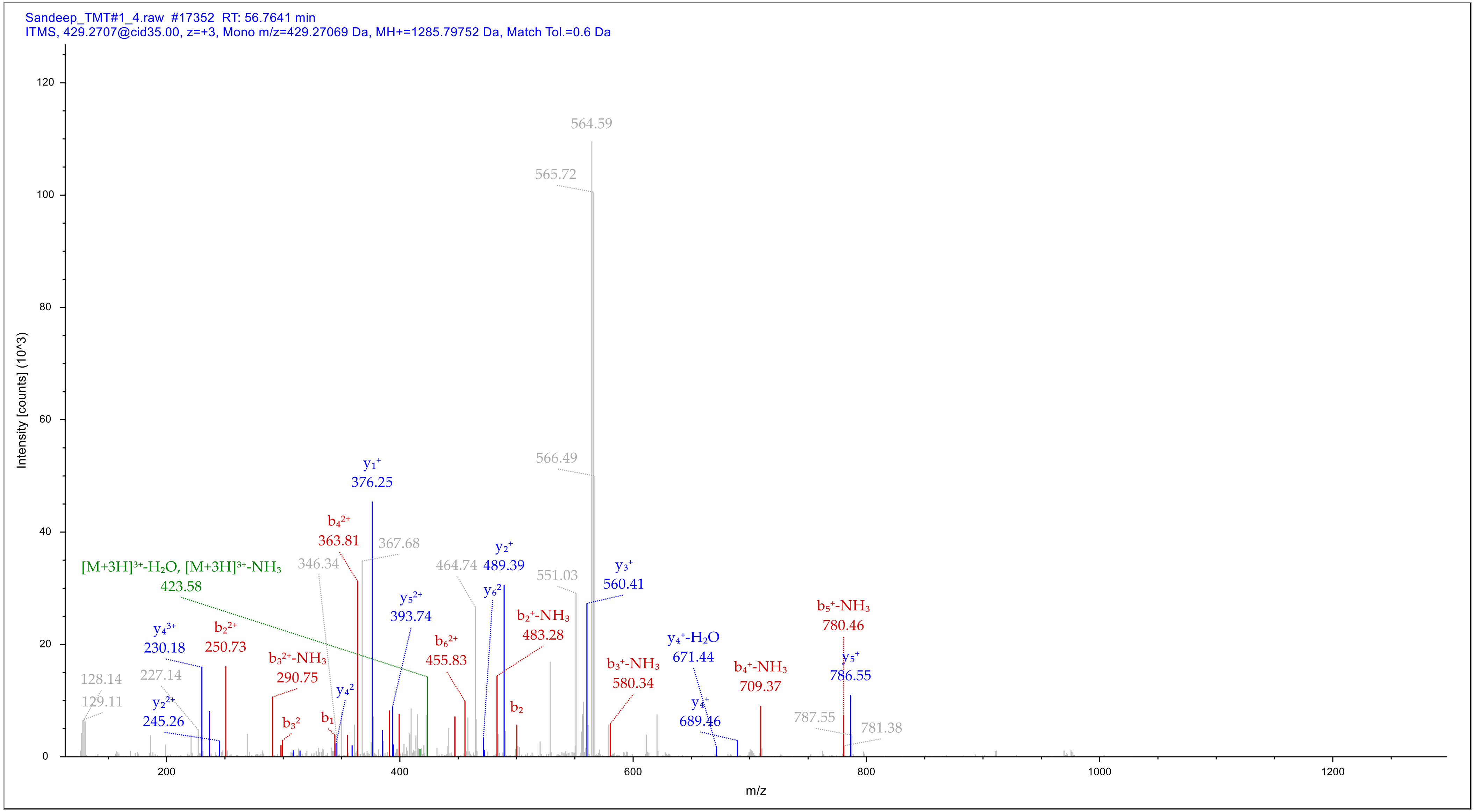
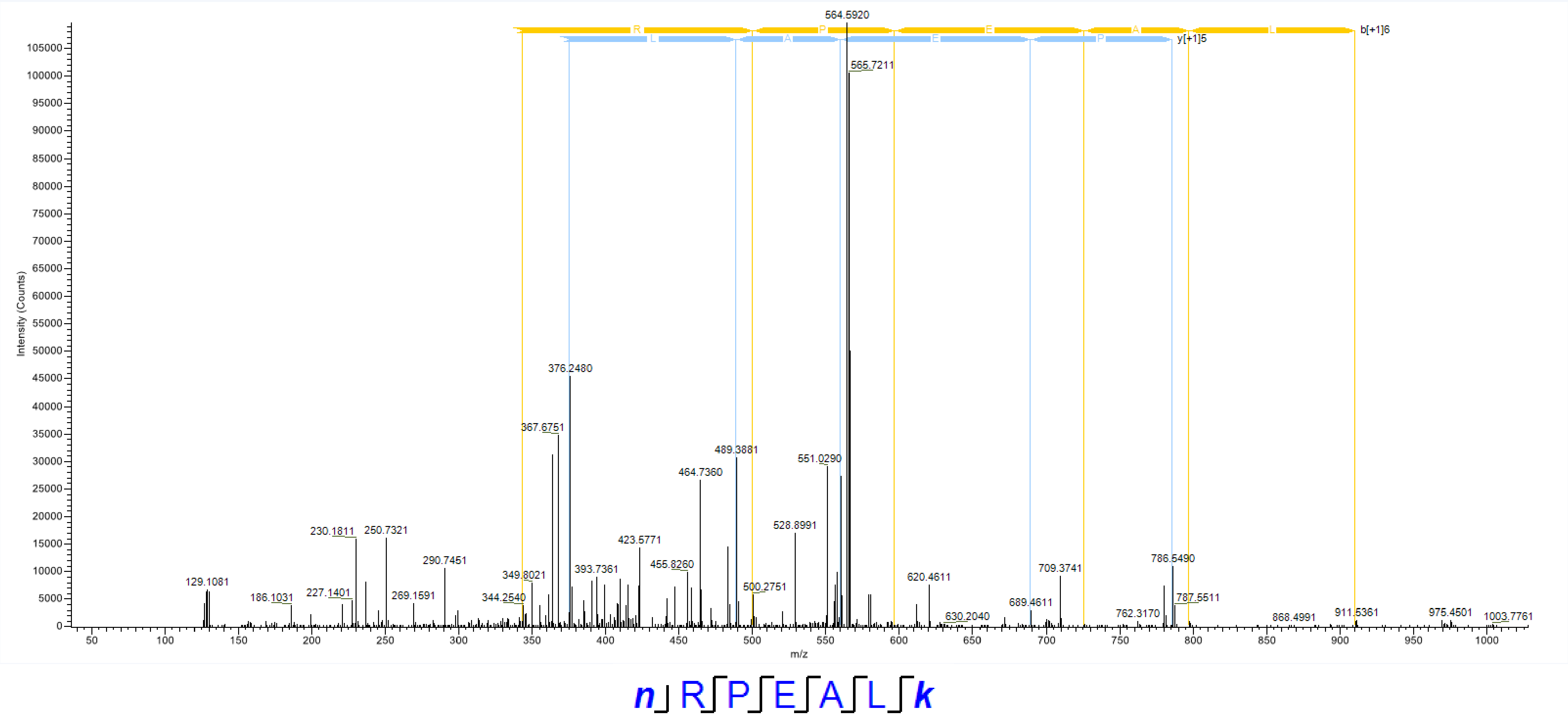
10000
15000
20000
25000
30000
35000
40000
45000
50000
55000
60000
65000
70000
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
1050
a S F V D E H T V R

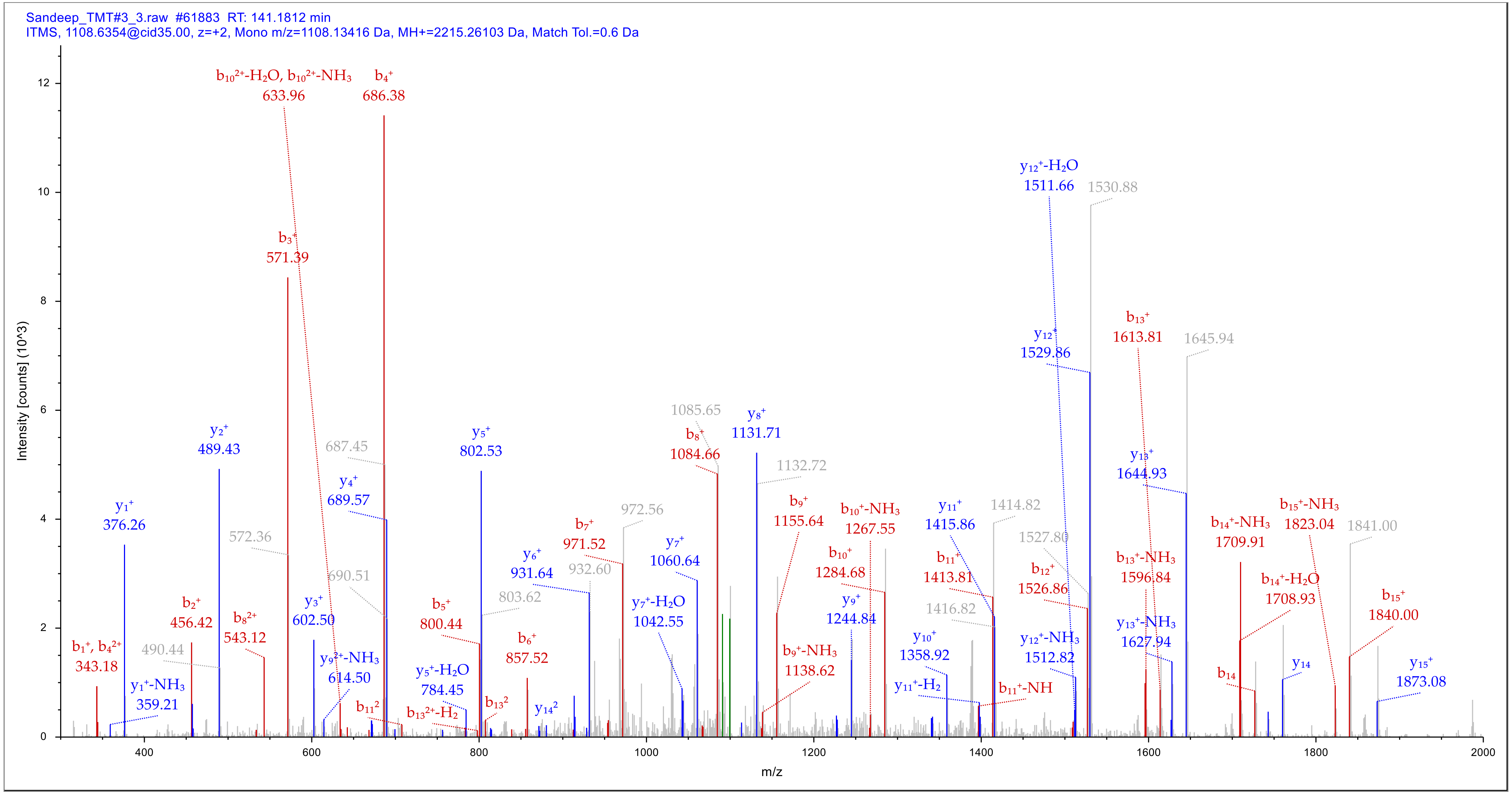
Sequence: NRPEALK, K7-TMT6plex (229.16293 Da), N1-TMT6plex (229.16293 Da)
Charge: +3,   Monoisotopic m/z: 429.27069 Da (-0.57 mmu/-1.34 ppm),   MH+: 1285.79752 Da,   RT: 56.7641 min,
Identified with: Sequest HT (v1.17); XCorr:2.87, Percolator q-Value:1.6e-3, Percolator PEP:1.4e-2, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): Methionine-R-sulfoxide reductase B1 OS=Mus musculus OX=10090 GN=Msrb1 PE=1 SV=3



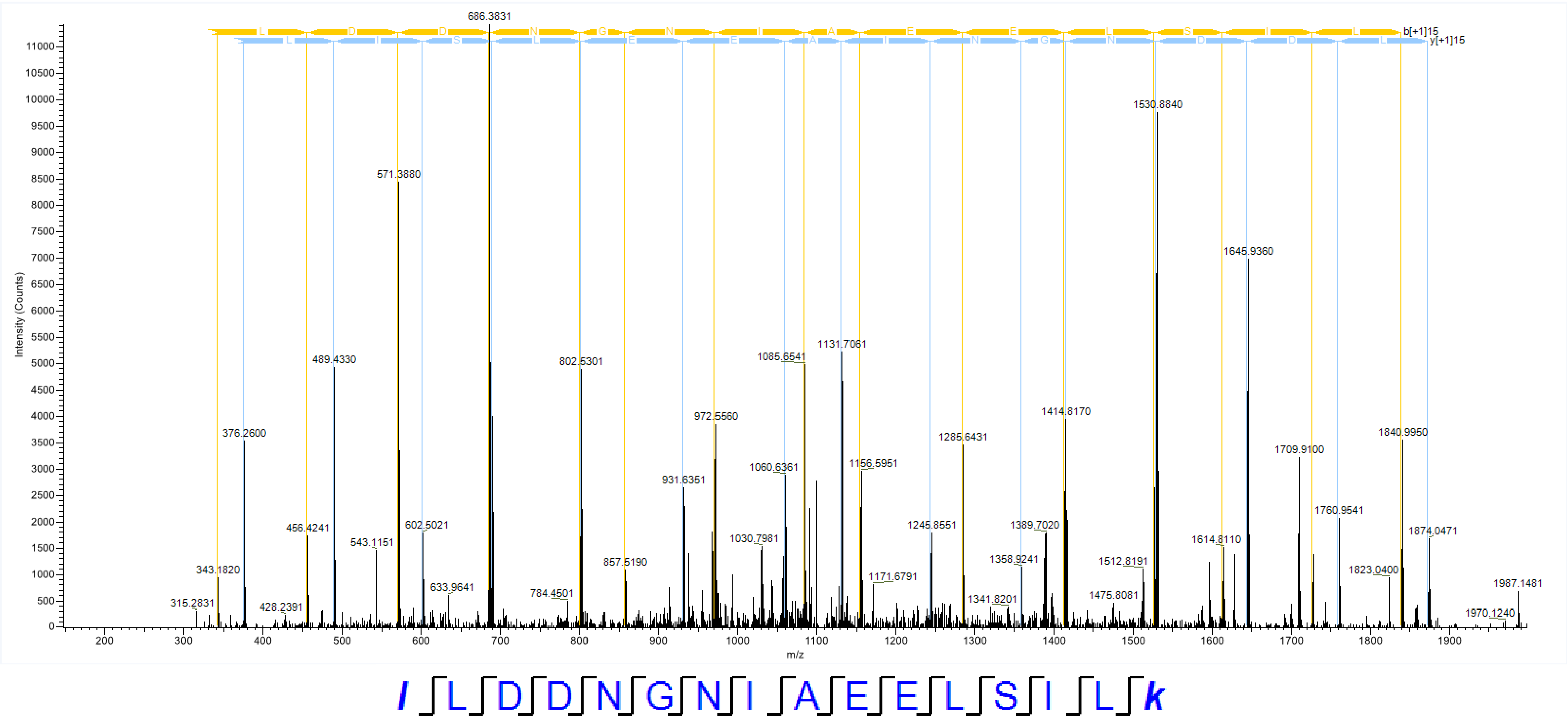
Peptide consensus view



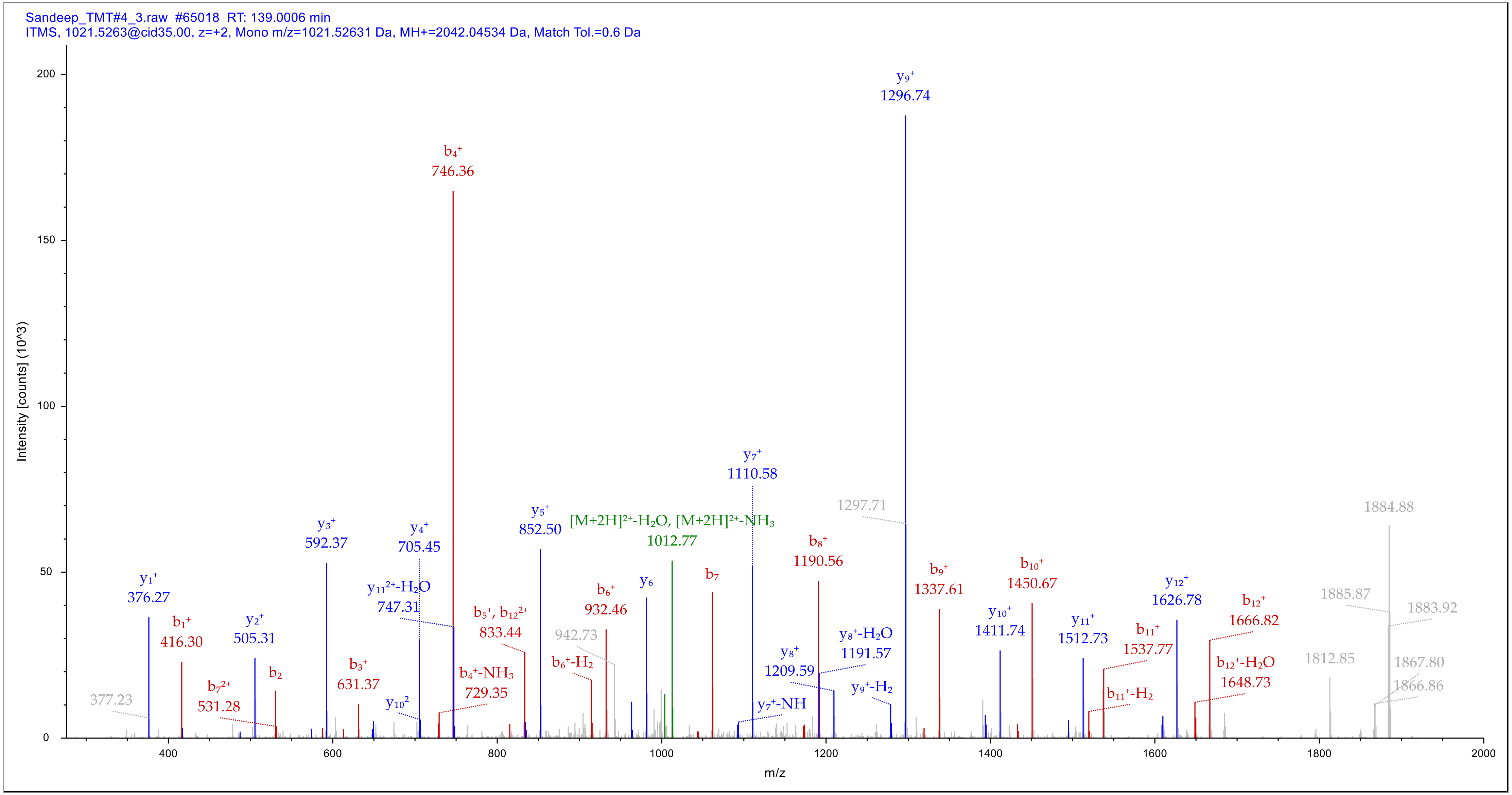
Sequence: LLDDNGNIAEELSILK, K16-TMT6plex (229.16293 Da), L1-TMT6plex (229.16293 Da)
Charge: +2, Monoisotopic m/z: 1108.13416 Da (+1.23 mmu/+1.11 ppm), MH+: 2215.26103 Da, RT: 141.1812 min,
Identified with: Sequest HT (v1.17); XCorr:6.81, Percolator q-Value:0.0e0, Percolator PEP:4.1e-7, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): Selenoprotein F OS=Mus musculus OX=10090 GN=Selenof PE=1 SV=3



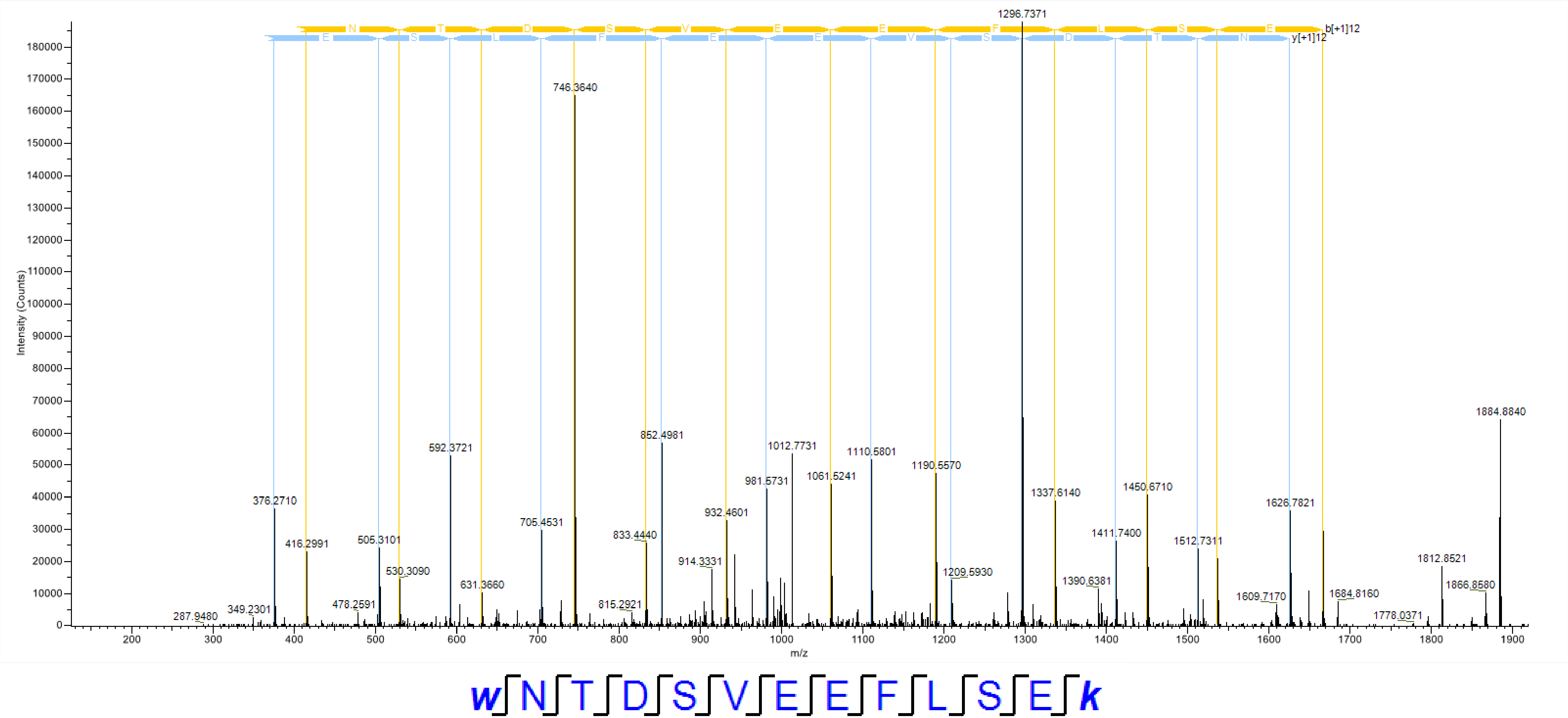
Peptide consensus view



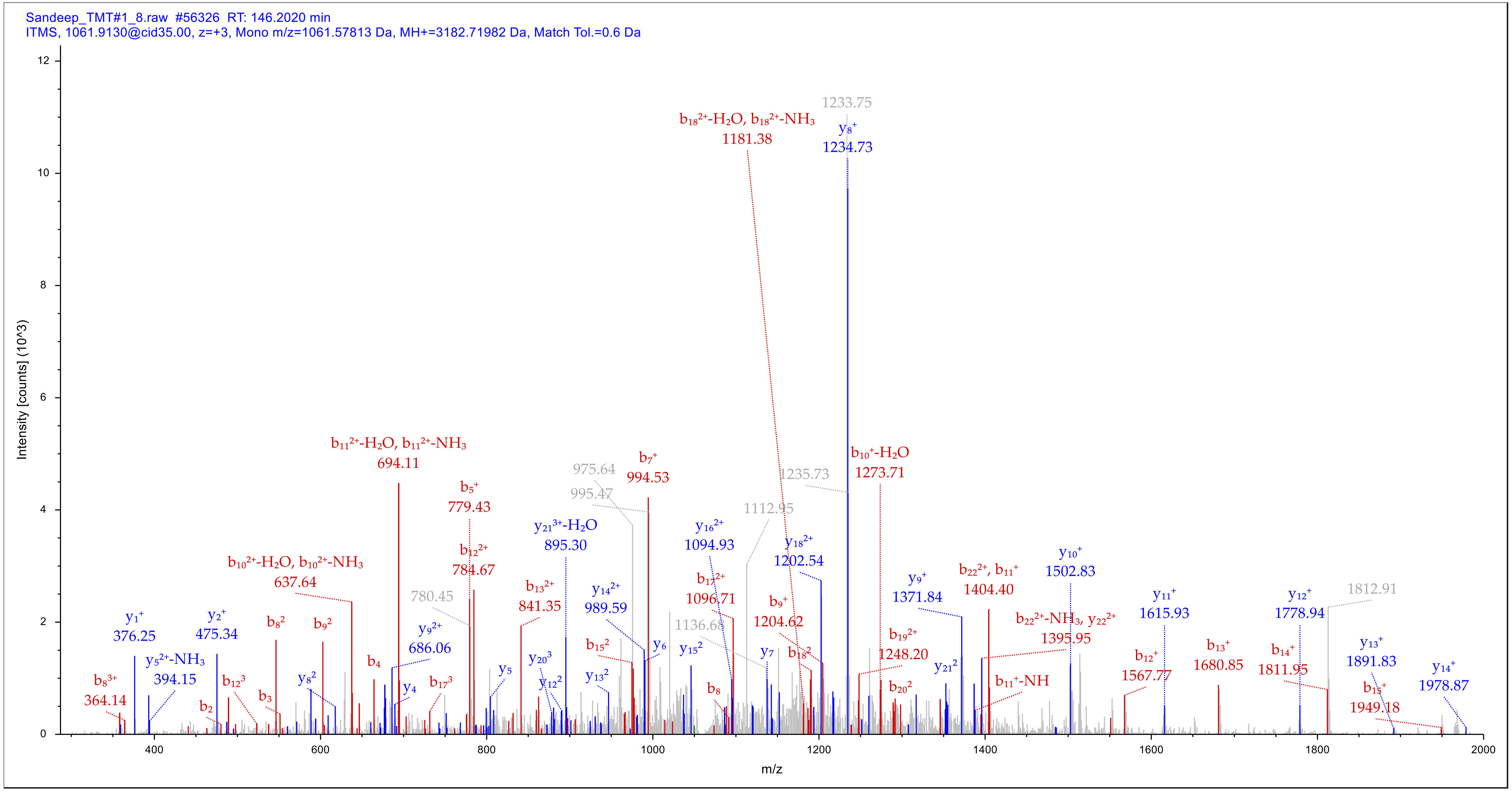
Sequence: WNTDSVEEFLSEK, K13-TMT6plex (229.16293 Da), W1-TMT6plex (229.16293 Da)
Charge: +2,   Monoisotopic m/z: 1021.52631 Da (-1.46 mmu/-1.43 ppm),   MH+: 2042.04534 Da,   RT: 139.0006 min,
Identified with: Sequest HT (v1.17); XCorr:6.13, Percolator q-Value:0.0e0, Percolator PEP:6.4e-7, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): Selenoprotein F OS=Mus musculus OX=10090 GN=Selenof PE=1 SV=3



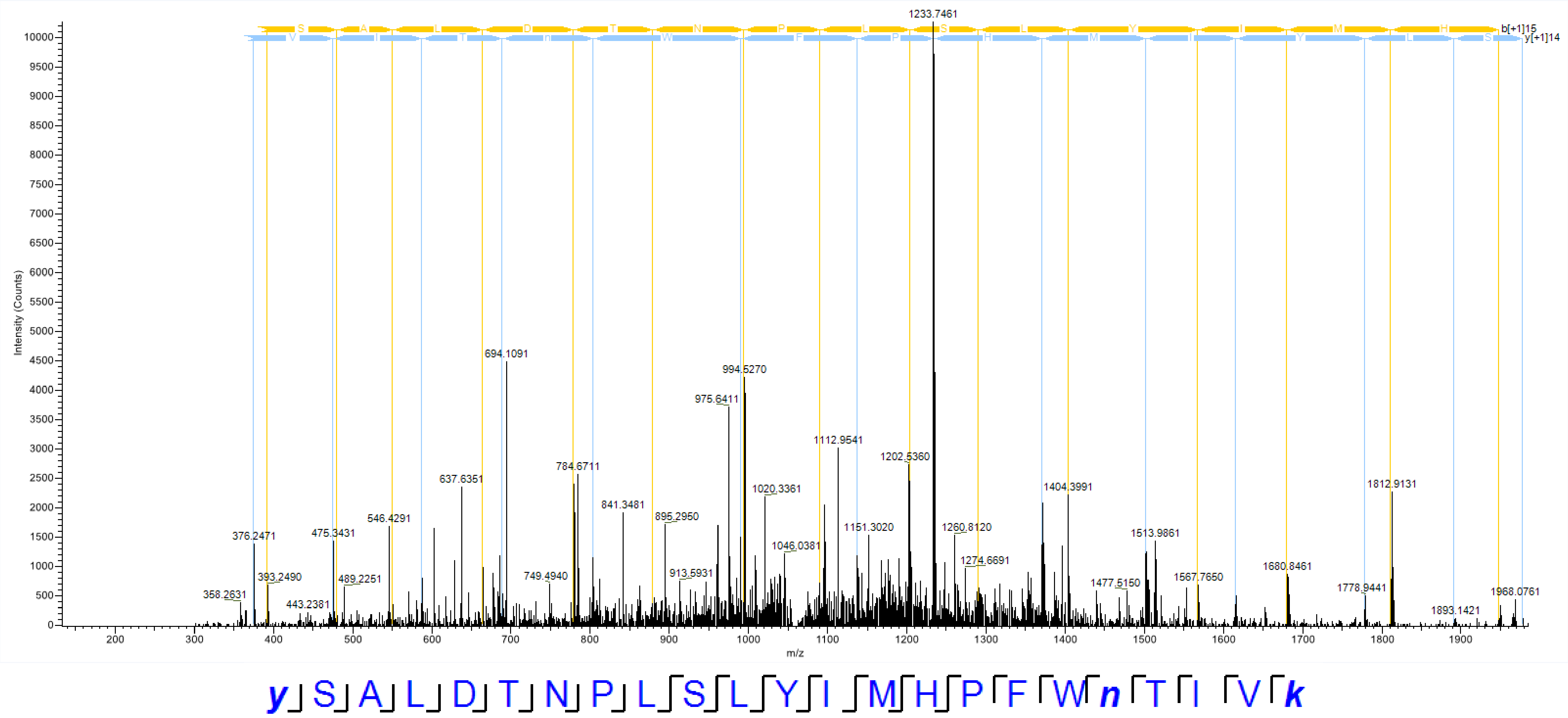
Peptide consensus view



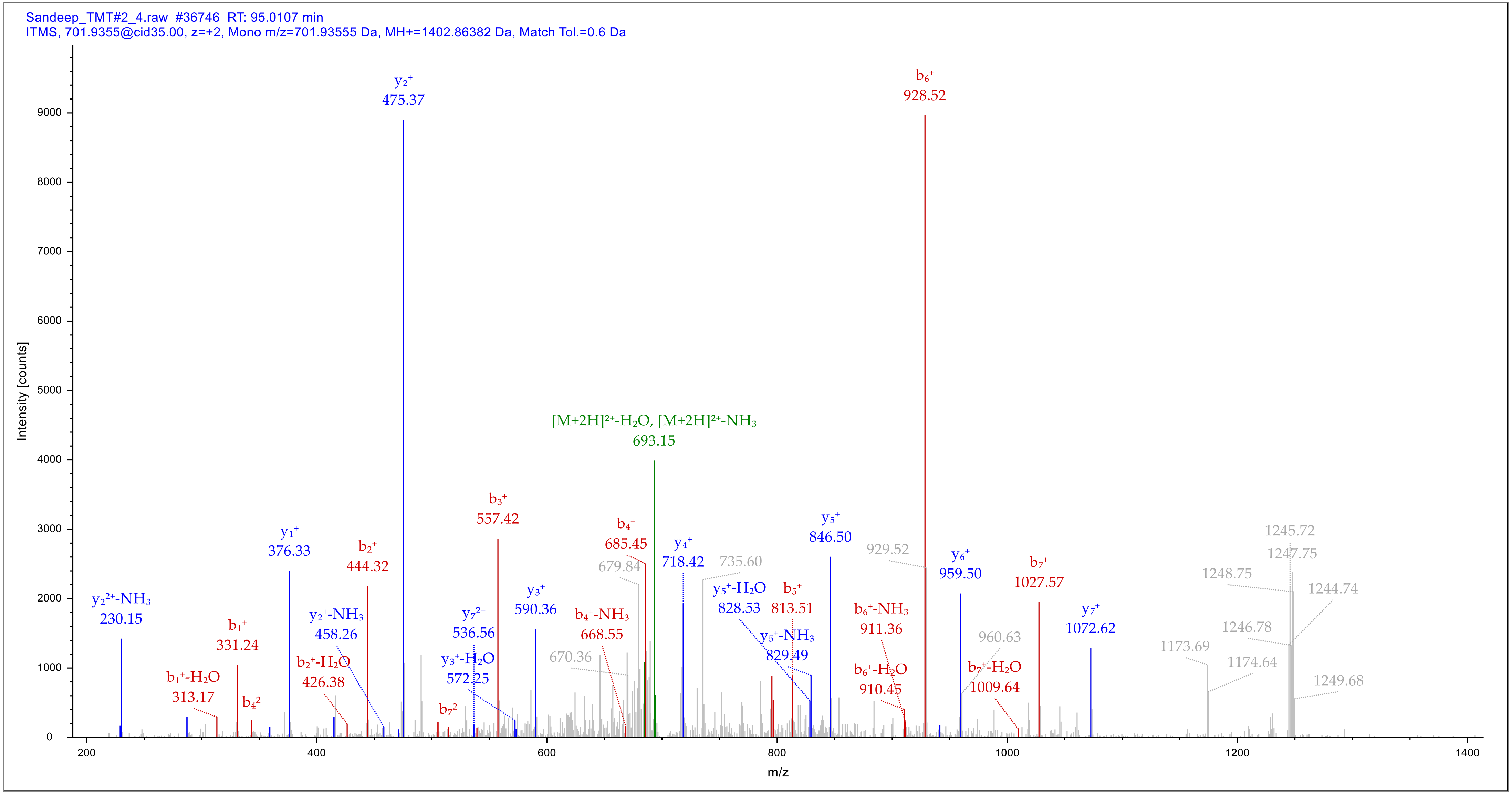
Sequence: YSALDTNPLSLYIMHPFWNTIVK, N19-Deamidated (0.98402 Da), K23-TMT6plex (229.16293 Da), Y1-TMT6plex (229.16293 Da)
Charge: +3, Monoisotopic m/z: 1061.57813 Da (+6.59 mmu/+6.21 ppm), MH+: 3182.71982 Da, RT: 146.2020 min,
Identified with: Sequest HT (v1.17); XCorr:6.85, Percolator q-Value:0.0e0, Percolator PEP:4.9e-6, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): Ethanolaminephosphotransferase 1 OS=Mus musculus OX=10090 GN=Selenoi PE=2 SV=3



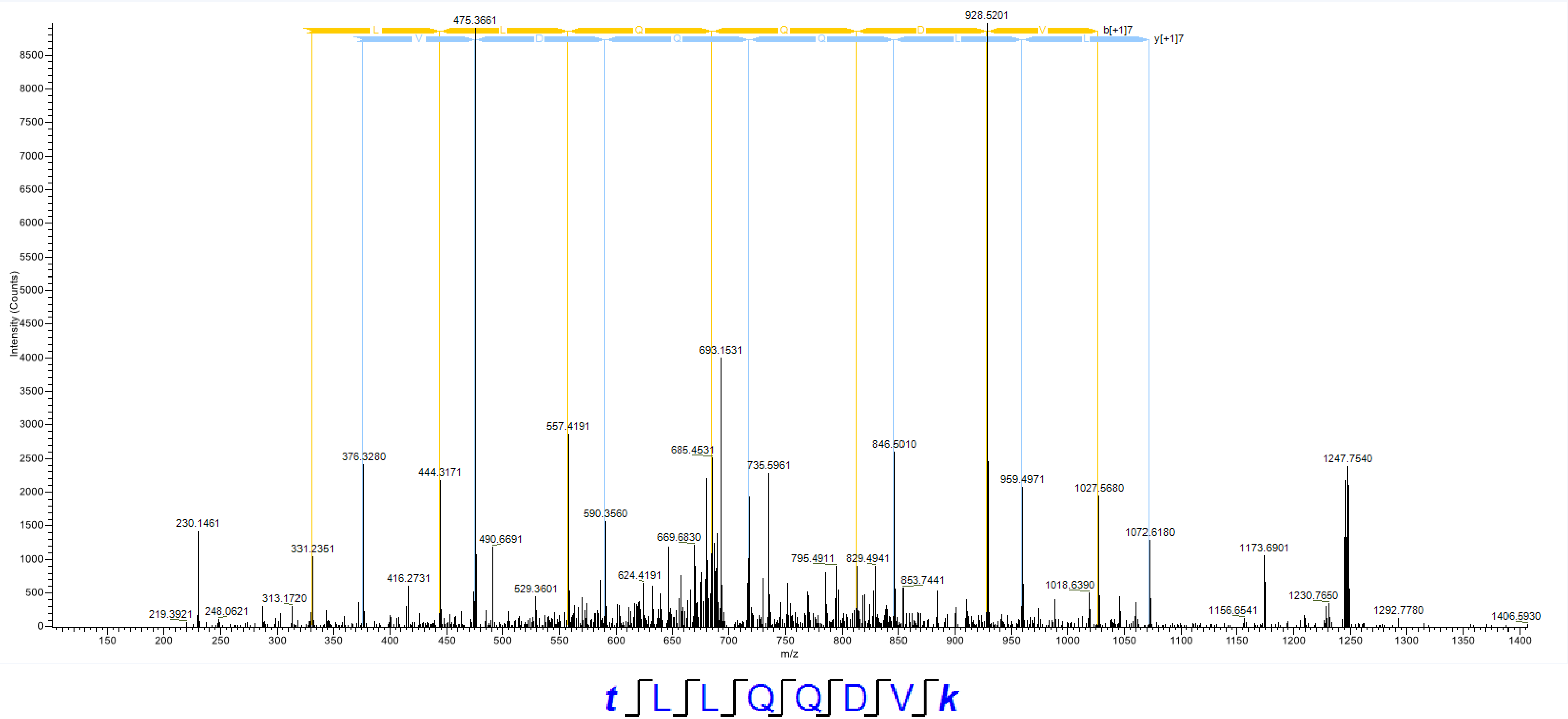
Peptide consensus view



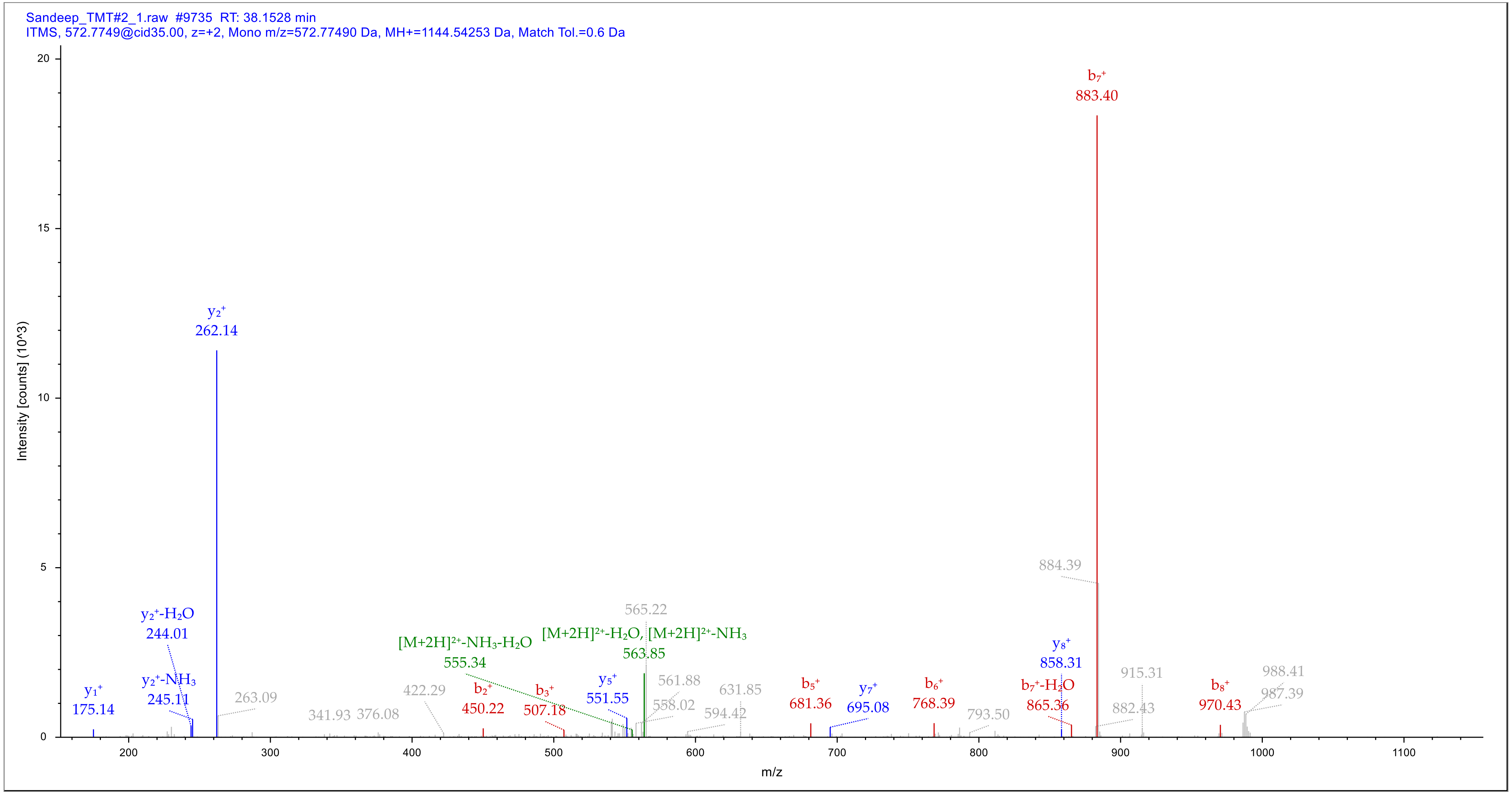
Sequence: TLLQQDVK, K8-TMT6plex (229.16293 Da), T1-TMT6plex (229.16293 Da)
Charge: +2, Monoisotopic m/z: 701.93555 Da (-1.59 mmu/-2.26 ppm), MH+: 1402.86382 Da, RT: 95.0107 min,
Identified with: Sequest HT (v1.17); XCorr:2.92, Percolator q-Value:9.8e-4, Percolator PEP:8.5e-3, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): Selenoprotein K OS=Mus musculus OX=10090 GN=Selenok PE=1 SV=3



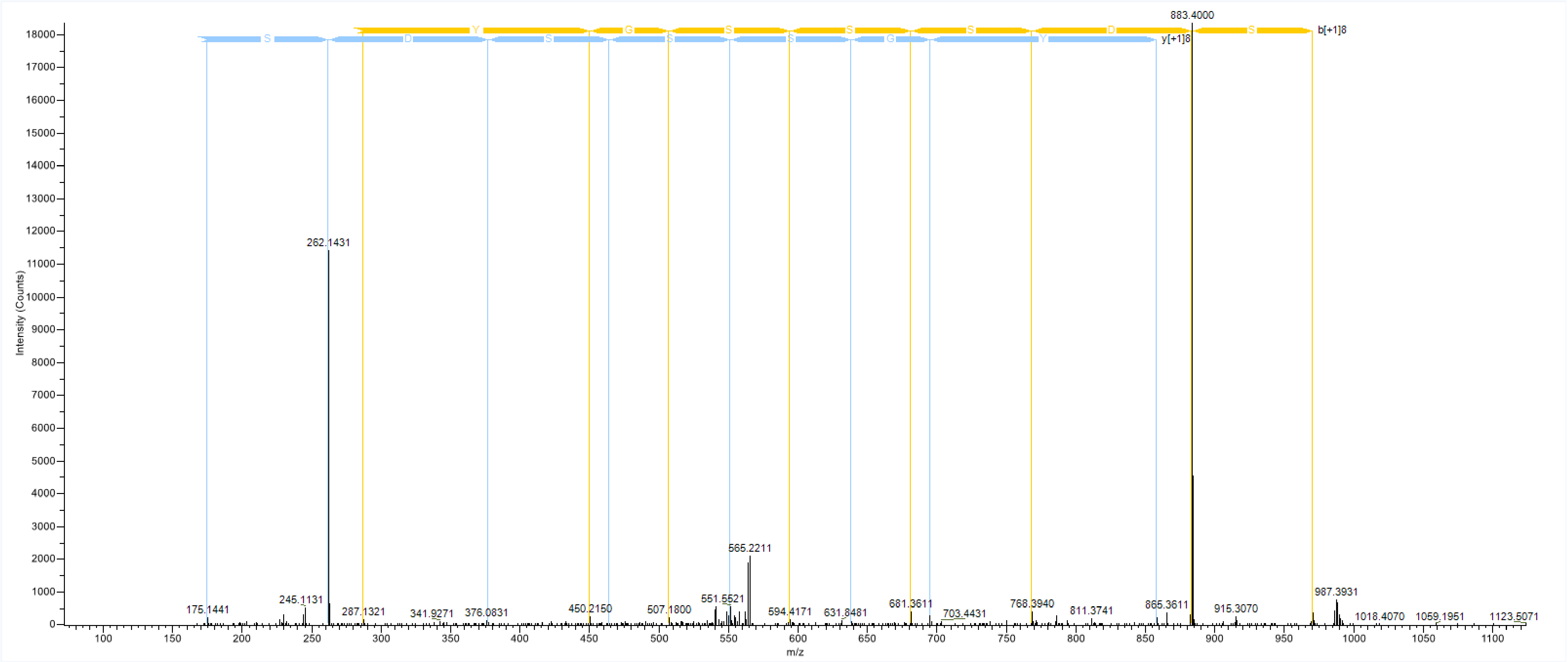
Peptide consensus view



Sequence: GYGSSSDSR, G1-TMT6plex (229.16293 Da)
Charge: +2, Monoisotopic m/z: 572.77490 Da (-0.33 mmu/-0.58 ppm), MH+: 1144.54253 Da, RT: 38.1528 min,
Identified with: Sequest HT (v1.17); XCorr:2.73, Percolator q-Value:2.3e-4, Percolator PEP:1.1e-3, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; y; y-H_2O; y-NH_3
Protein references (1): Selenoprotein K OS=Mus musculus OX=10090 GN=Selenok PE=1 SV=3

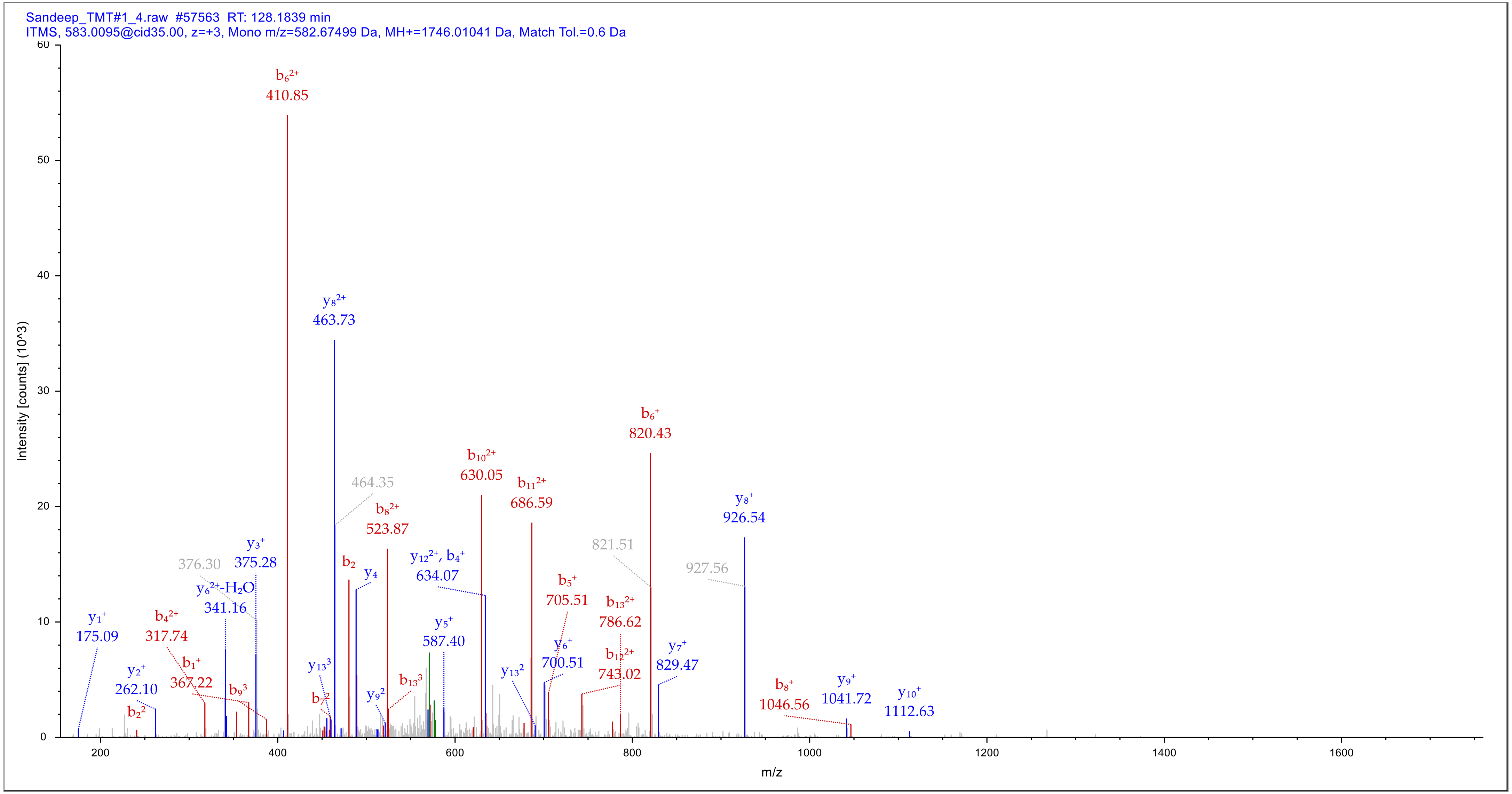


Peptide consensus view

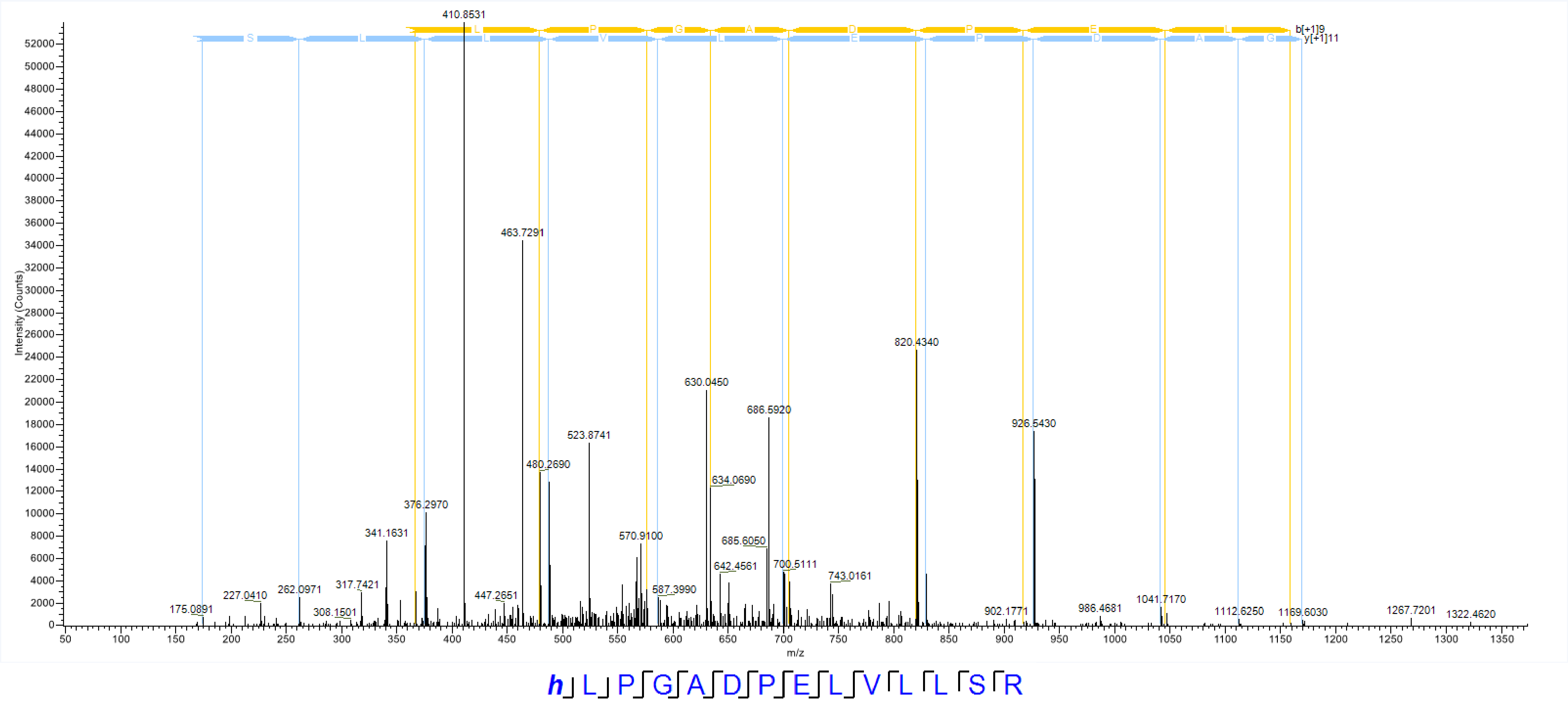


g∫Y∫G∫S∫S∫S∫D∫S∫R

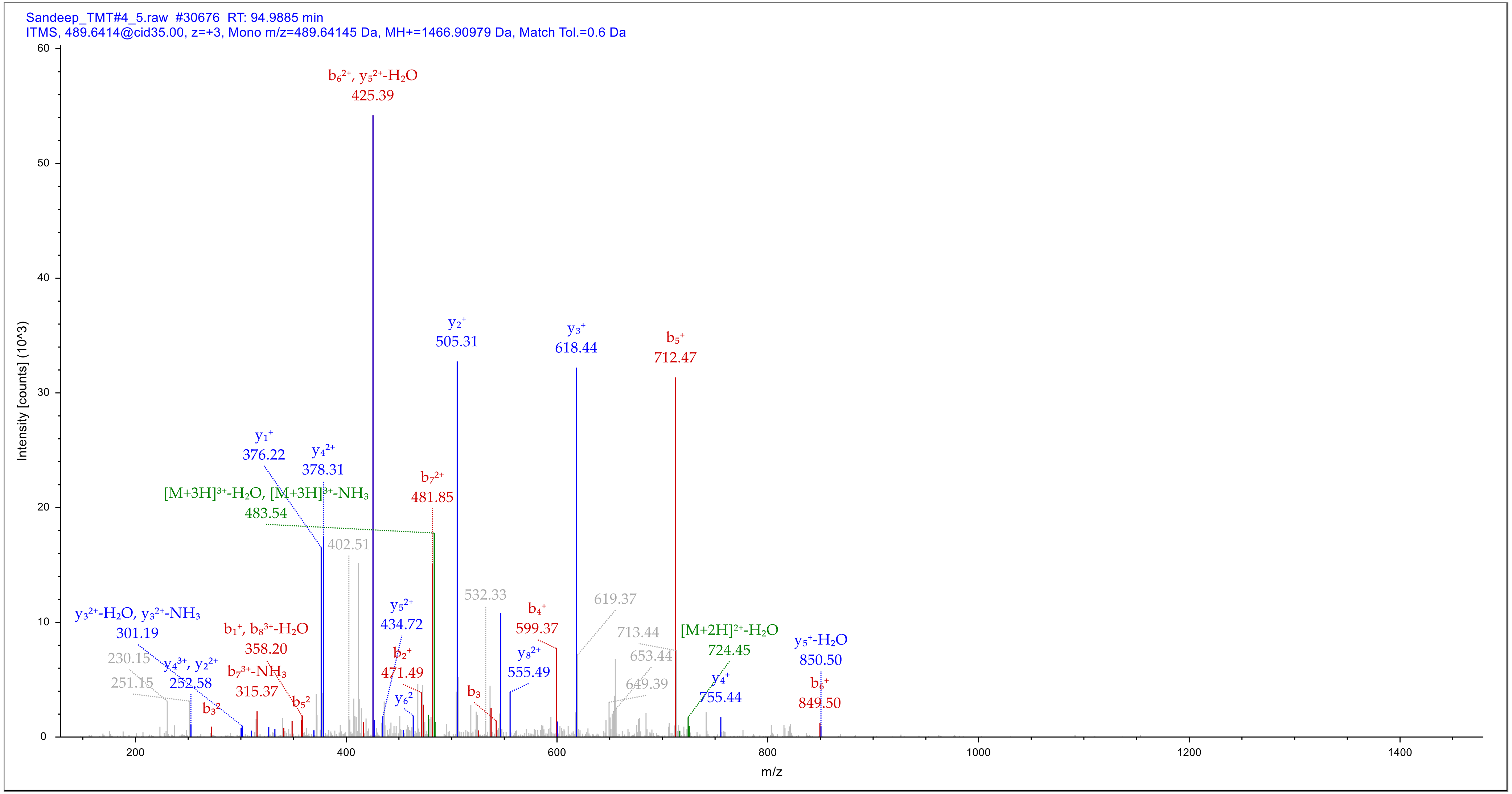
Sequence: HLPGADPELVLLSR, H1-TMT6plex (229.16293 Da)
Charge: +3, Monoisotopic m/z: 582.67499 Da (-0.24 mmu/-0.42 ppm), MH+: 1746.01041 Da, RT: 128.1839 min,
Identified with: Sequest HT (v1.17); XCorr:4.50, Percolator q-Value:2.5e-5, Percolator PEP:1.1e-4, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; y; y-H_2O; y-NH_3
Protein references (1): Selenoprotein M OS=Mus musculus OX=10090 GN=Selenom PE=1 SV=3



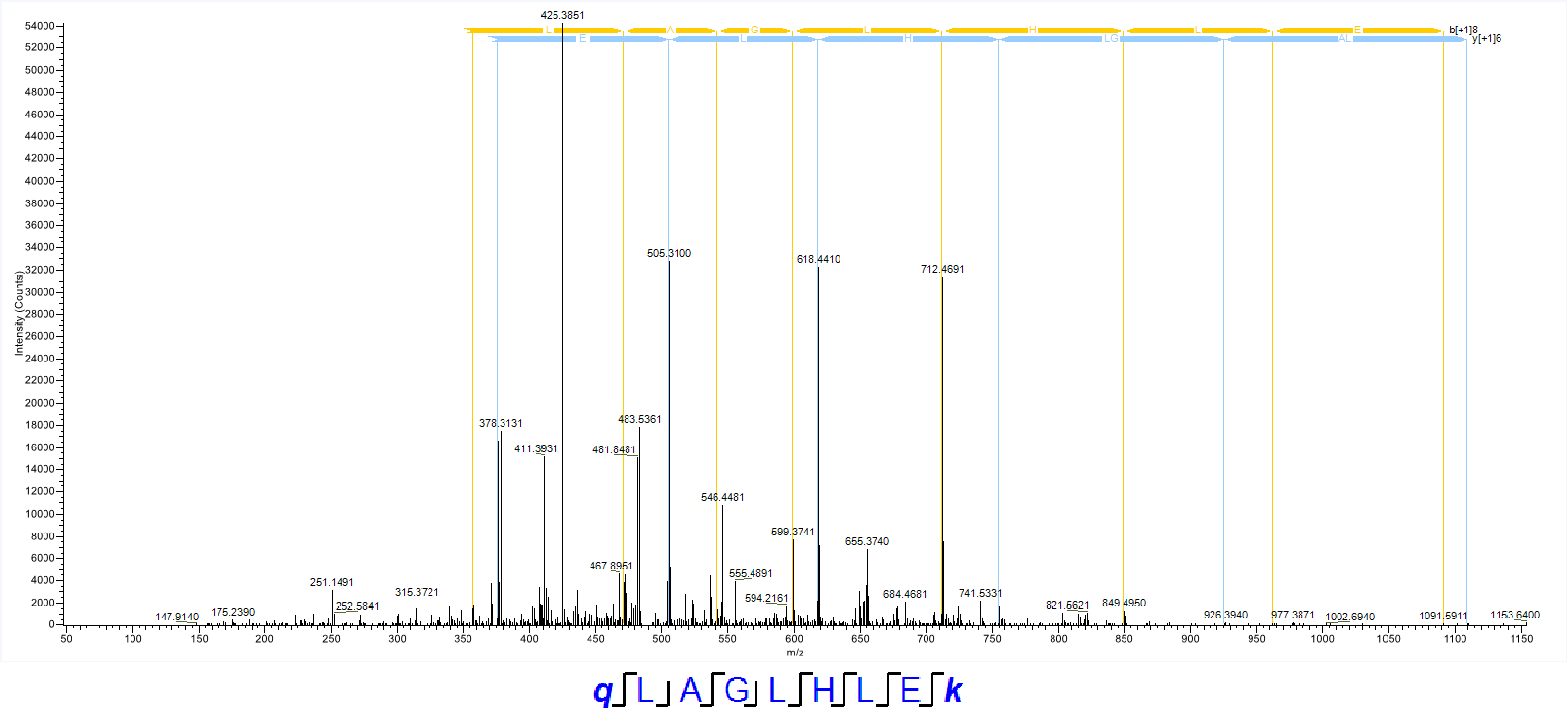
Peptide consensus view



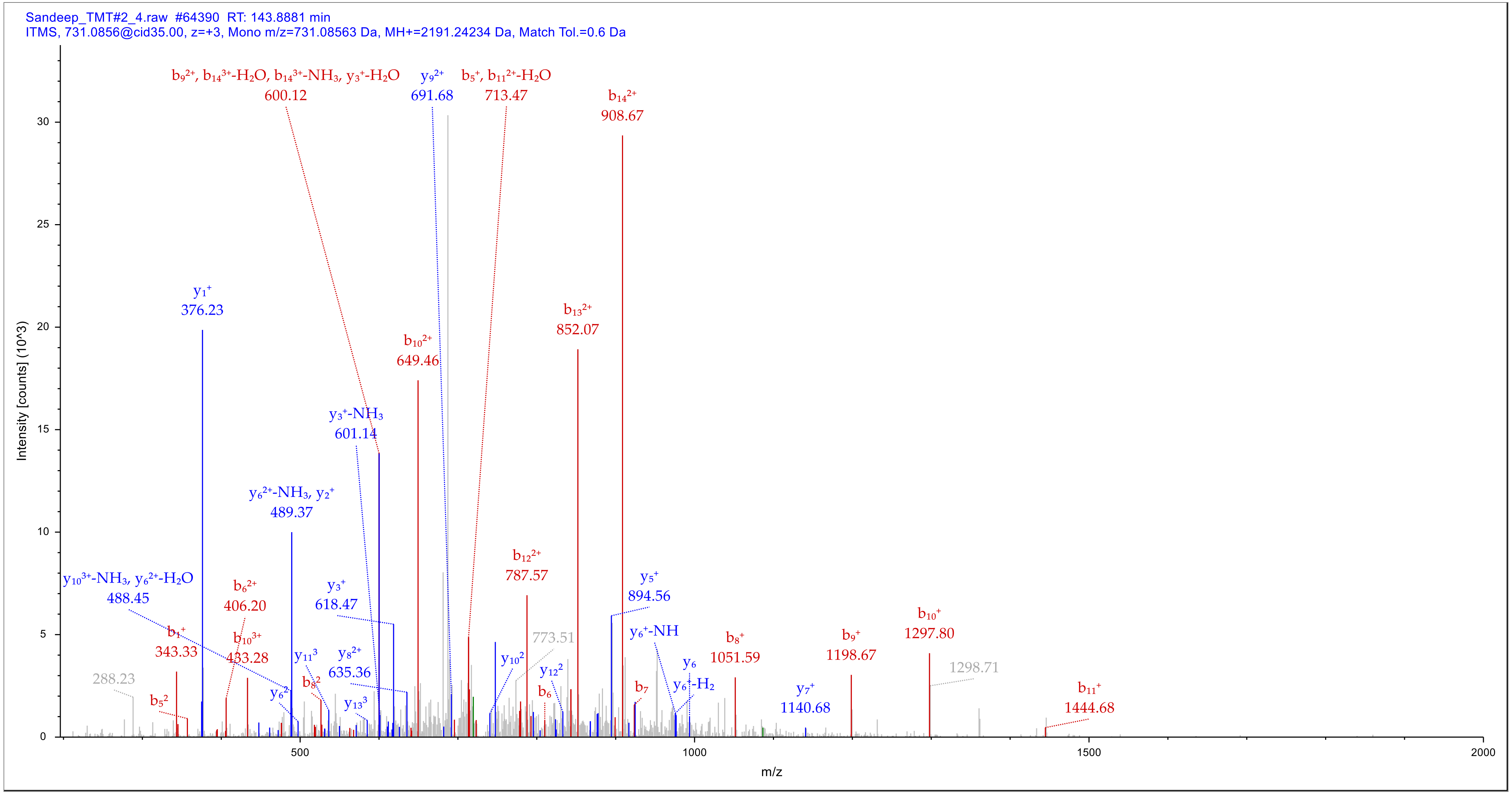
Sequence: QLAGLHLEK, K9-TMT6plex (229.16293 Da), Q1-TMT6plex (229.16293 Da)
Charge: +3, Monoisotopic m/z: 489.64145 Da (+0.09 mmu/+0.19 ppm), MH+: 1466.90979 Da, RT: 94.9885 min,
Identified with: Sequest HT (v1.17); XCorr:3.00, Percolator q-Value:8.5e-5, Percolator PEP:4.5e-4, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): Selenoprotein N OS=Mus musculus OX=10090 GN=Selenon PE=3 SV=2



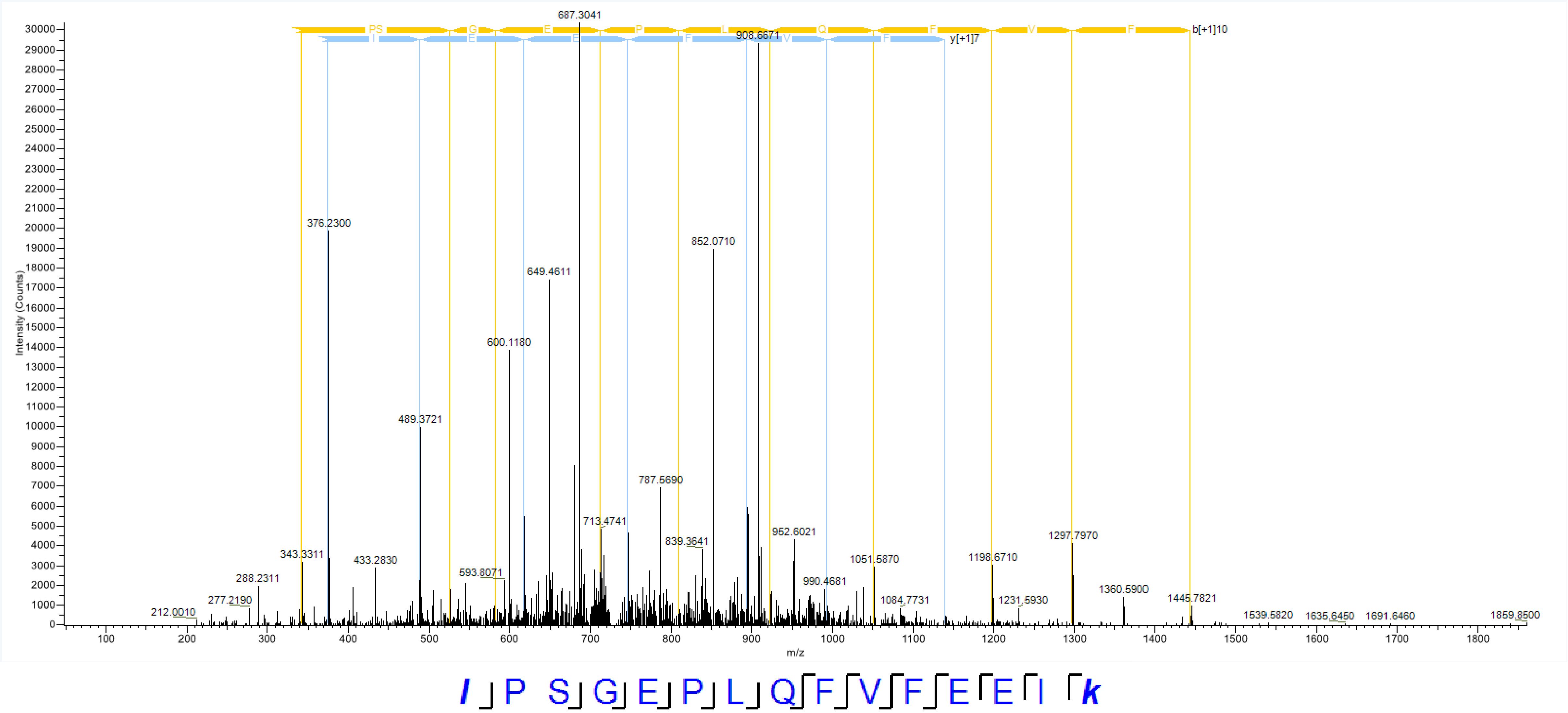
Peptide consensus view



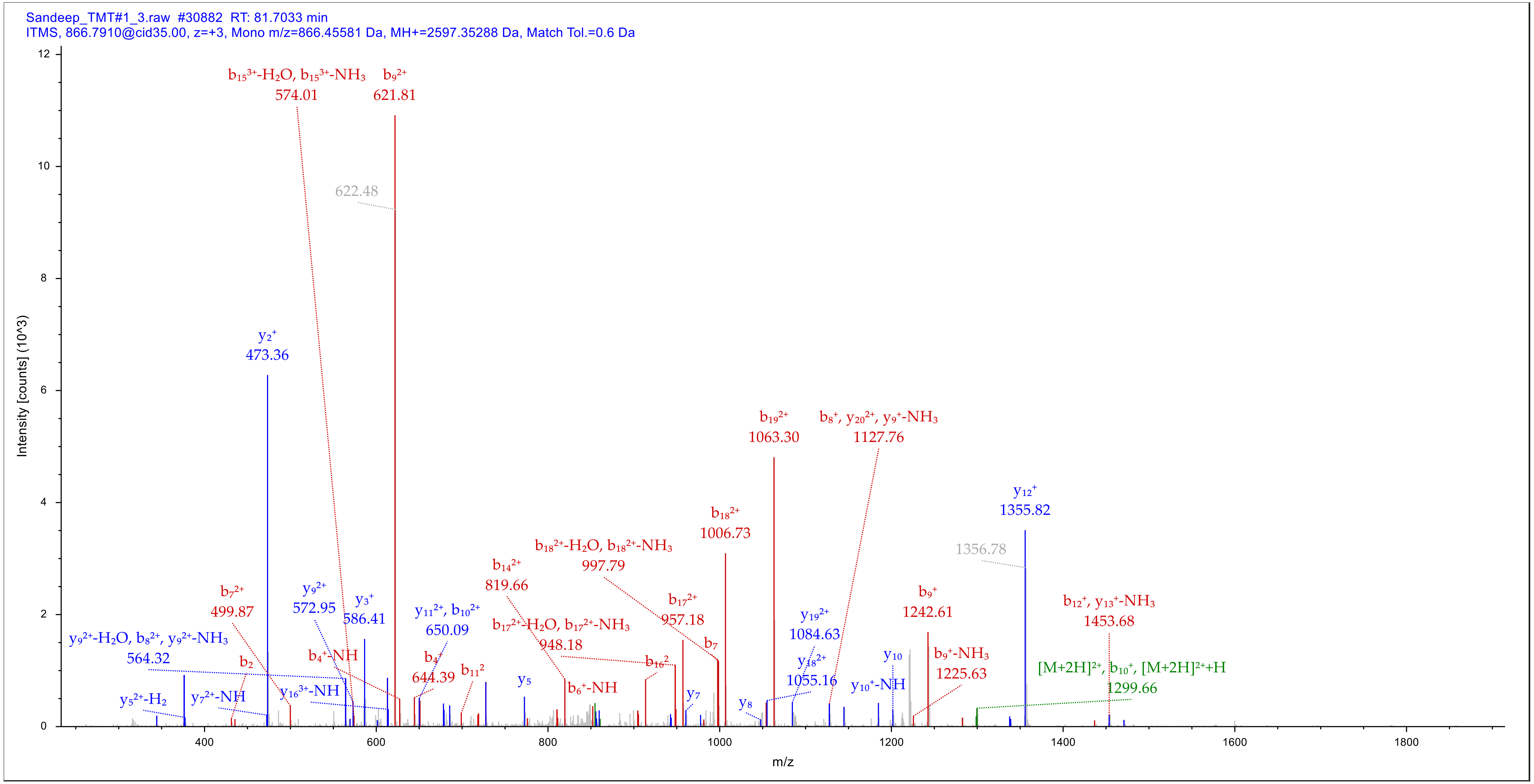
Sequence: LPSGEPLQFVFEEIK, K15-TMT6plex (229.16293 Da), L1-TMT6plex (229.16293 Da)
Charge: +3,   Monoisotopic m/z: 731.08563 Da (+0.29 mmu/+0.4 ppm),   MH+: 2191.24234 Da,   RT: 143.8881 min,
Identified with: Sequest HT (v1.17); XCorr:2.87, Percolator q-Value:3.7e-4, Percolator PEP:2.3e-3, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): Selenoprotein N OS=Mus musculus OX=10090 GN=Selenon PE=3 SV=2



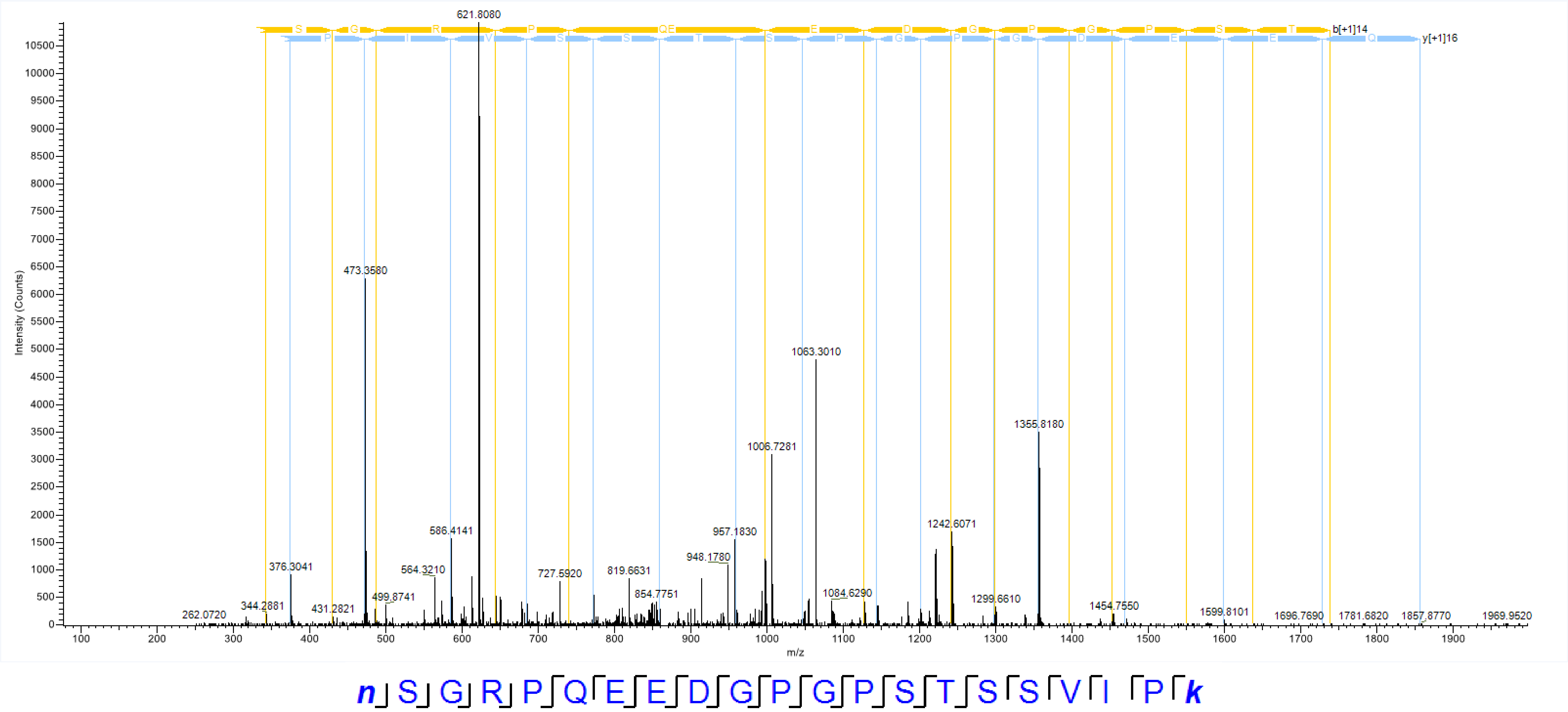
Peptide consensus view



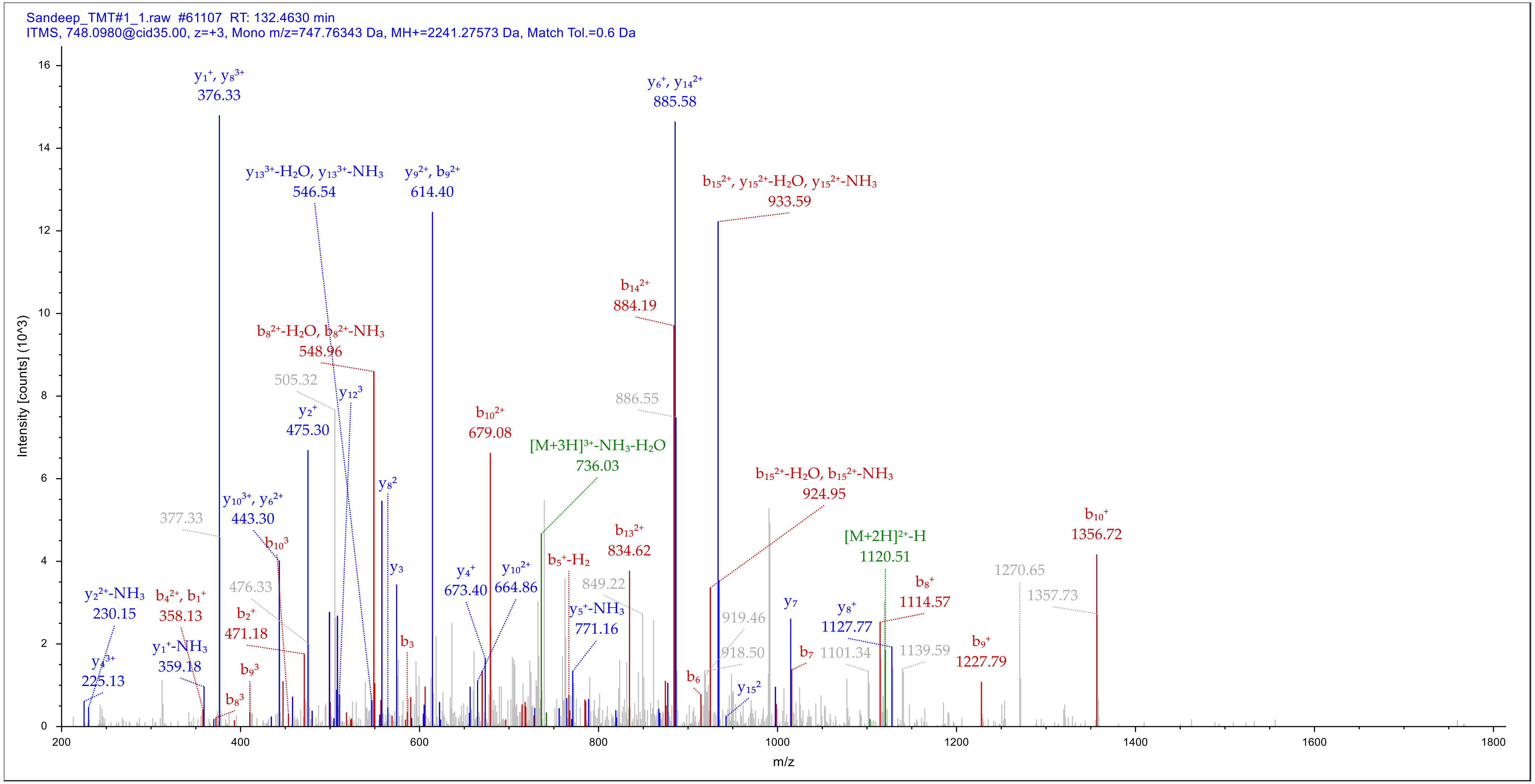
Sequence: NSGRPQEEDGPGPSTSSVIPK, K21-TMT6plex (229.16293 Da), N1-TMT6plex (229.16293 Da)
Charge: +3, Monoisotopic m/z: 866.45581 Da (-1.42 mmu/-1.64 ppm), MH+: 2597.35288 Da, RT: 81.7033 min,
Identified with: Sequest HT (v1.17); XCorr:4.85, Percolator q-Value:0.0e0, Percolator PEP:5.4e-7, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): Selenoprotein S OS=Mus musculus OX=10090 GN=Selenos PE=1 SV=3



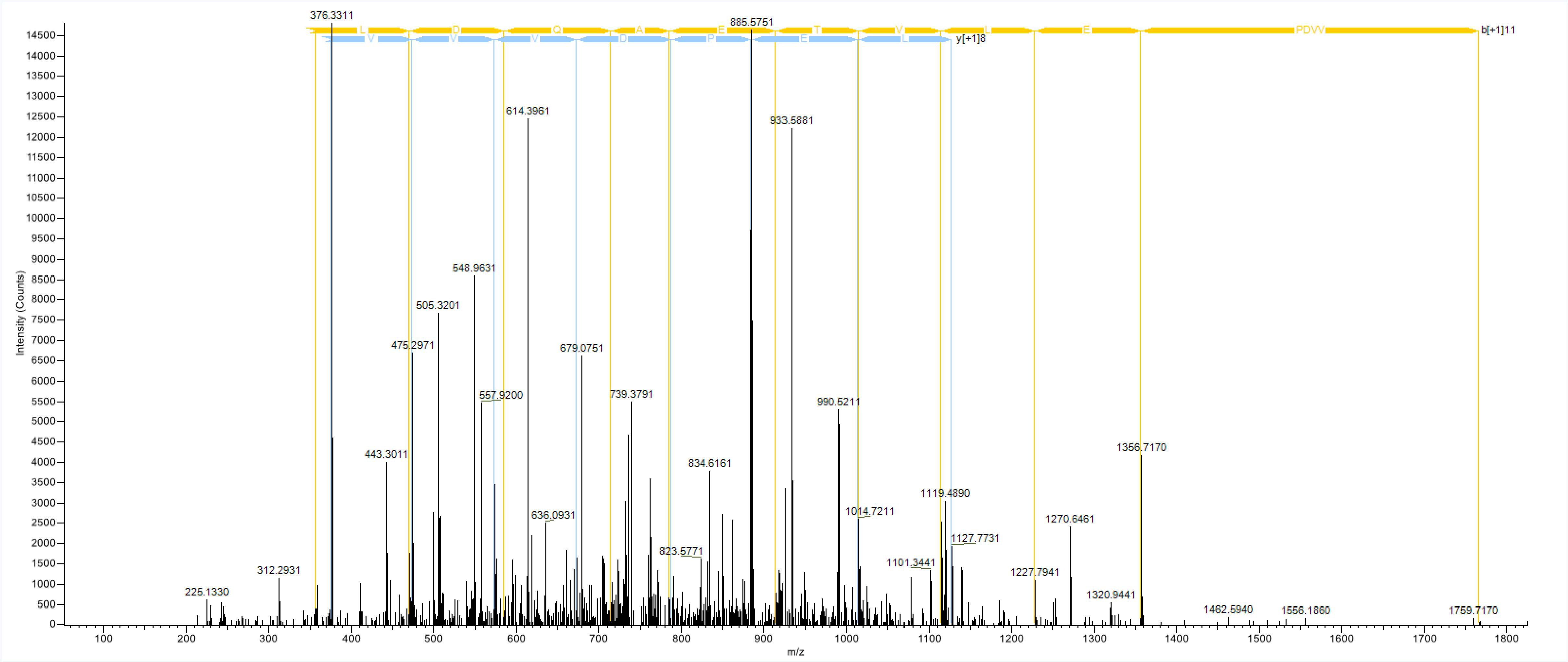
Peptide consensus view



Sequence: QLDQAETVLEPDVVVK, K16-TMT6plex (229.16293 Da), Q1-TMT6plex (229.16293 Da)
Charge: +3, Monoisotopic m/z: 747.76343 Da (+0.5 mmu/+0.67 ppm), MH+: 2241.27573 Da, RT: 132.4630 min,
Identified with: Sequest HT (v1.17); XCorr:4.22, Percolator q-Value:9.6e-4, Percolator PEP:6.8e-3, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): Selenoprotein S OS=Mus musculus OX=10090 GN=Selenos PE=1 SV=3

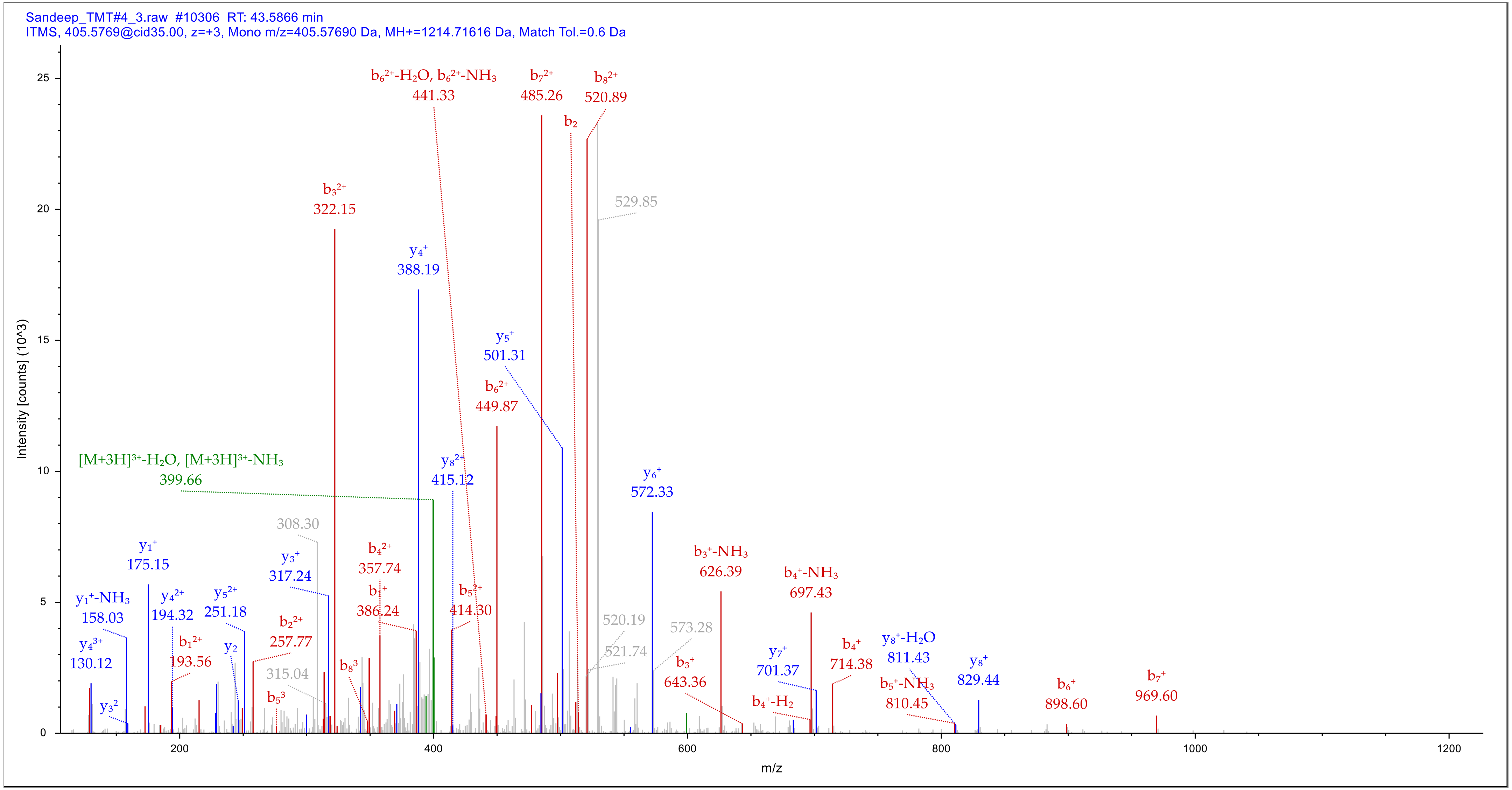


Peptide consensus view

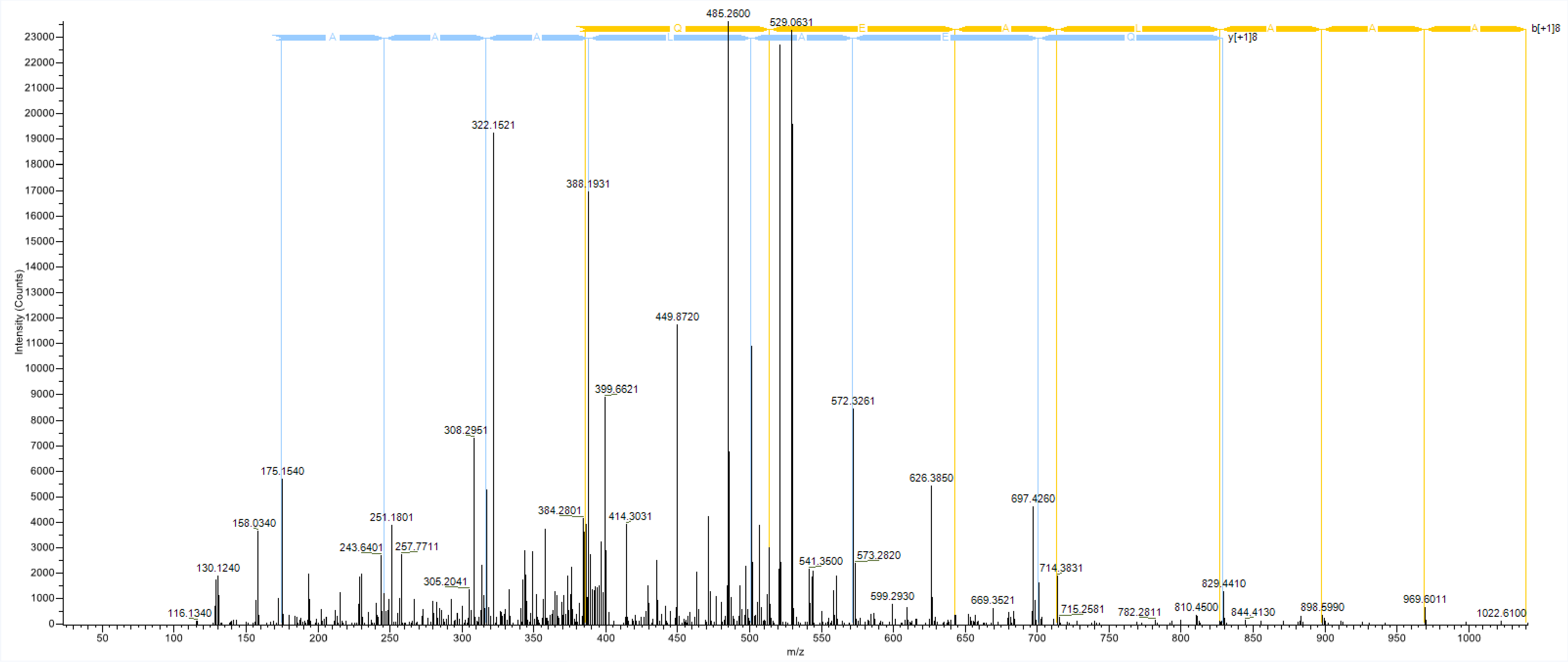


q L D Q A E T V L E P D V V V *k*

Sequence: RQEALAAAR, R1-TMT6plex (229.16293 Da)
Charge: +3, Monoisotopic m/z: 405.57690 Da (-0.18 mmu/-0.43 ppm), MH+: 1214.71616 Da, RT: 43.5866 min,
Identified with: Sequest HT (v1.17); XCorr:4.19, Percolator q-Value:0.0e0, Percolator PEP:1.1e-4, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): Selenoprotein S OS=Mus musculus OX=10090 GN=Selenos PE=1 SV=3

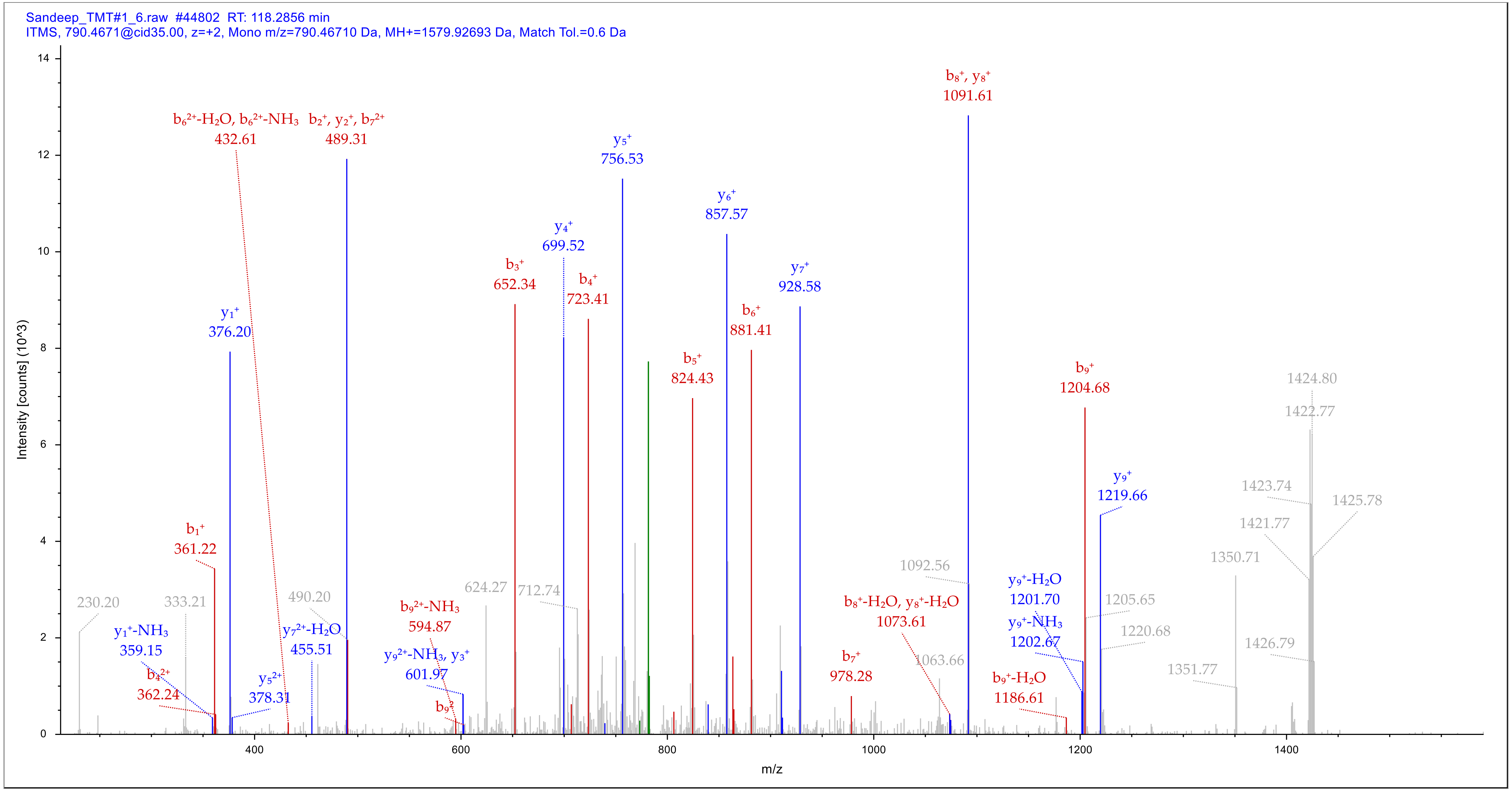


Peptide consensus view

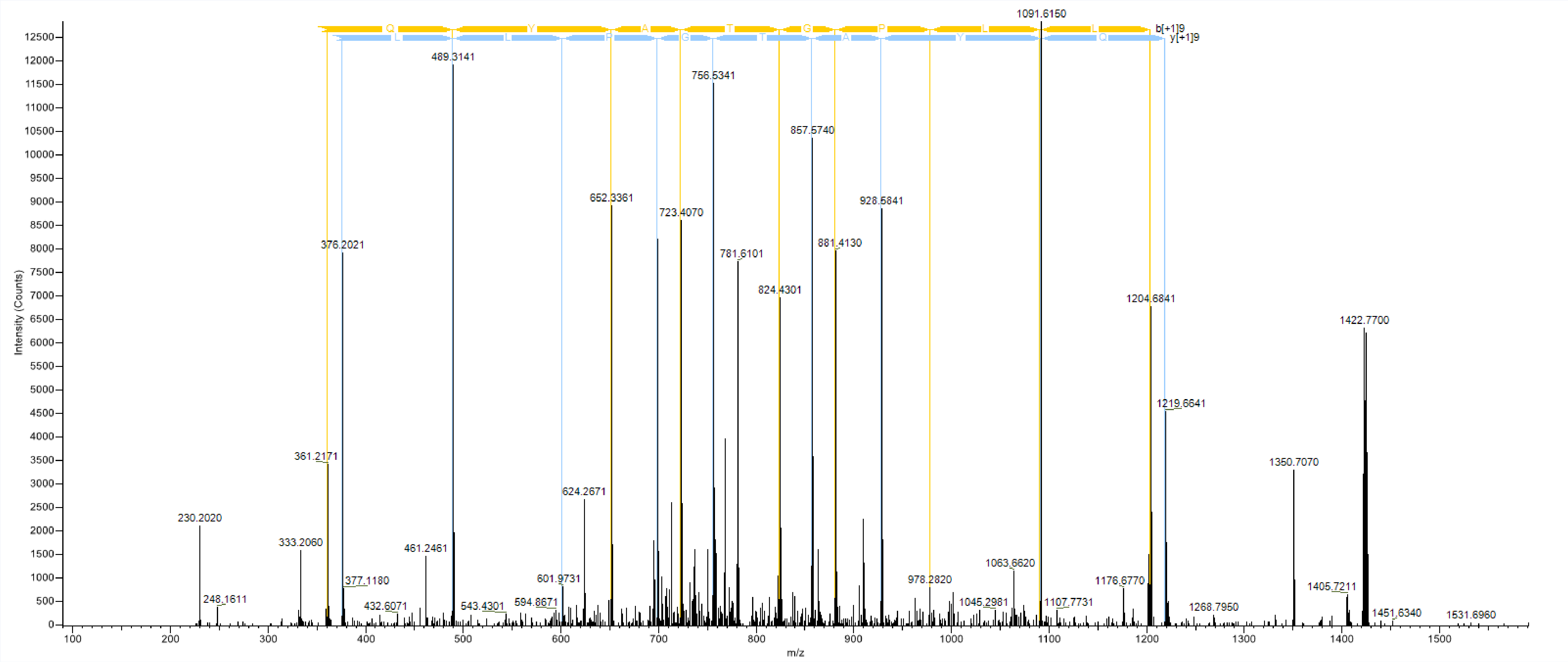


r QEALAAAR

Sequence: MQYATGPLLK, K10-TMT6plex (229.16293 Da), M1-TMT6plex (229.16293 Da)
Charge: +2, Monoisotopic m/z: 790.46710 Da (-0.64 mmu/-0.81 ppm), MH+: 1579.92693 Da, RT: 118.2856 min,
Identified with: Sequest HT (v1.17); XCorr:3.97, Percolator q-Value:1.6e-4, Percolator PEP:4.9e-4, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): Thioredoxin reductase-like selenoprotein T OS=Mus musculus OX=10090 GN=Selenot PE=1 SV=2

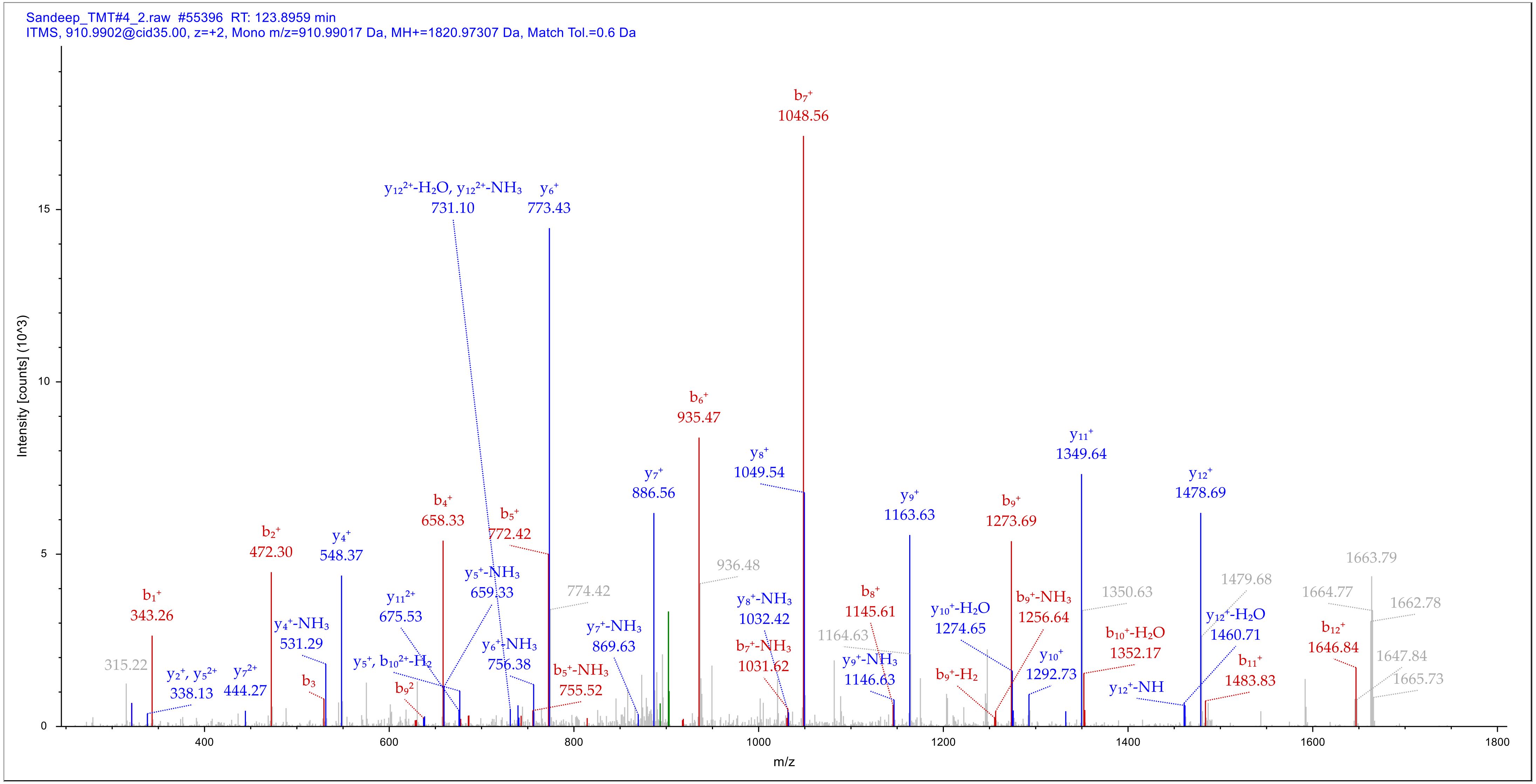


Peptide consensus view

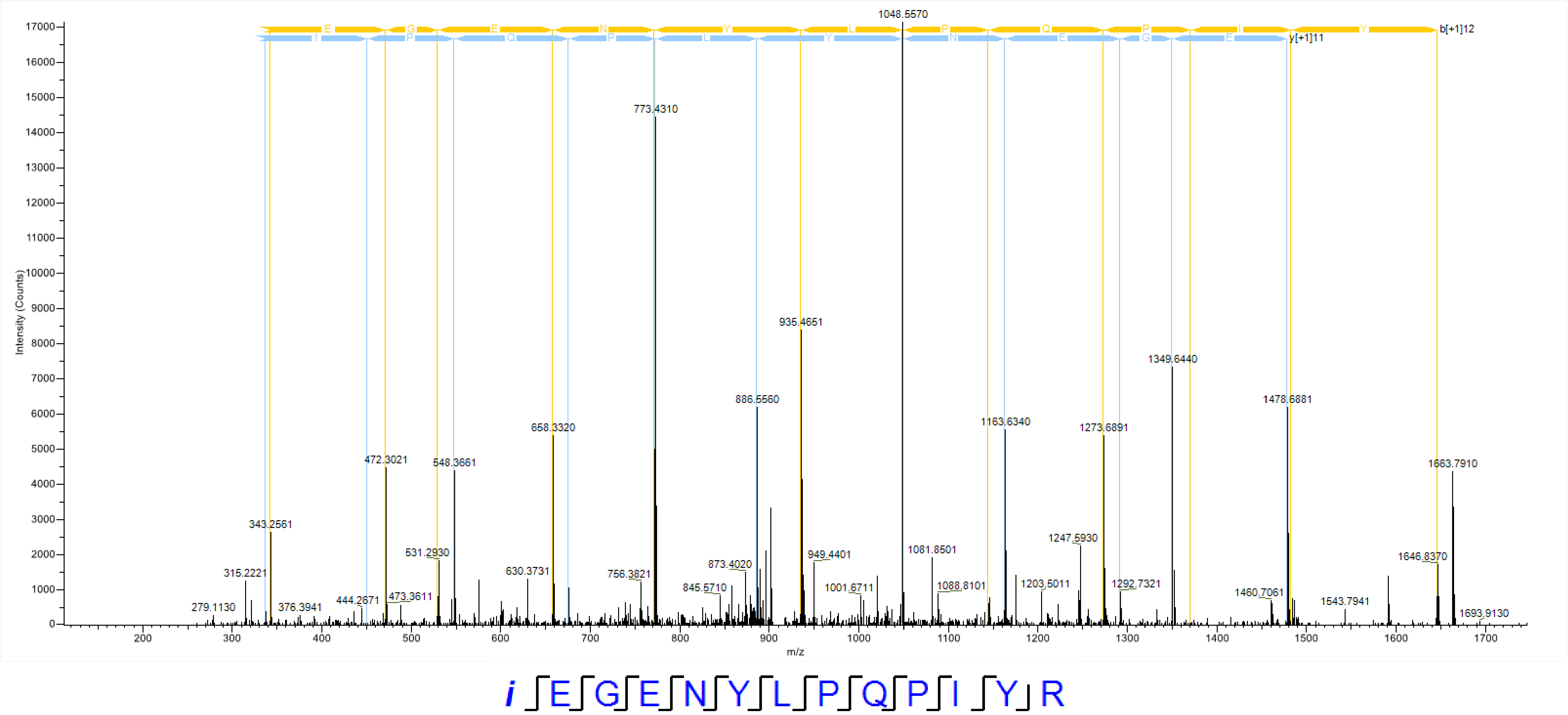


m Q Y A T G P L L ***k***

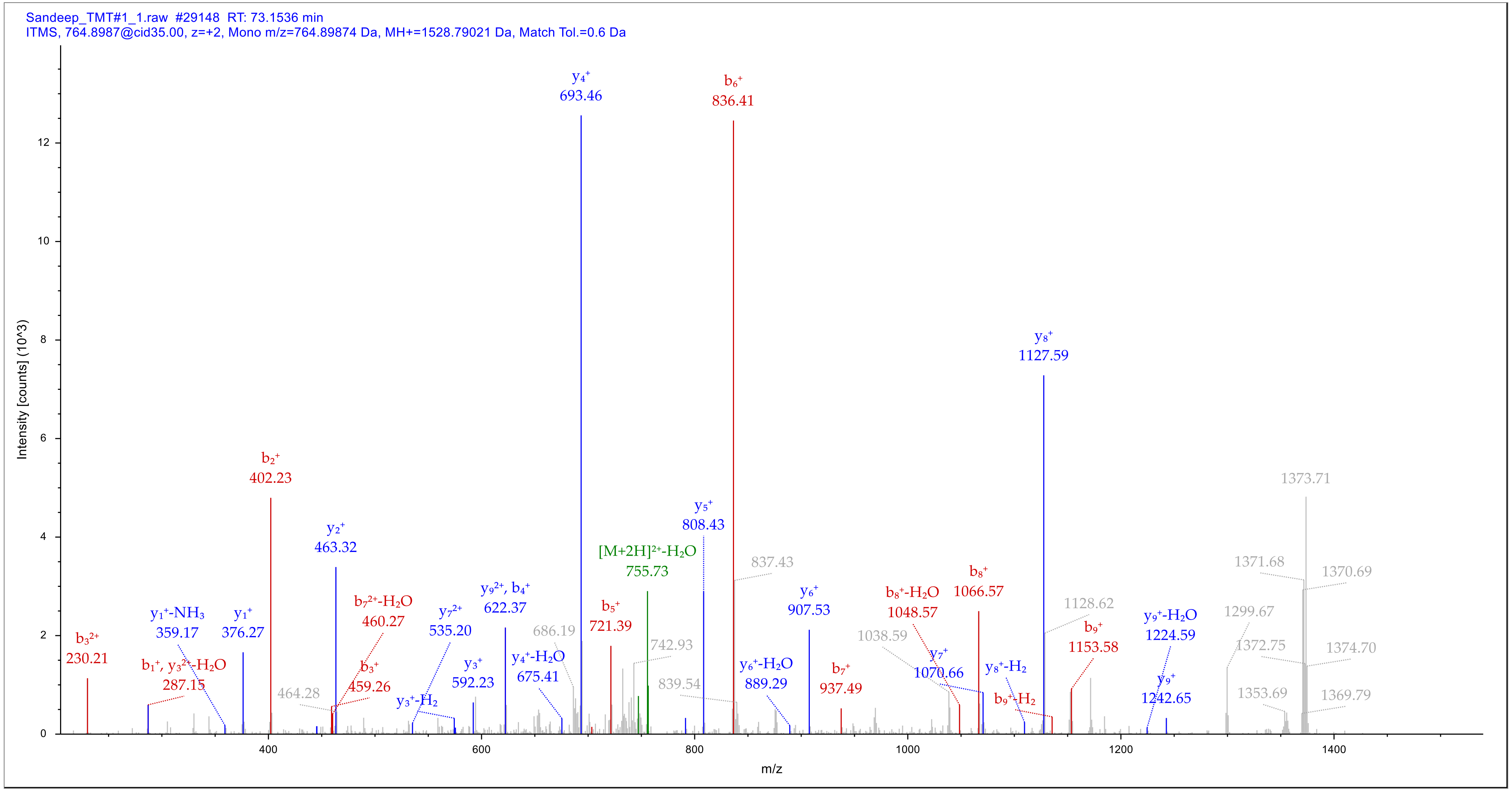
Sequence: IEGENYLPQPIYR, I1-TMT6plex (229.16293 Da)
Charge: +2, Monoisotopic m/z: 910.99017 Da (-0.67 mmu/-0.74 ppm), MH+: 1820.97307 Da, RT: 123.8959 min,
Identified with: Sequest HT (v1.17); XCorr:4.71, Percolator q-Value:0.0e0, Percolator PEP:5.7e-5, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; b-NH_3; y; y-H_2O; y-NH_3
Protein references (1): Thioredoxin reductase-like selenoprotein T OS=Mus musculus OX=10090 GN=Selenot PE=1 SV=2



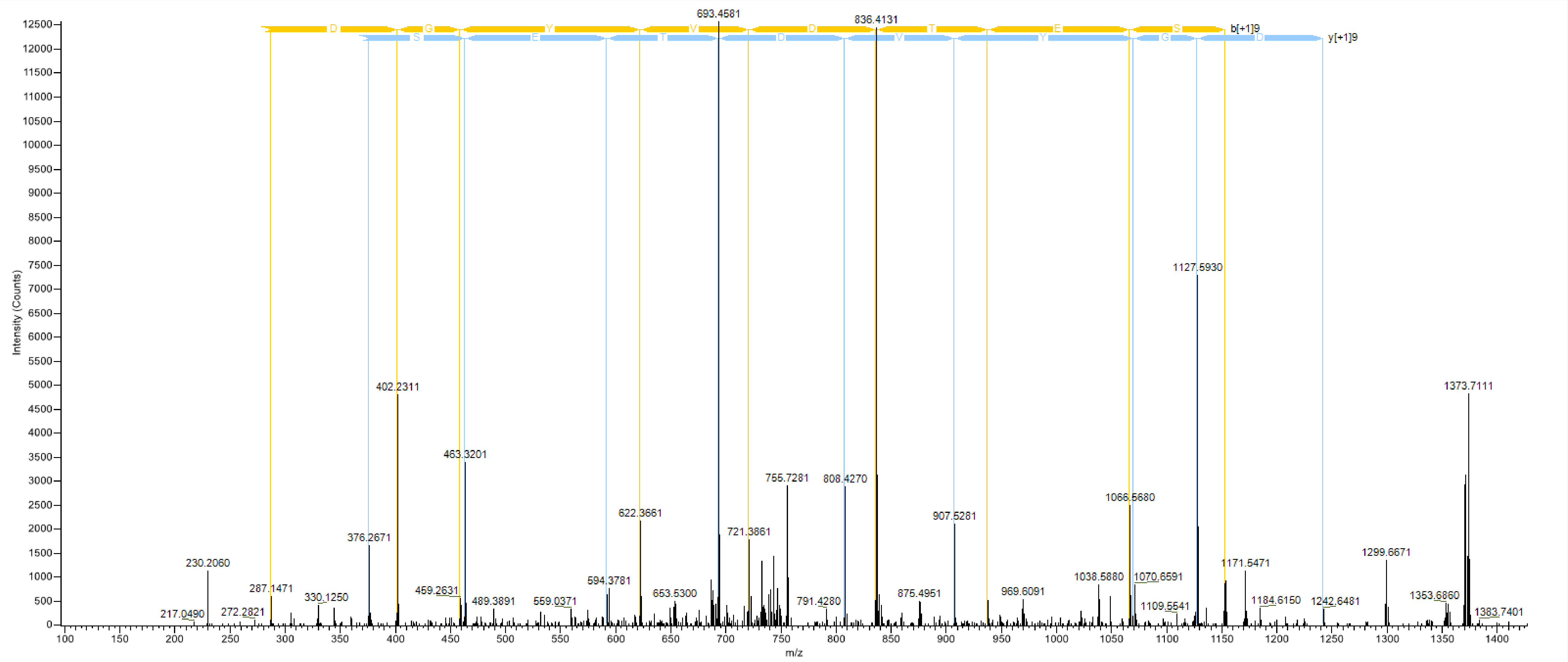
Peptide consensus view



Sequence: GDGYVDTESK, K10-TMT6plex (229.16293 Da), G1-TMT6plex (229.16293 Da)
Charge: +2, Monoisotopic m/z: 764.89874 Da (+0.34 mmu/+0.45 ppm), MH+: 1528.79021 Da, RT: 73.1536 min,
Identified with: Sequest HT (v1.17); XCorr:3.48, Percolator q-Value:1.4e-4, Percolator PEP:4.1e-4, Ions matched by search engine: 0/0
Fragment match tolerance used for search: 0.6 Da
Fragments used for search: b; b-H_2O; y; y-H_2O; y-NH_3
Protein references (1): - Selenoprotein W OS=Mus musculus OX=10090 GN=Selenow PE=1 SV=3



Peptide consensus view



g D G Y V D T E S ***k***