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Supporting Information

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Identification of Histone Lysine Acetoacetylation as a Dynamic Post-Translational Modification Regulated by HBO1

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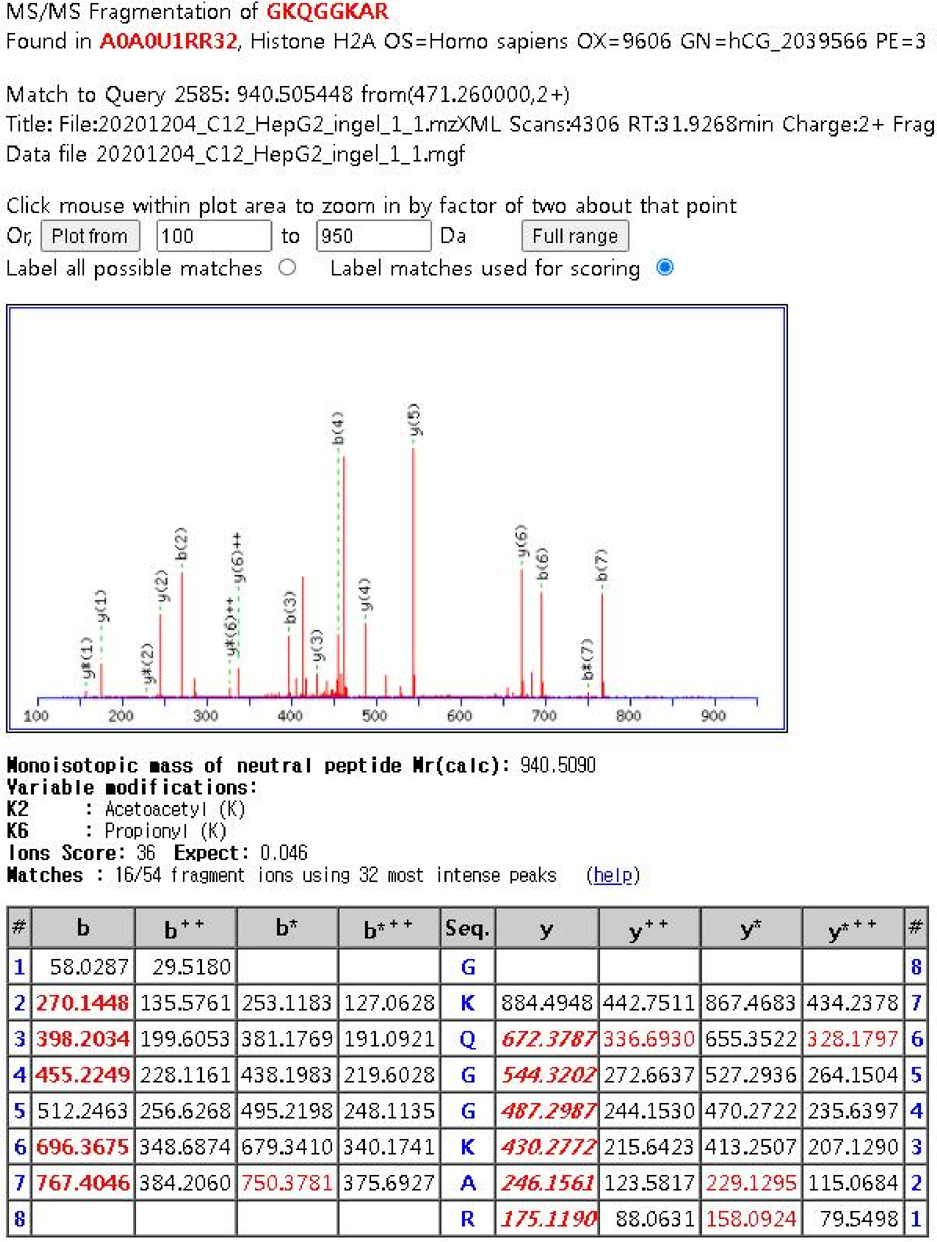
Figure S6. Representative MS^2 spectra of the identified 33 Kacac sites

H2AK5	**GKacacQGGKprAR**	**Human HepG2 cells**



MS/MS Fragmentation of **GKQGGKAR**
Found in **A0A0U1RR32**, Histone H2A OS=Homo sapiens OX=9606 GN=hCG_2039566 PE=3 SV=1

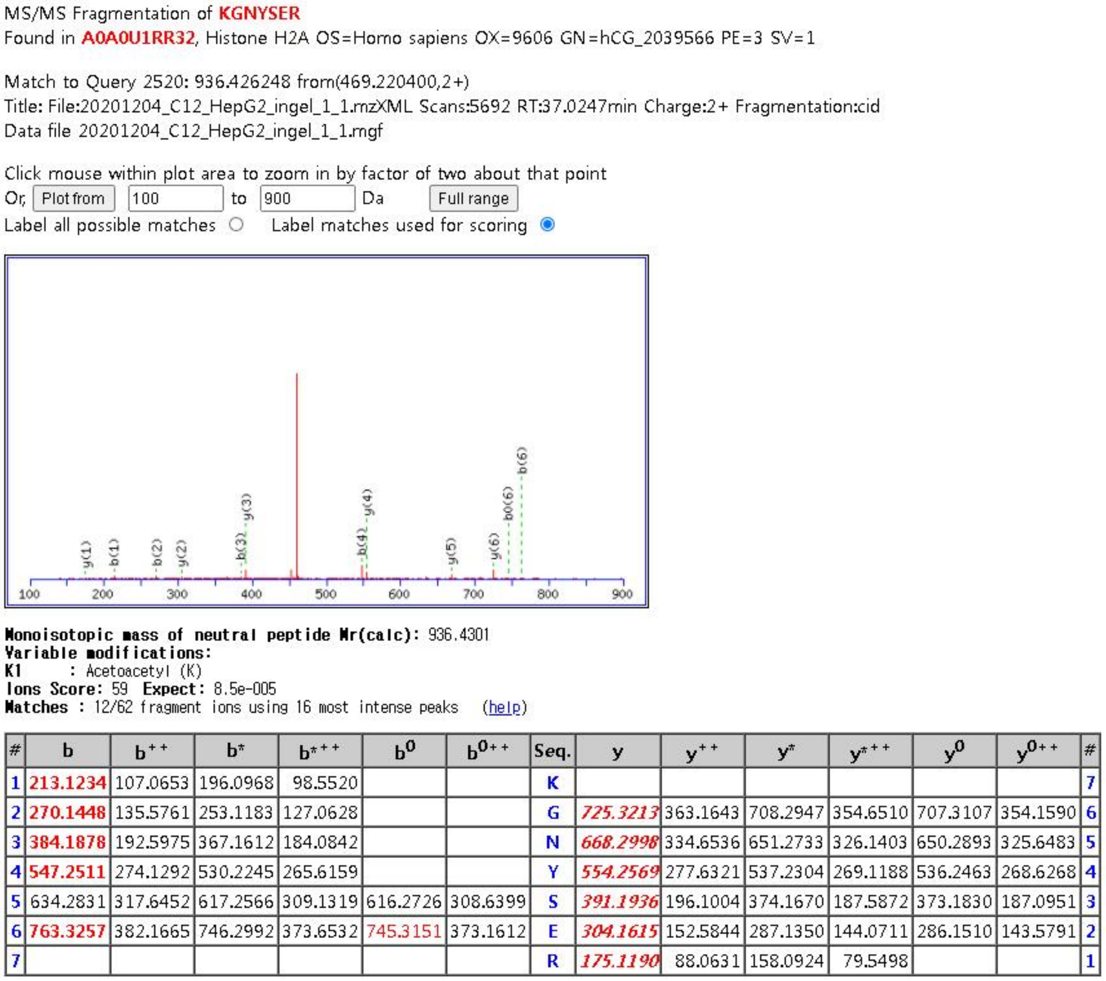
Match to Query 2585: 940.505448 from(471.260000,2+)
Title: File:20201204_C12_HepG2_ingel_1_1.mzXML Scans:4306 RT:31.9268min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_1_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 100 to 950 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 940.5090
Variable modifications:
K2 : Acetoacetyl (K)
K6 : Propionyl (K)
Ions Score: 36 **Expect:** 0.046
Matches : 16/54 fragment ions using 32 most intense peaks (help)

#	b	b^{++}	b^{*}	b^{*++}	Seq.	y	y^{++}	y^{*}	y^{*++}	#
1	58.0287	29.5180			G					8
2	**270.1448**	135.5761	253.1183	127.0628	K	884.4948	442.7511	867.4683	434.2378	7
3	**398.2034**	199.6053	381.1769	191.0921	Q	***672.3787***	336.6930	655.3522	328.1797	6
4	**455.2249**	228.1161	438.1983	219.6028	G	***544.3202***	272.6637	527.2936	264.1504	5
5	512.2463	256.6268	495.2198	248.1135	G	***487.2987***	244.1530	470.2722	235.6397	4
6	**696.3675**	348.6874	679.3410	340.1741	K	***430.2772***	215.6423	413.2507	207.1290	3
7	**767.4046**	384.2060	750.3781	375.6927	A	***246.1561***	123.5817	229.1295	115.0684	2
8					R	***175.1190***	88.0631	158.0924	79.5498	1

H2AK36	**KacacGNYSER**	**Human HepG2 cells**



MS/MS Fragmentation of **KGNYSER**
Found in **A0A0U1RR32**, Histone H2A OS=Homo sapiens OX=9606 GN=hCG_2039566 PE=3 SV=1

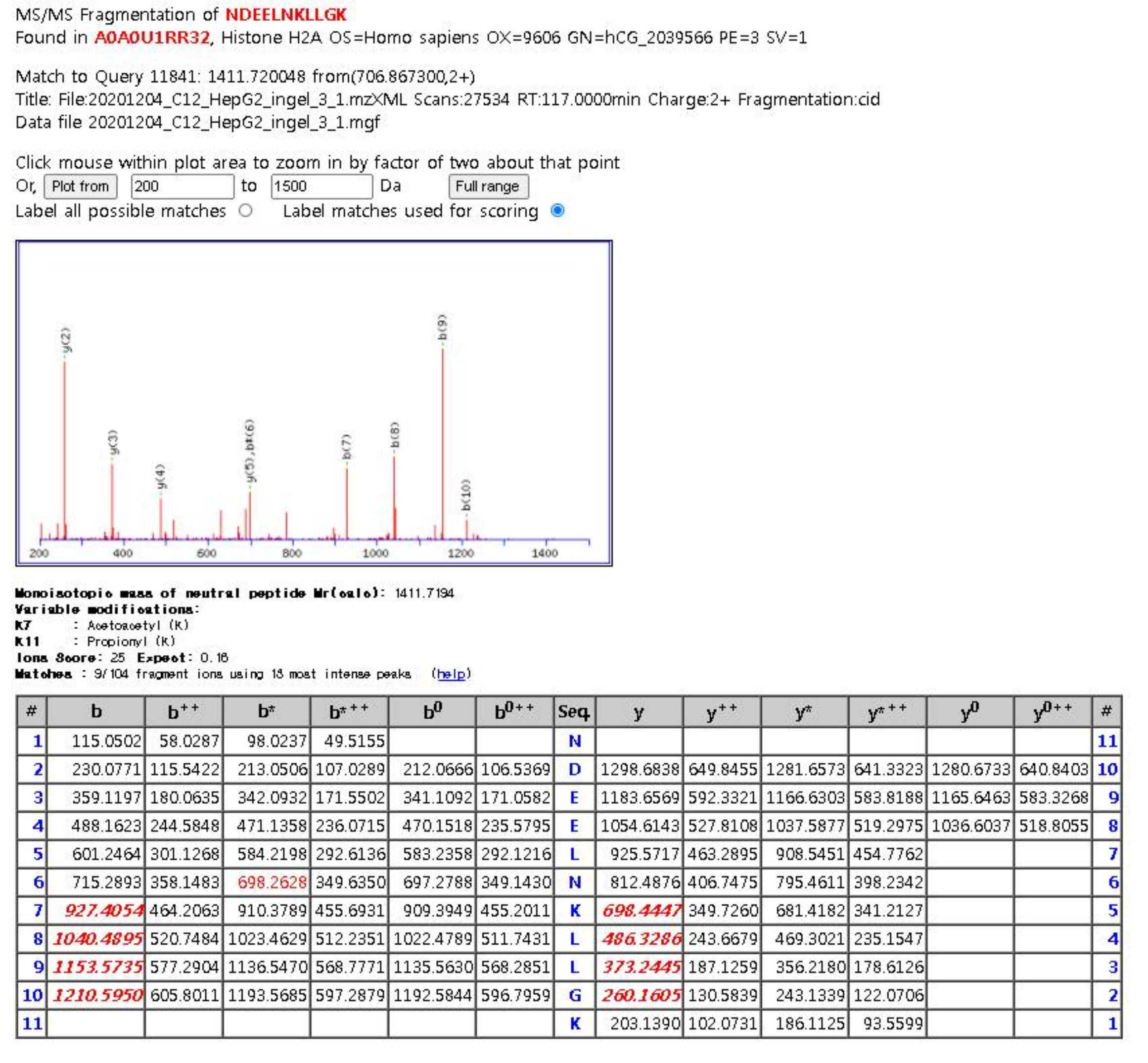
Match to Query 2520: 936.426248 from(469.220400,2+)
Title: File:20201204_C12_HepG2_ingel_1_1.mzXML Scans:5692 RT:37.0247min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_1_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 100 to 900 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 936.4301
Variable modifications:
K1 : Acetoacetyl (K)
Ions Score: 59 **Expect:** 8.5e-005
Matches : 12/62 fragment ions using 16 most intense peaks (help)

#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	**213.1234**	107.0653	196.0968	98.5520			K							7
2	**270.1448**	135.5761	253.1183	127.0628			G	*725.3213*	363.1643	708.2947	354.6510	707.3107	354.1590	6
3	**384.1878**	192.5975	367.1612	184.0842			N	*668.2998*	334.6536	651.2733	326.1403	650.2893	325.6483	5
4	**547.2511**	274.1292	530.2245	265.6159			Y	*554.2569*	277.6321	537.2304	269.1188	536.2463	268.6268	4
5	634.2831	317.6452	617.2566	309.1319	616.2726	308.6399	S	*391.1936*	196.1004	374.1670	187.5872	373.1830	187.0951	3
6	**763.3257**	382.1665	746.2992	373.6532	745.3151	373.1612	E	*304.1615*	152.5844	287.1350	144.0711	286.1510	143.5791	2
7							R	*175.1190*	88.0631	158.0924	79.5498			1

H2AK95	**NDEELNKacacLLGKpr**	**Human HepG2 cells**



MS/MS Fragmentation of **NDEELNKLLGK**
Found in **A0A0U1RR32**, Histone H2A OS=Homo sapiens OX=9606 GN=hCG_2039566 PE=3 SV=1

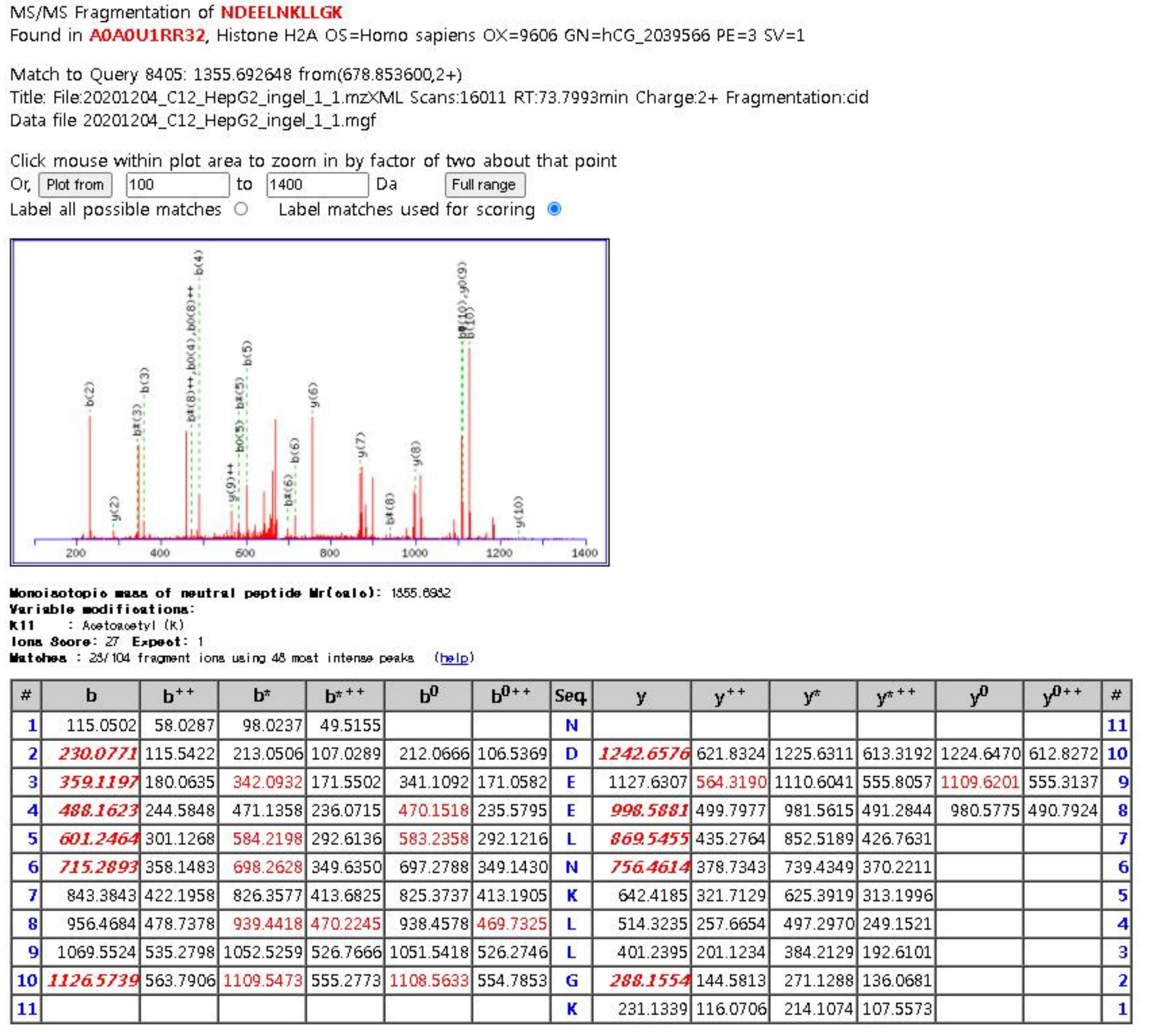
Match to Query 11841: 1411.720048 from(706.867300,2+)
Title: File:20201204_C12_HepG2_ingel_3_1.mzXML Scans:27534 RT:117.0000min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_3_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 200 to 1500 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 1411.7194
Variable modifications:
K7 : Acetoacetyl (K)
K11 : Propionyl (K)
Ions Score: 25 **Expect:** 0.16
Matches : 9/104 fragment ions using 18 most intense peaks (help)

#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	115.0502	58.0287	98.0237	49.5155			N							11
2	230.0771	115.5422	213.0506	107.0289	212.0666	106.5369	D	1298.6838	649.8455	1281.6573	641.3323	1280.6733	640.8403	10
3	359.1197	180.0635	342.0932	171.5502	341.1092	171.0582	E	1183.6569	592.3321	1166.6303	583.8188	1165.6463	583.3268	9
4	488.1623	244.5848	471.1358	236.0715	470.1518	235.5795	E	1054.6143	527.8108	1037.5877	519.2975	1036.6037	518.8055	8
5	601.2464	301.1268	584.2198	292.6136	583.2358	292.1216	L	925.5717	463.2895	908.5451	454.7762			7
6	715.2893	358.1483	698.2628	349.6350	697.2788	349.1430	N	812.4876	406.7475	795.4611	398.2342			6
7	***927.4054***	464.2063	910.3789	455.6931	909.3949	455.2011	K	***698.4447***	349.7260	681.4182	341.2127			5
8	***1040.4895***	520.7484	1023.4629	512.2351	1022.4789	511.7431	L	***486.3286***	243.6679	469.3021	235.1547			4
9	***1153.5735***	577.2904	1136.5470	568.7771	1135.5630	568.2851	L	***373.2445***	187.1259	356.2180	178.6126			3
10	***1210.5950***	605.8011	1193.5685	597.2879	1192.5844	596.7959	G	***260.1605***	130.5839	243.1339	122.0706			2
11							K	203.1390	102.0731	186.1125	93.5599			1

H2AK99	**NDEELNKLLGKacac**	**Human HepG2 cells**



MS/MS Fragmentation of **NDEELNKLLGK**
Found in **A0A0U1RR32**, Histone H2A OS=Homo sapiens OX=9606 GN=hCG_2039566 PE=3 SV=1

Match to Query 8405: 1355.692648 from(678.853600,2+)
Title: File:20201204_C12_HepG2_ingel_1_1.mzXML Scans:16011 RT:73.7993min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_1_1.mgf

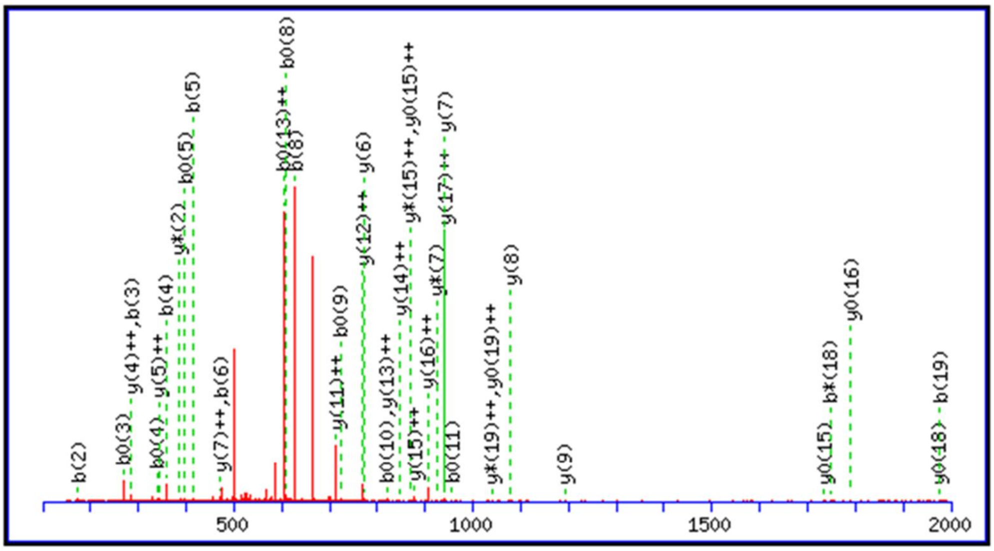
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 100 to 1400 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 1355.6932
Variable modifications:
K11 : Acetoacetyl (K)
Ions Score: 27 **Expect:** 1
Matches : 23/104 fragment ions using 48 most intense peaks (help)

#	b	b^{++}	b^*	b^{*++}	b^0	b^{0++}	Seq	y	y^{++}	y^*	y^{*++}	y^0	y^{0++}	#
1	115.0502	58.0287	98.0237	49.5155			N							11
2	**230.0771**	115.5422	213.0506	107.0289	212.0666	106.5369	D	**1242.6576**	621.8324	1225.6311	613.3192	1224.6470	612.8272	10
3	**359.1197**	180.0635	342.0932	171.5502	341.1092	171.0582	E	1127.6307	564.3190	1110.6041	555.8057	1109.6201	555.3137	9
4	**488.1623**	244.5848	471.1358	236.0715	470.1518	235.5795	E	**998.5881**	499.7977	981.5615	491.2844	980.5775	490.7924	8
5	**601.2464**	301.1268	584.2198	292.6136	583.2358	292.1216	L	**869.5455**	435.2764	852.5189	426.7631			7
6	**715.2893**	358.1483	698.2628	349.6350	697.2788	349.1430	N	**756.4614**	378.7343	739.4349	370.2211			6
7	843.3843	422.1958	826.3577	413.6825	825.3737	413.1905	K	642.4185	321.7129	625.3919	313.1996			5
8	956.4684	478.7378	939.4418	470.2245	938.4578	469.7325	L	514.3235	257.6654	497.2970	249.1521			4
9	1069.5524	535.2798	1052.5259	526.7666	1051.5418	526.2746	L	401.2395	201.1234	384.2129	192.6101			3
10	**1126.5739**	563.7906	1109.5473	555.2773	1108.5633	554.7853	G	**288.1554**	144.5813	271.1288	136.0681			2
11							K	231.1339	116.0706	214.1074	107.5573			1

H2AK118	**ATIAGGGVIPHIHKacSLIGKacacKac**	**Rat liver**

MS/MS Fragmentation of **ATIAGGGVIPHIHKSLIGKK**
Found in **A0A0A0MXW3**, Histone H2A OS=Rattus norvegicus OX=10116 GN=H2afz PE=3 SV=1
Match to Query 8799: 2164.270096 from(542.074800,4+)
Title: File:20200819_Histone_IP.mzXML Scans:13266 RT:53.8495min Charge:4+ Fragmentation:cid
Data file 20200819_Histone_IP_liver.mgf

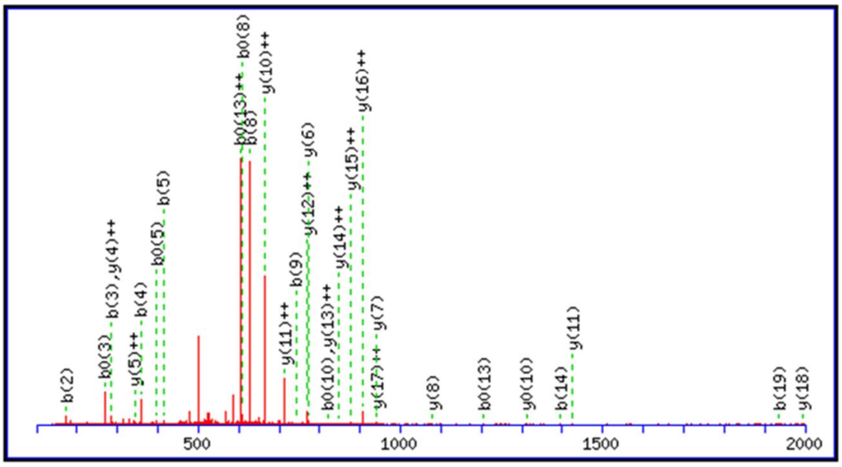


Monoisotopic mass of neutral peptide Mr(calc): 2164.2368
Variable modifications: K14 : Acetyl (K) **K19 :** Acetoacetyl (K) **K20 :** Acetyl (K)
Ions Score: 21 **Expect:** 0.16
Matches : 39/190 fragment ions using 126 most intense peaks

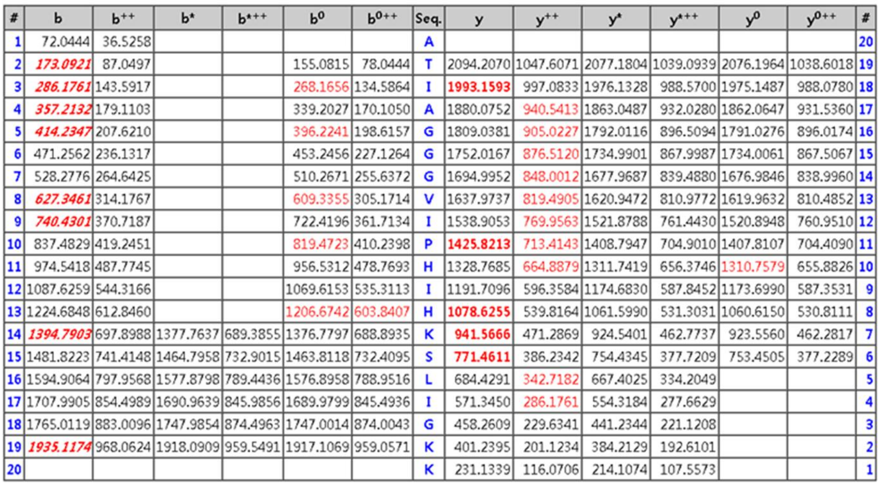
#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	72.0444	36.5258					A							20
2	**173.0921**	87.0497			155.0815	78.0444	T	2094.2070	1047.6071	2077.1804	1039.0939	2076.1964	1038.6018	19
3	**286.1761**	143.5917			268.1656	134.5864	I	1993.1593	997.0833	1976.1328	988.5700	1975.1487	988.0780	18
4	**357.2132**	179.1103			339.2027	170.1050	A	1880.0752	940.5413	1863.0487	932.0280	1862.0647	931.5360	17
5	**414.2347**	207.6210			396.2241	198.6157	G	1809.0381	905.0227	1792.0116	896.5094	1791.0276	896.0174	16
6	**471.2562**	236.1317			453.2456	227.1264	G	1752.0167	876.5120	1734.9901	867.9987	1734.0061	867.5067	15
7	528.2776	264.6425			510.2671	255.6372	G	1694.9952	848.0012	1677.9687	839.4880	1676.9846	838.9960	14
8	**627.3461**	314.1767			609.3355	305.1714	V	1637.9737	819.4905	1620.9472	810.9772	1619.9632	810.4852	13
9	740.4301	370.7187			722.4196	361.7134	I	1538.9053	769.9563	1521.8788	761.4430	1520.8948	760.9510	12
10	837.4829	419.2451			819.4723	410.2398	P	1425.8213	713.4143	1408.7947	704.9010	1407.8107	704.4090	11
11	974.5418	487.7745			956.5312	478.7693	H	1328.7685	664.8879	1311.7419	656.3746	1310.7579	655.8826	10
12	1087.6259	544.3166			1069.6153	535.3113	I	**1191.7096**	596.3584	1174.6830	587.8452	1173.6990	587.3531	9
13	1224.6848	612.8460			1206.6742	603.8407	H	**1078.6255**	539.8164	1061.5990	531.3031	1060.6150	530.8111	8
14	1394.7903	697.8988	1377.7637	689.3855	1376.7797	688.8935	K	**941.5666**	471.2869	924.5401	462.7737	923.5560	462.2817	7
15	1481.8223	741.4148	1464.7958	732.9015	1463.8118	732.4095	S	**771.4611**	386.2342	754.4345	377.7209	753.4505	377.2289	6
16	1594.9064	797.9568	1577.8798	789.4436	1576.8958	788.9516	L	684.4291	342.7182	667.4025	334.2049			5
17	1707.9905	854.4989	1690.9639	845.9856	1689.9799	845.4936	I	571.3450	286.1761	554.3184	277.6629			4
18	1765.0119	883.0096	1747.9854	874.4963	1747.0014	874.0043	G	458.2609	229.6341	441.2344	221.1208			3
19	**1977.1280**	989.0676	1960.1015	980.5544	1959.1174	980.0624	K	401.2395	201.1234	384.2129	192.6101			2
20							K	189.1234	95.0653	172.0968	86.5520			1

H2AK119	**ATIAGGGVIPHIHKacSLIGKacKacac**	**Rat liver**

MS/MS Fragmentation of **ATIAGGGVIPHIHKSLIGKK**
Found in **A0A0A0MXW3**, Histone H2A OS=Rattus norvegicus OX=10116 GN=H2afz PE=3 SV=1
Match to Query 7273: 2164.273696 from(542.075700,4+)
Title: File:20200819_Histone_IP_Kidney.mzXML Scans:11454 RT:51.3880min Charge:4+ Fragmentation:cid
Data file 20200819_Histone_IP_Kidney.mgf

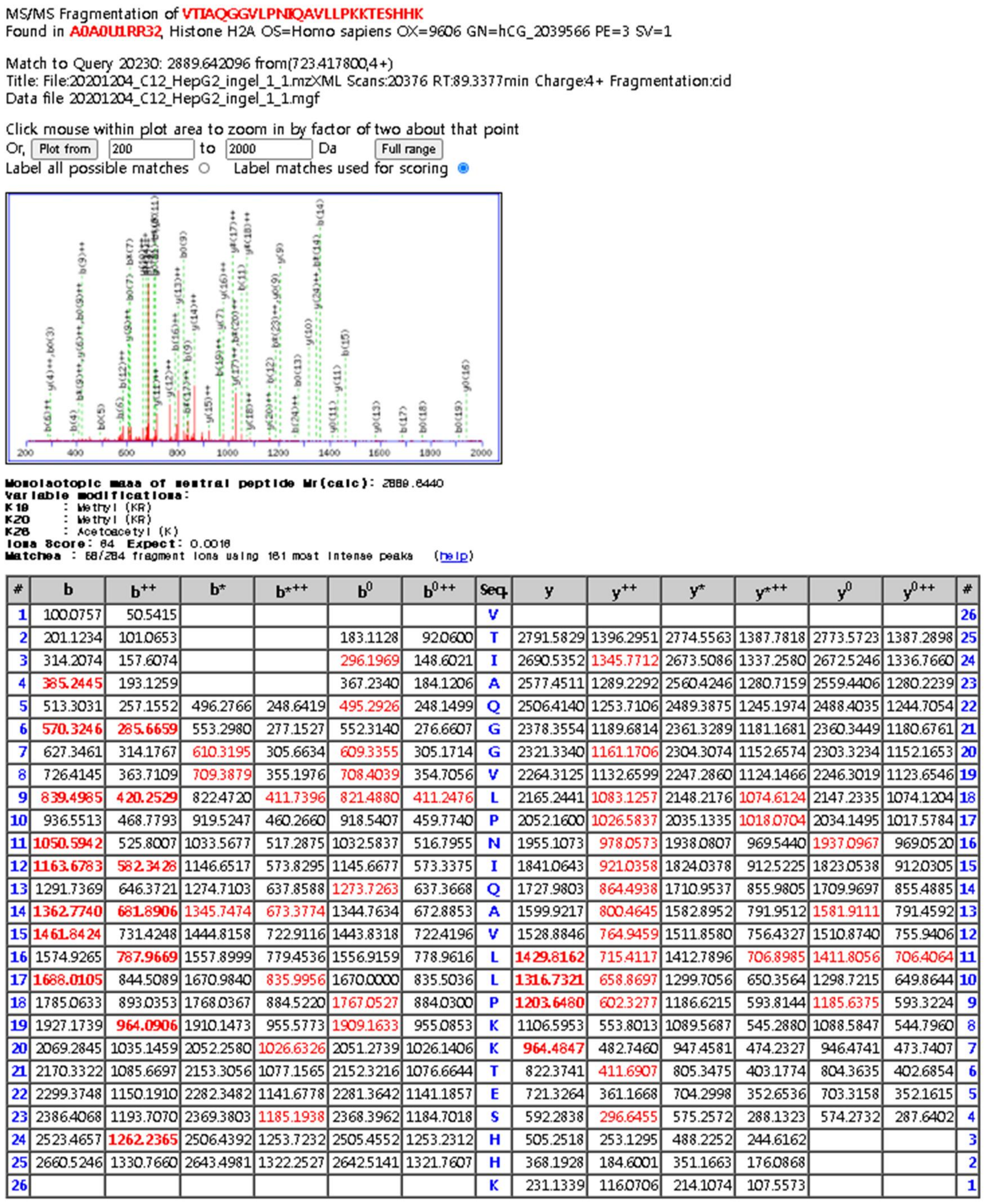


Monoisotopic mass of neutral peptide Mr(calc): 2164.2368
Variable modifications: K14 : Acetyl (K) **K19 :** Acetyl (K) **K20 : Acetoacetyl (K)**
Ions Score: 31 **Expect:** 0.038
Matches : 30/190 fragment ions using 86 most intense peaks



#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	72.0444	36.5258					A							20
2	***173.0921***	87.0497			155.0815	78.0444	T	2094.2070	1047.6071	2077.1804	1039.0939	2076.1964	1038.6018	19
3	***286.1761***	143.5917			268.1656	134.5864	I	**1993.1593**	997.0833	1976.1328	988.5700	1975.1487	988.0780	18
4	***357.2132***	179.1103			339.2027	170.1050	A	1880.0752	940.5413	1863.0487	932.0280	1862.0647	931.5360	17
5	***414.2347***	207.6210			396.2241	198.6157	G	1809.0381	905.0227	1792.0116	896.5094	1791.0276	896.0174	16
6	471.2562	236.1317			453.2456	227.1264	G	1752.0167	876.5120	1734.9901	867.9987	1734.0061	867.5067	15
7	528.2776	264.6425			510.2671	255.6372	G	1694.9952	848.0012	1677.9687	839.4880	1676.9846	838.9960	14
8	***627.3461***	314.1767			609.3355	305.1714	V	1637.9737	819.4905	1620.9472	810.9772	1619.9632	810.4852	13
9	***740.4301***	370.7187			722.4196	361.7134	I	1538.9053	769.9563	1521.8788	761.4430	1520.8948	760.9510	12
10	837.4829	419.2451			819.4723	410.2398	P	**1425.8213**	713.4143	1408.7947	704.9010	1407.8107	704.4090	11
11	974.5418	487.7745			956.5312	478.7693	H	1328.7685	664.8879	1311.7419	656.3746	1310.7579	655.8826	10
12	1087.6259	544.3166			1069.6153	535.3113	I	1191.7096	596.3584	1174.6830	587.8452	1173.6990	587.3531	9
13	1224.6848	612.8460			1206.6742	603.8407	H	**1078.6255**	539.8164	1061.5990	531.3031	1060.6150	530.8111	8
14	***1394.7903***	697.8988	1377.7637	689.3855	1376.7797	688.8935	K	**941.5666**	471.2869	924.5401	462.7737	923.5560	462.2817	7
15	1481.8223	741.4148	1464.7958	732.9015	1463.8118	732.4095	S	**771.4611**	386.2342	754.4345	377.7209	753.4505	377.2289	6
16	1594.9064	797.9568	1577.8798	789.4436	1576.8958	788.9516	L	684.4291	342.7182	667.4025	334.2049			5
17	1707.9905	854.4989	1690.9639	845.9856	1689.9799	845.4936	I	571.3450	286.1761	554.3184	277.6629			4
18	1765.0119	883.0096	1747.9854	874.4963	1747.0014	874.0043	G	458.2609	229.6341	441.2344	221.1208			3
19	***1935.1174***	968.0624	1918.0909	959.5491	1917.1069	959.0571	K	401.2395	201.1234	384.2129	192.6101			2
20							K	231.1339	116.0706	214.1074	107.5573			1

H2AK125	**VTIAQGGVLPNIQAVLLPKmeKmeTESHHKacac**	**Human HepG2 cells**



MS/MS Fragmentation of VTIAQGGVLPNIQAVLLPKKTESHHK
Found in A0A0U1RR32, Histone H2A OS=Homo sapiens OX=9606 GN=hCG_2039566 PE=3 SV=1

Match to Query 20230: 2889.642096 from(723.417800,4+)
Title: File:20201204_C12_HepG2_ingel_1_1.mzXML Scans:20376 RT:89.3377min Charge:4+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_1_1.mgf

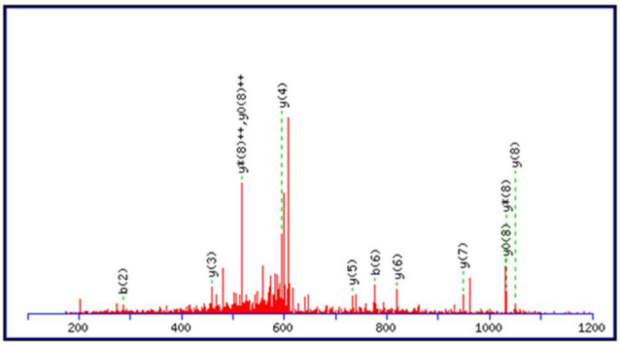
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 200 to 2000 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 2888.6440
Variable modifications:
K19 : Methyl (KR)
K20 : Methyl (KR)
K26 : Acetoacetyl (K)
Ions Score: 64 Expect: 0.0018
Matches : 68/284 fragment ions using 181 most intense peaks (help)

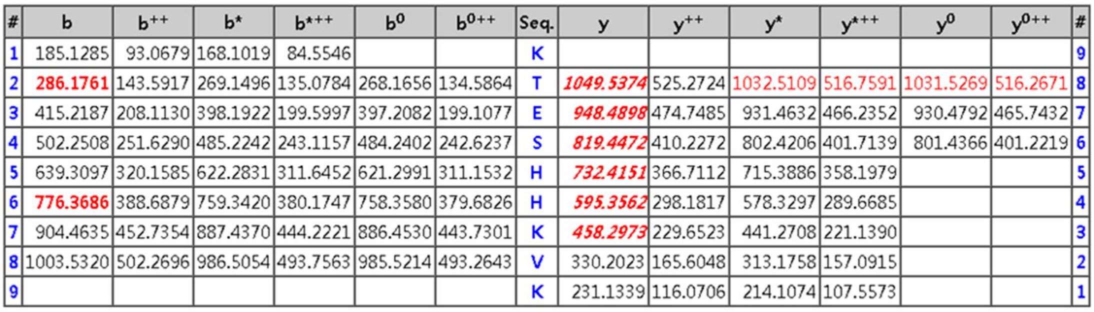
#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	100.0757	50.5415					V							26
2	201.1234	101.0653			183.1128	92.0600	T	2791.5829	1396.2951	2774.5563	1387.7818	2773.5723	1387.2898	25
3	314.2074	157.6074			296.1969	148.6021	I	2690.5352	1345.7712	2673.5086	1337.2580	2672.5246	1336.7660	24
4	**385.2445**	193.1259			367.2340	184.1206	A	2577.4511	1289.2292	2560.4246	1280.7159	2559.4406	1280.2239	23
5	513.3031	257.1552	496.2766	248.6419	495.2926	248.1499	Q	2506.4140	1253.7106	2489.3875	1245.1974	2488.4035	1244.7054	22
6	**570.3246**	**285.6659**	553.2980	277.1527	552.3140	276.6607	G	2378.3554	1189.6814	2361.3289	1181.1681	2360.3449	1180.6761	21
7	627.3461	314.1767	610.3195	305.6634	609.3355	305.1714	G	2321.3340	1161.1706	2304.3074	1152.6574	2303.3234	1152.1653	20
8	726.4145	363.7109	709.3879	355.1976	708.4039	354.7056	V	2264.3125	1132.6599	2247.2860	1124.1466	2246.3019	1123.6546	19
9	**839.4985**	**420.2529**	822.4720	411.7396	821.4880	411.2476	L	2165.2441	1083.1257	2148.2176	1074.6124	2147.2335	1074.1204	18
10	936.5513	468.7793	919.5247	460.2660	918.5407	459.7740	P	2052.1600	1026.5837	2035.1335	1018.0704	2034.1495	1017.5784	17
11	**1050.5942**	525.8007	1033.5677	517.2875	1032.5837	516.7955	N	1955.1073	978.0573	1938.0807	969.5440	1937.0967	969.0520	16
12	**1163.6783**	**582.3428**	1146.6517	573.8295	1145.6677	573.3375	I	1841.0643	921.0358	1824.0378	912.5225	1823.0538	912.0305	15
13	1291.7369	646.3721	1274.7103	637.8588	1273.7263	637.3668	Q	1727.9803	864.4938	1710.9537	855.9805	1709.9697	855.4885	14
14	**1362.7740**	**681.8906**	1345.7474	673.3774	1344.7634	672.8853	A	1599.9217	800.4645	1582.8952	791.9512	1581.9111	791.4592	13
15	**1461.8424**	731.4248	1444.8158	722.9116	1443.8318	722.4196	V	1528.8846	764.9459	1511.8580	756.4327	1510.8740	755.9406	12
16	1574.9265	**787.9669**	1557.8999	779.4536	1556.9159	778.9616	L	**1429.8162**	715.4117	1412.7896	706.8985	1411.8056	706.4064	11
17	**1688.0105**	844.5089	1670.9840	835.9956	1670.0000	835.5036	L	**1316.7321**	658.8697	1299.7056	650.3564	1298.7215	649.8644	10
18	1785.0633	893.0353	1768.0367	884.5220	1767.0527	884.0300	P	**1203.6480**	602.3277	1186.6215	593.8144	1185.6375	593.3224	9
19	1927.1739	**964.0906**	1910.1473	955.5773	1909.1633	955.0853	K	1106.5953	553.8013	1089.5687	545.2880	1088.5847	544.7960	8
20	2069.2845	1035.1459	2052.2580	1026.6326	2051.2739	1026.1406	K	**964.4847**	482.7460	947.4581	474.2327	946.4741	473.7407	7
21	2170.3322	1085.6697	2153.3056	1077.1565	2152.3216	1076.6644	T	822.3741	411.6907	805.3475	403.1774	804.3635	402.6854	6
22	2299.3748	1150.1910	2282.3482	1141.6778	2281.3642	1141.1857	E	721.3264	361.1668	704.2998	352.6536	703.3158	352.1615	5
23	2386.4068	1193.7070	2369.3803	1185.1938	2368.3962	1184.7018	S	592.2838	296.6455	575.2572	288.1323	574.2732	287.6402	4
24	2523.4657	**1262.2365**	2506.4392	1253.7232	2505.4552	1253.2312	H	505.2518	253.1295	488.2252	244.6162			3
25	2660.5246	1330.7660	2643.4981	1322.2527	2642.5141	1321.7607	H	368.1928	184.6001	351.1663	176.0868			2
26							K	231.1339	116.0706	214.1074	107.5573			1

H2AK127	**KprTESHHKVKacac**	**Rat liver**

MS/MS Fragmentation of **KTESHHKVK**
Found in **M0RDM4**, Histone H2A OS=Rattus norvegicus OX=10116 GN=LOC680322 PE=3 SV=1
Match to Query 3046: 1232.654248 from(617.334400,2+)
Title: File:20200819_Histone_IP.mzXML Scans:1001 RT:6.0979min Charge:2+ Fragmentation:cid
Data file 20200819_Histone_IP_liver.mgf

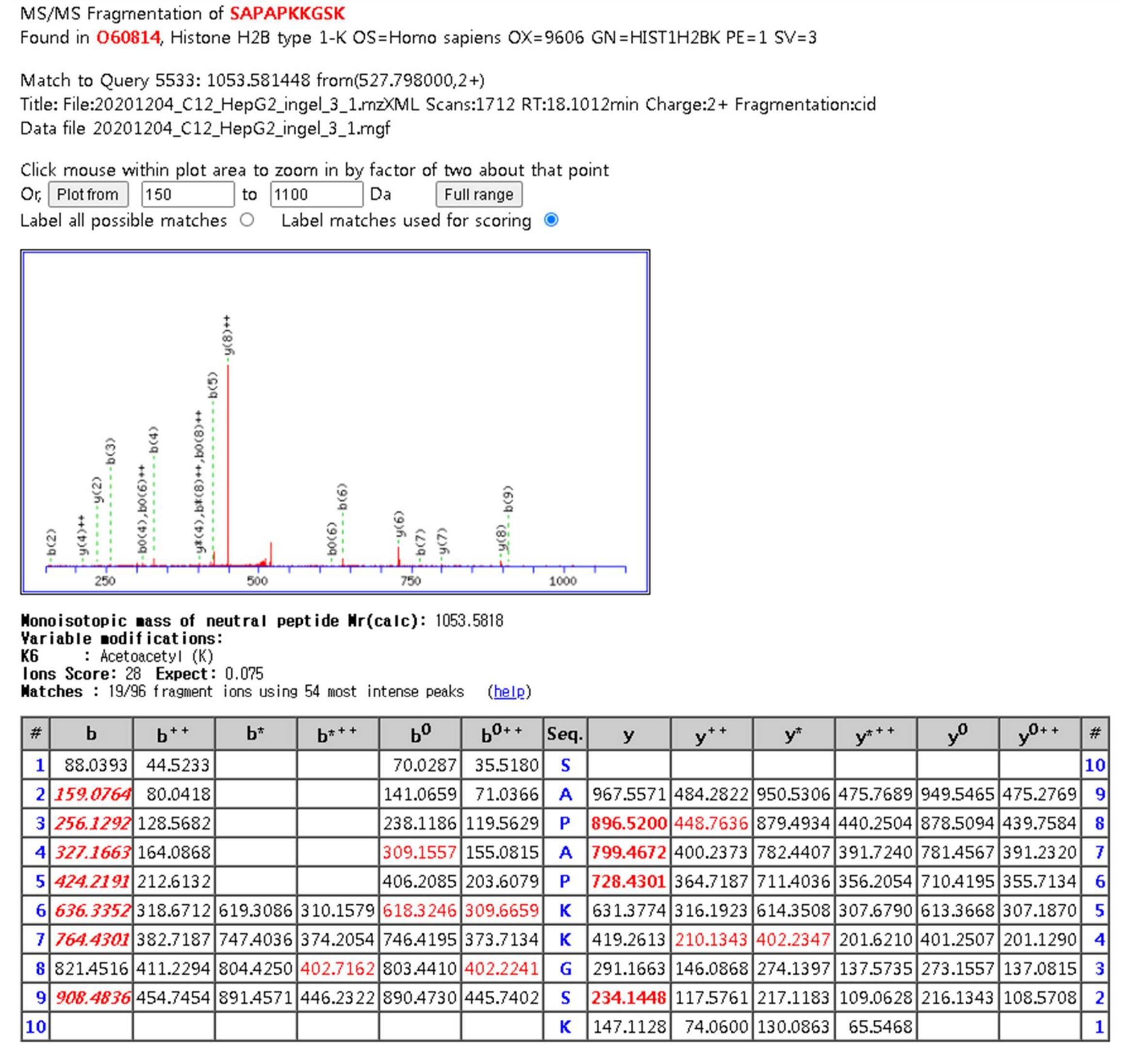


Monoisotopic mass of neutral peptide Mr(calc): 1232.6513 **Variable modifications: K1 :** Propionyl (K) **K9 :** Acetoacetyl (K) **Ions Score:** 24 **Expect:** 1.2 **Matches :** 12/84 fragment ions using 33 most intense peaks



#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	185.1285	93.0679	168.1019	84.5546			K							9
2	**286.1761**	143.5917	269.1496	135.0784	268.1656	134.5864	T	***1049.5374***	525.2724	1032.5109	516.7591	1031.5269	516.2671	8
3	415.2187	208.1130	398.1922	199.5997	397.2082	199.1077	E	***948.4898***	474.7485	931.4632	466.2352	930.4792	465.7432	7
4	502.2508	251.6290	485.2242	243.1157	484.2402	242.6237	S	***819.4472***	410.2272	802.4206	401.7139	801.4366	401.2219	6
5	639.3097	320.1585	622.2831	311.6452	621.2991	311.1532	H	***732.4151***	366.7112	715.3886	358.1979			5
6	**776.3686**	388.6879	759.3420	380.1747	758.3580	379.6826	H	***595.3562***	298.1817	578.3297	289.6685			4
7	904.4635	452.7354	887.4370	444.2221	886.4530	443.7301	K	***458.2973***	229.6523	441.2708	221.1390			3
8	1003.5320	502.2696	986.5054	493.7563	985.5214	493.2643	V	330.2023	165.6048	313.1758	157.0915			2
9							K	231.1339	116.0706	214.1074	107.5573			1

H2BK11	SAPAPKacacKGSK	Human HepG2 cells



MS/MS Fragmentation of **SAPAPKKGSK**
Found in **O60814**, Histone H2B type 1-K OS=Homo sapiens OX=9606 GN=HIST1H2BK PE=1 SV=3

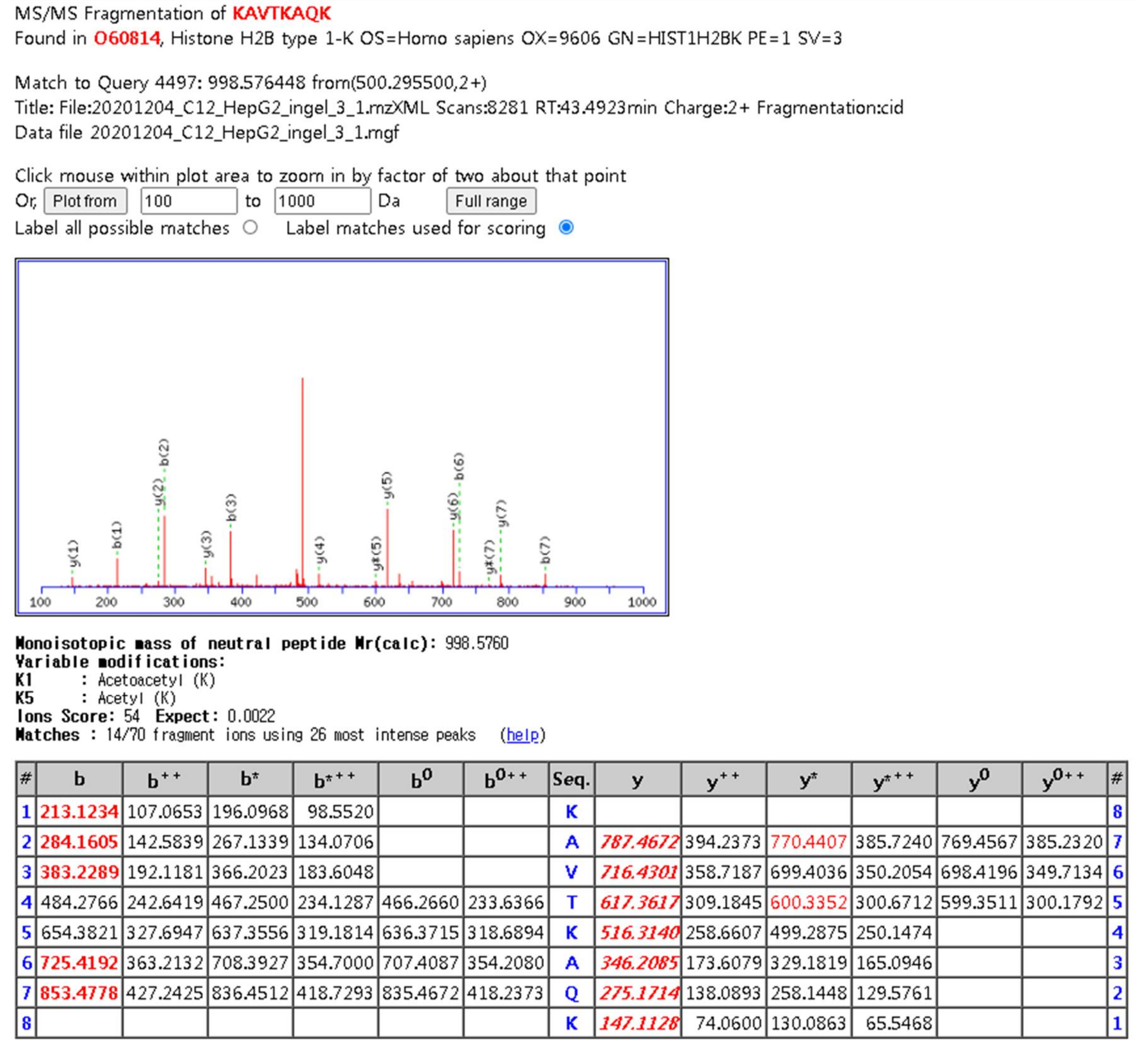
Match to Query 5533: 1053.581448 from(527.798000,2+)
Title: File:20201204_C12_HepG2_ingel_3_1.mzXML Scans:1712 RT:18.1012min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_3_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 150 to 1100 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 1053.5818
Variable modifications:
K6 : Acetoacetyl (K)
Ions Score: 28 **Expect:** 0.075
Matches : 19/96 fragment ions using 54 most intense peaks (help)

#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	88.0393	44.5233			70.0287	35.5180	S							10
2	***159.0764***	80.0418			141.0659	71.0366	A	967.5571	484.2822	950.5306	475.7689	949.5465	475.2769	9
3	***256.1292***	128.5682			238.1186	119.5629	P	**896.5200**	448.7636	879.4934	440.2504	878.5094	439.7584	8
4	***327.1663***	164.0868			309.1557	155.0815	A	**799.4672**	400.2373	782.4407	391.7240	781.4567	391.2320	7
5	***424.2191***	212.6132			406.2085	203.6079	P	**728.4301**	364.7187	711.4036	356.2054	710.4195	355.7134	6
6	***636.3352***	318.6712	619.3086	310.1579	618.3246	309.6659	K	631.3774	316.1923	614.3508	307.6790	613.3668	307.1870	5
7	***764.4301***	382.7187	747.4036	374.2054	746.4195	373.7134	K	419.2613	210.1343	402.2347	201.6210	401.2507	201.1290	4
8	821.4516	411.2294	804.4250	402.7162	803.4410	402.2241	G	291.1663	146.0868	274.1397	137.5735	273.1557	137.0815	3
9	***908.4836***	454.7454	891.4571	446.2322	890.4730	445.7402	S	**234.1448**	117.5761	217.1183	109.0628	216.1343	108.5708	2
10							K	147.1128	74.0600	130.0863	65.5468			1

H2BK16	KacacAVTKacAQK	**Human HepG2 cells**



MS/MS Fragmentation of KAVTKAQK
Found in O60814, Histone H2B type 1-K OS=Homo sapiens OX=9606 GN=HIST1H2BK PE=1 SV=3

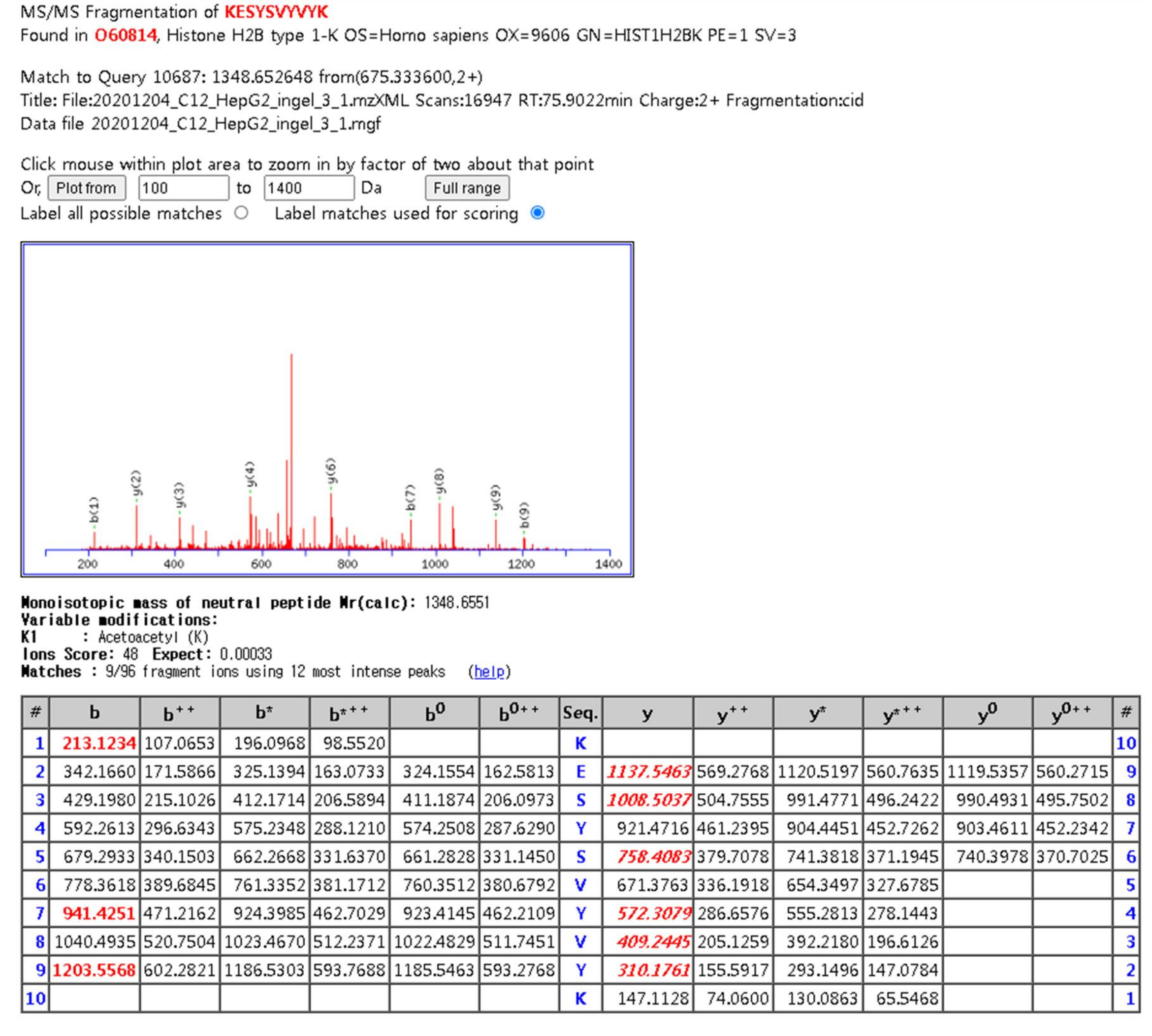
Match to Query 4497: 998.576448 from(500.295500,2+)
Title: File:20201204_C12_HepG2_ingel_3_1.mzXML Scans:8281 RT:43.4923min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_3_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 100 to 1000 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 998.5760
Variable modifications:
K1 : Acetoacetyl (K)
K5 : Acetyl (K)
Ions Score: 54 **Expect:** 0.0022
Matches : 14/70 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	213.1234	107.0653	196.0968	98.5520			K							8
2	284.1605	142.5839	267.1339	134.0706			A	*787.4672*	394.2373	770.4407	385.7240	769.4567	385.2320	7
3	383.2289	192.1181	366.2023	183.6048			V	*716.4301*	358.7187	699.4036	350.2054	698.4196	349.7134	6
4	484.2766	242.6419	467.2500	234.1287	466.2660	233.6366	T	*617.3617*	309.1845	600.3352	300.6712	599.3511	300.1792	5
5	654.3821	327.6947	637.3556	319.1814	636.3715	318.6894	K	*516.3140*	258.6607	499.2875	250.1474			4
6	725.4192	363.2132	708.3927	354.7000	707.4087	354.2080	A	*346.2085*	173.6079	329.1819	165.0946			3
7	853.4778	427.2425	836.4512	418.7293	835.4672	418.2373	Q	*275.1714*	138.0893	258.1448	129.5761			2
8							K	*147.1128*	74.0600	130.0863	65.5468			1

H2BK34	**KacacESYSVYVYK**	**Human HepG2 cells**



MS/MS Fragmentation of **KESYSVYVYK**
Found in **O60814**, Histone H2B type 1-K OS=Homo sapiens OX=9606 GN=HIST1H2BK PE=1 SV=3

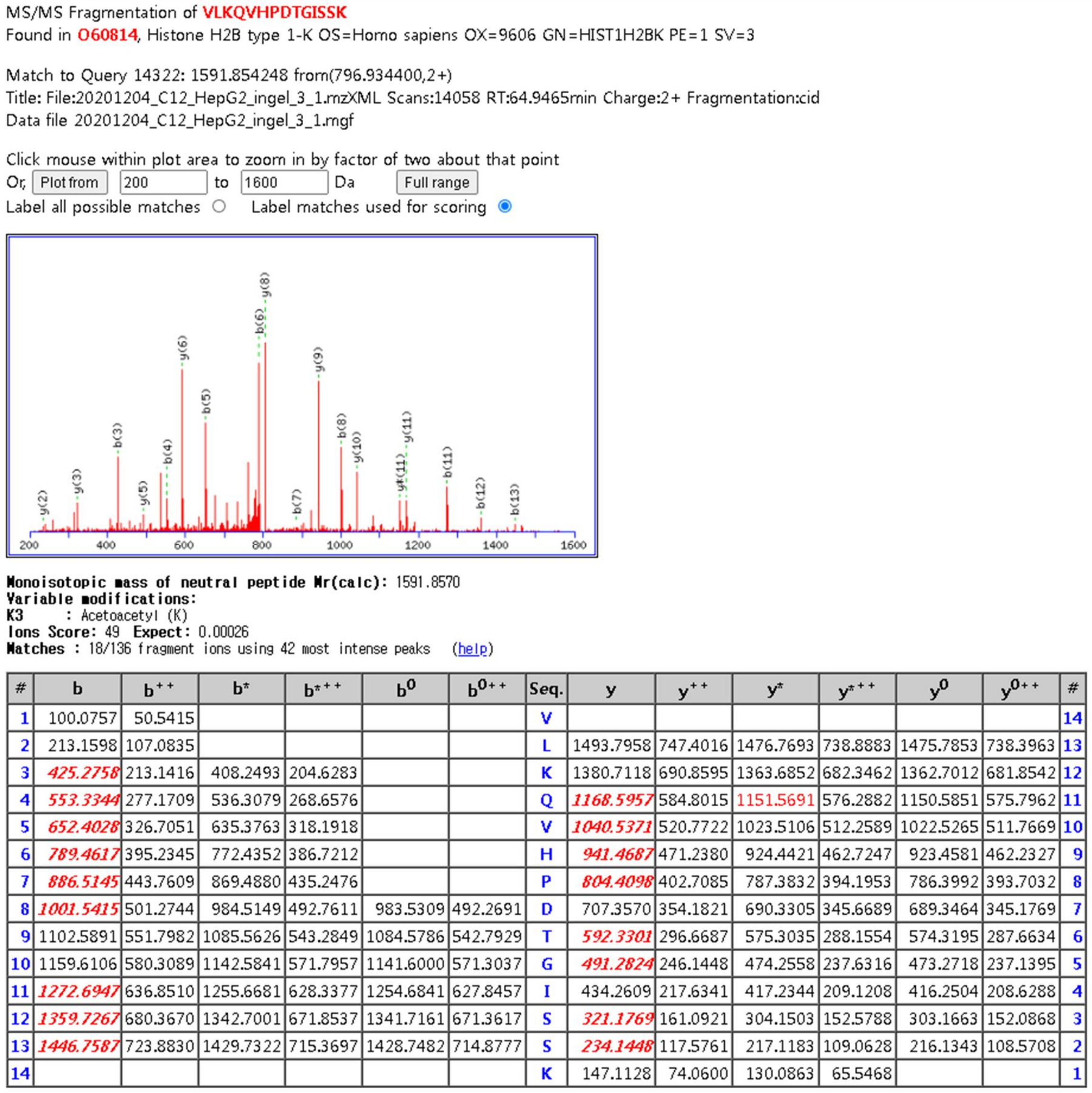
Match to Query 10687: 1348.652648 from(675.333600,2+)
Title: File:20201204_C12_HepG2_ingel_3_1.mzXML Scans:16947 RT:75.9022min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_3_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 100 to 1400 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 1348.6551
Variable modifications:
K1 : Acetoacetyl (K)
Ions Score: 48 **Expect:** 0.00033
Matches : 9/96 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	**213.1234**	107.0653	196.0968	98.5520			K							10
2	342.1660	171.5866	325.1394	163.0733	324.1554	162.5813	E	***1137.5463***	569.2768	1120.5197	560.7635	1119.5357	560.2715	9
3	429.1980	215.1026	412.1714	206.5894	411.1874	206.0973	S	***1008.5037***	504.7555	991.4771	496.2422	990.4931	495.7502	8
4	592.2613	296.6343	575.2348	288.1210	574.2508	287.6290	Y	921.4716	461.2395	904.4451	452.7262	903.4611	452.2342	7
5	679.2933	340.1503	662.2668	331.6370	661.2828	331.1450	S	***758.4083***	379.7078	741.3818	371.1945	740.3978	370.7025	6
6	778.3618	389.6845	761.3352	381.1712	760.3512	380.6792	V	671.3763	336.1918	654.3497	327.6785			5
7	**941.4251**	471.2162	924.3985	462.7029	923.4145	462.2109	Y	***572.3079***	286.6576	555.2813	278.1443			4
8	1040.4935	520.7504	1023.4670	512.2371	1022.4829	511.7451	V	***409.2445***	205.1259	392.2180	196.6126			3
9	**1203.5568**	602.2821	1186.5303	593.7688	1185.5463	593.2768	Y	***310.1761***	155.5917	293.1496	147.0784			2
10							K	147.1128	74.0600	130.0863	65.5468			1

H2BK46	VLKacacQVHPDTGISSK	Human HepG2 cells



MS/MS Fragmentation of VLKQVHPDTGISSK
Found in O60814, Histone H2B type 1-K OS=Homo sapiens OX=9606 GN=HIST1H2BK PE=1 SV=3

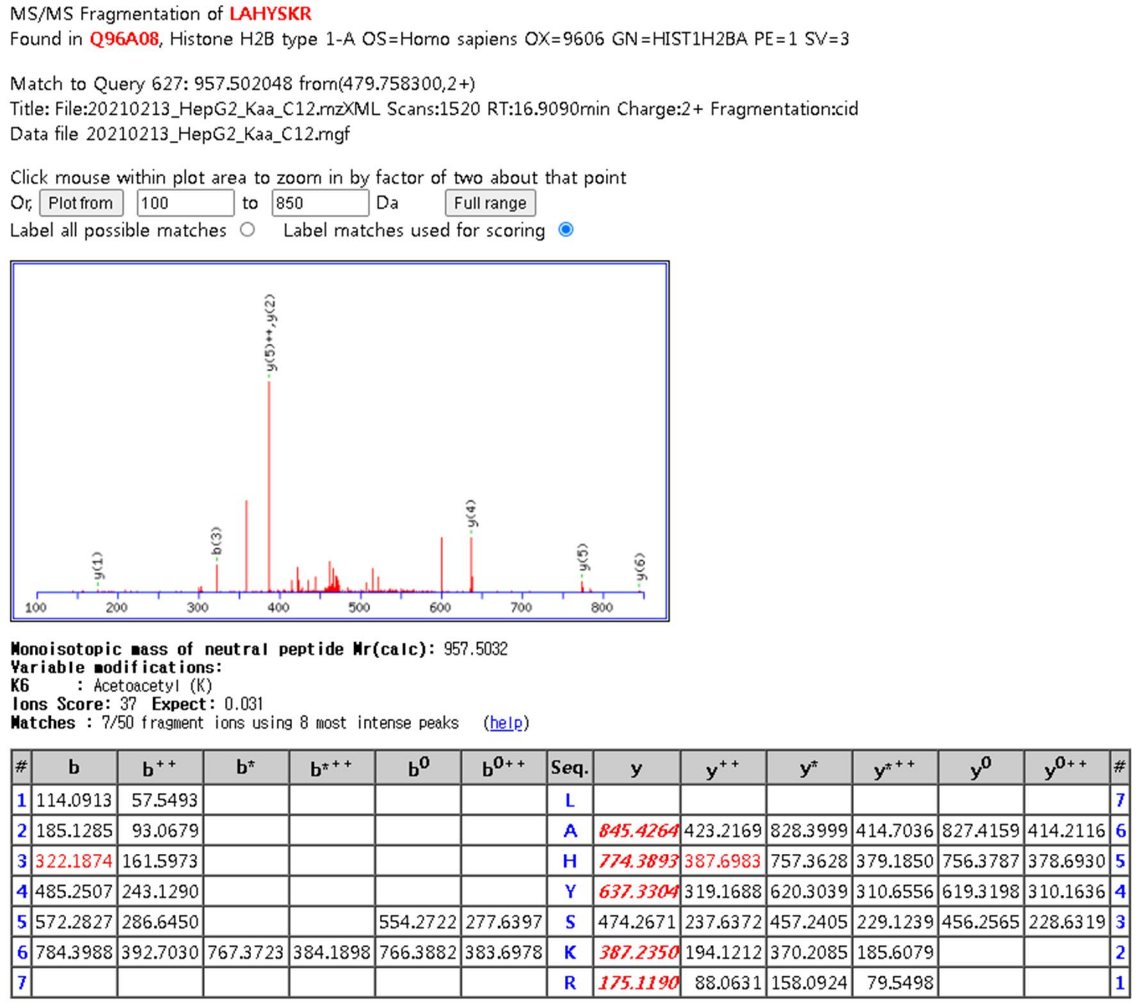
Match to Query 14322: 1591.854248 from(796.934400,2+)
Title: File:20201204_C12_HepG2_ingel_3_1.mzXML Scans:14058 RT:64.9465min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_3_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 200 to 1600 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 1591.8570
Variable modifications:
K3 : Acetoacetyl (K)
Ions Score: 49 **Expect:** 0.00026
Matches : 18/136 fragment ions using 42 most intense peaks (help)

#	b	b++	b*	b*++	b0	b0++	Seq.	y	y++	y*	y*++	y0	y0++	#
1	100.0757	50.5415					V							14
2	213.1598	107.0835					L	1493.7958	747.4016	1476.7693	738.8883	1475.7853	738.3963	13
3	*425.2758*	213.1416	408.2493	204.6283			K	1380.7118	690.8595	1363.6852	682.3462	1362.7012	681.8542	12
4	*553.3344*	277.1709	536.3079	268.6576			Q	*1168.5957*	584.8015	1151.5691	576.2882	1150.5851	575.7962	11
5	*652.4028*	326.7051	635.3763	318.1918			V	*1040.5371*	520.7722	1023.5106	512.2589	1022.5265	511.7669	10
6	*789.4617*	395.2345	772.4352	386.7212			H	*941.4687*	471.2380	924.4421	462.7247	923.4581	462.2327	9
7	*886.5145*	443.7609	869.4880	435.2476			P	*804.4098*	402.7085	787.3832	394.1953	786.3992	393.7032	8
8	*1001.5415*	501.2744	984.5149	492.7611	983.5309	492.2691	D	707.3570	354.1821	690.3305	345.6689	689.3464	345.1769	7
9	1102.5891	551.7982	1085.5626	543.2849	1084.5786	542.7929	T	*592.3301*	296.6687	575.3035	288.1554	574.3195	287.6634	6
10	1159.6106	580.3089	1142.5841	571.7957	1141.6000	571.3037	G	*491.2824*	246.1448	474.2558	237.6316	473.2718	237.1395	5
11	*1272.6947*	636.8510	1255.6681	628.3377	1254.6841	627.8457	I	434.2609	217.6341	417.2344	209.1208	416.2504	208.6288	4
12	*1359.7267*	680.3670	1342.7001	671.8537	1341.7161	671.3617	S	*321.1769*	161.0921	304.1503	152.5788	303.1663	152.0868	3
13	*1446.7587*	723.8830	1429.7322	715.3697	1428.7482	714.8777	S	*234.1448*	117.5761	217.1183	109.0628	216.1343	108.5708	2
14							K	147.1128	74.0600	130.0863	65.5468			1

H2BK86	LAHYSKacacR	Human HepG2 cells



MS/MS Fragmentation of LAHYSKR
Found in Q96A08, Histone H2B type 1-A OS=Homo sapiens OX=9606 GN=HIST1H2BA PE=1 SV=3

Match to Query 627: 957.502048 from(479.758300,2+)
Title: File:20210213_HepG2_Kaa_C12.mzXML Scans:1520 RT:16.9090min Charge:2+ Fragmentation:cid
Data file 20210213_HepG2_Kaa_C12.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, 100 to 850 Da
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 957.5032
Variable modifications:
K6 : Acetoacetyl (K)
Ions Score: 37 **Expect:** 0.031
Matches : 7/50 fragment ions using 8 most intense peaks (help)

#	b	b++	b*	b*++	b0	b0++	Seq.	y	y++	y*	y*++	y0	y0++	#
1	114.0913	57.5493					L							7
2	185.1285	93.0679					A	*845.4264*	423.2169	828.3999	414.7036	827.4159	414.2116	6
3	322.1874	161.5973					H	*774.3893*	387.6983	757.3628	379.1850	756.3787	378.6930	5
4	485.2507	243.1290					Y	*637.3304*	319.1688	620.3039	310.6556	619.3198	310.1636	4
5	572.2827	286.6450			554.2722	277.6397	S	474.2671	237.6372	457.2405	229.1239	456.2565	228.6319	3
6	784.3988	392.7030	767.3723	384.1898	766.3882	383.6978	K	*387.2350*	194.1212	370.2085	185.6079			2
7							R	*175.1190*	88.0631	158.0924	79.5498			1

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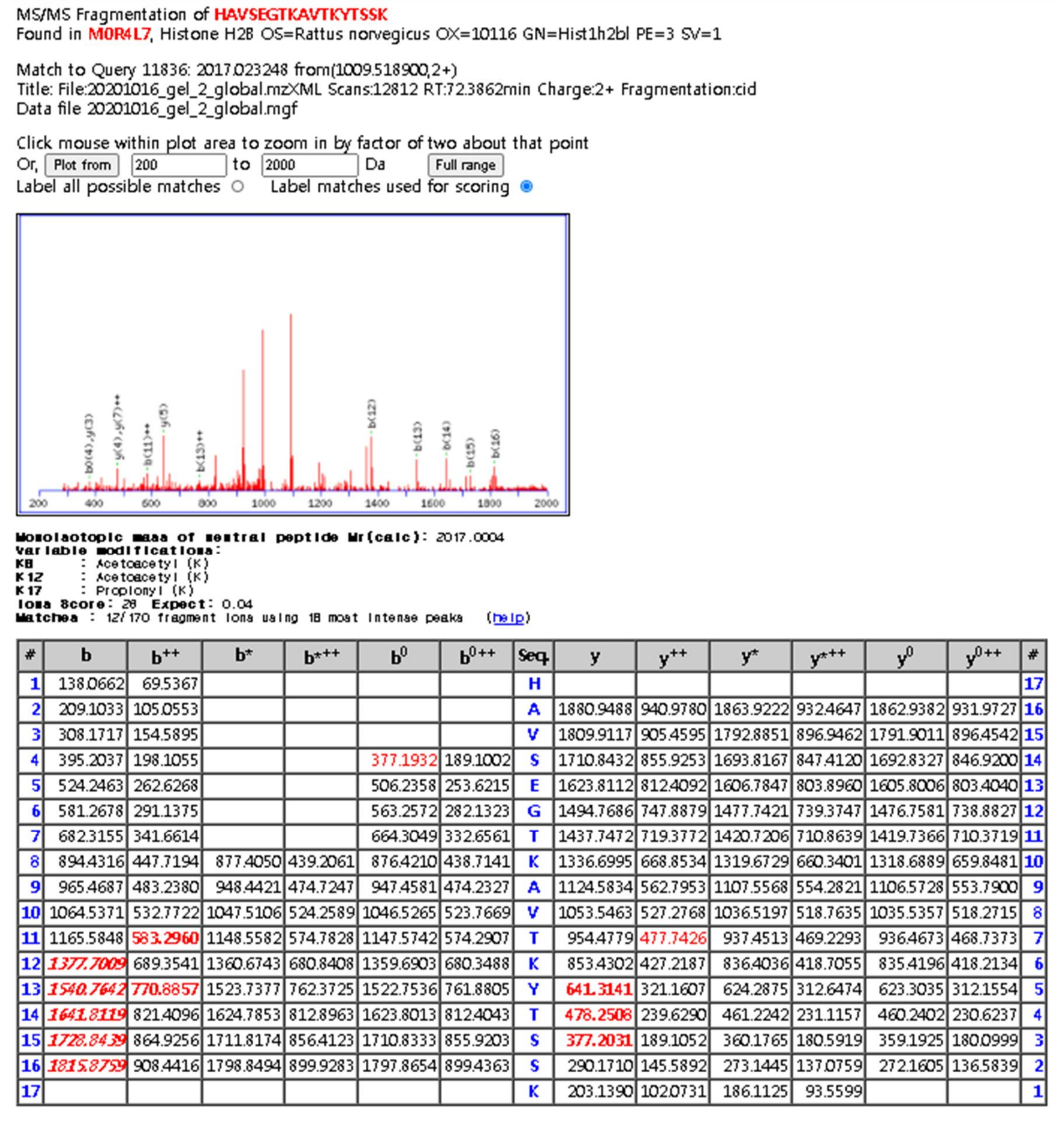
H2BK116	HAVSEGTKacacAVTKacacYTSSKpr	Rat liver



MS/MS Fragmentation of HAVSEGTKAVTKYTSSK
Found in M0R4L7, Histone H2B OS=Rattus norvegicus OX=10116 GN=Hist1h2bl PE=3 SV=1

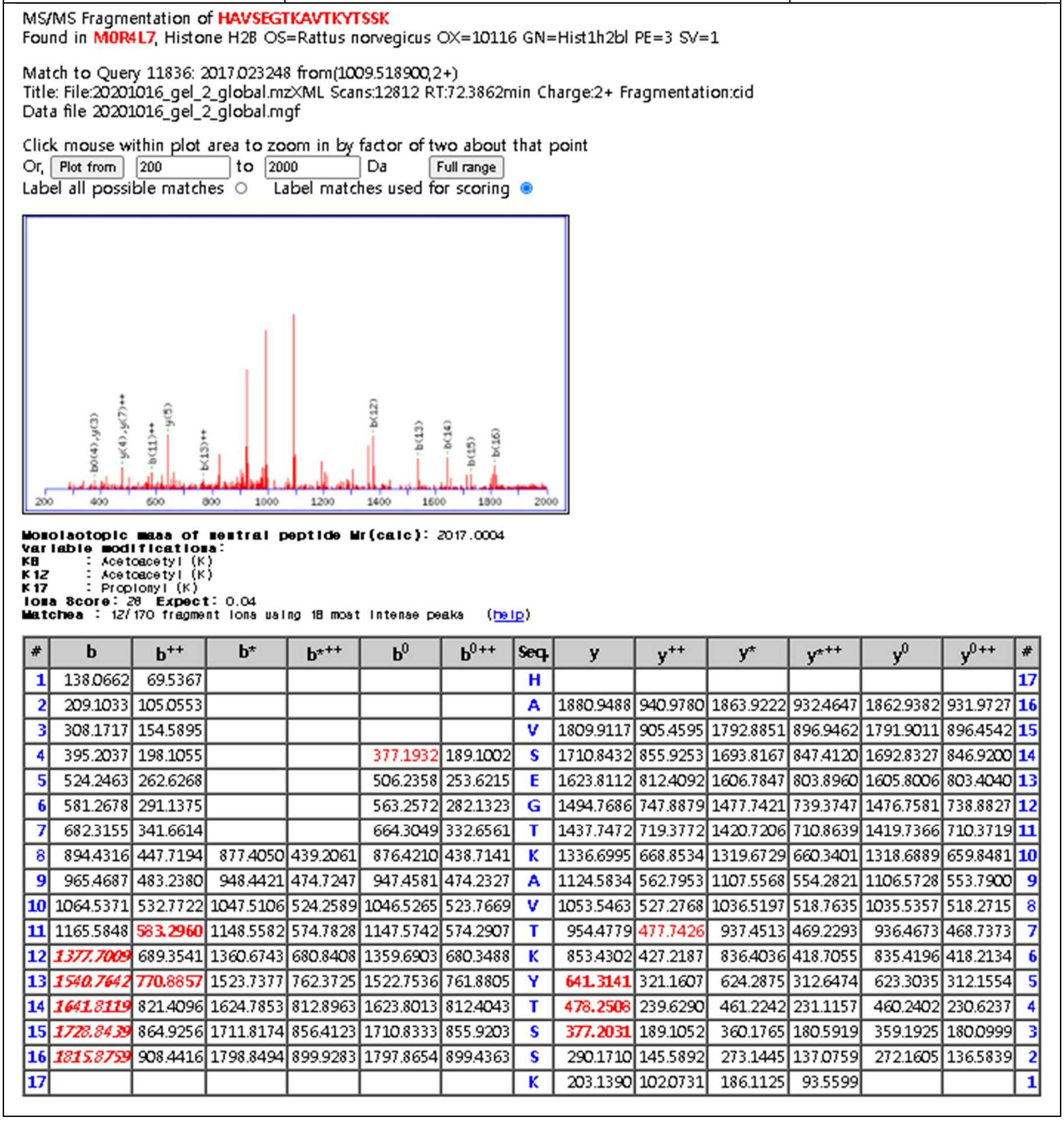
Match to Query 11836: 2017.023248 from(1009.518900,2+)
Title: File:20201016_gel_2_global.mzXML Scans:12812 RT:72.3862min Charge:2+ Fragmentation:cid
Data file 20201016_gel_2_global.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 200 to 2000 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 2017.0004
Variable modifications:
K8 : Acetoacetyl (K)
K12 : Acetoacetyl (K)
K17 : Propionyl (K)
Ions Score: 28 **Expect:** 0.04
Matches : 12/170 fragment ions using 18 most intense peaks (help)

#	b	b++	b*	b*++	b0	b0++	Seq.	y	y++	y*	y*++	y0	y0++	#
1	138.0662	69.5367					H							17
2	209.1033	105.0553					A	1880.9488	940.9780	1863.9222	932.4647	1862.9382	931.9727	16
3	308.1717	154.5895					V	1809.9117	905.4595	1792.8851	896.9462	1791.9011	896.4542	15
4	395.2037	198.1055			377.1932	189.1002	S	1710.8432	855.9253	1693.8167	847.4120	1692.8327	846.9200	14
5	524.2463	262.6268			506.2358	253.6215	E	1623.8112	812.4092	1606.7847	803.8960	1605.8006	803.4040	13
6	581.2678	291.1375			563.2572	282.1323	G	1494.7686	747.8879	1477.7421	739.3747	1476.7581	738.8827	12
7	682.3155	341.6614			664.3049	332.6561	T	1437.7472	719.3772	1420.7206	710.8639	1419.7366	710.3719	11
8	894.4316	447.7194	877.4050	439.2061	876.4210	438.7141	K	1336.6995	668.8534	1319.6729	660.3401	1318.6889	659.8481	10
9	965.4687	483.2380	948.4421	474.7247	947.4581	474.2327	A	1124.5834	562.7953	1107.5568	554.2821	1106.5728	553.7900	9
10	1064.5371	532.7722	1047.5106	524.2589	1046.5265	523.7669	V	1053.5463	527.2768	1036.5197	518.7635	1035.5357	518.2715	8
11	1165.5848	**583.2960**	1148.5582	574.7828	1147.5742	574.2907	T	954.4779	477.7426	937.4513	469.2293	936.4673	468.7373	7
12	***1377.7009***	689.3541	1360.6743	680.8408	1359.6903	680.3488	K	853.4302	427.2187	836.4036	418.7055	835.4196	418.2134	6
13	***1540.7642***	**770.8857**	1523.7377	762.3725	1522.7536	761.8805	Y	**641.3141**	321.1607	624.2875	312.6474	623.3035	312.1554	5
14	***1641.8119***	821.4096	1624.7853	812.8963	1623.8013	812.4043	T	**478.2508**	239.6290	461.2242	231.1157	460.2402	230.6237	4
15	***1728.8439***	864.9256	1711.8174	856.4123	1710.8333	855.9203	S	**377.2031**	189.1052	360.1765	180.5919	359.1925	180.0999	3
16	***1815.8759***	908.4416	1798.8494	899.9283	1797.8654	899.4363	S	290.1710	145.5892	273.1445	137.0759	272.1605	136.5839	2
17							K	203.1390	102.0731	186.1125	93.5599			1

H2BK120	**HAVSEGTKacacAVTKacacYTSSKpr**	**Rat liver**



MS/MS Fragmentation of **HAVSEGTKAVTKYTSSK**
Found in **M0R4L7**, Histone H2B OS=Rattus norvegicus OX=10116 GN=Hist1h2bl PE=3 SV=1

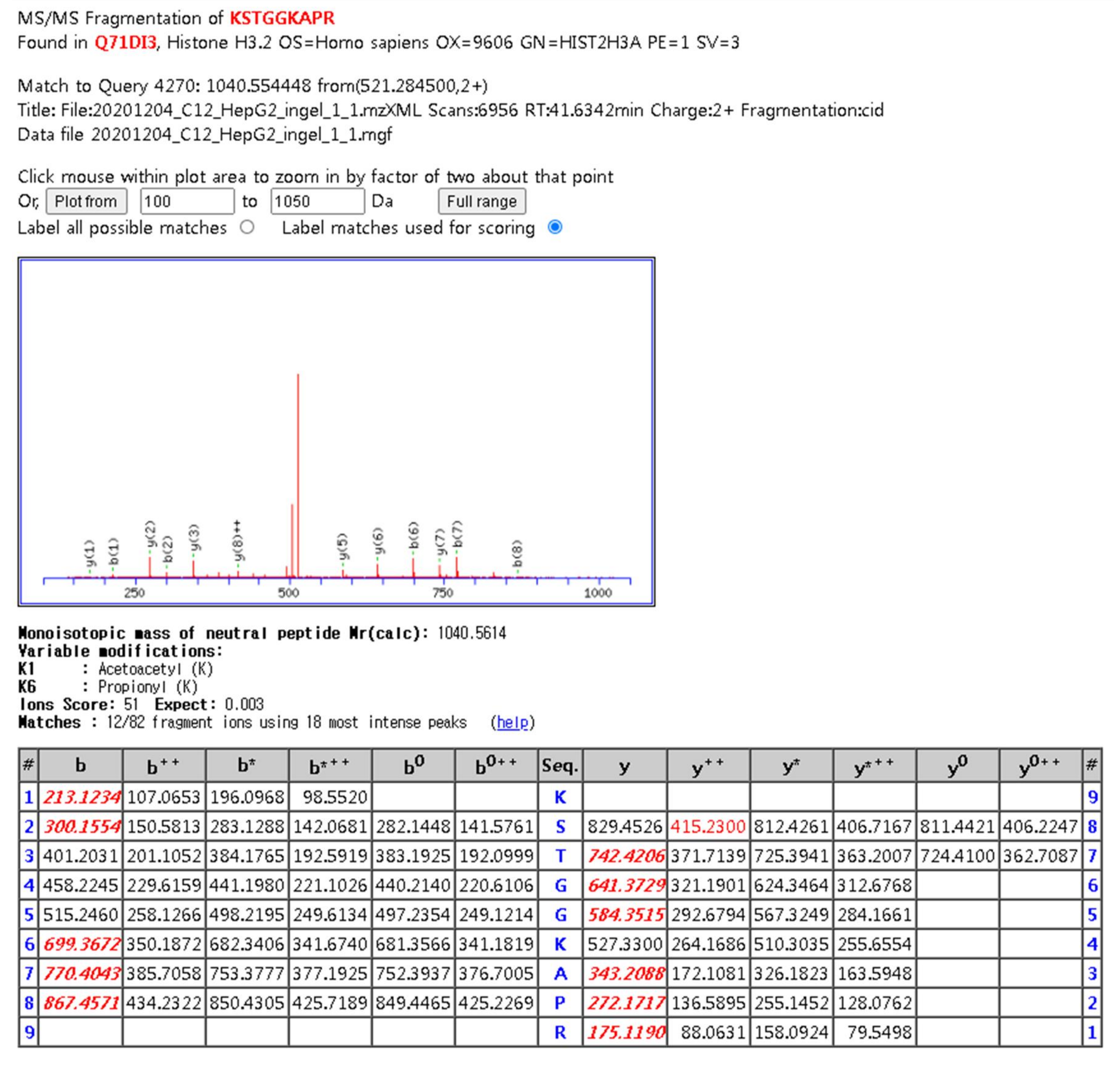
Match to Query 11836: 2017.023248 from(1009.518900,2+)
Title: File:20201016_gel_2_global.mzXML Scans:12812 RT:72.3862min Charge:2+ Fragmentation:cid
Data file 20201016_gel_2_global.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 200 to 2000 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 2017.0004
Variable modifications:
K8 : Acetoacetyl (K)
K12 : Acetoacetyl (K)
K17 : Propionyl (K)
Ions Score: 28 **Expect:** 0.04
Matches : 12/170 fragment ions using 18 most intense peaks (help)

#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	138.0662	69.5367					H							17
2	209.1033	105.0553					A	1880.9488	940.9780	1863.9222	932.4647	1862.9382	931.9727	16
3	308.1717	154.5895					V	1809.9117	905.4595	1792.8851	896.9462	1791.9011	896.4542	15
4	395.2037	198.1055			377.1932	189.1002	S	1710.8432	855.9253	1693.8167	847.4120	1692.8327	846.9200	14
5	524.2463	262.6268			506.2358	253.6215	E	1623.8112	812.4092	1606.7847	803.8960	1605.8006	803.4040	13
6	581.2678	291.1375			563.2572	282.1323	G	1494.7686	747.8879	1477.7421	739.3747	1476.7581	738.8827	12
7	682.3155	341.6614			664.3049	332.6561	T	1437.7472	719.3772	1420.7206	710.8639	1419.7366	710.3719	11
8	894.4316	447.7194	877.4050	439.2061	876.4210	438.7141	K	1336.6995	668.8534	1319.6729	660.3401	1318.6889	659.8481	10
9	965.4687	483.2380	948.4421	474.7247	947.4581	474.2327	A	1124.5834	562.7953	1107.5568	554.2821	1106.5728	553.7900	9
10	1064.5371	532.7722	1047.5106	524.2589	1046.5265	523.7669	V	1053.5463	527.2768	1036.5197	518.7635	1035.5357	518.2715	8
11	1165.5848	**583.2960**	1148.5582	574.7828	1147.5742	574.2907	T	954.4779	477.7426	937.4513	469.2293	936.4673	468.7373	7
12	***1377.7009***	689.3541	1360.6743	680.8408	1359.6903	680.3488	K	853.4302	427.2187	836.4036	418.7055	835.4196	418.2134	6
13	***1540.7642***	***770.8857***	1523.7377	762.3725	1522.7536	761.8805	Y	**641.3141**	321.1607	624.2875	312.6474	623.3035	312.1554	5
14	***1641.8119***	821.4096	1624.7853	812.8963	1623.8013	812.4043	T	**478.2508**	239.6290	461.2242	231.1157	460.2402	230.6237	4
15	***1728.8439***	864.9256	1711.8174	856.4123	1710.8333	855.9203	S	**377.2031**	189.1052	360.1765	180.5919	359.1925	180.0999	3
16	***1815.8759***	908.4416	1798.8494	899.9283	1797.8654	899.4363	S	290.1710	145.5892	273.1445	137.0759	272.1605	136.5839	2
17							K	203.1390	102.0731	186.1125	93.5599			1

H3K9	KacacSTGGKprAPR	Human HepG2 cells



MS/MS Fragmentation of KSTGGKAPR
Found in Q71DI3, Histone H3.2 OS=Homo sapiens OX=9606 GN=HIST2H3A PE=1 SV=3

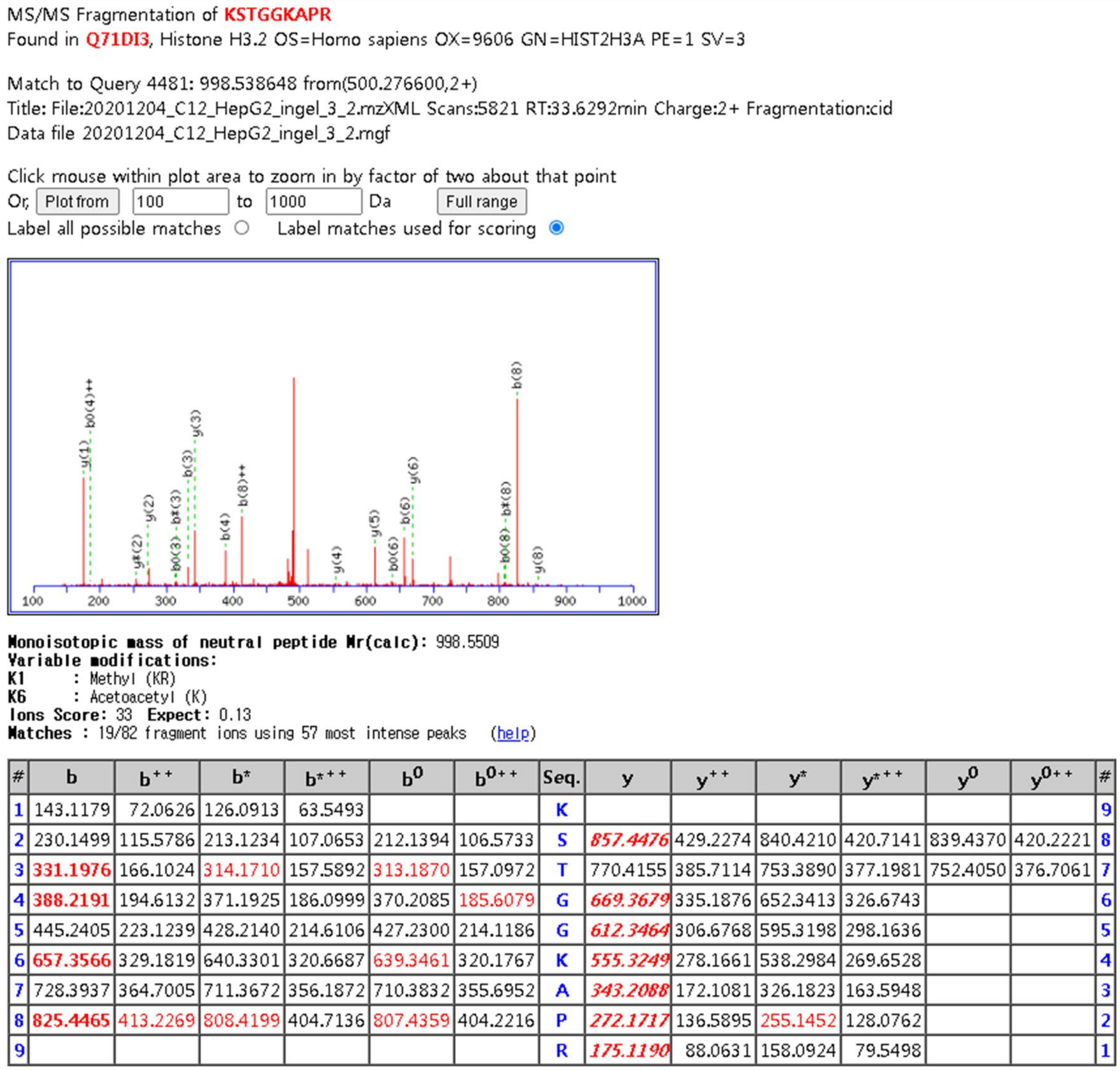
Match to Query 4270: 1040.554448 from(521.284500,2+)
Title: File:20201204_C12_HepG2_ingel_1_1.mzXML Scans:6956 RT:41.6342min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_1_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 100 to 1050 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 1040.5614
Variable modifications:
K1 : Acetoacetyl (K)
K6 : Propionyl (K)
Ions Score: 51 **Expect:** 0.003
Matches : 12/82 fragment ions using 18 most intense peaks (help)

#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	213.1234	107.0653	196.0968	98.5520			K							9
2	300.1554	150.5813	283.1288	142.0681	282.1448	141.5761	S	829.4526	415.2300	812.4261	406.7167	811.4421	406.2247	8
3	401.2031	201.1052	384.1765	192.5919	383.1925	192.0999	T	742.4206	371.7139	725.3941	363.2007	724.4100	362.7087	7
4	458.2245	229.6159	441.1980	221.1026	440.2140	220.6106	G	641.3729	321.1901	624.3464	312.6768			6
5	515.2460	258.1266	498.2195	249.6134	497.2354	249.1214	G	584.3515	292.6794	567.3249	284.1661			5
6	699.3672	350.1872	682.3406	341.6740	681.3566	341.1819	K	527.3300	264.1686	510.3035	255.6554			4
7	770.4043	385.7058	753.3777	377.1925	752.3937	376.7005	A	343.2088	172.1081	326.1823	163.5948			3
8	867.4571	434.2322	850.4305	425.7189	849.4465	425.2269	P	272.1717	136.5895	255.1452	128.0762			2
9							R	175.1190	88.0631	158.0924	79.5498			1

H3K14	**KmeSTGGKacacAPR**	**Human HepG2 cells**



MS/MS Fragmentation of KSTGGKAPR
Found in Q71DI3, Histone H3.2 OS=Homo sapiens OX=9606 GN=HIST2H3A PE=1 SV=3

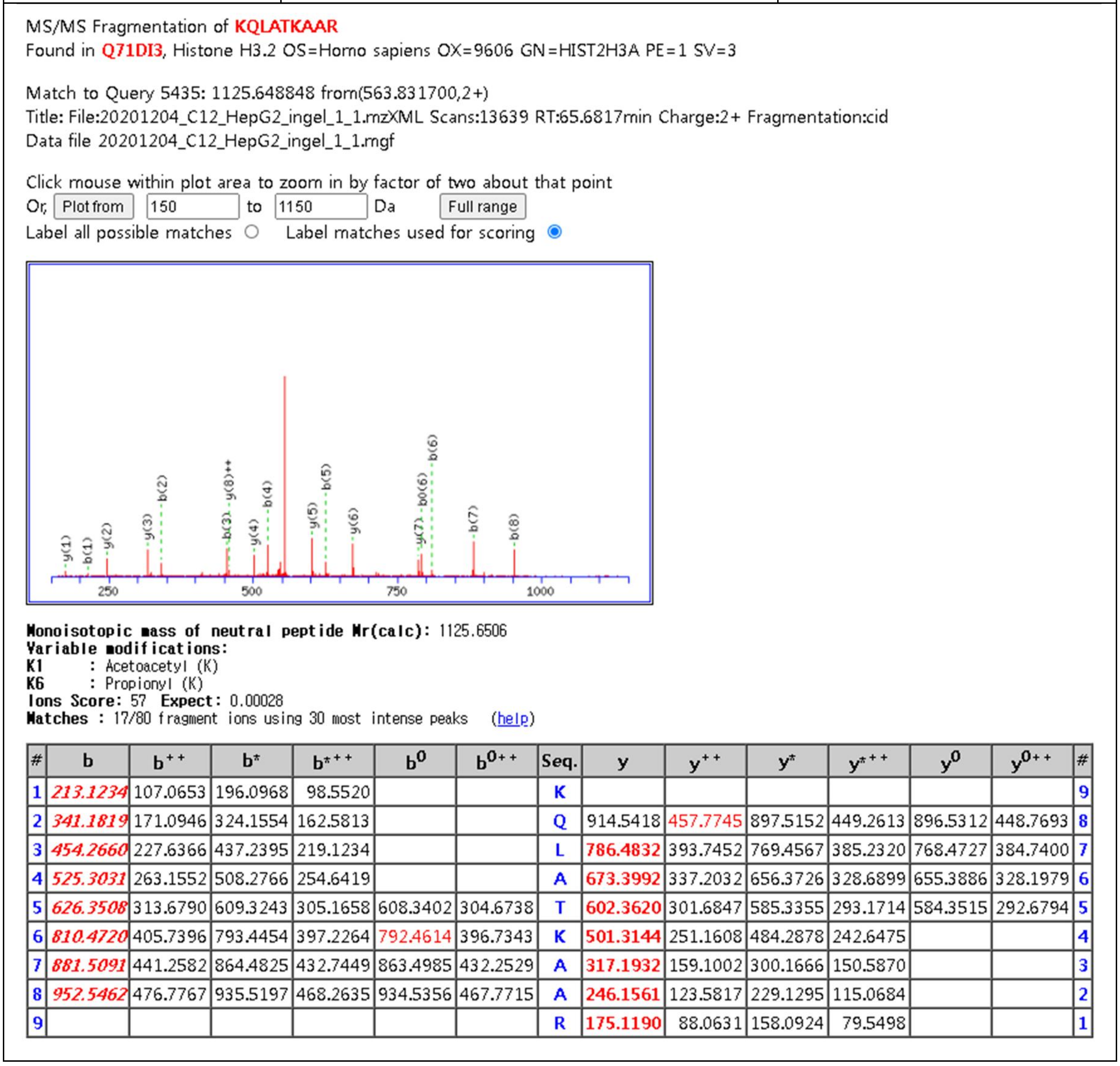
Match to Query 4481: 998.538648 from(500.276600,2+)
Title: File:20201204_C12_HepG2_ingel_3_2.mzXML Scans:5821 RT:33.6292min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_3_2.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 100 to 1000 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 998.5509
Variable modifications:
K1 : Methyl (KR)
K6 : Acetoacetyl (K)
Ions Score: 33 **Expect:** 0.13
Matches : 19/82 fragment ions using 57 most intense peaks (help)

#	b	b⁺⁺	b*	b*⁺⁺	b⁰	b⁰⁺⁺	Seq.	y	y⁺⁺	y*	y*⁺⁺	y⁰	y⁰⁺⁺	#
1	143.1179	72.0626	126.0913	63.5493			K							9
2	230.1499	115.5786	213.1234	107.0653	212.1394	106.5733	S	*857.4476*	429.2274	840.4210	420.7141	839.4370	420.2221	8
3	**331.1976**	166.1024	314.1710	157.5892	313.1870	157.0972	T	770.4155	385.7114	753.3890	377.1981	752.4050	376.7061	7
4	**388.2191**	194.6132	371.1925	186.0999	370.2085	185.6079	G	*669.3679*	335.1876	652.3413	326.6743			6
5	445.2405	223.1239	428.2140	214.6106	427.2300	214.1186	G	*612.3464*	306.6768	595.3198	298.1636			5
6	**657.3566**	329.1819	640.3301	320.6687	639.3461	320.1767	K	*555.3249*	278.1661	538.2984	269.6528			4
7	728.3937	364.7005	711.3672	356.1872	710.3832	355.6952	A	*343.2088*	172.1081	326.1823	163.5948			3
8	**825.4465**	413.2269	808.4199	404.7136	807.4359	404.2216	P	*272.1717*	136.5895	255.1452	128.0762			2
9							R	*175.1190*	88.0631	158.0924	79.5498			1

H3K18	KacacQLATKprAAR	Human HepG2 cells



MS/MS Fragmentation of KQLATKAAR
Found in Q71DI3, Histone H3.2 OS=Homo sapiens OX=9606 GN=HIST2H3A PE=1 SV=3

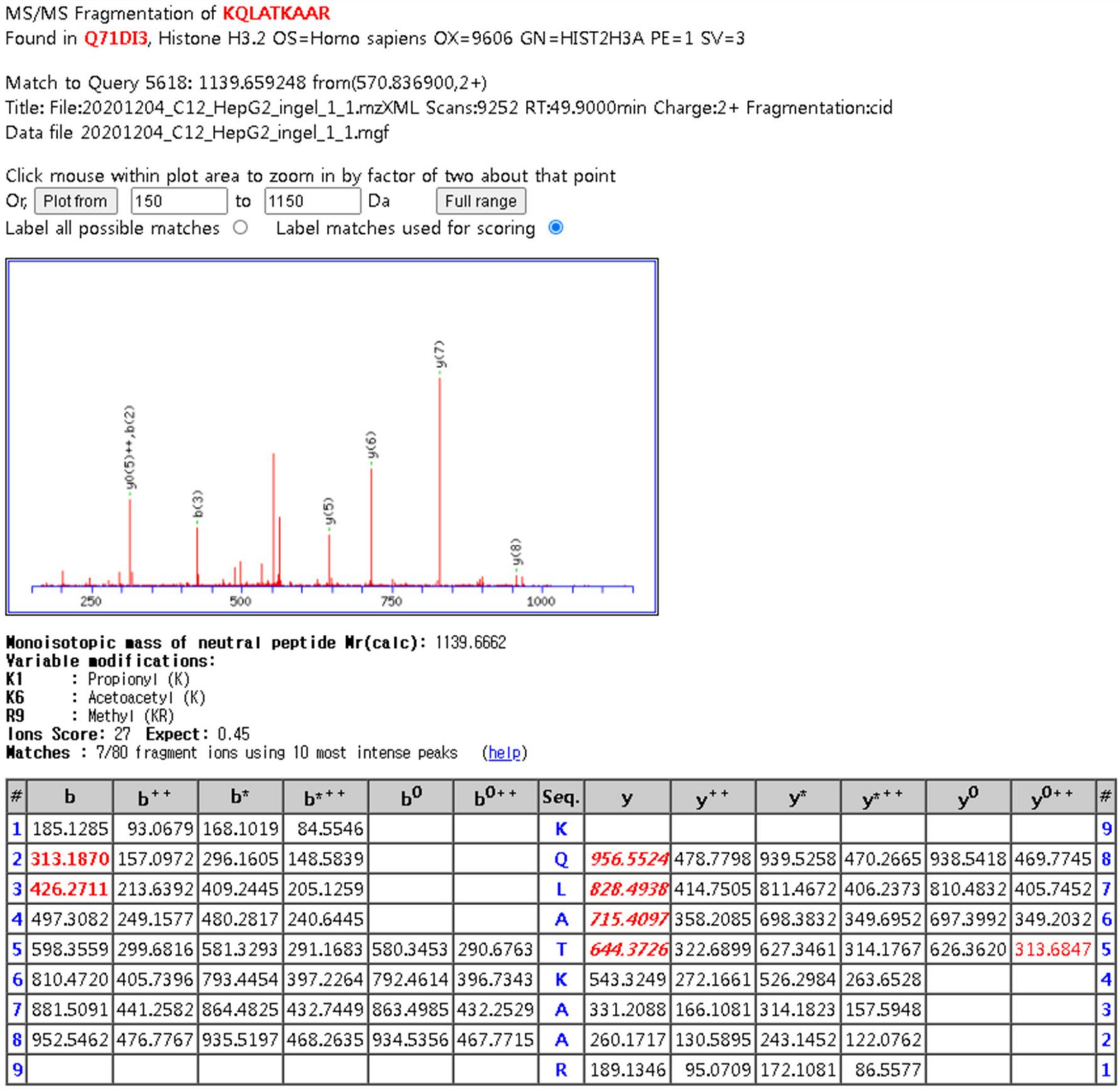
Match to Query 5435: 1125.648848 from(563.831700,2+)
Title: File:20201204_C12_HepG2_ingel_1_1.mzXML Scans:13639 RT:65.6817min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_1_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 150 to 1150 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 1125.6506
Variable modifications:
K1 : Acetoacetyl (K)
K6 : Propionyl (K)
Ions Score: 57 **Expect:** 0.00028
Matches : 17/80 fragment ions using 30 most intense peaks (help)

#	b	b++	b*	b*++	b0	b0++	Seq.	y	y++	y*	y*++	y0	y0++	#
1	213.1234	107.0653	196.0968	98.5520			K							9
2	341.1819	171.0946	324.1554	162.5813			Q	914.5418	457.7745	897.5152	449.2613	896.5312	448.7693	8
3	454.2660	227.6366	437.2395	219.1234			L	786.4832	393.7452	769.4567	385.2320	768.4727	384.7400	7
4	525.3031	263.1552	508.2766	254.6419			A	673.3992	337.2032	656.3726	328.6899	655.3886	328.1979	6
5	626.3508	313.6790	609.3243	305.1658	608.3402	304.6738	T	602.3620	301.6847	585.3355	293.1714	584.3515	292.6794	5
6	810.4720	405.7396	793.4454	397.2264	792.4614	396.7343	K	501.3144	251.1608	484.2878	242.6475			4
7	881.5091	441.2582	864.4825	432.7449	863.4985	432.2529	A	317.1932	159.1002	300.1666	150.5870			3
8	952.5462	476.7767	935.5197	468.2635	934.5356	467.7715	A	246.1561	123.5817	229.1295	115.0684			2
9							R	175.1190	88.0631	158.0924	79.5498			1

H3K23	**KprQLATKacacAARme**	**Human HepG2 cells**


MS/MS Fragmentation of **KQLATKAAR**
Found in **Q71DI3**, Histone H3.2 OS=Homo sapiens OX=9606 GN=HIST2H3A PE=1 SV=3

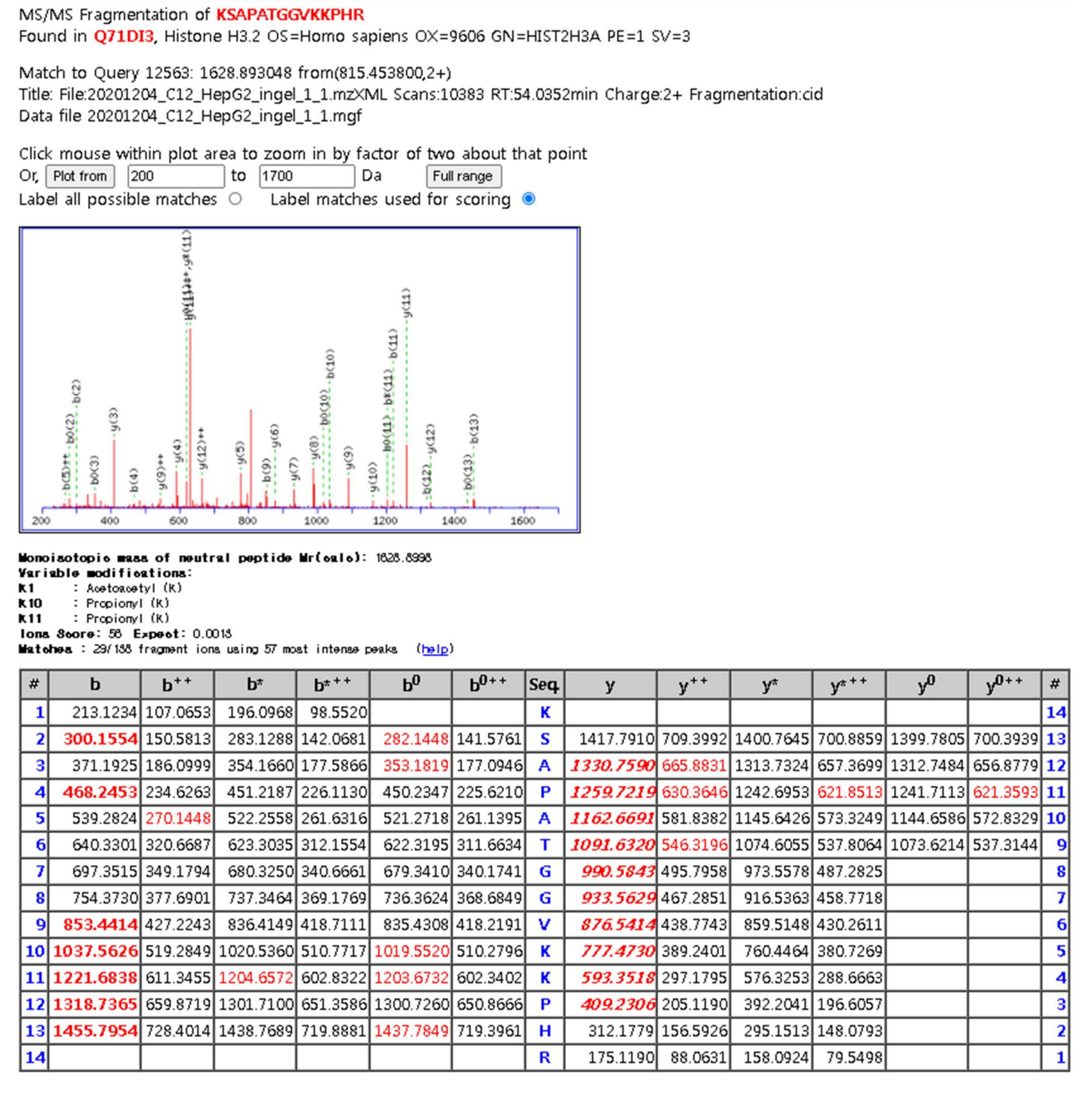
Match to Query 5618: 1139.659248 from(570.836900,2+)
Title: File:20201204_C12_HepG2_ingel_1_1.mzXML Scans:9252 RT:49.9000min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_1_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 150 to 1150 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 1139.6662
Variable modifications:
K1 : Propionyl (K)
K6 : Acetoacetyl (K)
R9 : Methyl (KR)
Ions Score: 27 **Expect:** 0.45
Matches : 7/80 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	185.1285	93.0679	168.1019	84.5546			K							9
2	**313.1870**	157.0972	296.1605	148.5839			Q	***956.5524***	478.7798	939.5258	470.2665	938.5418	469.7745	8
3	**426.2711**	213.6392	409.2445	205.1259			L	***828.4938***	414.7505	811.4672	406.2373	810.4832	405.7452	7
4	497.3082	249.1577	480.2817	240.6445			A	***715.4097***	358.2085	698.3832	349.6952	697.3992	349.2032	6
5	598.3559	299.6816	581.3293	291.1683	580.3453	290.6763	T	***644.3726***	322.6899	627.3461	314.1767	626.3620	313.6847	5
6	810.4720	405.7396	793.4454	397.2264	792.4614	396.7343	K	543.3249	272.1661	526.2984	263.6528			4
7	881.5091	441.2582	864.4825	432.7449	863.4985	432.2529	A	331.2088	166.1081	314.1823	157.5948			3
8	952.5462	476.7767	935.5197	468.2635	934.5356	467.7715	A	260.1717	130.5895	243.1452	122.0762			2
9							R	189.1346	95.0709	172.1081	86.5577			1

H3K27	**KacacSAPATGGVKprKprPHR**	**Human HepG2 cells**



MS/MS Fragmentation of **KSAPATGGVKKPHR**
Found in **Q71DI3**, Histone H3.2 OS=Homo sapiens OX=9606 GN=HIST2H3A PE=1 SV=3

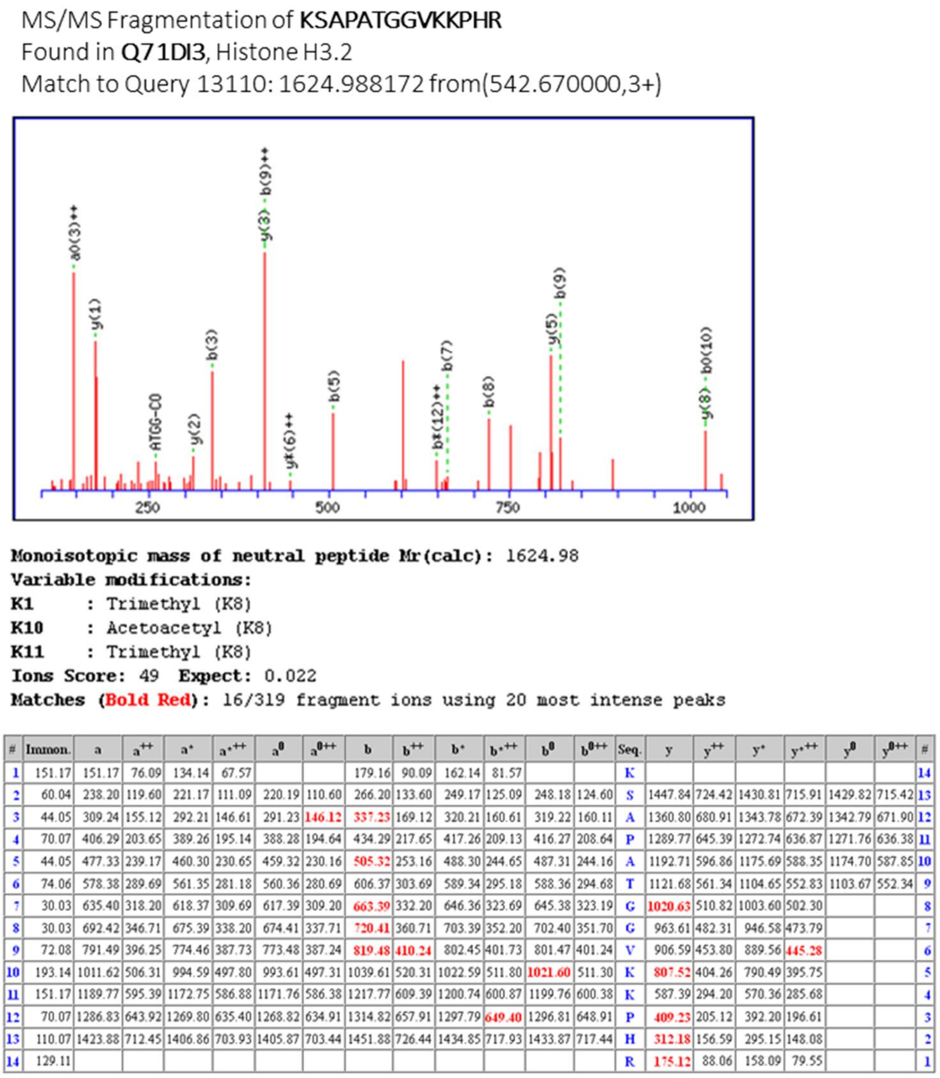
Match to Query 12563: 1628.893048 from(815.453800,2+)
Title: File:20201204_C12_HepG2_ingel_1_1.mzXML Scans:10383 RT:54.0352min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_1_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 200 to 1700 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 1628.8998
Variable modifications:
K1 : Acetoacetyl (K)
K10 : Propionyl (K)
K11 : Propionyl (K)
Ions Score: 58 **Expect:** 0.0018
Matches : 29/188 fragment ions using 57 most intense peaks (help)

#	b	b++	b*	b*++	b0	b0++	Seq	y	y++	y*	y*++	y0	y0++	#
1	213.1234	107.0653	196.0968	98.5520			K							14
2	**300.1554**	150.5813	283.1288	142.0681	282.1448	141.5761	S	1417.7910	709.3992	1400.7645	700.8859	1399.7805	700.3939	13
3	371.1925	186.0999	354.1660	177.5866	353.1819	177.0946	A	***1330.7590***	665.8831	1313.7324	657.3699	1312.7484	656.8779	12
4	**468.2453**	234.6263	451.2187	226.1130	450.2347	225.6210	P	***1259.7219***	630.3646	1242.6953	621.8513	1241.7113	621.3593	11
5	539.2824	270.1448	522.2558	261.6316	521.2718	261.1395	A	***1162.6691***	581.8382	1145.6426	573.3249	1144.6586	572.8329	10
6	640.3301	320.6687	623.3035	312.1554	622.3195	311.6634	T	***1091.6320***	546.3196	1074.6055	537.8064	1073.6214	537.3144	9
7	697.3515	349.1794	680.3250	340.6661	679.3410	340.1741	G	***990.5843***	495.7958	973.5578	487.2825			8
8	754.3730	377.6901	737.3464	369.1769	736.3624	368.6849	G	***933.5629***	467.2851	916.5363	458.7718			7
9	**853.4414**	427.2243	836.4149	418.7111	835.4308	418.2191	V	***876.5414***	438.7743	859.5148	430.2611			6
10	**1037.5626**	519.2849	1020.5360	510.7717	1019.5520	510.2796	K	***777.4730***	389.2401	760.4464	380.7269			5
11	**1221.6838**	611.3455	1204.6572	602.8322	1203.6732	602.3402	K	***593.3518***	297.1795	576.3253	288.6663			4
12	**1318.7365**	659.8719	1301.7100	651.3586	1300.7260	650.8666	P	***409.2306***	205.1190	392.2041	196.6057			3
13	**1455.7954**	728.4014	1438.7689	719.8881	1437.7849	719.3961	H	312.1779	156.5926	295.1513	148.0793			2
14							R	175.1190	88.0631	158.0924	79.5498			1

H3K36	**KacacSAPATGGVKacacKacPHR**	**Human MCF-7cell**

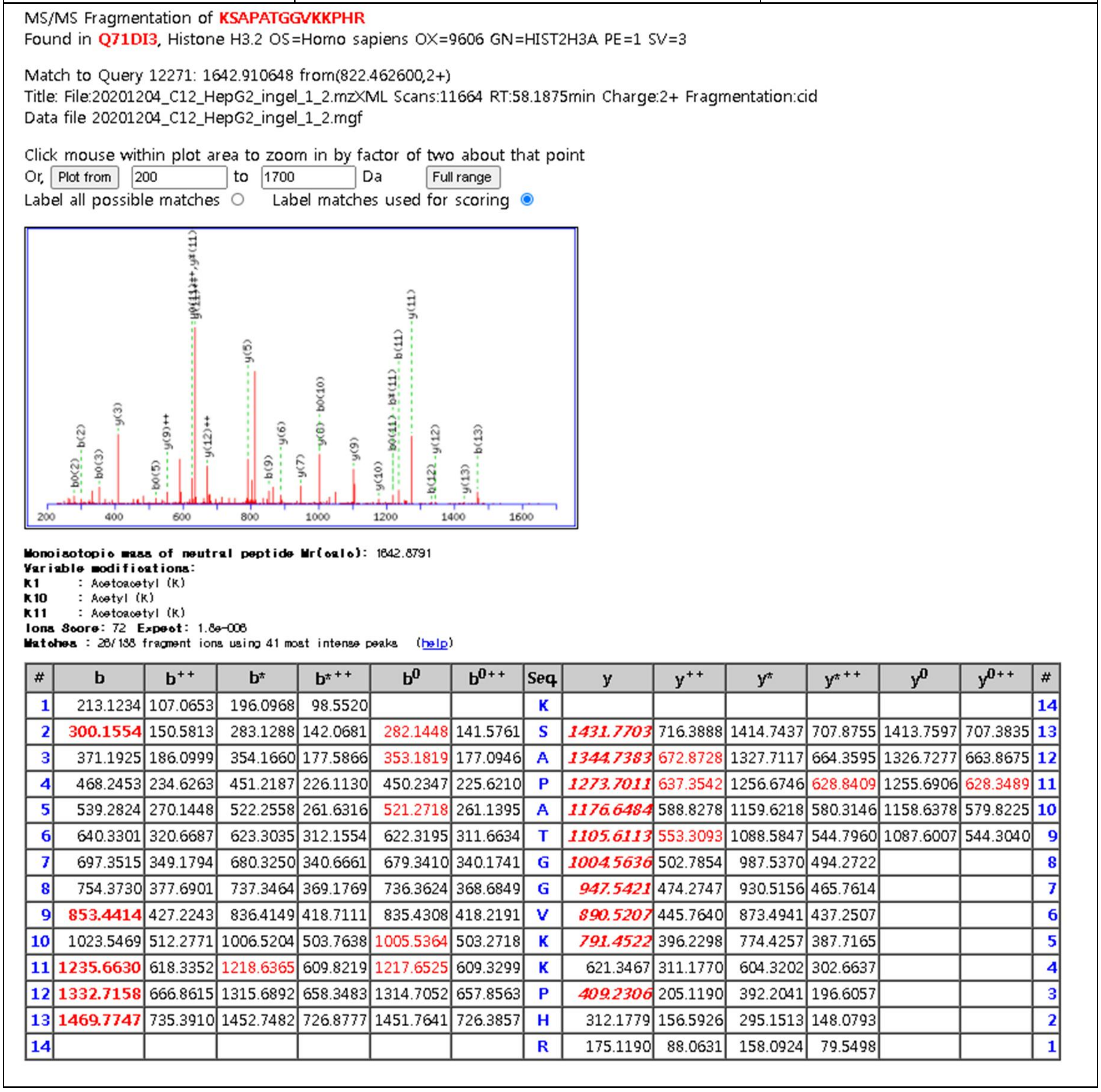


MS/MS Fragmentation of **KSAPATGGVKKPHR**
Found in **Q71DI3**, Histone H3.2
Match to Query 13110: 1624.988172 from(542.670000,3+)

Monoisotopic mass of neutral peptide Mr(calc): 1624.98
Variable modifications:
K1 : Trimethyl (K8)
K10 : Acetoacetyl (K8)
K11 : Trimethyl (K8)
Ions Score: 49 **Expect:** 0.022
Matches (Bold Red): 16/319 fragment ions using 20 most intense peaks

#	Immon.	a	a^{++}	a^*	a^{*++}	a^0	a^{0++}	b	b^{++}	b^*	b^{*++}	b^0	b^{0++}	Seq.	y	y^{++}	y^*	y^{*++}	y^0	y^{0++}	#
1	151.17	151.17	76.09	134.14	67.57			179.16	90.09	162.14	81.57			K							14
2	60.04	238.20	119.60	221.17	111.09	220.19	110.60	266.20	133.60	249.17	125.09	248.18	124.60	S	1447.84	724.42	1430.81	715.91	1429.82	715.42	13
3	44.05	309.24	155.12	292.21	146.61	291.23	**146.12**	**337.23**	169.12	320.21	160.61	319.22	160.11	A	1360.80	680.91	1343.78	672.39	1342.79	671.90	12
4	70.07	406.29	203.65	389.26	195.14	388.28	194.64	434.29	217.65	417.26	209.13	416.27	208.64	P	1289.77	645.39	1272.74	636.87	1271.76	636.38	11
5	44.05	477.33	239.17	460.30	230.65	459.32	230.16	**505.32**	253.16	488.30	244.65	487.31	244.16	A	1192.71	596.86	1175.69	588.35	1174.70	587.85	10
6	74.06	578.38	289.69	561.35	281.18	560.36	280.69	606.37	303.69	589.34	295.18	588.36	294.68	T	1121.68	561.34	1104.65	552.83	1103.67	552.34	9
7	30.03	635.40	318.20	618.37	309.69	617.39	309.20	**663.39**	332.20	646.36	323.69	645.38	323.19	G	**1020.63**	510.82	1003.60	502.30			8
8	30.03	692.42	346.71	675.39	338.20	674.41	337.71	**720.41**	360.71	703.39	352.20	702.40	351.70	G	963.61	482.31	946.58	473.79			7
9	72.08	791.49	396.25	774.46	387.73	773.48	387.24	**819.48**	**410.24**	802.45	401.73	801.47	401.24	V	906.59	453.80	889.56	**445.28**			6
10	193.14	1011.62	506.31	994.59	497.80	993.61	497.31	1039.61	520.31	1022.59	511.80	**1021.60**	511.30	K	**807.52**	404.26	790.49	395.75			5
11	151.17	1189.77	595.39	1172.75	586.88	1171.76	586.38	1217.77	609.39	1200.74	600.87	1199.76	600.38	K	587.39	294.20	570.36	285.68			4
12	70.07	1286.83	643.92	1269.80	635.40	1268.82	634.91	1314.82	657.91	1297.79	**649.40**	1296.81	648.91	P	**409.23**	205.12	392.20	196.61			3
13	110.07	1423.88	712.45	1406.86	703.93	1405.87	703.44	1451.88	726.44	1434.85	717.93	1433.87	717.44	H	**312.18**	156.59	295.15	148.08			2
14	129.11													R	**175.12**	88.06	158.09	79.55			1

H3K37	**KacacSAPATGGVKacKacacPHR**	**Human HepG2 cells**



MS/MS Fragmentation of **KSAPATGGVKKPHR**
Found in **Q71DI3**, Histone H3.2 OS=Homo sapiens OX=9606 GN=HIST2H3A PE=1 SV=3

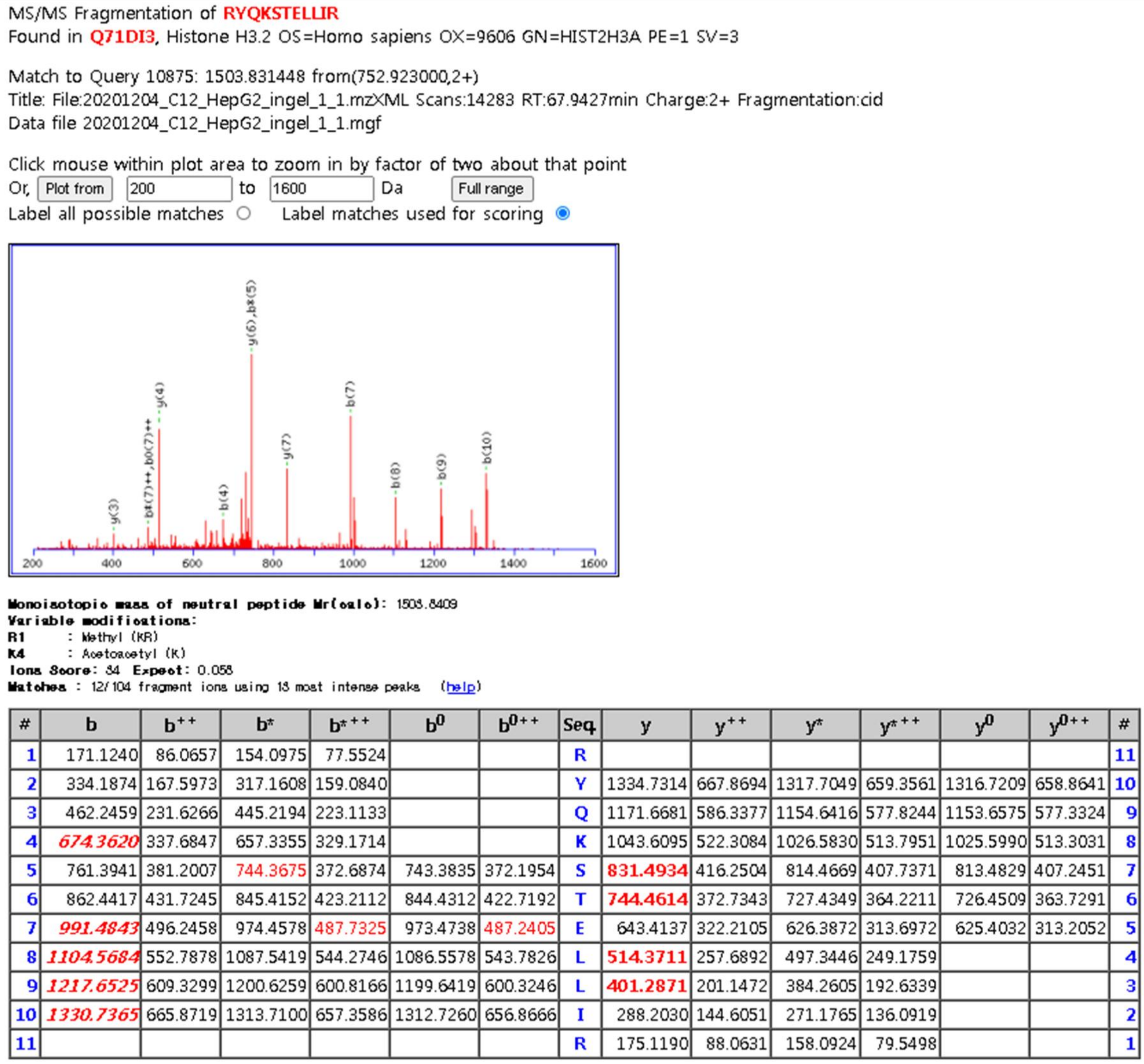
Match to Query 12271: 1642.910648 from(822.462600,2+)
Title: File:20201204_C12_HepG2_ingel_1_2.mzXML Scans:11664 RT:58.1875min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_1_2.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 200 to 1700 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 1642.8791
Variable modifications:
K1 : Acetoacetyl (K)
K10 : Acetyl (K)
K11 : Acetoacetyl (K)
Ions Score: 72 **Expect:** 1.8e-008
Matches : 28/138 fragment ions using 41 most intense peaks (help)

#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	213.1234	107.0653	196.0968	98.5520			K							14
2	**300.1554**	150.5813	283.1288	142.0681	282.1448	141.5761	S	***1431.7703***	716.3888	1414.7437	707.8755	1413.7597	707.3835	13
3	371.1925	186.0999	354.1660	177.5866	353.1819	177.0946	A	***1344.7383***	672.8728	1327.7117	664.3595	1326.7277	663.8675	12
4	468.2453	234.6263	451.2187	226.1130	450.2347	225.6210	P	***1273.7011***	637.3542	1256.6746	628.8409	1255.6906	628.3489	11
5	539.2824	270.1448	522.2558	261.6316	521.2718	261.1395	A	***1176.6484***	588.8278	1159.6218	580.3146	1158.6378	579.8225	10
6	640.3301	320.6687	623.3035	312.1554	622.3195	311.6634	T	***1105.6113***	553.3093	1088.5847	544.7960	1087.6007	544.3040	9
7	697.3515	349.1794	680.3250	340.6661	679.3410	340.1741	G	***1004.5636***	502.7854	987.5370	494.2722			8
8	754.3730	377.6901	737.3464	369.1769	736.3624	368.6849	G	***947.5421***	474.2747	930.5156	465.7614			7
9	**853.4414**	427.2243	836.4149	418.7111	835.4308	418.2191	V	***890.5207***	445.7640	873.4941	437.2507			6
10	1023.5469	512.2771	1006.5204	503.7638	1005.5364	503.2718	K	***791.4522***	396.2298	774.4257	387.7165			5
11	**1235.6630**	618.3352	1218.6365	609.8219	1217.6525	609.3299	K	621.3467	311.1770	604.3202	302.6637			4
12	**1332.7158**	666.8615	1315.6892	658.3483	1314.7052	657.8563	P	***409.2306***	205.1190	392.2041	196.6057			3
13	**1469.7747**	735.3910	1452.7482	726.8777	1451.7641	726.3857	H	312.1779	156.5926	295.1513	148.0793			2
14							R	175.1190	88.0631	158.0924	79.5498			1

H3K56	**RmeYQKacacSTELLIR**	**Human HepG2 cells**



MS/MS Fragmentation of **RYQKSTELLIR**
Found in **Q71DI3**, Histone H3.2 OS=Homo sapiens OX=9606 GN=HIST2H3A PE=1 SV=3

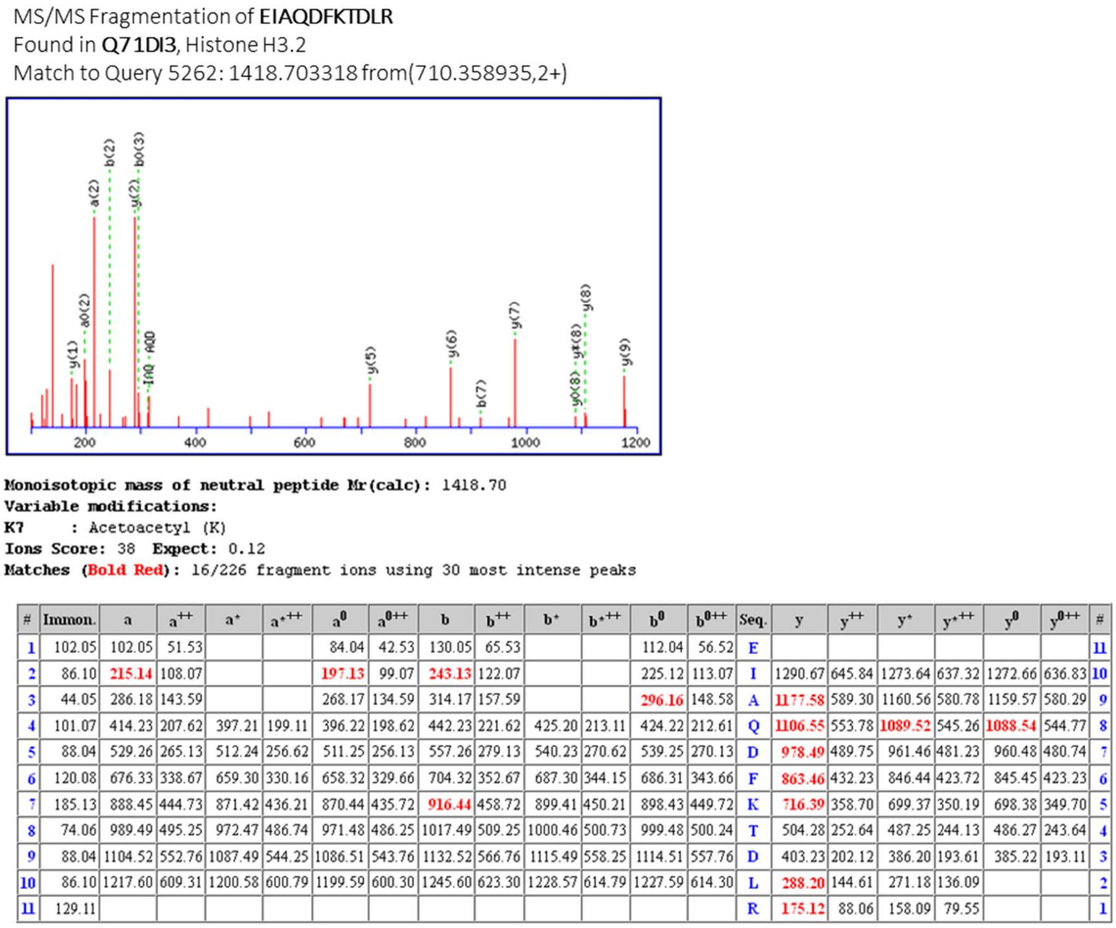
Match to Query 10875: 1503.831448 from(752.923000,2+)
Title: File:20201204_C12_HepG2_ingel_1_1.mzXML Scans:14283 RT:67.9427min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_1_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 200 to 1600 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 1503.8409
Variable modifications:
R1 : Methyl (KR)
K4 : Acetoacetyl (K)
Ions Score: 34 **Expect:** 0.058
Matches : 12/104 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	171.1240	86.0657	154.0975	77.5524			R							11
2	334.1874	167.5973	317.1608	159.0840			Y	1334.7314	667.8694	1317.7049	659.3561	1316.7209	658.8641	10
3	462.2459	231.6266	445.2194	223.1133			Q	1171.6681	586.3377	1154.6416	577.8244	1153.6575	577.3324	9
4	***674.3620***	337.6847	657.3355	329.1714			K	1043.6095	522.3084	1026.5830	513.7951	1025.5990	513.3031	8
5	761.3941	381.2007	744.3675	372.6874	743.3835	372.1954	S	**831.4934**	416.2504	814.4669	407.7371	813.4829	407.2451	7
6	862.4417	431.7245	845.4152	423.2112	844.4312	422.7192	T	**744.4614**	372.7343	727.4349	364.2211	726.4509	363.7291	6
7	***991.4843***	496.2458	974.4578	487.7325	973.4738	487.2405	E	643.4137	322.2105	626.3872	313.6972	625.4032	313.2052	5
8	***1104.5684***	552.7878	1087.5419	544.2746	1086.5578	543.7826	L	**514.3711**	257.6892	497.3446	249.1759			4
9	***1217.6525***	609.3299	1200.6259	600.8166	1199.6419	600.3246	L	**401.2871**	201.1472	384.2605	192.6339			3
10	***1330.7365***	665.8719	1313.7100	657.3586	1312.7260	656.8666	I	288.2030	144.6051	271.1765	136.0919			2
11							R	175.1190	88.0631	158.0924	79.5498			1

H3K79	**EIAQDFKacacTDLR**	**Human MCF-7 cells**

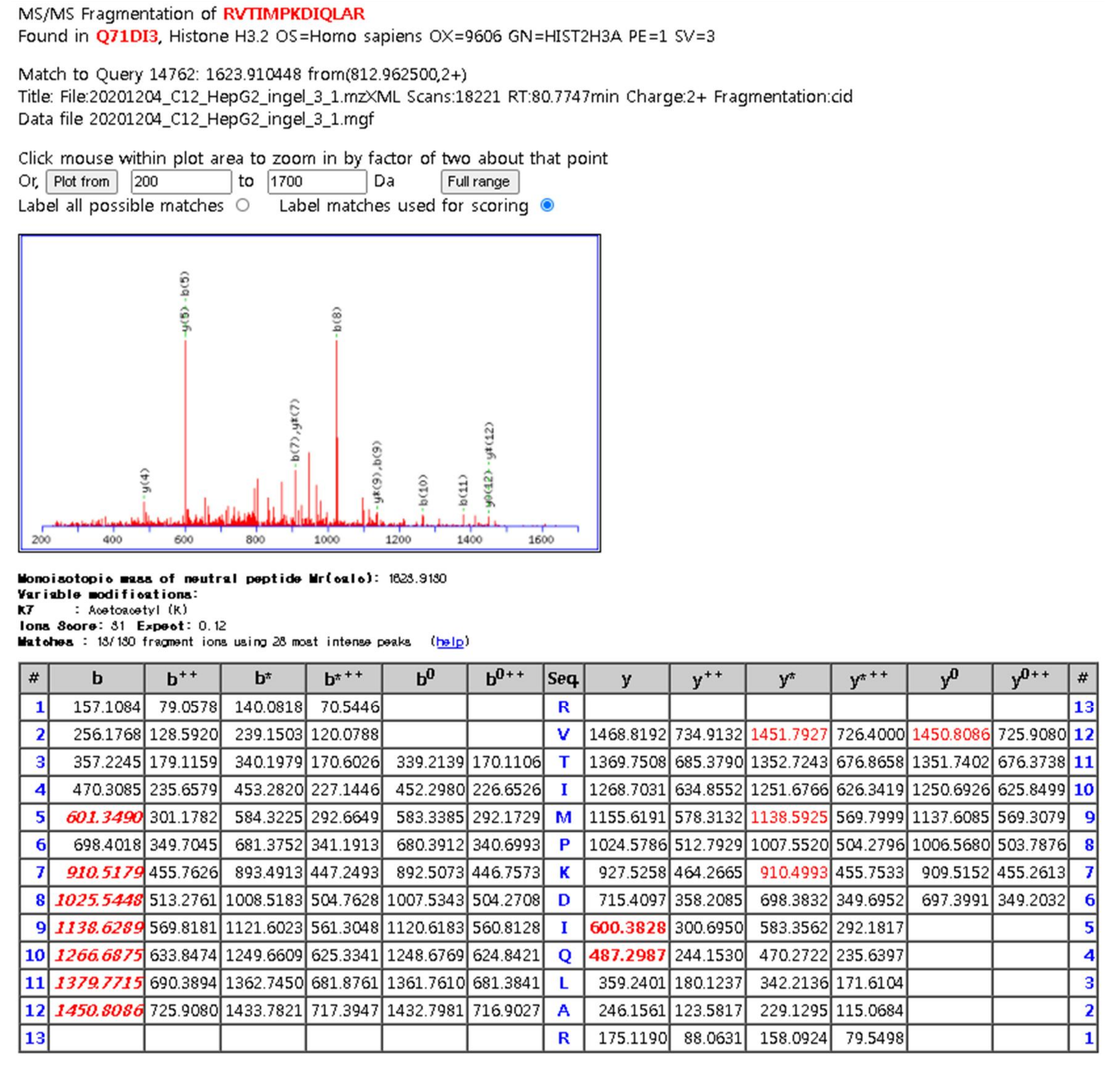


MS/MS Fragmentation of **EIAQDFKTDLR**
Found in **Q71DI3**, Histone H3.2
Match to Query 5262: 1418.703318 from(710.358935,2+)

Monoisotopic mass of neutral peptide Mr(calc): 1418.70
Variable modifications:
K7 : Acetoacetyl (K)
Ions Score: 38 **Expect:** 0.12
Matches (Bold Red): 16/226 fragment ions using 30 most intense peaks

#	Immon.	a	a^{++}	a^{*}	a^{*++}	a^{0}	a^{0++}	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	102.05	102.05	51.53			84.04	42.53	130.05	65.53			112.04	56.52	E							11
2	86.10	**215.14**	108.07			**197.13**	99.07	**243.13**	122.07			225.12	113.07	I	1290.67	645.84	1273.64	637.32	1272.66	636.83	10
3	44.05	286.18	143.59			268.17	134.59	314.17	157.59			**296.16**	148.58	A	**1177.58**	589.30	1160.56	580.78	1159.57	580.29	9
4	101.07	414.23	207.62	397.21	199.11	396.22	198.62	442.23	221.62	425.20	213.11	424.22	212.61	Q	**1106.55**	553.78	**1089.52**	545.26	**1088.54**	544.77	8
5	88.04	529.26	265.13	512.24	256.62	511.25	256.13	557.26	279.13	540.23	270.62	539.25	270.13	D	**978.49**	489.75	961.46	481.23	960.48	480.74	7
6	120.08	676.33	338.67	659.30	330.16	658.32	329.66	704.32	352.67	687.30	344.15	686.31	343.66	F	**863.46**	432.23	846.44	423.72	845.45	423.23	6
7	185.13	888.45	444.73	871.42	436.21	870.44	435.72	**916.44**	458.72	899.41	450.21	898.43	449.72	K	**716.39**	358.70	699.37	350.19	698.38	349.70	5
8	74.06	989.49	495.25	972.47	486.74	971.48	486.25	1017.49	509.25	1000.46	500.73	999.48	500.24	T	504.28	252.64	487.25	244.13	486.27	243.64	4
9	88.04	1104.52	552.76	1087.49	544.25	1086.51	543.76	1132.52	566.76	1115.49	558.25	1114.51	557.76	D	403.23	202.12	386.20	193.61	385.22	193.11	3
10	86.10	1217.60	609.31	1200.58	600.79	1199.59	600.30	1245.60	623.30	1228.57	614.79	1227.59	614.30	L	**288.20**	144.61	271.18	136.09			2
11	129.11													R	**175.12**	88.06	158.09	79.55			1

H3K122	**RVTIMPKacacDIQLAR**	**Human HepG2 cells**



MS/MS Fragmentation of **RVTIMPKDIQLAR**
Found in **Q71DI3**, Histone H3.2 OS=Homo sapiens OX=9606 GN=HIST2H3A PE=1 SV=3

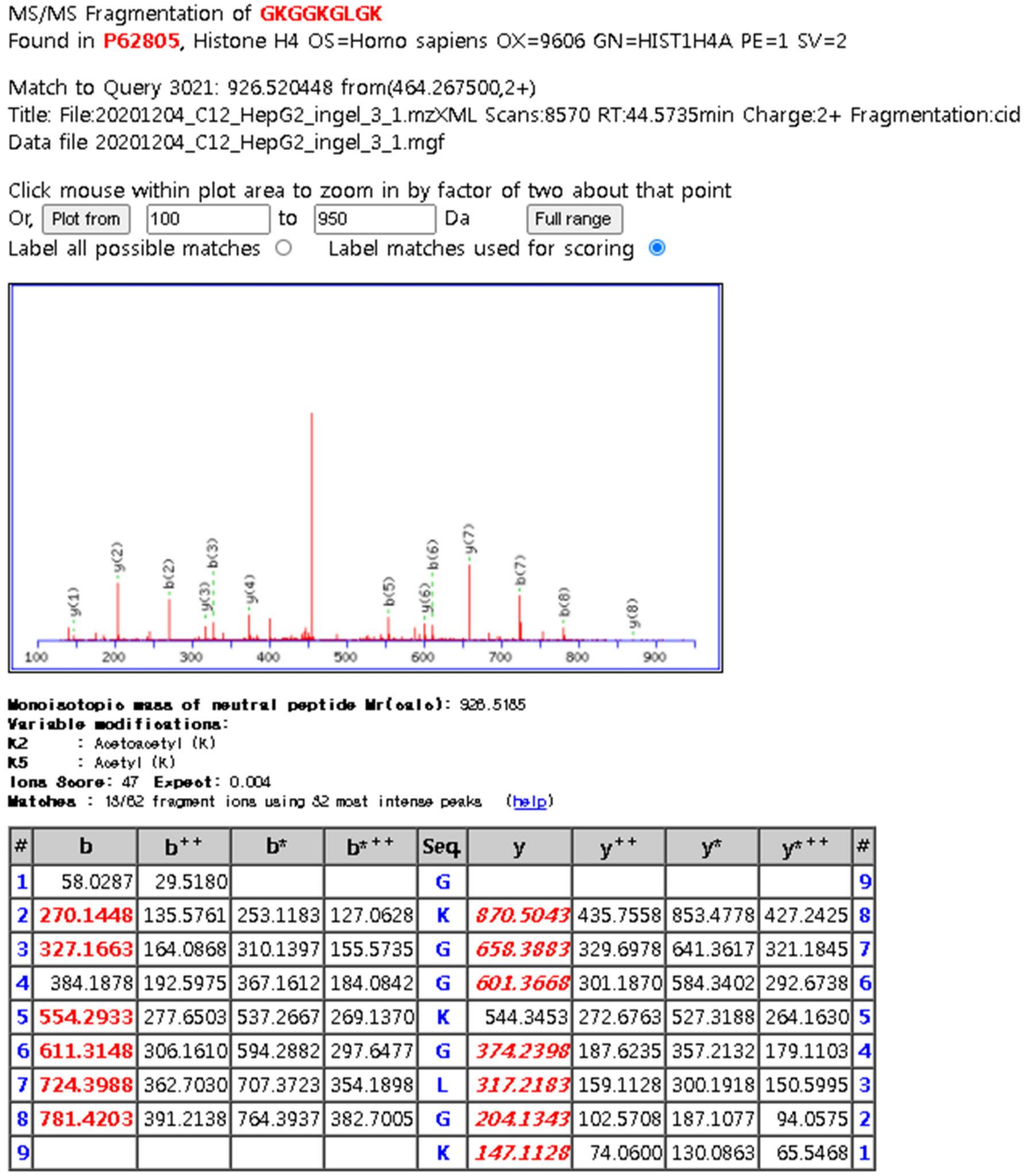
Match to Query 14762: 1623.910448 from(812.962500,2+)
Title: File:20201204_C12_HepG2_ingel_3_1.mzXML Scans:18221 RT:80.7747min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_3_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 200 to 1700 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 1623.9130
Variable modifications:
K7 : Acetoacetyl (K)
Ions Score: 31 **Expect:** 0.12
Matches : 13/130 fragment ions using 28 most intense peaks (help)

#	b	b⁺⁺	b*	b*⁺⁺	b⁰	b⁰⁺⁺	Seq	y	y⁺⁺	y*	y*⁺⁺	y⁰	y⁰⁺⁺	#
1	157.1084	79.0578	140.0818	70.5446			R							13
2	256.1768	128.5920	239.1503	120.0788			V	1468.8192	734.9132	1451.7927	726.4000	1450.8086	725.9080	12
3	357.2245	179.1159	340.1979	170.6026	339.2139	170.1106	T	1369.7508	685.3790	1352.7243	676.8658	1351.7402	676.3738	11
4	470.3085	235.6579	453.2820	227.1446	452.2980	226.6526	I	1268.7031	634.8552	1251.6766	626.3419	1250.6926	625.8499	10
5	***601.3490***	301.1782	584.3225	292.6649	583.3385	292.1729	M	1155.6191	578.3132	1138.5925	569.7999	1137.6085	569.3079	9
6	698.4018	349.7045	681.3752	341.1913	680.3912	340.6993	P	1024.5786	512.7929	1007.5520	504.2796	1006.5680	503.7876	8
7	***910.5179***	455.7626	893.4913	447.2493	892.5073	446.7573	K	927.5258	464.2665	910.4993	455.7533	909.5152	455.2613	7
8	***1025.5448***	513.2761	1008.5183	504.7628	1007.5343	504.2708	D	715.4097	358.2085	698.3832	349.6952	697.3991	349.2032	6
9	***1138.6289***	569.8181	1121.6023	561.3048	1120.6183	560.8128	I	**600.3828**	300.6950	583.3562	292.1817			5
10	***1266.6875***	633.8474	1249.6609	625.3341	1248.6769	624.8421	Q	**487.2987**	244.1530	470.2722	235.6397			4
11	***1379.7715***	690.3894	1362.7450	681.8761	1361.7610	681.3841	L	359.2401	180.1237	342.2136	171.6104			3
12	***1450.8086***	725.9080	1433.7821	717.3947	1432.7981	716.9027	A	246.1561	123.5817	229.1295	115.0684			2
13							R	175.1190	88.0631	158.0924	79.5498			1

H4K5	**GKacacGGKacGLGK**	**Human HepG2 cells**



MS/MS Fragmentation of **GKGGKGLGK**
Found in **P62805**, Histone H4 OS=Homo sapiens OX=9606 GN=HIST1H4A PE=1 SV=2

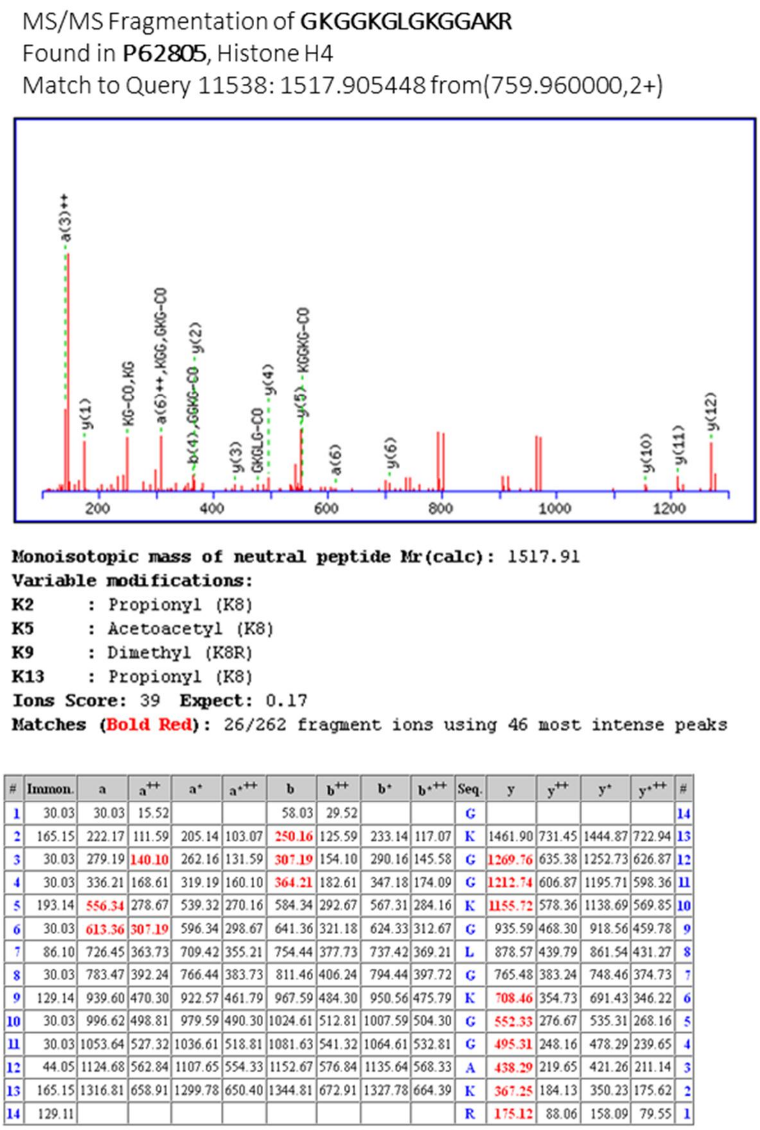
Match to Query 3021: 926.520448 from(464.267500,2+)
Title: File:20201204_C12_HepG2_ingel_3_1.mzXML Scans:8570 RT:44.5735min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_3_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 100 to 950 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 926.5185
Variable modifications:
K2 : Acetoacetyl (K)
K5 : Acetyl (K)
Ions Score: 47 **Expect:** 0.004
Matches : 13/62 fragment ions using 32 most intense peaks (help)

#	b	b⁺⁺	b*	b*⁺⁺	Seq	y	y⁺⁺	y*	y*⁺⁺	#
1	58.0287	29.5180			G					9
2	**270.1448**	135.5761	253.1183	127.0628	K	*870.5043*	435.7558	853.4778	427.2425	8
3	**327.1663**	164.0868	310.1397	155.5735	G	*658.3883*	329.6978	641.3617	321.1845	7
4	384.1878	192.5975	367.1612	184.0842	G	*601.3668*	301.1870	584.3402	292.6738	6
5	**554.2933**	277.6503	537.2667	269.1370	K	544.3453	272.6763	527.3188	264.1630	5
6	**611.3148**	306.1610	594.2882	297.6477	G	*374.2398*	187.6235	357.2132	179.1103	4
7	**724.3988**	362.7030	707.3723	354.1898	L	*317.2183*	159.1128	300.1918	150.5995	3
8	**781.4203**	391.2138	764.3937	382.7005	G	*204.1343*	102.5708	187.1077	94.0575	2
9					K	*147.1128*	74.0600	130.0863	65.5468	1

H4K8	**GKprGGKacacGLGKdiGGAKprR**	**Human MCF-7 cells**

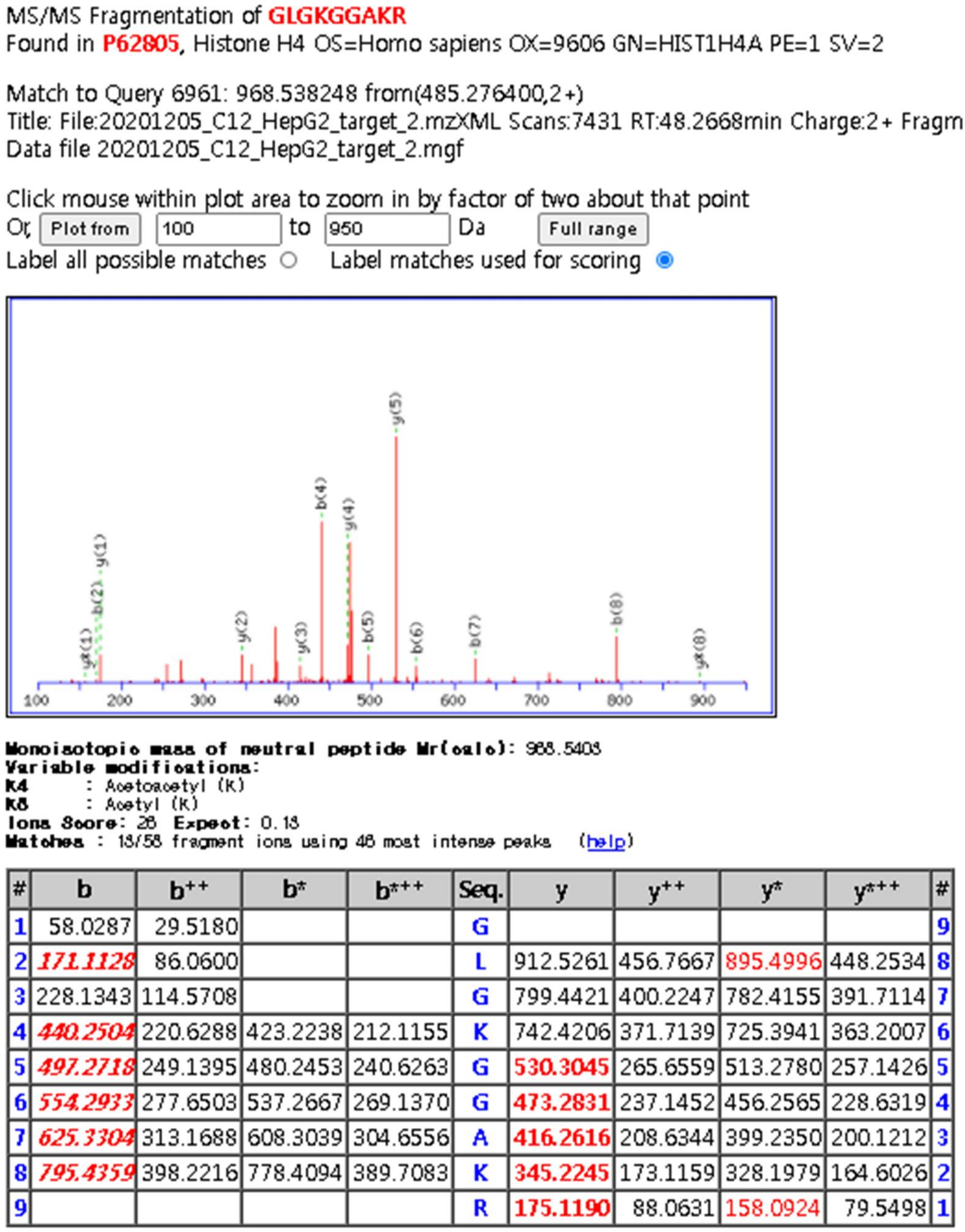


MS/MS Fragmentation of **GKGGKGLGKGGAKR**
Found in **P62805**, Histone H4
Match to Query 11538: 1517.905448 from(759.960000,2+)

Monoisotopic mass of neutral peptide Mr(calc): 1517.91
Variable modifications:
K2 : Propionyl (K8)
K5 : Acetoacetyl (K8)
K9 : Dimethyl (K8R)
K13 : Propionyl (K8)
Ions Score: 39 **Expect:** 0.17
Matches (Bold Red): 26/262 fragment ions using 46 most intense peaks

#	Immon.	a	a^{++}	a^{*}	a^{*++}	b	b^{++}	b^{*}	b^{*++}	Seq.	y	y^{++}	y^{*}	y^{*++}	#
1	30.03	30.03	15.52			58.03	29.52			G					14
2	165.15	222.17	111.59	205.14	103.07	**250.16**	125.59	233.14	117.07	K	1461.90	731.45	1444.87	722.94	13
3	30.03	279.19	**140.10**	262.16	131.59	**307.19**	154.10	290.16	145.58	G	**1269.76**	635.38	1252.73	626.87	12
4	30.03	336.21	168.61	319.19	160.10	**364.21**	182.61	347.18	174.09	G	**1212.74**	606.87	1195.71	598.36	11
5	193.14	**556.34**	278.67	539.32	270.16	584.34	292.67	567.31	284.16	K	**1155.72**	578.36	1138.69	569.85	10
6	30.03	**613.36**	**307.19**	596.34	298.67	641.36	321.18	624.33	312.67	G	935.59	468.30	918.56	459.78	9
7	86.10	726.45	363.73	709.42	355.21	754.44	377.73	737.42	369.21	L	878.57	439.79	861.54	431.27	8
8	30.03	783.47	392.24	766.44	383.73	811.46	406.24	794.44	397.72	G	765.48	383.24	748.46	374.73	7
9	129.14	939.60	470.30	922.57	461.79	967.59	484.30	950.56	475.79	K	**708.46**	354.73	691.43	346.22	6
10	30.03	996.62	498.81	979.59	490.30	1024.61	512.81	1007.59	504.30	G	**552.33**	276.67	535.31	268.16	5
11	30.03	1053.64	527.32	1036.61	518.81	1081.63	541.32	1064.61	532.81	G	**495.31**	248.16	478.29	239.65	4
12	44.05	1124.68	562.84	1107.65	554.33	1152.67	576.84	1135.64	568.33	A	**438.29**	219.65	421.26	211.14	3
13	165.15	1316.81	658.91	1299.78	650.40	1344.81	672.91	1327.78	664.39	K	**367.25**	184.13	350.23	175.62	2
14	129.11									R	**175.12**	88.06	158.09	79.55	1

H4K12	**GLGKacacGGAKacR**	**Human HepG2 cells**



MS/MS Fragmentation of GLGKGGAKR
Found in P62805, Histone H4 OS=Homo sapiens OX=9606 GN=HIST1H4A PE=1 SV=2

Match to Query 6961: 968.538248 from(485.276400,2+)
Title: File:20201205_C12_HepG2_target_2.mzXML Scans:7431 RT:48.2668min Charge:2+ Fragmentation:cid
Data file 20201205_C12_HepG2_target_2.mgf

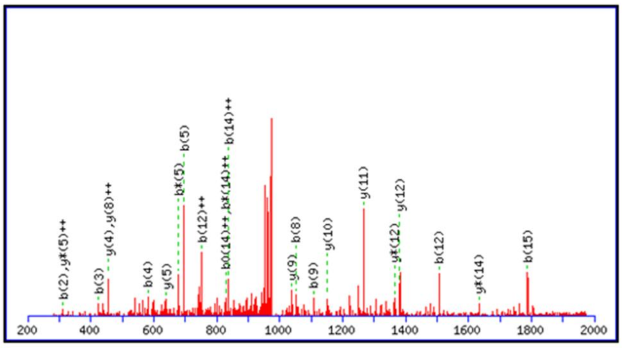
Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 100 to 950 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 968.5403
Variable modifications:
K4 : Acetoacetyl (K)
K8 : Acetyl (K)
Ions Score: 28 **Expect:** 0.18
Matches : 13/58 fragment ions using 48 most intense peaks (help)

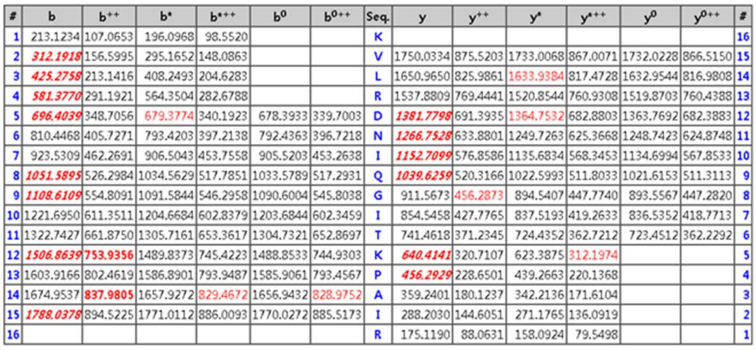
#	b	b++	b*	b*++	Seq.	y	y++	y*	y*++	#
1	58.0287	29.5180			G					9
2	*171.1128*	86.0600			L	912.5261	456.7667	895.4996	448.2534	8
3	228.1343	114.5708			G	799.4421	400.2247	782.4155	391.7114	7
4	*440.2504*	220.6288	423.2238	212.1155	K	742.4206	371.7139	725.3941	363.2007	6
5	*497.2718*	249.1395	480.2453	240.6263	G	**530.3045**	265.6559	513.2780	257.1426	5
6	*554.2933*	277.6503	537.2667	269.1370	G	**473.2831**	237.1452	456.2565	228.6319	4
7	*625.3304*	313.1688	608.3039	304.6556	A	**416.2616**	208.6344	399.2350	200.1212	3
8	*795.4359*	398.2216	778.4094	389.7083	K	**345.2245**	173.1159	328.1979	164.6026	2
9					R	**175.1190**	88.0631	158.0924	79.5498	1

H4K20	**KacacVLRDNIQGITKprPAIR**	**Rat liver**

MS/MS Fragmentation of **KVLRDNIQGITKPAIR**
Found in **P62804**, Histone H4 OS=Rattus norvegicus OX=10116 GN=Hist1h4b PE=1 SV=2
Match to Query 11928: 1961.172848 from(981.593700,2+)
Title: File:20201016_gel_6_global.mzXML Scans:11564 RT:62.4307min Charge:2+ Fragmentation:cid
Data file 20201016_gel_6_global.mgf

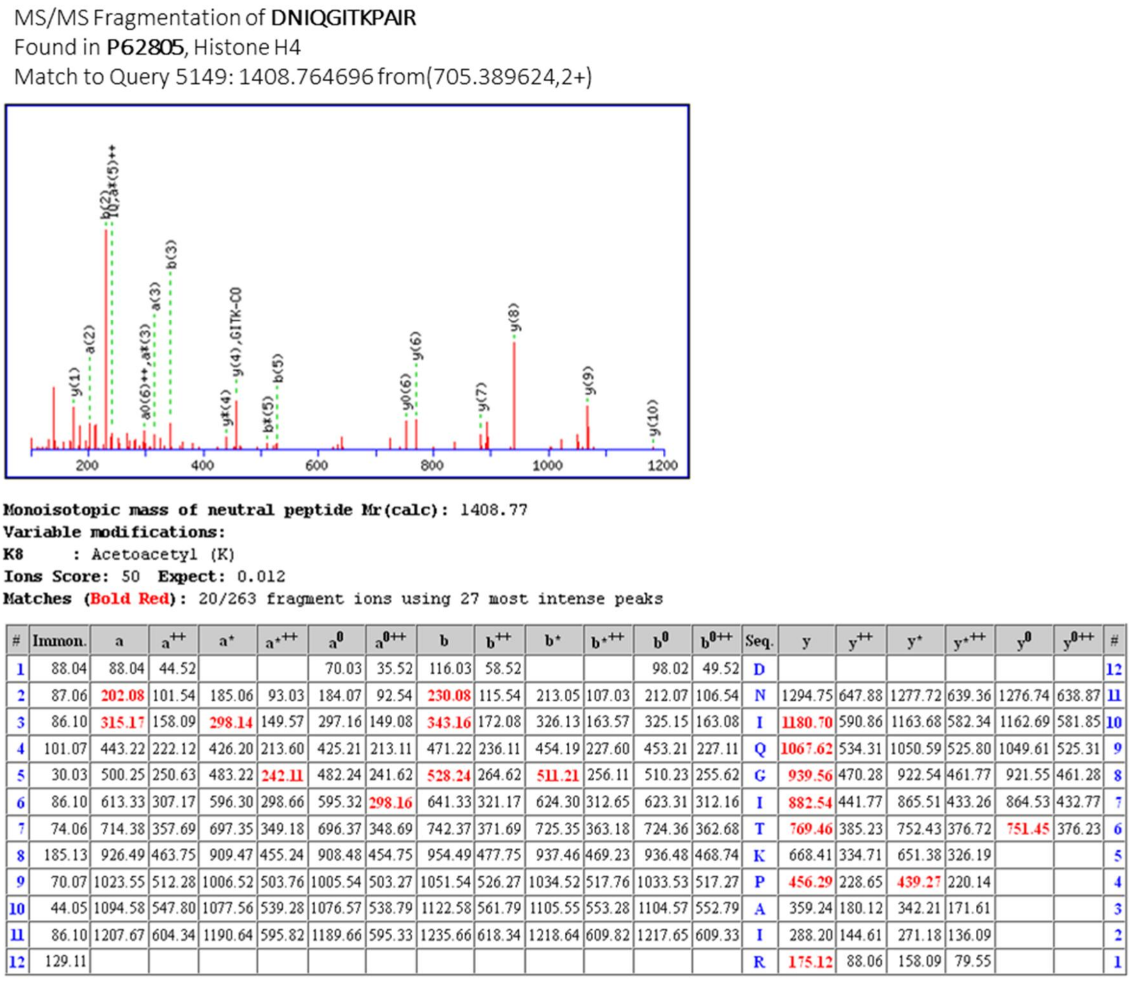


Monoisotopic mass of neutral peptide Mr(calc): 1961.1422
Variable modifications:
K1 : Acetoacetyl (K)
K12 : Propionyl (K)
Ions Score: 53 Expect: 0.00021
Matches : 23/162 fragment ions using 34 most intense peaks



#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	213.1234	107.0653	196.0968	98.5520			K							16
2	**312.1918**	156.5995	295.1652	148.0863			V	1750.0334	875.5203	1733.0068	867.0071	1732.0228	866.5150	15
3	**425.2758**	213.1416	408.2493	204.6283			L	1650.9650	825.9861	1633.9384	817.4728	1632.9544	816.9808	14
4	**581.3770**	291.1921	564.3504	282.6788			R	1537.8809	769.4441	1520.8544	760.9308	1519.8703	760.4388	13
5	**696.4039**	348.7056	679.3774	340.1923	678.3933	339.7003	D	**1381.7798**	691.3935	1364.7532	682.8803	1363.7692	682.3883	12
6	810.4468	405.7271	793.4203	397.2138	792.4363	396.7218	N	**1266.7528**	633.8801	1249.7263	625.3668	1248.7423	624.8748	11
7	923.5309	462.2691	906.5043	453.7558	905.5203	453.2638	I	**1152.7099**	576.8586	1135.6834	568.3453	1134.6994	567.8533	10
8	**1051.5895**	526.2984	1034.5629	517.7851	1033.5789	517.2931	Q	**1039.6259**	520.3166	1022.5993	511.8033	1021.6153	511.3113	9
9	**1108.6109**	554.8091	1091.5844	546.2958	1090.6004	545.8038	G	911.5673	456.2873	894.5407	447.7740	893.5567	447.2820	8
10	1221.6950	611.3511	1204.6684	602.8379	1203.6844	602.3459	I	854.5458	427.7765	837.5193	419.2633	836.5352	418.7713	7
11	1322.7427	661.8750	1305.7161	653.3617	1304.7321	652.8697	T	741.4618	371.2345	724.4352	362.7212	723.4512	362.2292	6
12	**1506.8639**	**753.9356**	1489.8373	745.4223	1488.8533	744.9303	K	**640.4141**	320.7107	623.3875	312.1974			5
13	1603.9166	802.4619	1586.8901	793.9487	1585.9061	793.4567	P	**456.2929**	228.6501	439.2663	220.1368			4
14	1674.9537	**837.9805**	1657.9272	829.4672	1656.9432	828.9752	A	359.2401	180.1237	342.2136	171.6104			3
15	**1788.0378**	894.5225	1771.0112	886.0093	1770.0272	885.5173	I	288.2030	144.6051	271.1765	136.0919			2
16							R	175.1190	88.0631	158.0924	79.5498			1

H4K31	**DNIQGITKacacPAIR**	**Human MCF-7 cell**

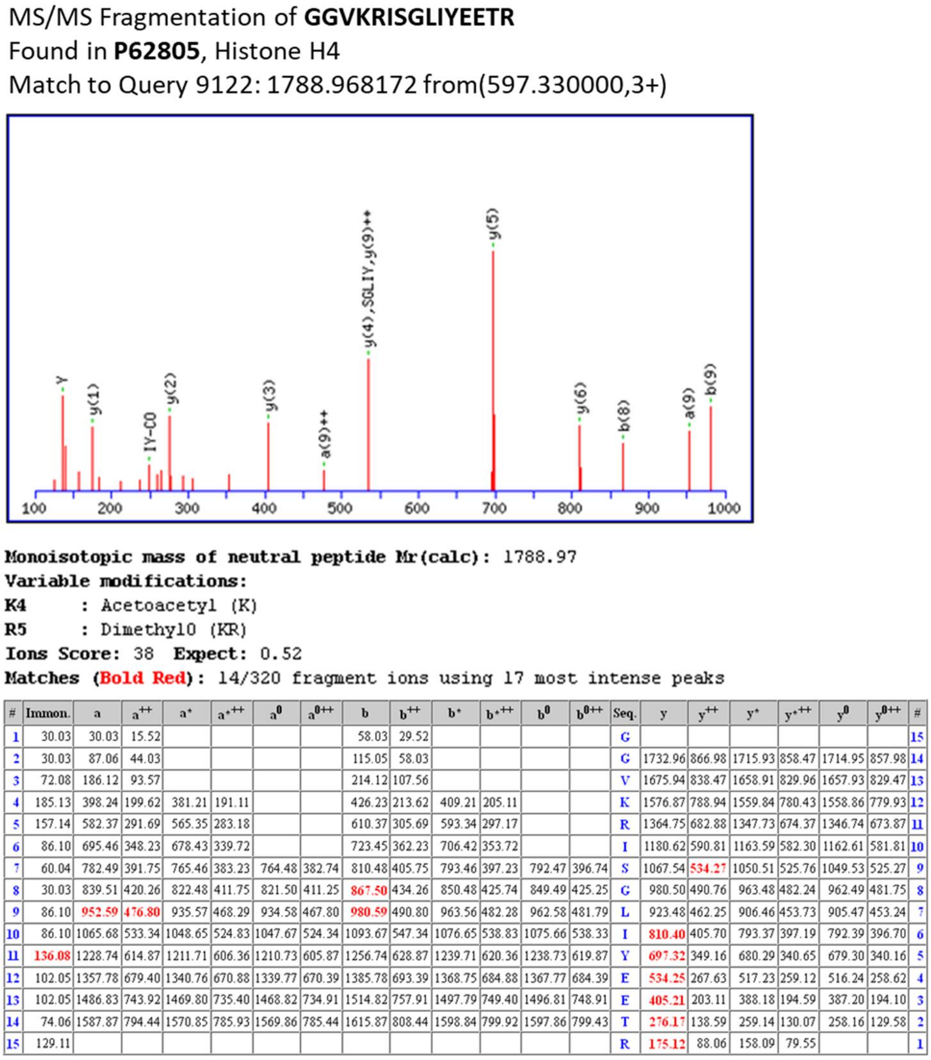


MS/MS Fragmentation of **DNIQGITKPAIR**
Found in **P62805**, Histone H4
Match to Query 5149: 1408.764696 from(705.389624,2+)

Monoisotopic mass of neutral peptide Mr(calc): 1408.77
Variable modifications:
K8 : Acetoacetyl (K)
Ions Score: 50 **Expect:** 0.012
Matches (Bold Red): 20/263 fragment ions using 27 most intense peaks

#	Immon.	a	a^{++}	a^{*}	a^{*++}	a^{0}	a^{0++}	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	88.04	88.04	44.52			70.03	35.52	116.03	58.52			98.02	49.52	D							12
2	87.06	**202.08**	101.54	185.06	93.03	184.07	92.54	**230.08**	115.54	213.05	107.03	212.07	106.54	N	1294.75	647.88	1277.72	639.36	1276.74	638.87	11
3	86.10	**315.17**	158.09	**298.14**	149.57	297.16	149.08	**343.16**	172.08	326.13	163.57	325.15	163.08	I	**1180.70**	590.86	1163.68	582.34	1162.69	581.85	10
4	101.07	443.22	222.12	426.20	213.60	425.21	213.11	471.22	236.11	454.19	227.60	453.21	227.11	Q	**1067.62**	534.31	1050.59	525.80	1049.61	525.31	9
5	30.03	500.25	250.63	483.22	**242.11**	482.24	241.62	**528.24**	264.62	**511.21**	256.11	510.23	255.62	G	**939.56**	470.28	922.54	461.77	921.55	461.28	8
6	86.10	613.33	307.17	596.30	298.66	595.32	**298.16**	641.33	321.17	624.30	312.65	623.31	312.16	I	**882.54**	441.77	865.51	433.26	864.53	432.77	7
7	74.06	714.38	357.69	697.35	349.18	696.37	348.69	742.37	371.69	725.35	363.18	724.36	362.68	T	**769.46**	385.23	752.43	376.72	**751.45**	376.23	6
8	185.13	926.49	463.75	909.47	455.24	908.48	454.75	954.49	477.75	937.46	469.23	936.48	468.74	K	668.41	334.71	651.38	326.19			5
9	70.07	1023.55	512.28	1006.52	503.76	1005.54	503.27	1051.54	526.27	1034.52	517.76	1033.53	517.27	P	**456.29**	228.65	**439.27**	220.14			4
10	44.05	1094.58	547.80	1077.56	539.28	1076.57	538.79	1122.58	561.79	1105.55	553.28	1104.57	552.79	A	359.24	180.12	342.21	171.61			3
11	86.10	1207.67	604.34	1190.64	595.82	1189.66	595.33	1235.66	618.34	1218.64	609.82	1217.65	609.33	I	288.20	144.61	271.18	136.09			2
12	129.11													R	**175.12**	88.06	158.09	79.55			1

H4K44	**GGVKacacRdiISGLIYEETR**	**Human HeLa cells**

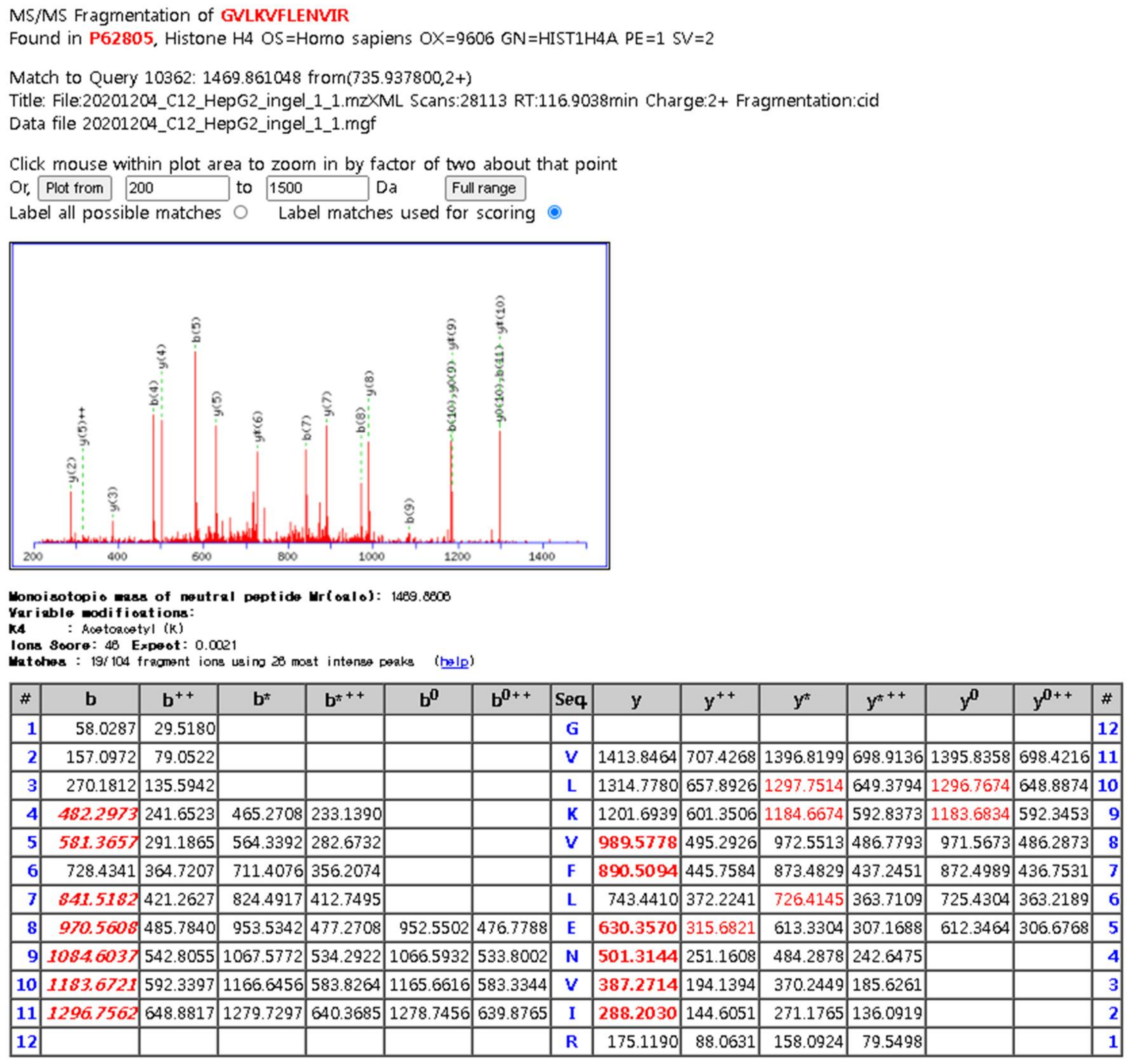


MS/MS Fragmentation of **GGVKRISGLIYEETR**
Found in **P62805**, Histone H4
Match to Query 9122: 1788.968172 from(597.330000,3+)

Monoisotopic mass of neutral peptide Mr(calc): 1788.97
Variable modifications:
K4 : Acetoacetyl (K)
R5 : Dimethyl0 (KR)
Ions Score: 38 **Expect:** 0.52
Matches (Bold Red): 14/320 fragment ions using 17 most intense peaks

#	Immon.	a	a^{++}	a^{*}	a^{*++}	a^{0}	a^{0++}	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq.	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	30.03	30.03	15.52					58.03	29.52					G							15
2	30.03	87.06	44.03					115.05	58.03					G	1732.96	866.98	1715.93	858.47	1714.95	857.98	14
3	72.08	186.12	93.57					214.12	107.56					V	1675.94	838.47	1658.91	829.96	1657.93	829.47	13
4	185.13	398.24	199.62	381.21	191.11			426.23	213.62	409.21	205.11			K	1576.87	788.94	1559.84	780.43	1558.86	779.93	12
5	157.14	582.37	291.69	565.35	283.18			610.37	305.69	593.34	297.17			R	1364.75	682.88	1347.73	674.37	1346.74	673.87	11
6	86.10	695.46	348.23	678.43	339.72			723.45	362.23	706.42	353.72			I	1180.62	590.81	1163.59	582.30	1162.61	581.81	10
7	60.04	782.49	391.75	765.46	383.23	764.48	382.74	810.48	405.75	793.46	397.23	792.47	396.74	S	1067.54	**534.27**	1050.51	525.76	1049.53	525.27	9
8	30.03	839.51	420.26	822.48	411.75	821.50	411.25	**867.50**	434.26	850.48	425.74	849.49	425.25	G	980.50	490.76	963.48	482.24	962.49	481.75	8
9	86.10	**952.59**	**476.80**	935.57	468.29	934.58	467.80	**980.59**	490.80	963.56	482.28	962.58	481.79	L	923.48	462.25	906.46	453.73	905.47	453.24	7
10	86.10	1065.68	533.34	1048.65	524.83	1047.67	524.34	1093.67	547.34	1076.65	538.83	1075.66	538.33	I	**810.40**	405.70	793.37	397.19	792.39	396.70	6
11	**136.08**	1228.74	614.87	1211.71	606.36	1210.73	605.87	1256.74	628.87	1239.71	620.36	1238.73	619.87	Y	**697.32**	349.16	680.29	340.65	679.30	340.16	5
12	102.05	1357.78	679.40	1340.76	670.88	1339.77	670.39	1385.78	693.39	1368.75	684.88	1367.77	684.39	E	**534.25**	267.63	517.23	259.12	516.24	258.62	4
13	102.05	1486.83	743.92	1469.80	735.40	1468.82	734.91	1514.82	757.91	1497.79	749.40	1496.81	748.91	E	**405.21**	203.11	388.18	194.59	387.20	194.10	3
14	74.06	1587.87	794.44	1570.85	785.93	1569.86	785.44	1615.87	808.44	1598.84	799.92	1597.86	799.43	T	**276.17**	138.59	259.14	130.07	258.16	129.58	2
15	129.11													R	**175.12**	88.06	158.09	79.55			1

H4K59	**GVLKacacVFLENVIR**	**Human HepG2 cells**



MS/MS Fragmentation of GVLKVFLENVIR
Found in P62805, Histone H4 OS=Homo sapiens OX=9606 GN=HIST1H4A PE=1 SV=2

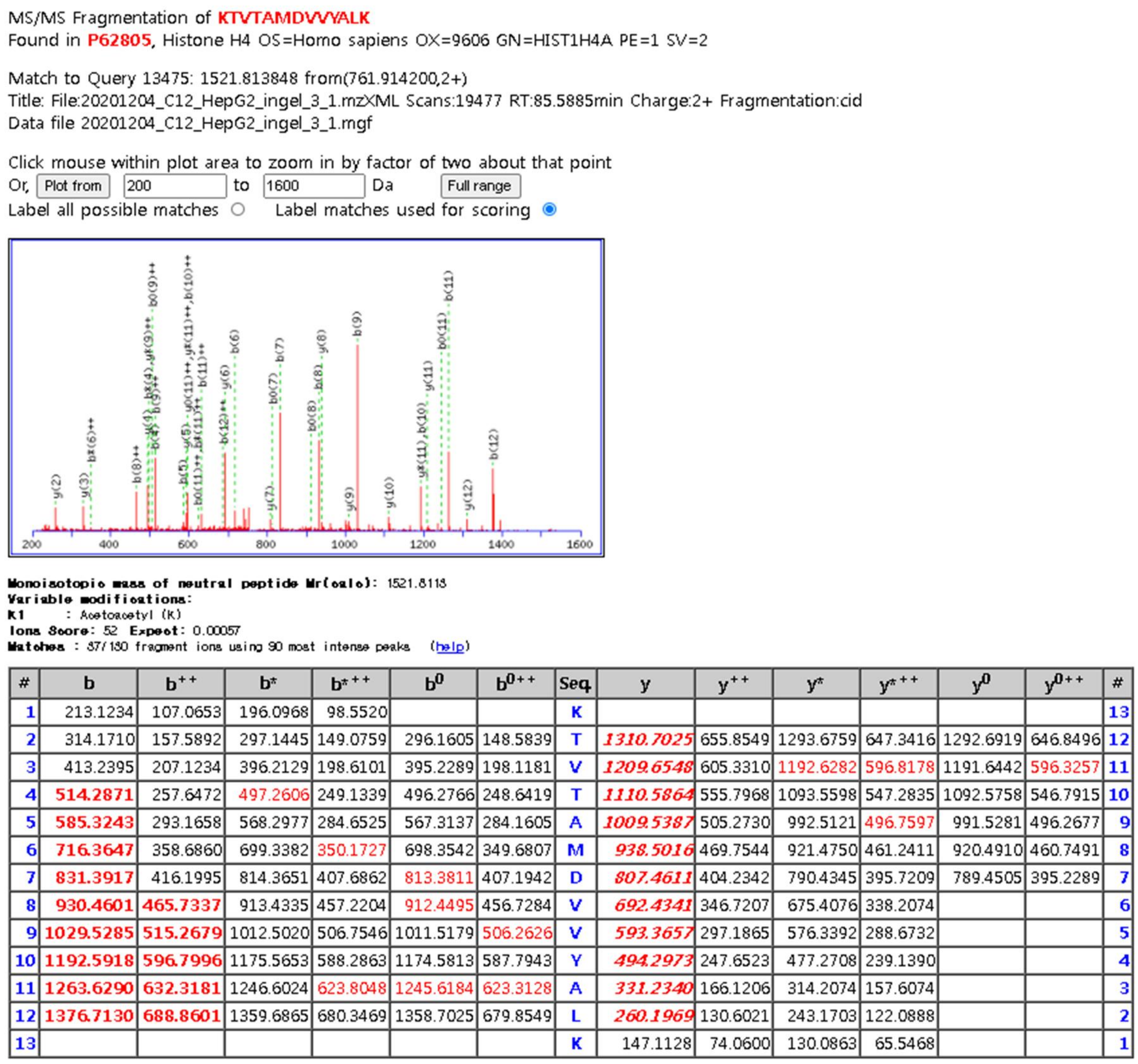
Match to Query 10362: 1469.861048 from(735.937800,2+)
Title: File:20201204_C12_HepG2_ingel_1_1.mzXML Scans:28113 RT:116.9038min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_1_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 200 to 1500 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 1469.8608
Variable modifications:
K4 : Acetoacetyl (K)
Ions Score: 48 **Expect:** 0.0021
Matches : 19/104 fragment ions using 28 most intense peaks (help)

#	b	b^{++}	b^{*}	b^{*++}	b^{0}	b^{0++}	Seq	y	y^{++}	y^{*}	y^{*++}	y^{0}	y^{0++}	#
1	58.0287	29.5180					G							12
2	157.0972	79.0522					V	1413.8464	707.4268	1396.8199	698.9136	1395.8358	698.4216	11
3	270.1812	135.5942					L	1314.7780	657.8926	1297.7514	649.3794	1296.7674	648.8874	10
4	482.2973	241.6523	465.2708	233.1390			K	1201.6939	601.3506	1184.6674	592.8373	1183.6834	592.3453	9
5	581.3657	291.1865	564.3392	282.6732			V	989.5778	495.2926	972.5513	486.7793	971.5673	486.2873	8
6	728.4341	364.7207	711.4076	356.2074			F	890.5094	445.7584	873.4829	437.2451	872.4989	436.7531	7
7	841.5182	421.2627	824.4917	412.7495			L	743.4410	372.2241	726.4145	363.7109	725.4304	363.2189	6
8	970.5608	485.7840	953.5342	477.2708	952.5502	476.7788	E	630.3570	315.6821	613.3304	307.1688	612.3464	306.6768	5
9	1084.6037	542.8055	1067.5772	534.2922	1066.5932	533.8002	N	501.3144	251.1608	484.2878	242.6475			4
10	1183.6721	592.3397	1166.6456	583.8264	1165.6616	583.3344	V	387.2714	194.1394	370.2449	185.6261			3
11	1296.7562	648.8817	1279.7297	640.3685	1278.7456	639.8765	I	288.2030	144.6051	271.1765	136.0919			2
12							R	175.1190	88.0631	158.0924	79.5498			1

H4K79	**KacacTVTAMDVVYALK**	**Human HepG2 cells**



MS/MS Fragmentation of **KTVTAMDVVYALK**
Found in **P62805**, Histone H4 OS=Homo sapiens OX=9606 GN=HIST1H4A PE=1 SV=2

Match to Query 13475: 1521.813848 from(761.914200,2+)
Title: File:20201204_C12_HepG2_ingel_3_1.mzXML Scans:19477 RT:85.5885min Charge:2+ Fragmentation:cid
Data file 20201204_C12_HepG2_ingel_3_1.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 200 to 1600 Da Full range
Label all possible matches ○ Label matches used for scoring ●

Monoisotopic mass of neutral peptide Mr(calc): 1521.8113
Variable modifications:
K1 : Acetoacetyl (K)
Ions Score: 52 **Expect:** 0.00057
Matches : 37/130 fragment ions using 90 most intense peaks (help)

#	b	b++	b*	b*++	b0	b0++	Seq	y	y++	y*	y*++	y0	y0++	#
1	213.1234	107.0653	196.0968	98.5520			K							13
2	314.1710	157.5892	297.1445	149.0759	296.1605	148.5839	T	1310.7025	655.8549	1293.6759	647.3416	1292.6919	646.8496	12
3	413.2395	207.1234	396.2129	198.6101	395.2289	198.1181	V	1209.6548	605.3310	1192.6282	596.8178	1191.6442	596.3257	11
4	514.2871	257.6472	497.2606	249.1339	496.2766	248.6419	T	1110.5864	555.7968	1093.5598	547.2835	1092.5758	546.7915	10
5	585.3243	293.1658	568.2977	284.6525	567.3137	284.1605	A	1009.5387	505.2730	992.5121	496.7597	991.5281	496.2677	9
6	716.3647	358.6860	699.3382	350.1727	698.3542	349.6807	M	938.5016	469.7544	921.4750	461.2411	920.4910	460.7491	8
7	831.3917	416.1995	814.3651	407.6862	813.3811	407.1942	D	807.4611	404.2342	790.4345	395.7209	789.4505	395.2289	7
8	930.4601	465.7337	913.4335	457.2204	912.4495	456.7284	V	692.4341	346.7207	675.4076	338.2074			6
9	1029.5285	515.2679	1012.5020	506.7546	1011.5179	506.2626	V	593.3657	297.1865	576.3392	288.6732			5
10	1192.5918	596.7996	1175.5653	588.2863	1174.5813	587.7943	Y	494.2973	247.6523	477.2708	239.1390			4
11	1263.6290	632.3181	1246.6024	623.8048	1245.6184	623.3128	A	331.2340	166.1206	314.2074	157.6074			3
12	1376.7130	688.8601	1359.6865	680.3469	1358.7025	679.8549	L	260.1969	130.6021	243.1703	122.0888			2
13							K	147.1128	74.0600	130.0863	65.5468			1