

Supplemental Figure 3.

MS/MS *de novo* sequencing of neuropeptides detected in ESI experiments.

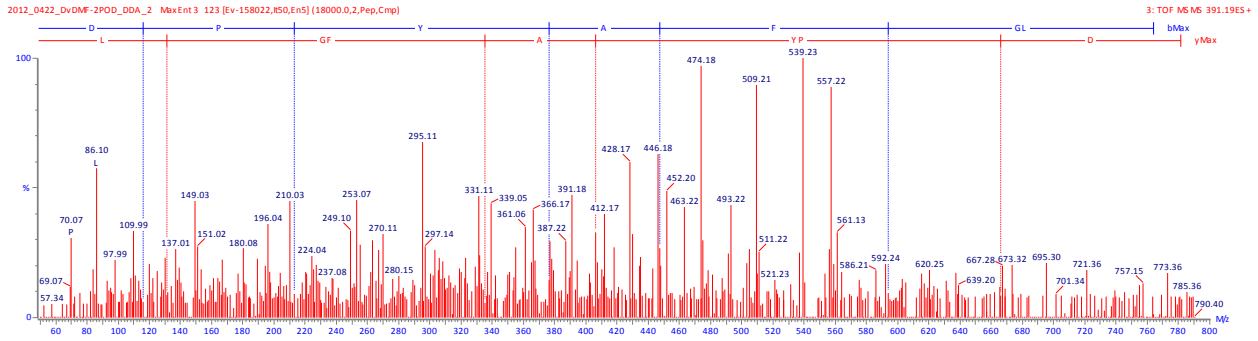
PepSeq software was used to process *de novo* data.

MS/MS *de novo* sequences of peptides in table 1 (pg 2 – 33)

MS/MS of CPRP ($[M+1]^+ = 3837$) (pg 34 – 35)

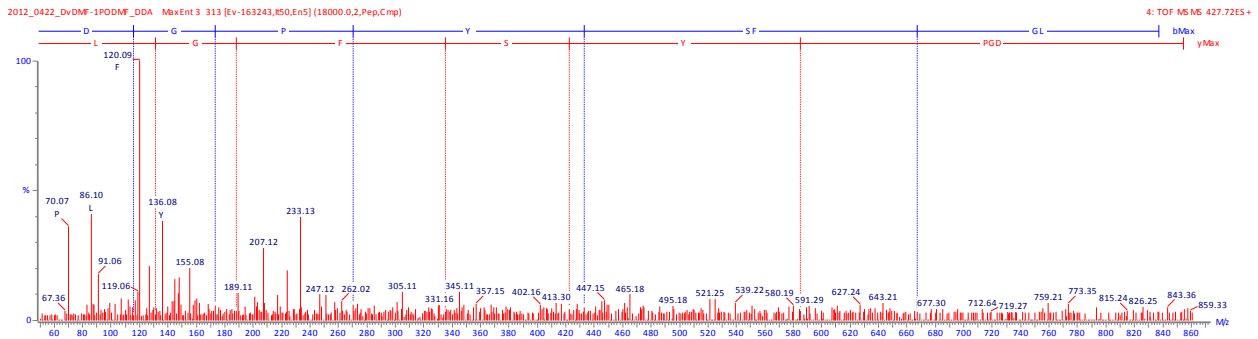
AST-A DPYAFGLa (m/z 781.3879)

MS/MS of m/z 391.19⁺² (PepSeq score = 44)



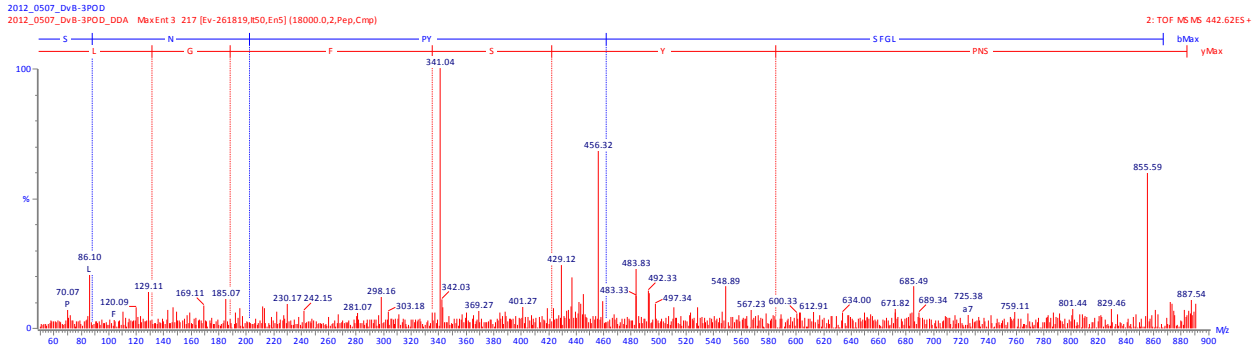
AST-A DGPYSFGLa (m/z 854.4458)

MS/MS of m/z 427.72⁺² (PepSeq score = 20)



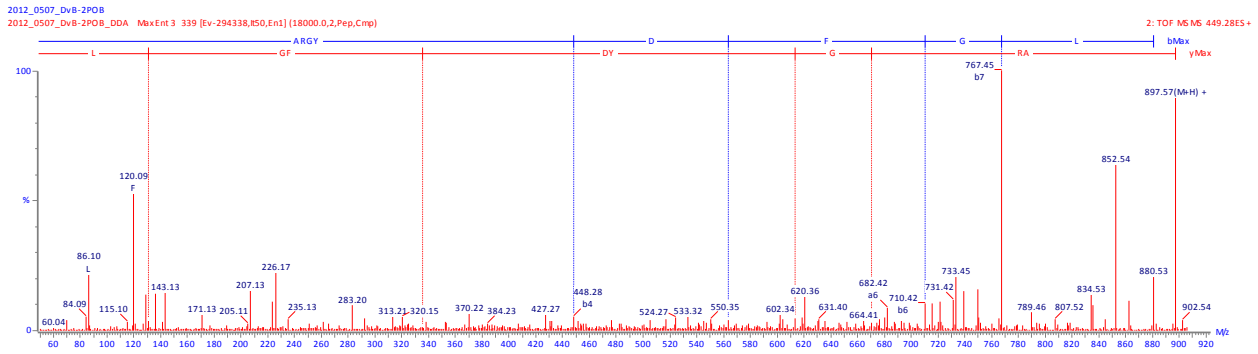
AST-A SNPYSFGLa (m/z 883.4308)

MS/MS of m/z 442.62⁺² (PepSeq score = 19)



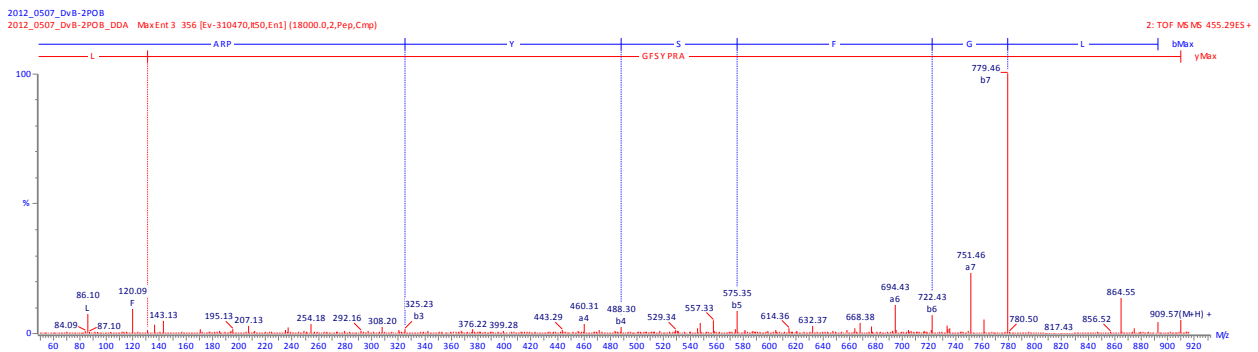
AST-A ARGYDFGLa (m/z 897.4577)

MS/MS of m/z 449.28⁺ (PepSeq score = 63)



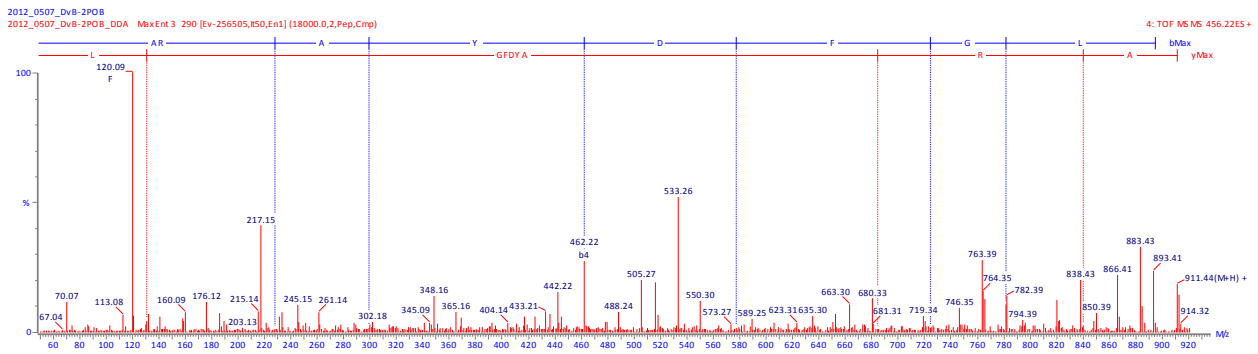
AST-A ARPYSFGLa (m/z 909.4941)

MS/MS of m/z 455.29⁺ (PepSeq score = 28)



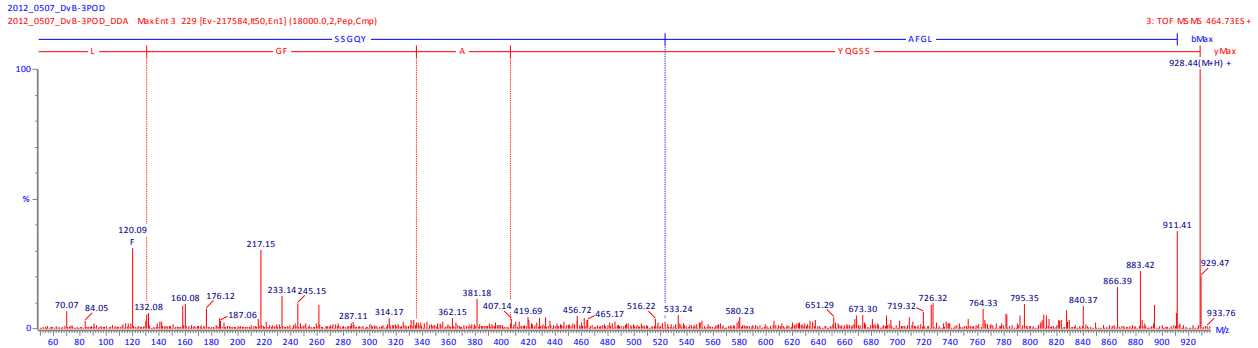
AST-A ARAYDFGLa (m/z 911.4734)

MS/MS of m/z 456.22⁺ (PepSeq score = 21)



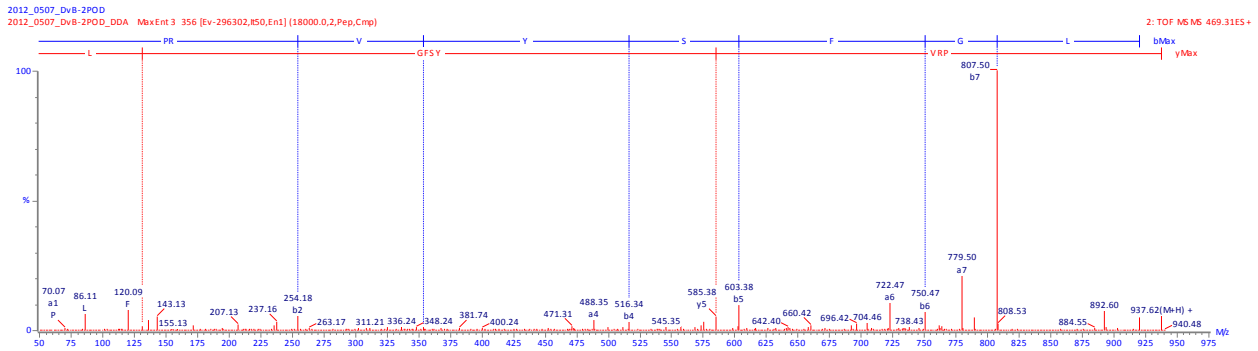
AST-A SSGQYAFGLa (m/z 928.4523)

MS/MS of m/z 464.73⁺² (PepSeq score =4)



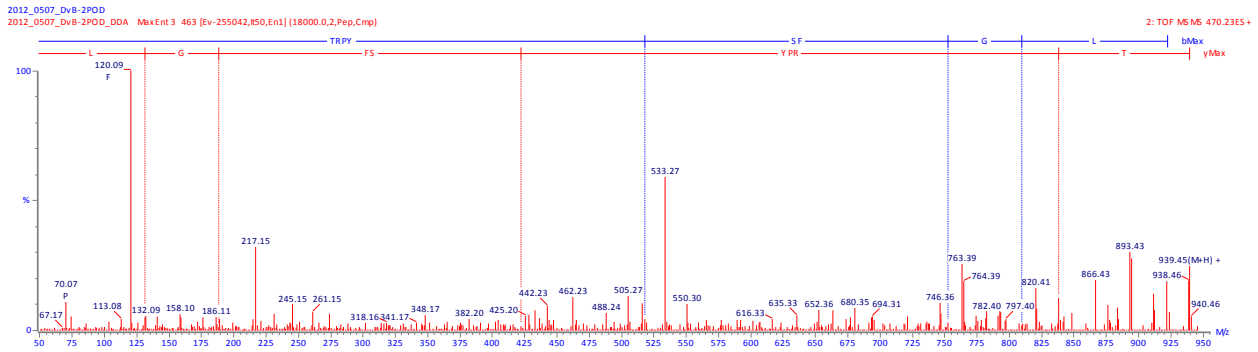
AST-A PRVYSFGLa (m/z 937.5254)

MS/MS of m/z 469.31⁺² (PepSeq score = 52)



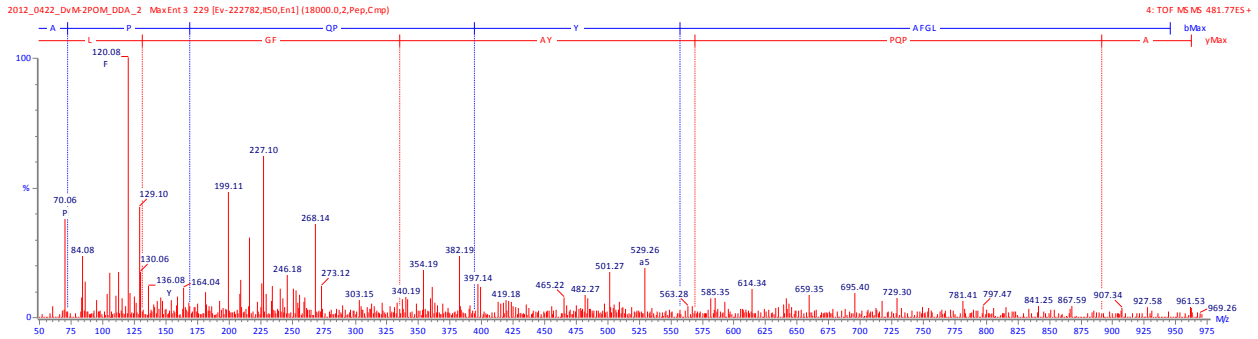
AST-A TRPYSFGLa (m/z 939.5047)

MS/MS of m/z 470.23⁺² (PepSeq score = 7)



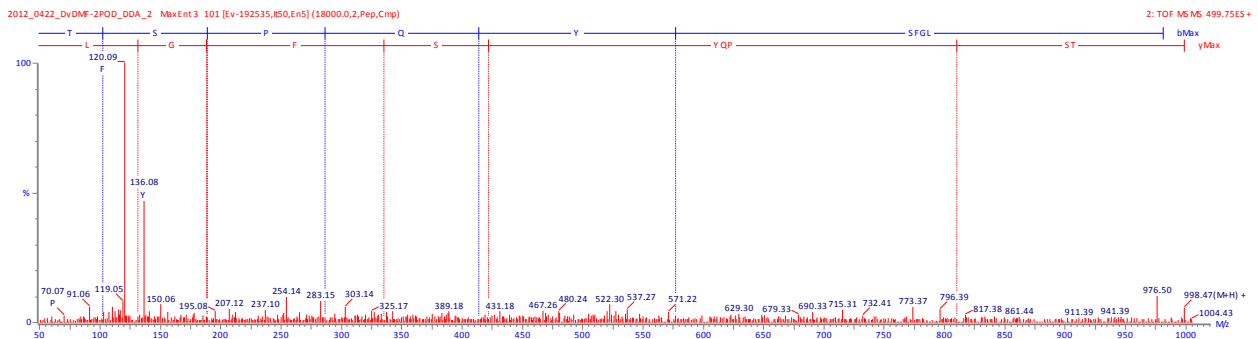
AST-A APQPYAFGLa (m/z 962.5094)

MS/MS of m/z 455.29⁺² (PepSeq score = 11)



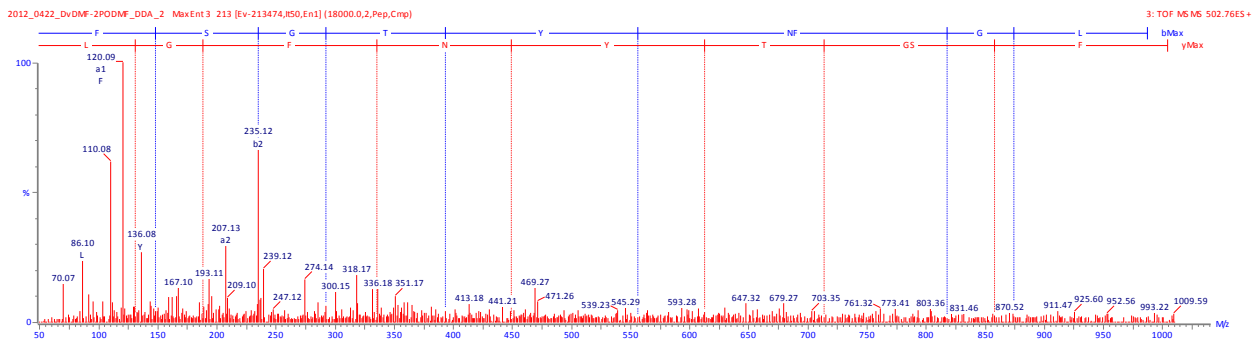
AST-A TSPQYSFGLa (m/z 998.4942)

MS/MS of m/z 499.75⁺² (PepSeq score = 8)



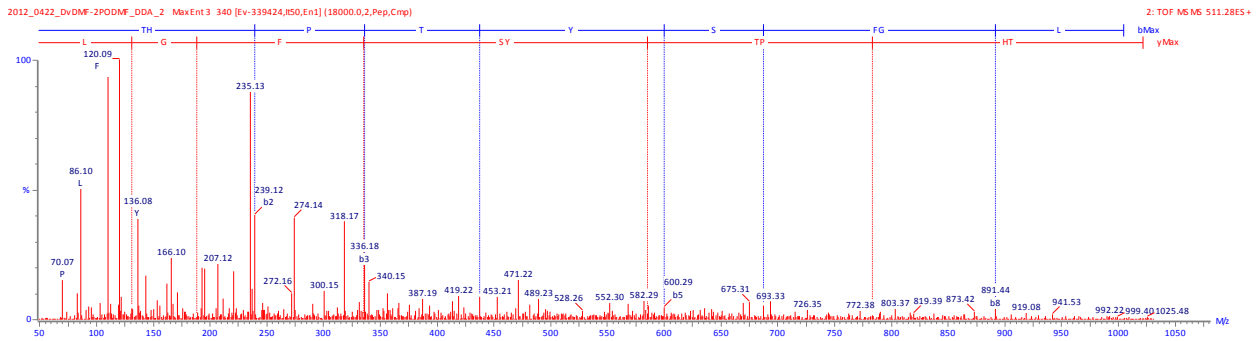
AST-A FSGTYNFGLa (m/z 1004.4836)

MS/MS of m/z 502.76⁺² (PepSeq score = 108)



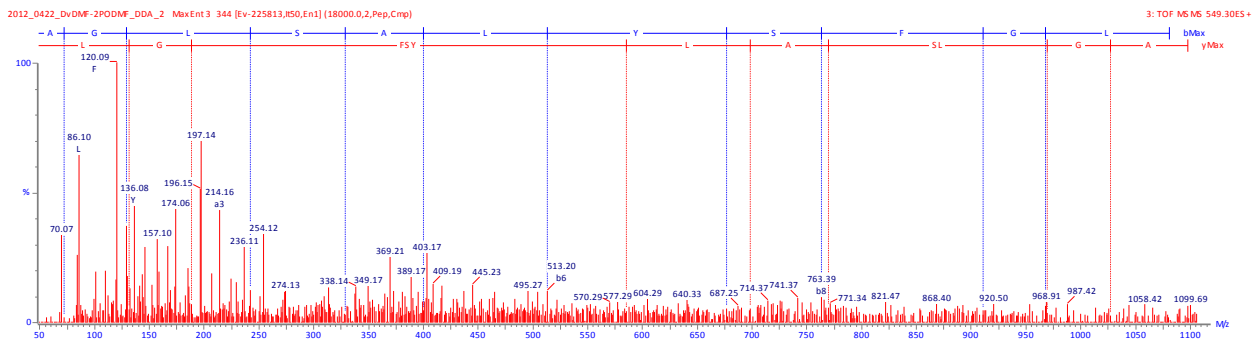
AST-A THPTYSFGLa (m/z 1021.5102)

MS/MS of m/z 511.28⁺² (PepSeq score = 87)



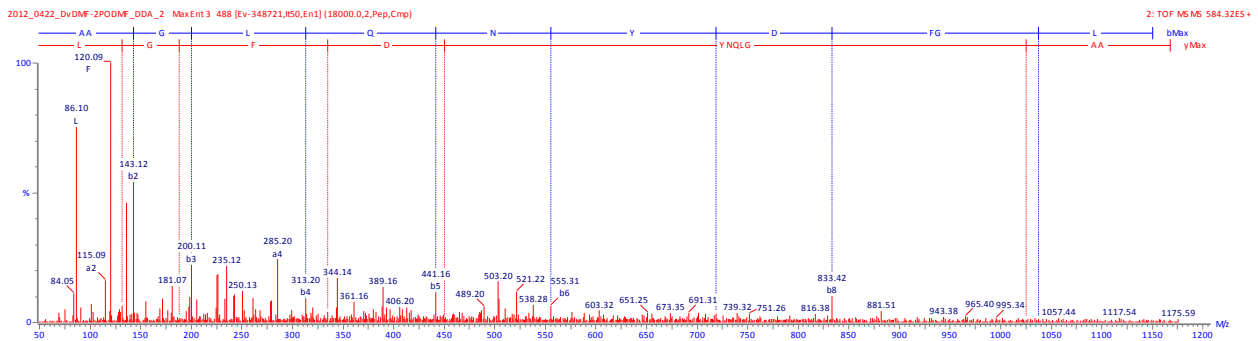
AST-A AGLSALYSFGLa (m/z 1097.5990)

MS/MS of m/z 549.30⁺² (PepSeq score = 180)



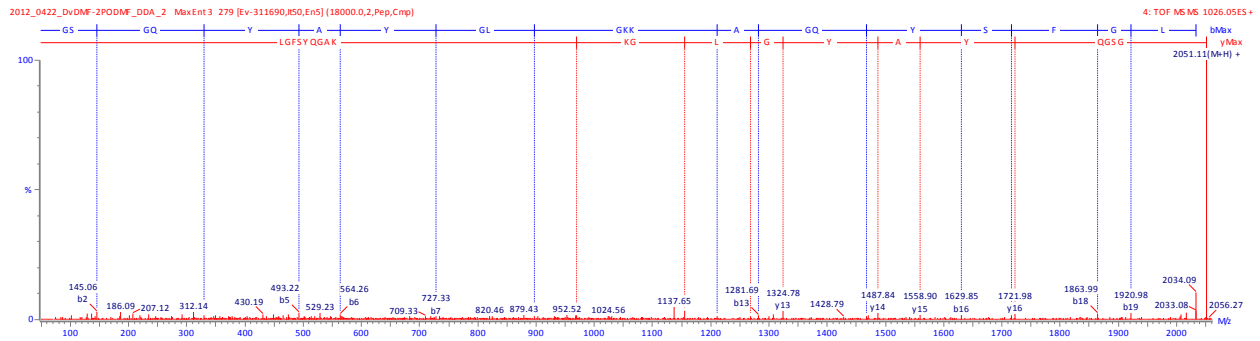
AST-A AAGLQNYDFGLa (m/z 1167.5793)

MS/MS of m/z 584.32⁺² (PepSeq score = 127)



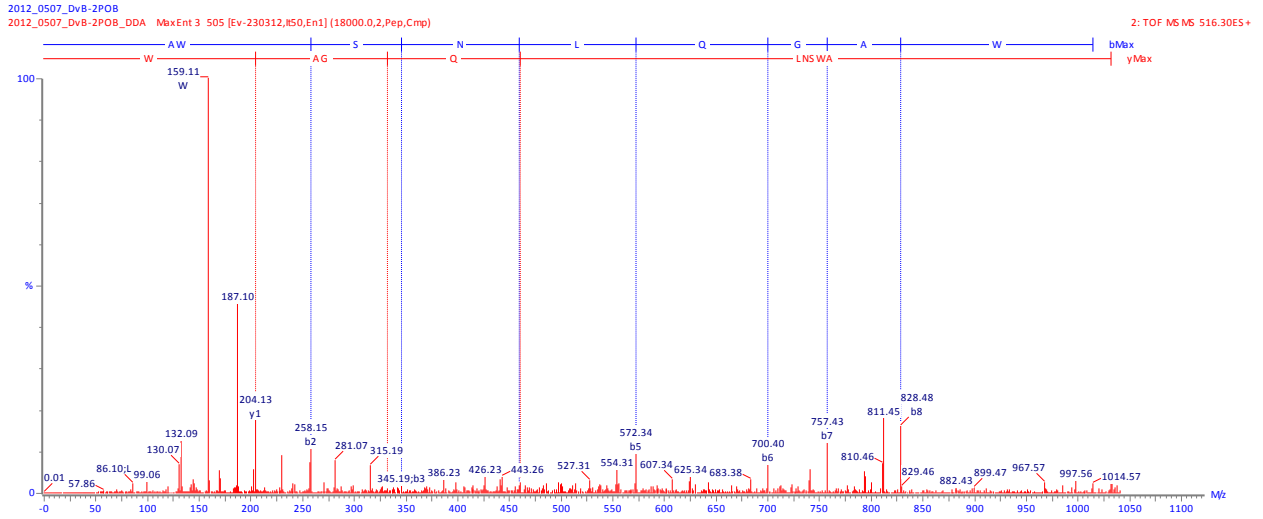
AST-A GSGQYAYGLGKKAGQYSFGLa (*m/z* 2051.0345)

MS/MS of *m/z* 1028.05⁺² (PepSeq score = 302)



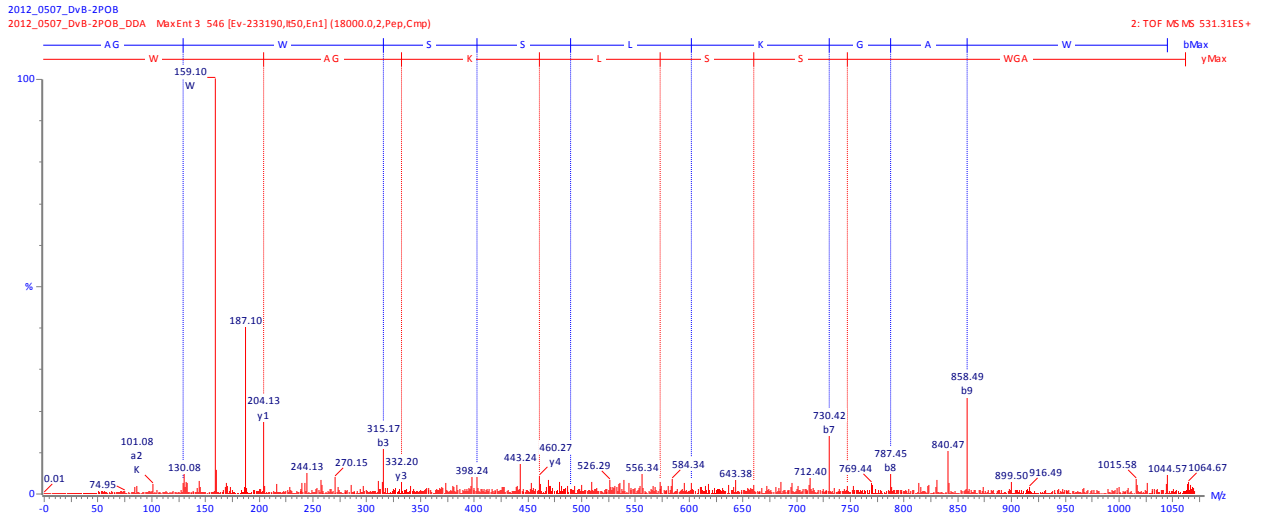
AST-B AWSNLQGAWa (m/z 1031.5057)

MS/MS of m/z 516.30 (PepSeq score = 54)



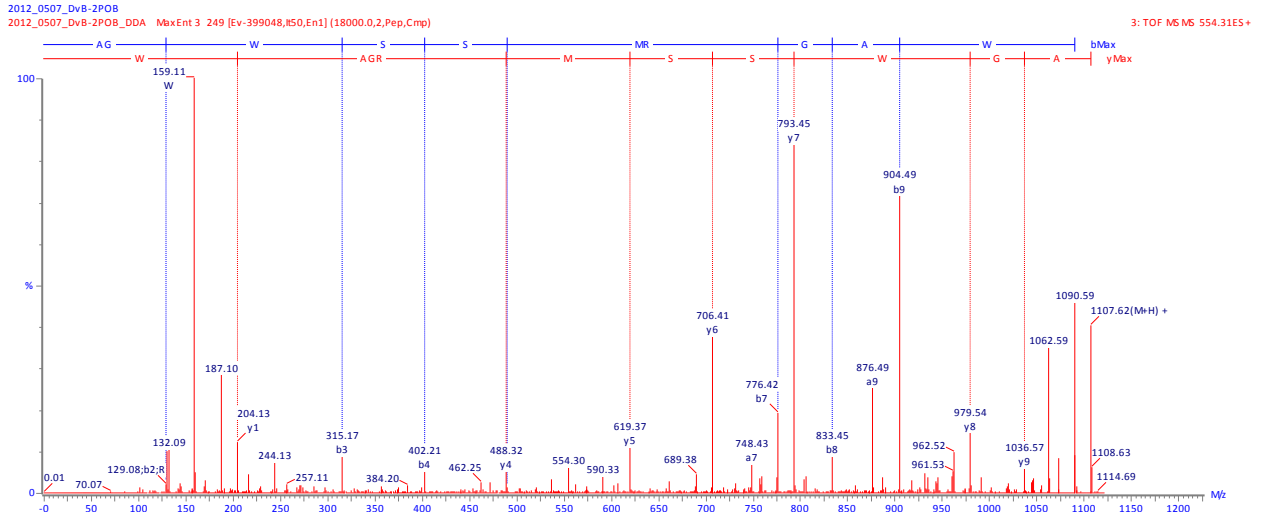
AST-B AGWSSLKGAWa (m/z 1061.5527)

MS/MS of m/z 531.28 (PepSeq score = 98)



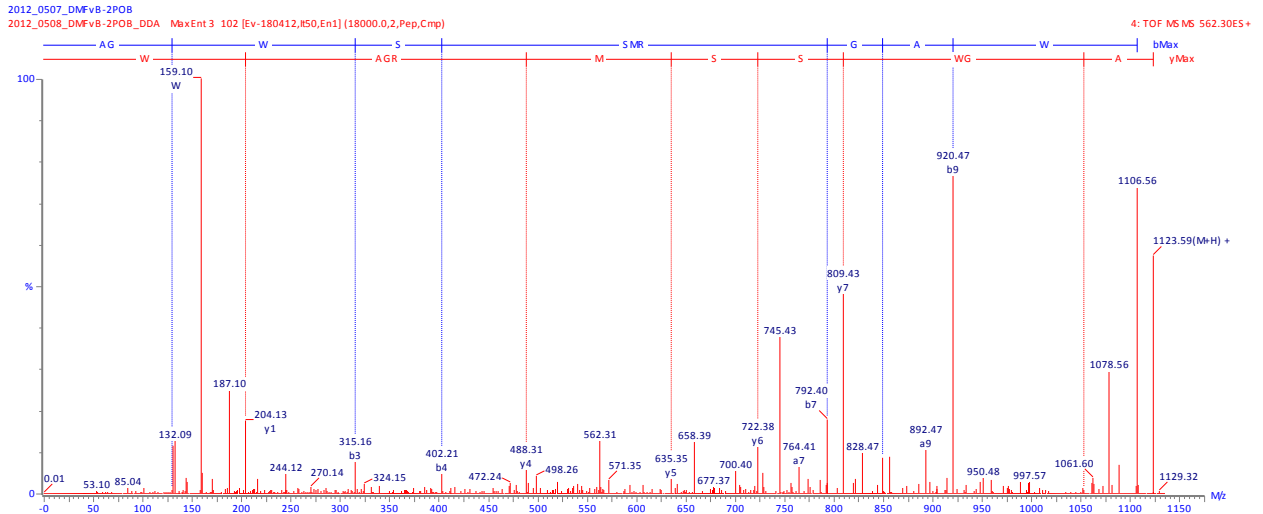
AST-B AGWSSMRGAWa (m/z 1107.5153)

MS/MS of m/z 554.26 (PepSeq score = 225)



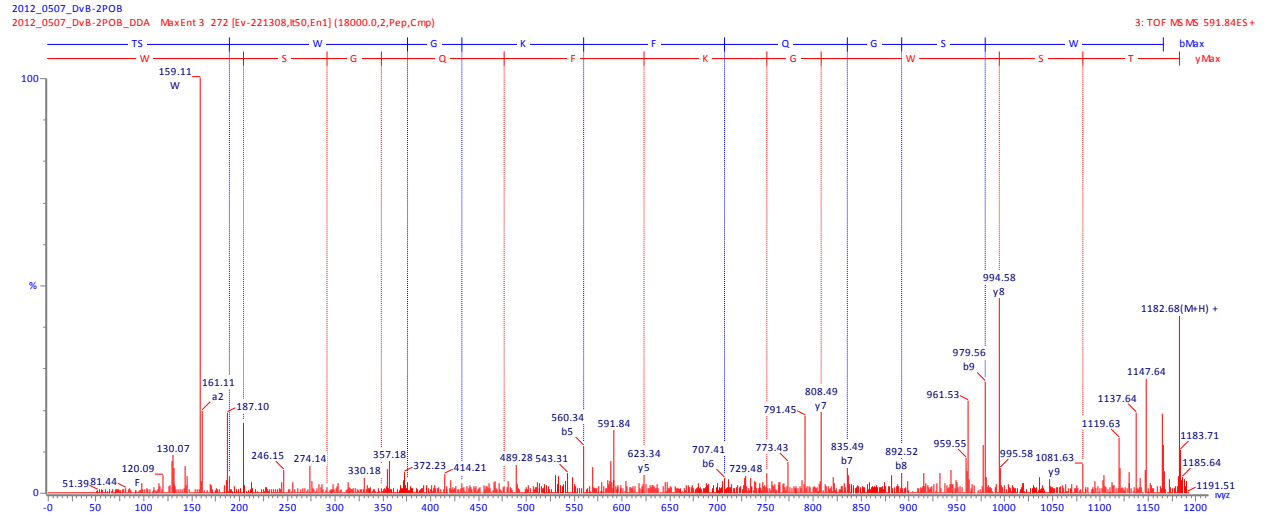
AST-B AGWSSM(O)RGAWa (m/z 1123.5102)

MS/MS of m/z 562.26 (PepSeq score = 119)



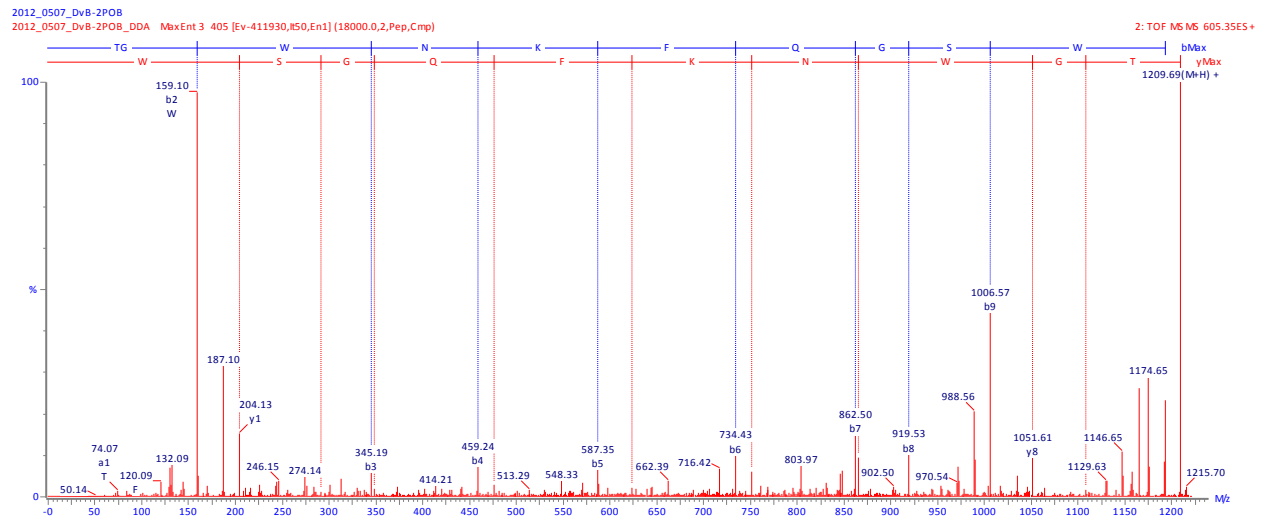
AST-B TSWGKFQGSWa (m/z 1182.5691)

MS/MS of m/z 591.78 (PepSeq score = 161)



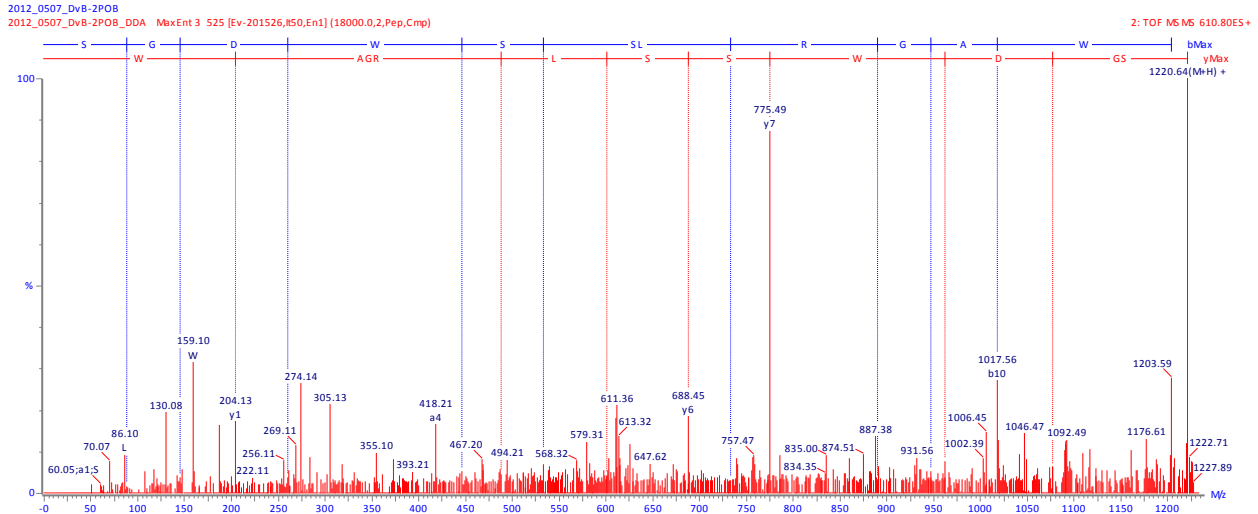
AST-B TGWNKFQGSWa (m/z 1209.5800)

MS/MS of m/z 605.29 (PepSeq score = 278)



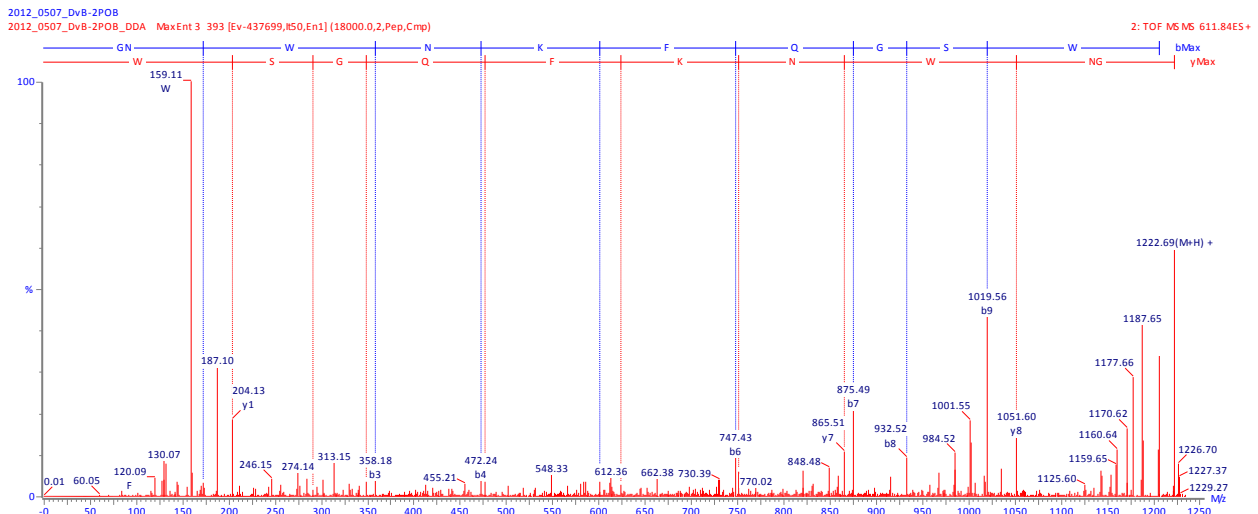
AST-B SGDWSSLRGAWa (m/z 1220.5807)

MS/MS of m/z 610.79 (PepSeq score = 331)



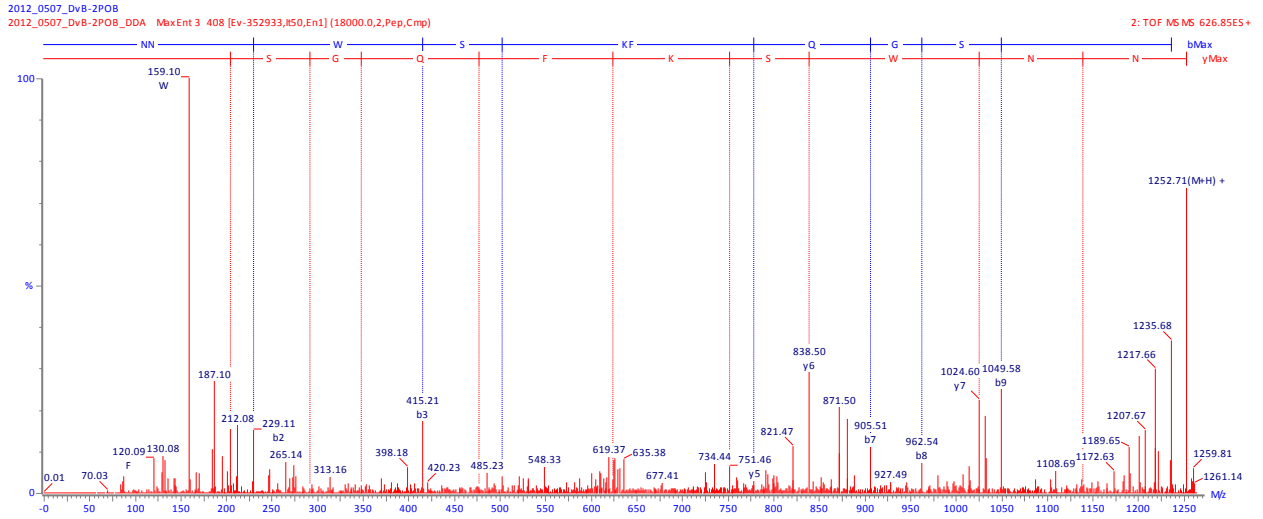
AST-B GNWNKFQGSWa (m/z 1222.5752)

MS/MS of m/z 611.79 (PepSeq score = 157)



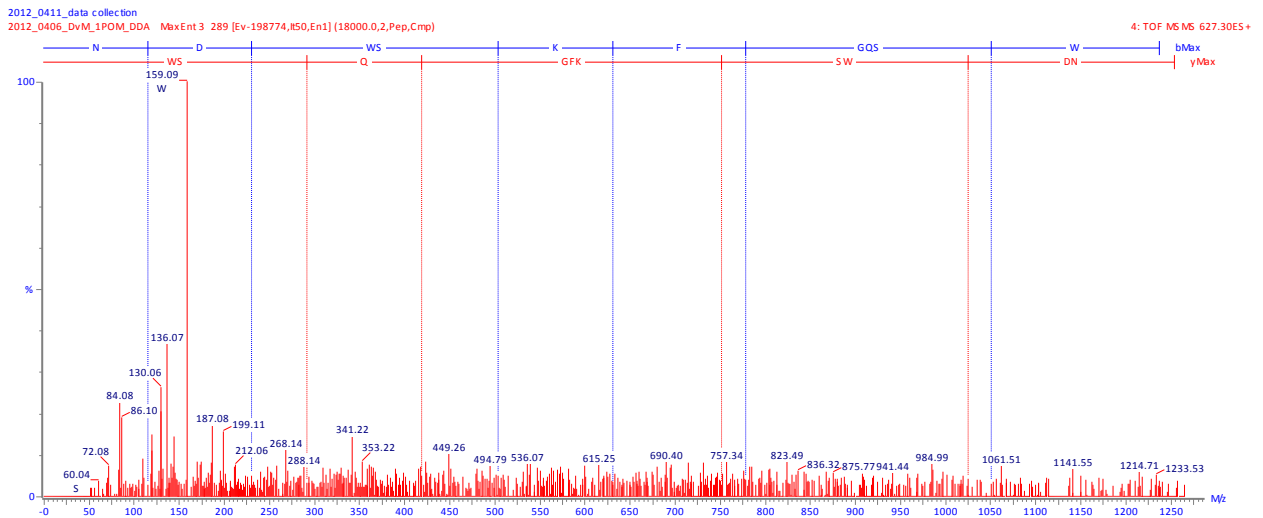
AST-B NNWSKFQGSWa (m/z 1252.5858)

MS/MS of m/z 626.79 (PepSeq score = 220)



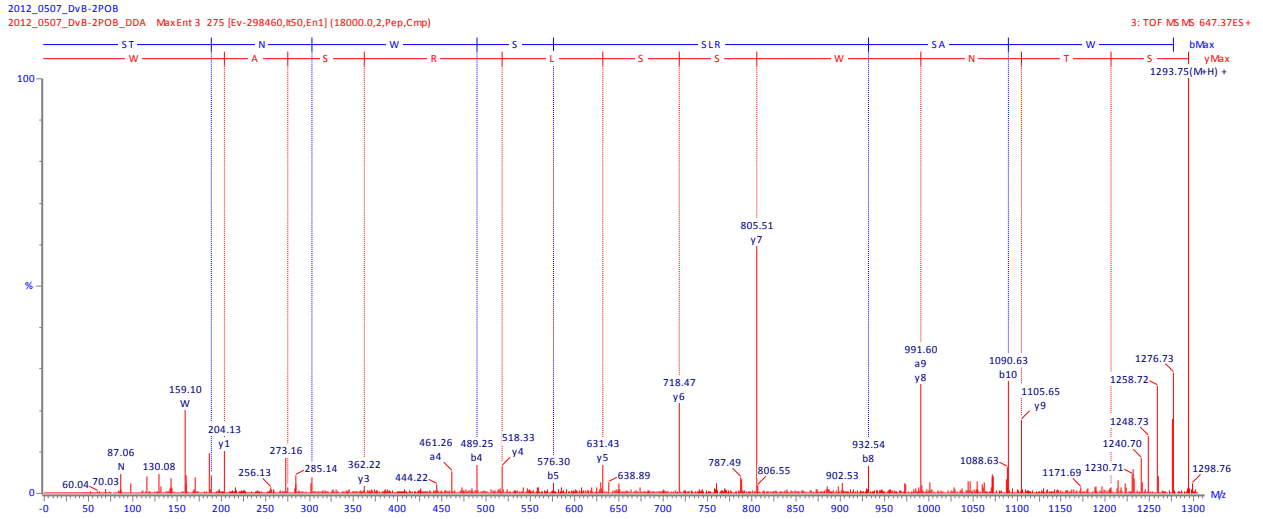
AST-B NDWSKFGQSWa (m/z 1253.5698)

MS/MS of m/z 627.28 (PepSeq score = 20)



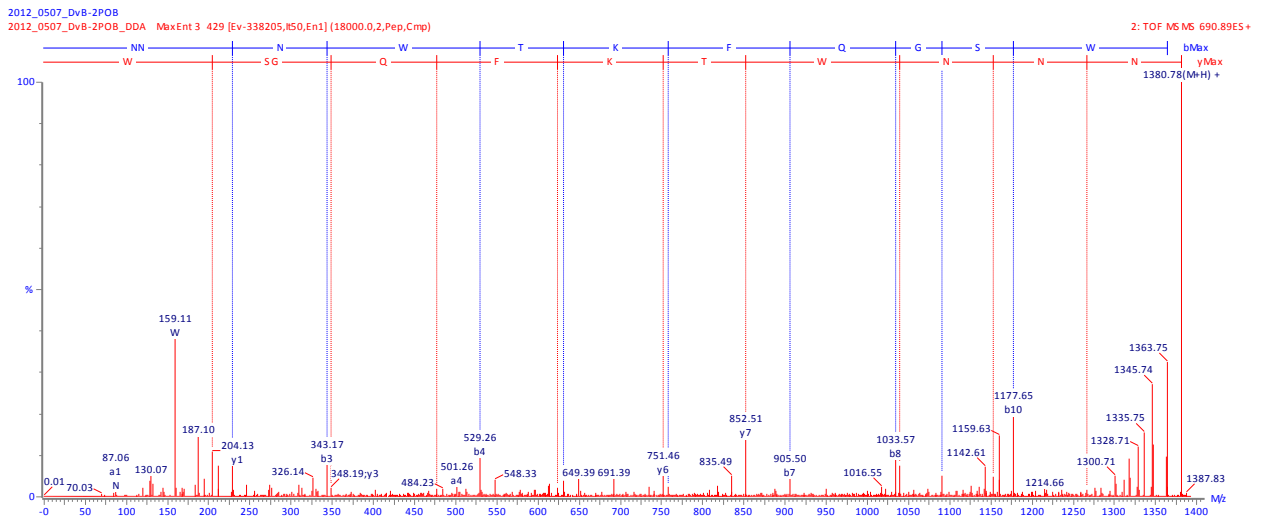
AST-B STNWSSLRSaW (m/z 1293.6335)

MS/MS of m/z 647.32 (PepSeq score = 282)



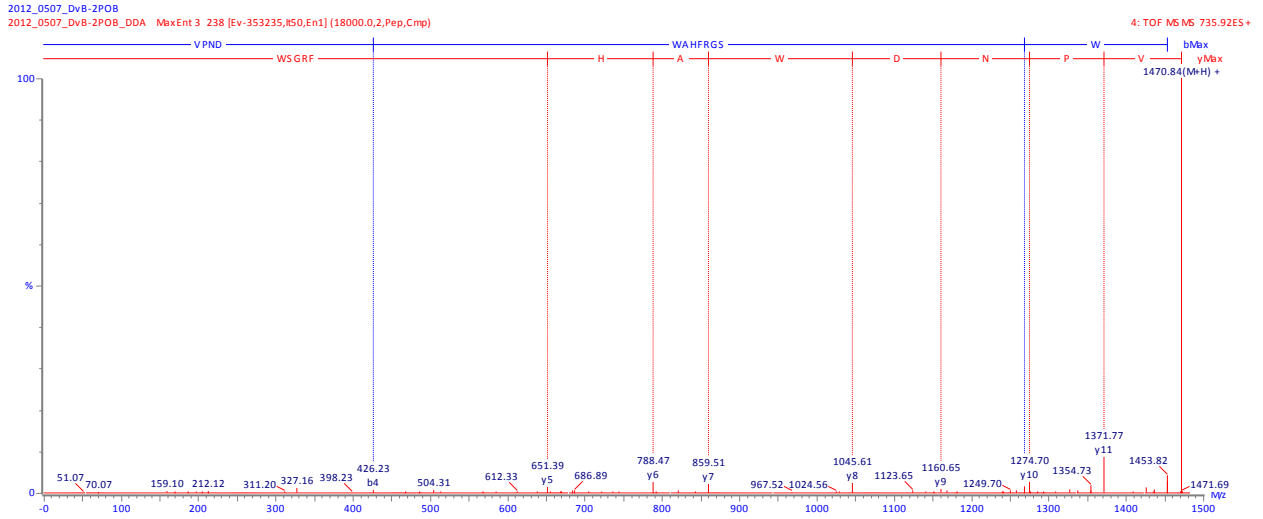
AST-B NNNWTKFQGSWa (m/z 1380.6444)

MS/MS of m/z 690.82 (PepSeq score = 329)



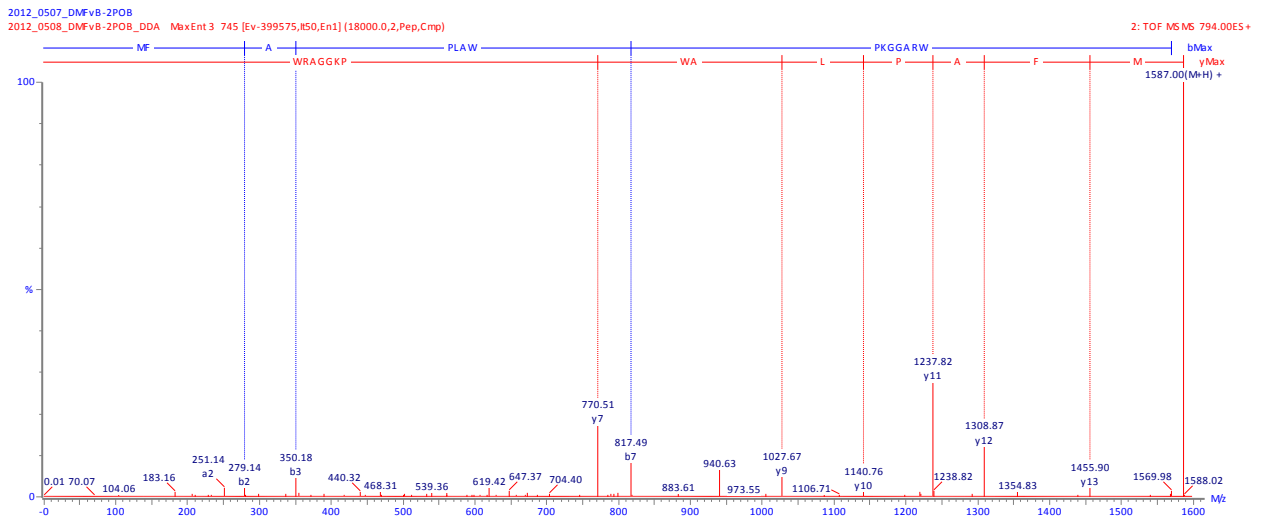
AST-B VPNDWAHFRGSWa (m/z 1470.7025)

MS/MS of m/z 735.85 (PepSeq score = 29)



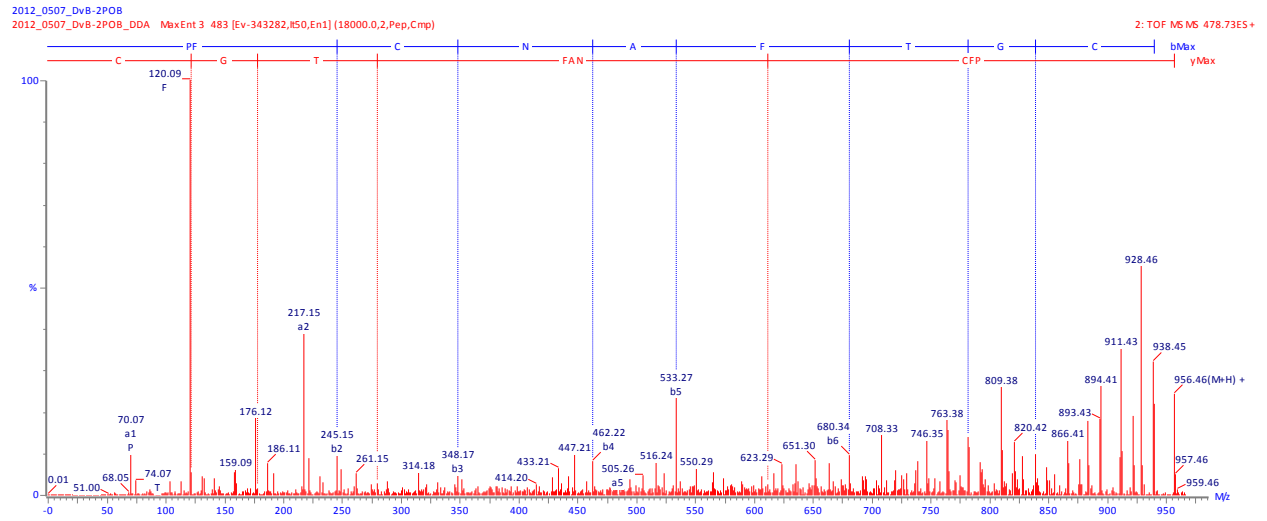
AST-B MFAPLAWPKGGARWAa (m/z 1586.8413)

MS/MS of m/z 793.92 (PepSeq score = 29)



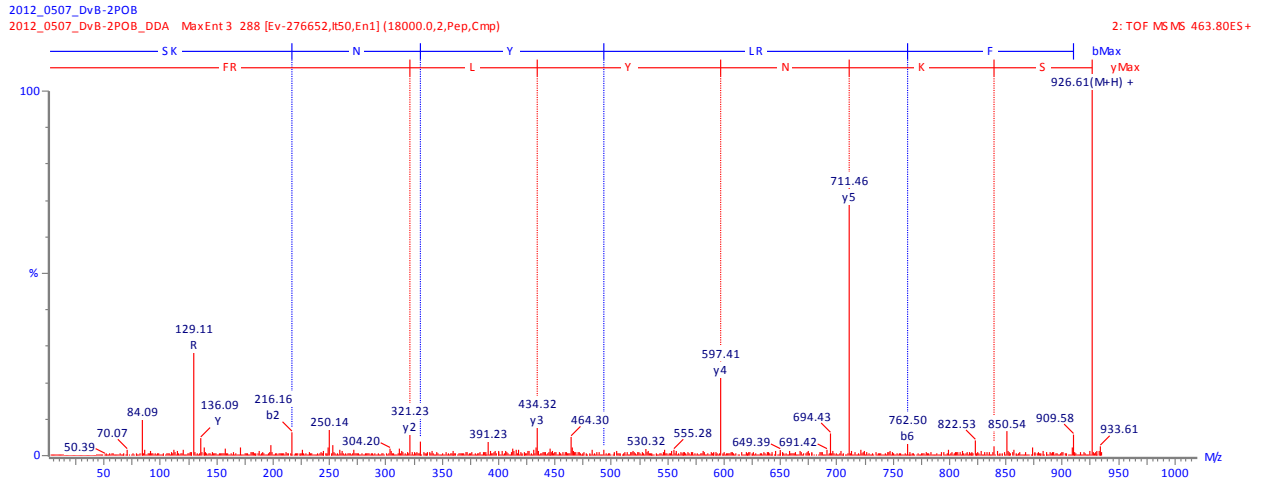
CCAP PFCNAFTGCa (m/z 956.3753)

MS/MS of m/z 478.69 (PepSeq score = 63)



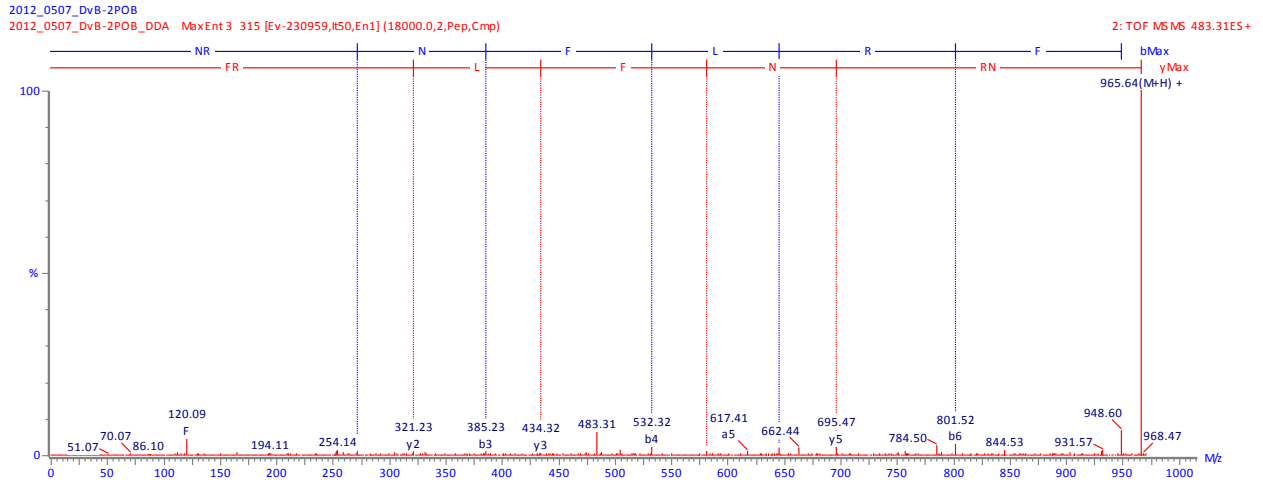
FLP-SKNYLRF (m/z 926.5207)

MS/MS of m/z 463.80²⁺ (PepSeq score = 62)



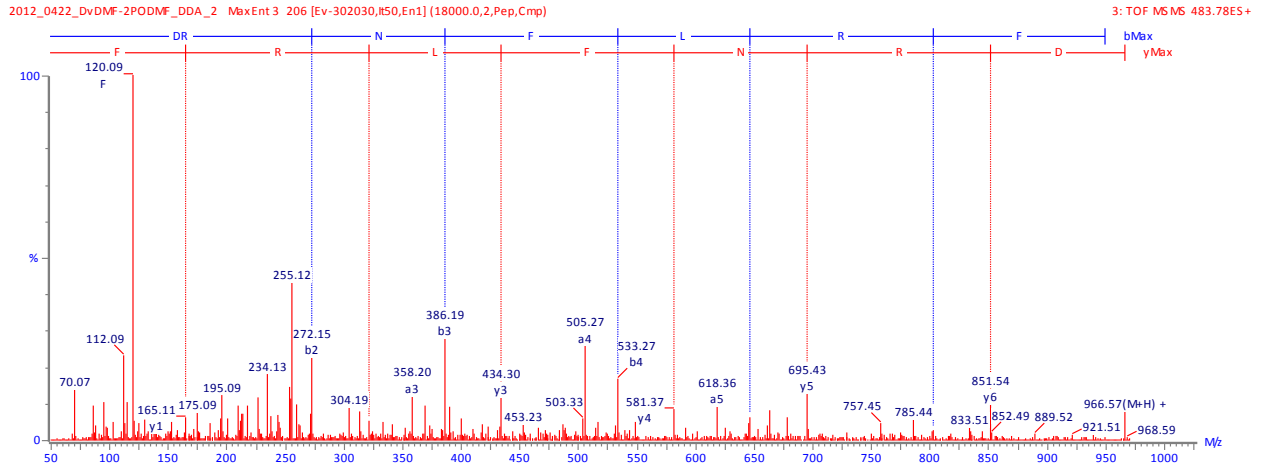
FLP-NRNFLRFa (m/z 965.5428)

MS/MS of m/z 483.31²⁺ (PepSeq score = 53)



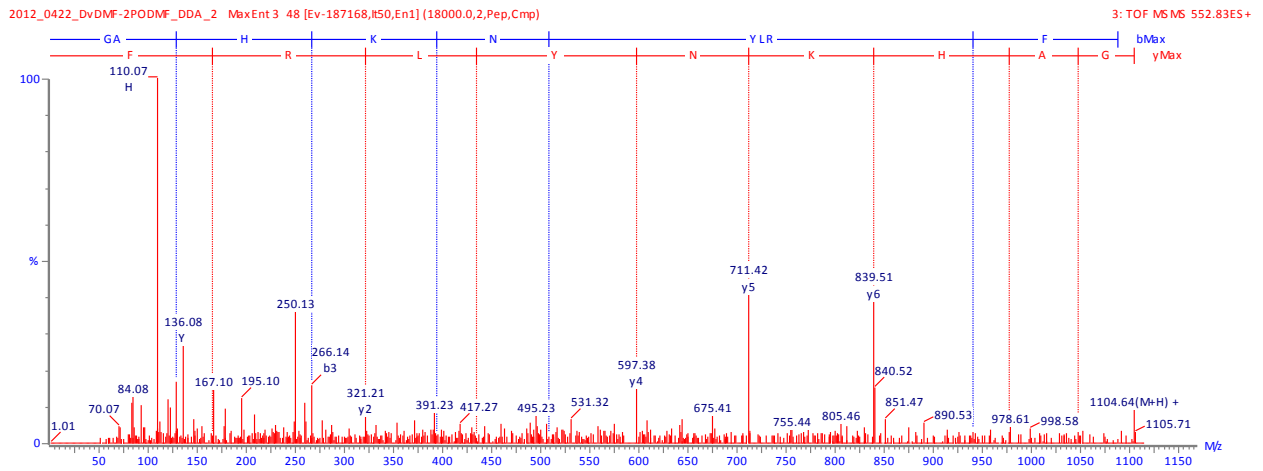
FLP-DRNFLRFa (m/z 966.5268)

MS/MS of m/z 483.78²⁺ (PepSeq score = 135)



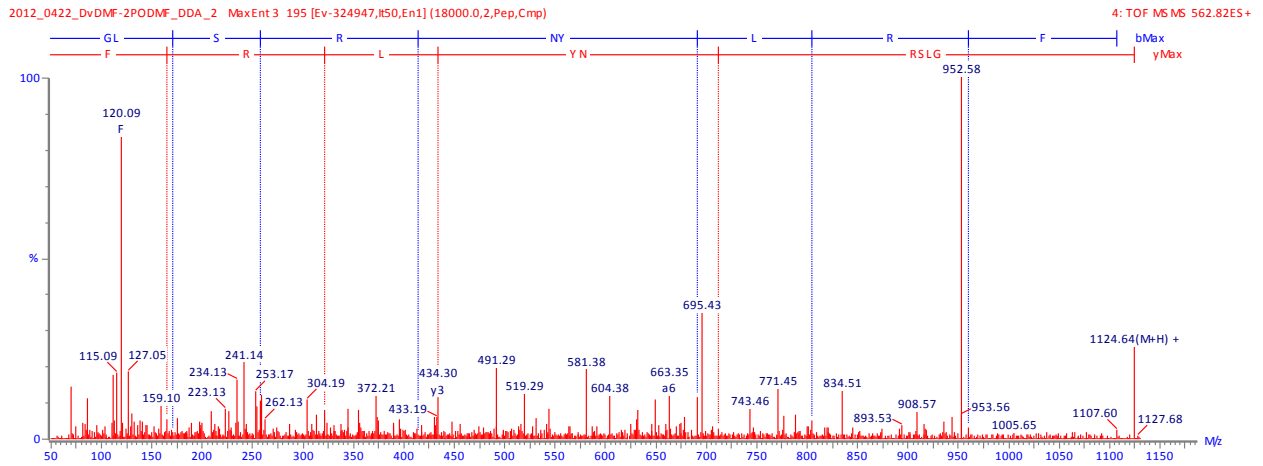
FLP-GAHKNYLRFa (m/z 1104.6061)

MS/MS of m/z 552.83²⁺ (PepSeq score = 132)



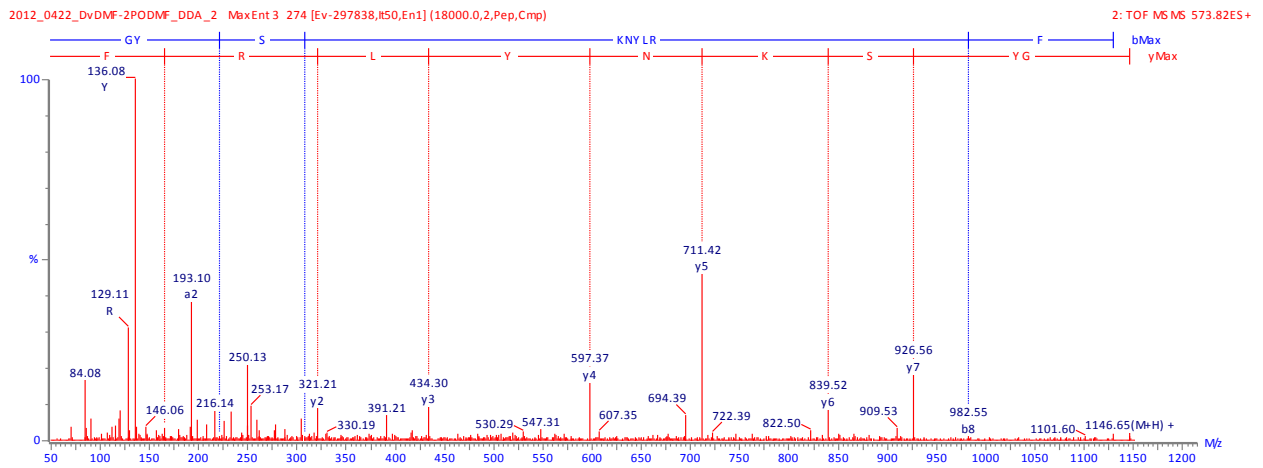
FLP-GLSRNYLRFa (m/z 1124.6323)

MS/MS of m/z 562.82²⁺ (PepSeq score = 47)



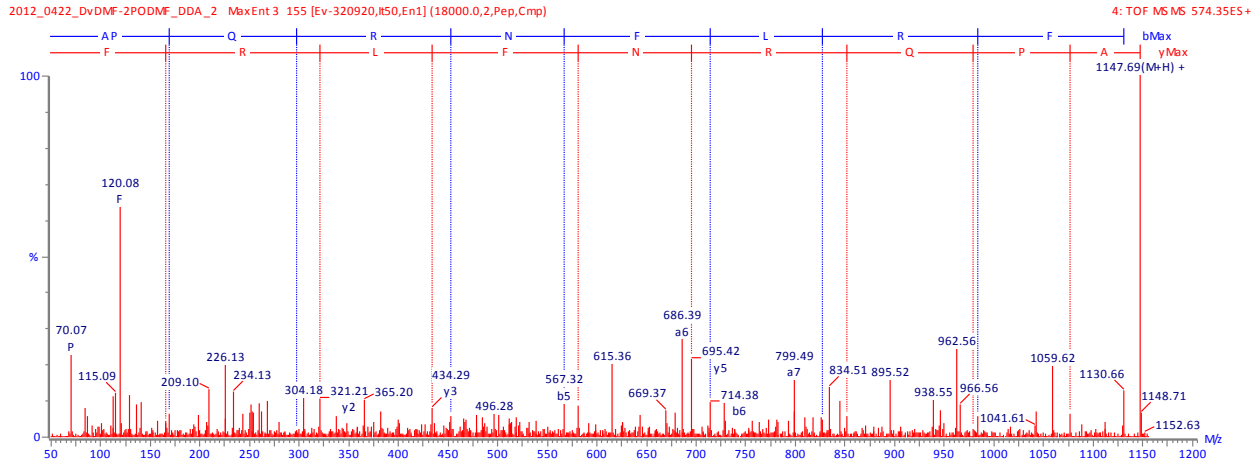
FLP-GYSKNYLRFa (m/z 1146.6055)

MS/MS of m/z 573.82²⁺ (PepSeq score = 73)



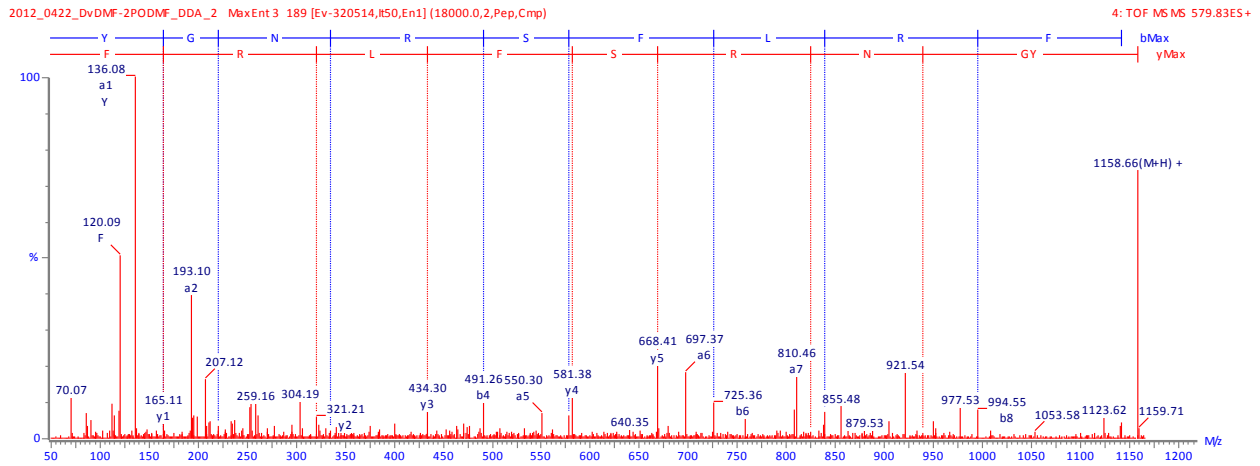
FLP-APQRNFLRFa (m/z 1147.6483)

MS/MS of m/z 574.3242²⁺ (PepSeq score = 259)



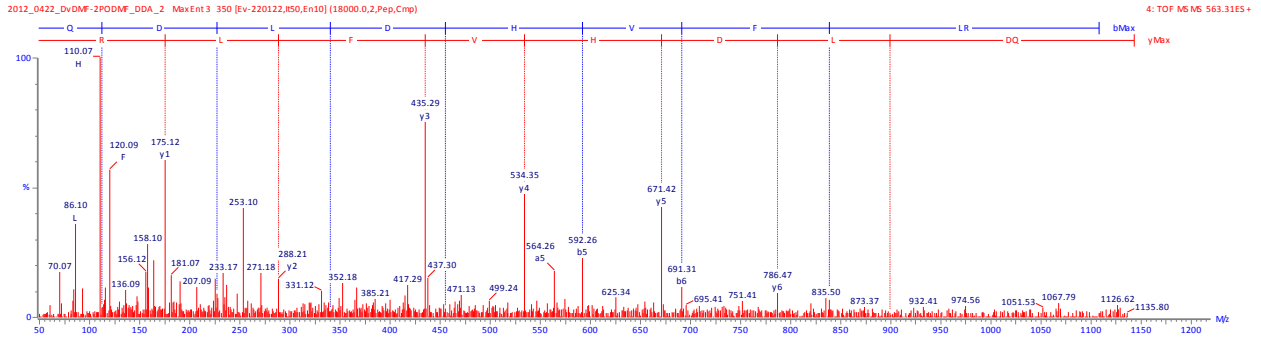
FLP-YGNRSFLRFa (m/z 1158.6167)

MS/MS of m/z 579.82²⁺ (PepSeq score = 142)



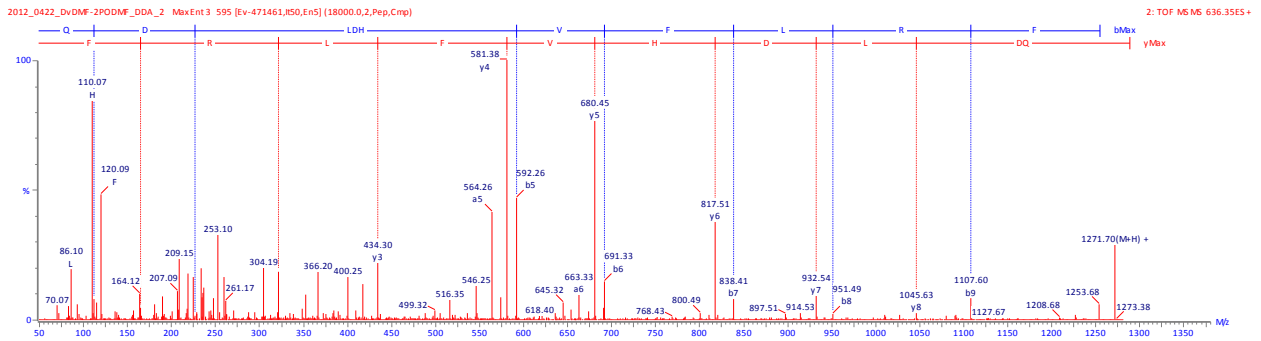
Myosuppressin pQLDHSVFLR (m/z 1125.5687)

MS/MS of m/z 563.31 (PepSeq score = 434)



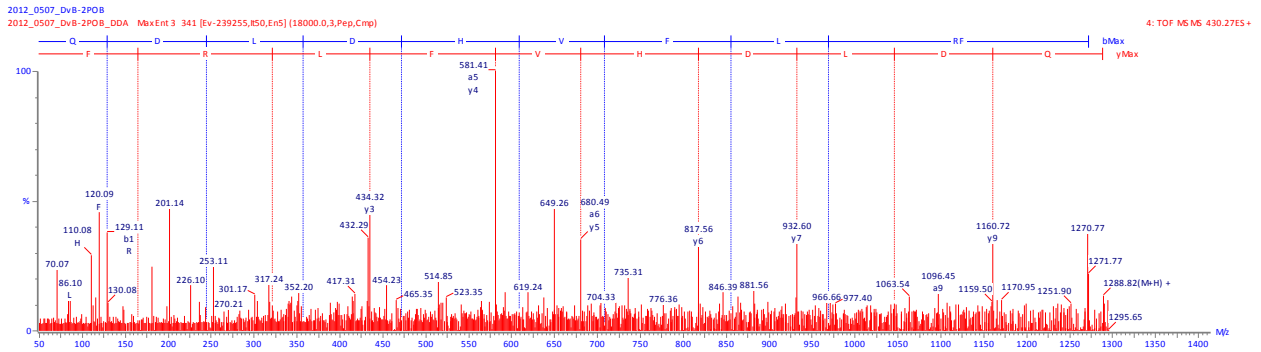
Myosuppressin pQLDHSVFLRFa (m/z 1271.6531)

MS/MS of m/z 636.35 (PepSeq score = 213)



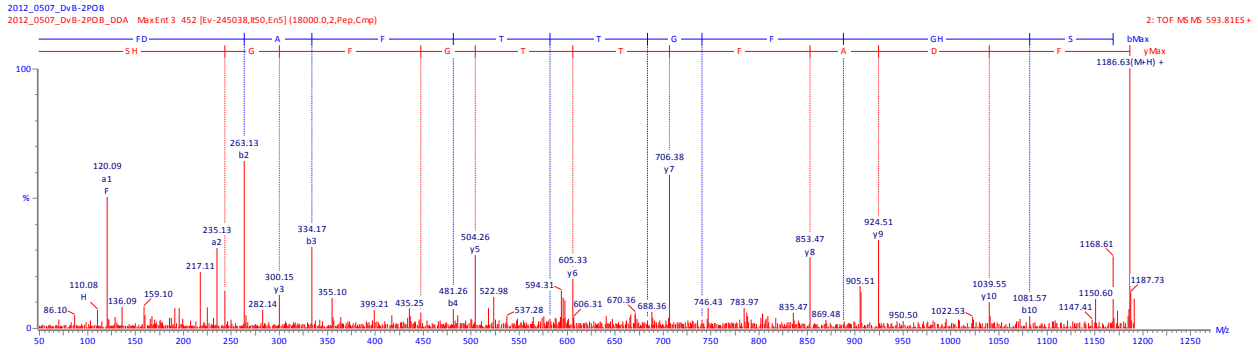
Myosuppressin QLDHVFLRFa (m/z 1288.6797)

MS/MS of m/z 430.27 (PepSeq score = 581)



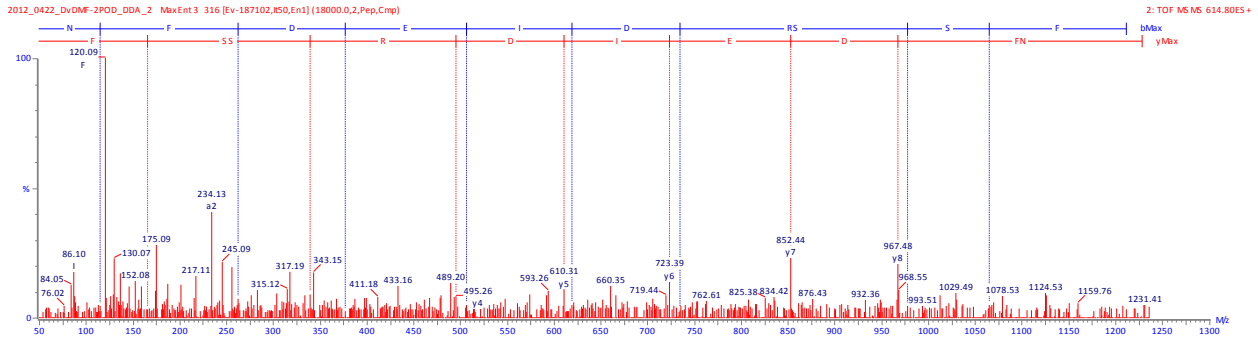
Orcomyotropin FDAFTTGFHGS (m/z 1186.5164)

MS/MS of m/z 593.81 (PepSeq score = 623)



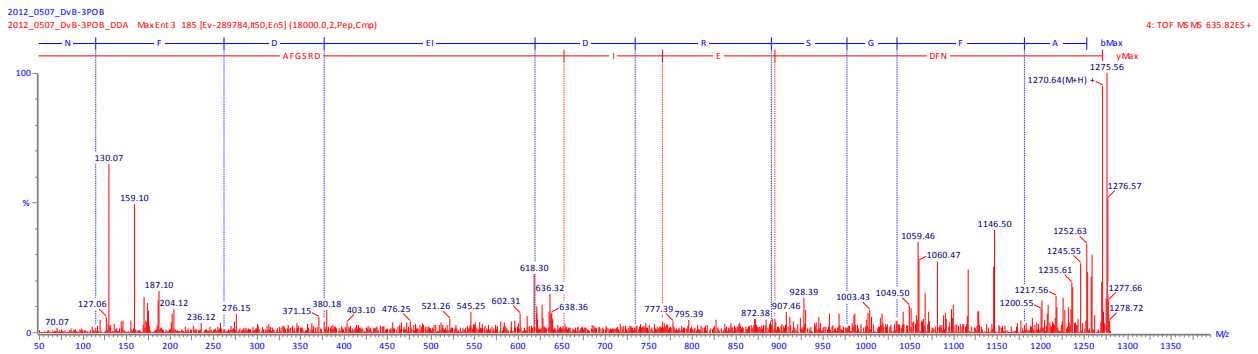
Orcokinin NFDEIDRSSFa (m/z 1228.5593)

MS/MS of m/z 614.80 (PepSeq score = 171)



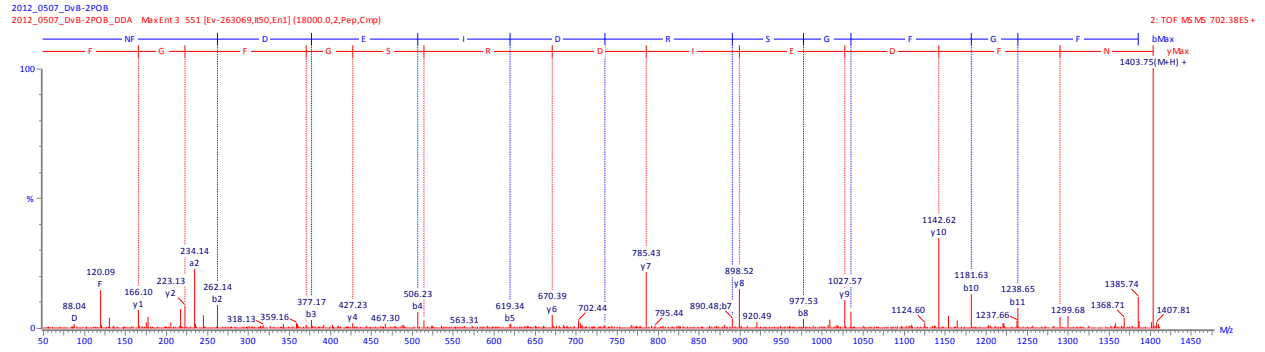
Orcokinin NFDEIDRSGFA (m/z 1270.5699)

MS/MS of m/z 635.82 (PepSeq score = 21)



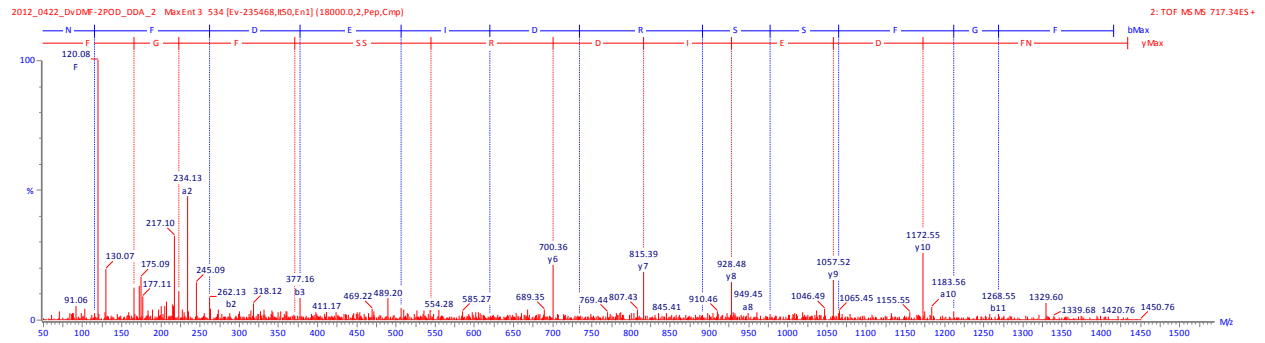
Orcokinin NFDEIDRSGFGF (m/z 1403.6226)

MS/MS of m/z 702.38 (PepSeq score = 480)



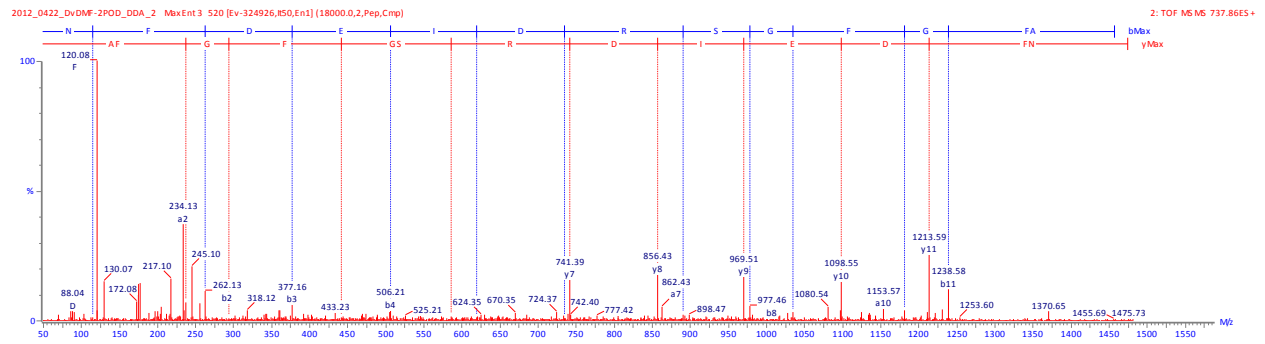
Orcokinin NFDEIDRSSFGF (m/z 1433.6332)

MS/MS of m/z 717.34 (PepSeq score = 354)



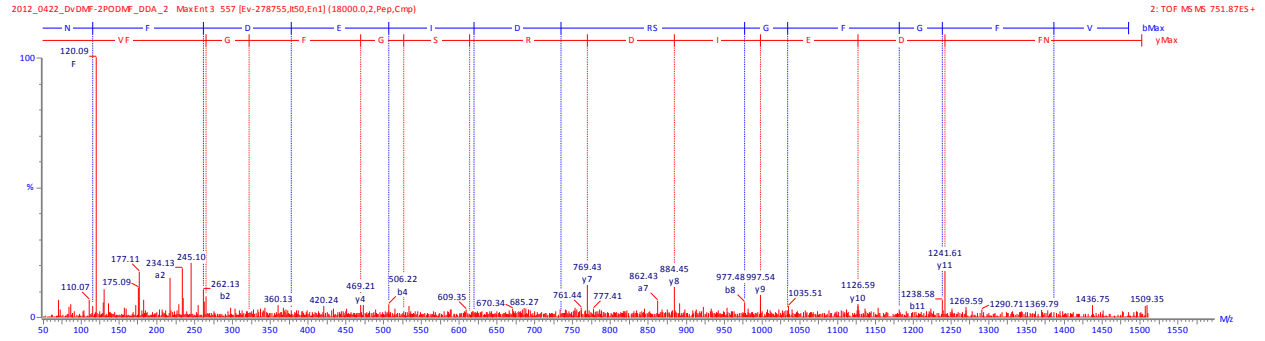
Orcokinin NFDEIDRSGFGFA (m/z 1474.6597)

MS/MS of m/z 737.86 (PepSeq score = 204)



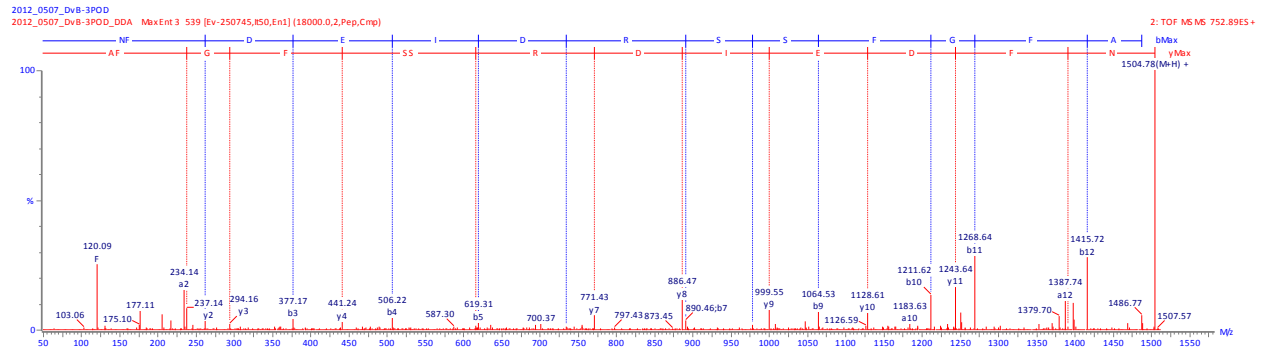
Orcokinin NFDEIDRSGFGFV (m/z 1502.6910)

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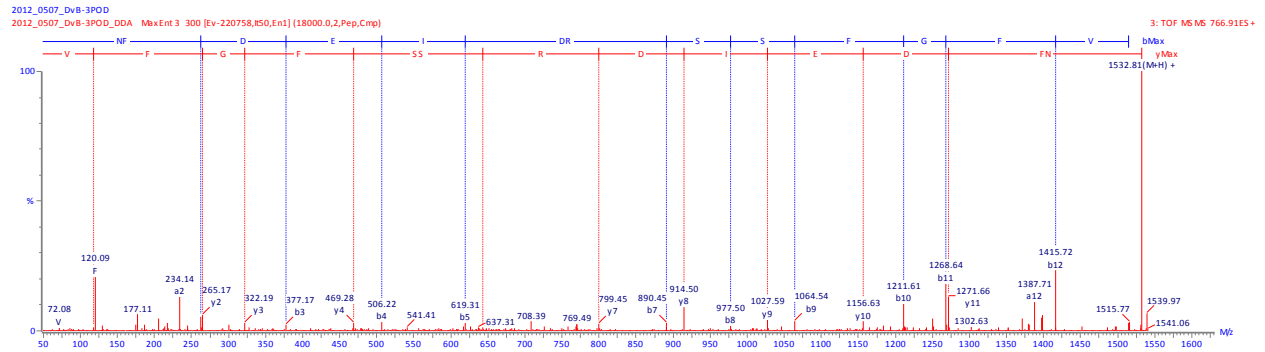
Orcokinin NFDEIDRSSFGFA (m/z 1504.6703)

MS/MS of m/z 752.89 (PepSeq score = 403)



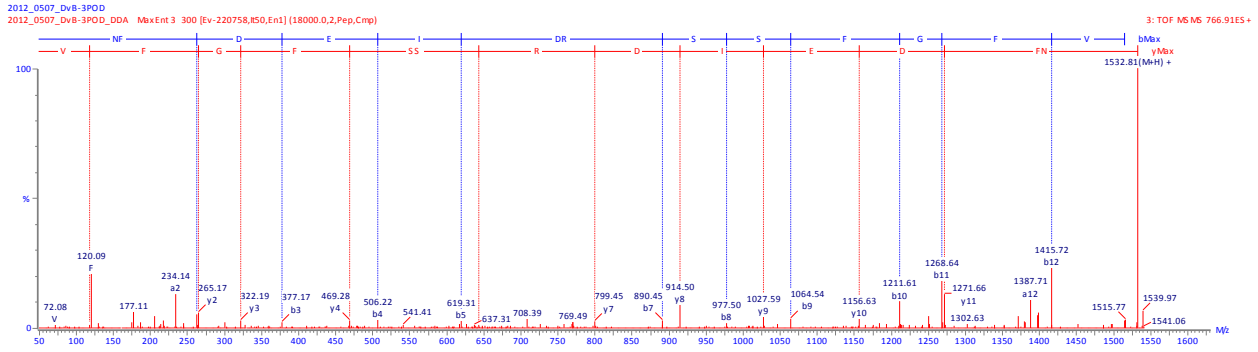
Orcokinin NFDEIDRSSFGFV (m/z 1532.7016)

MS/MS of m/z 766.91 (PepSeq score = 313)



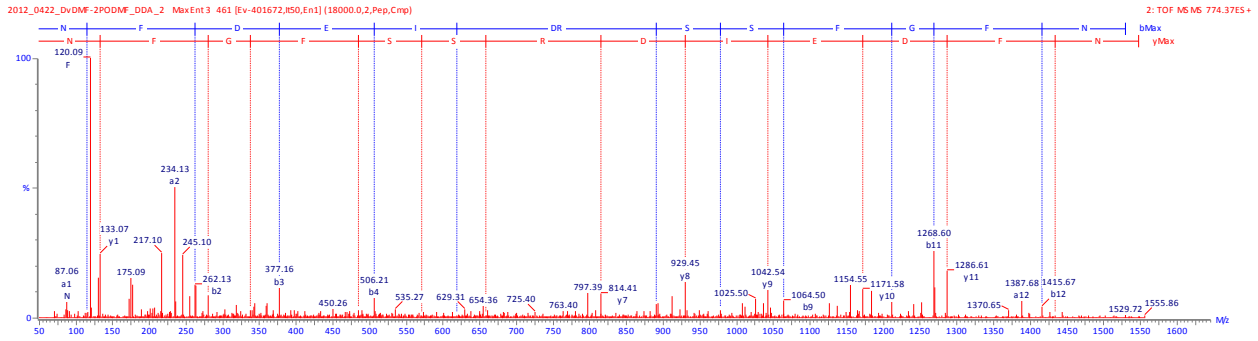
Orcokinin NFDEIDRSSFGFV (m/z 1532.7016)

MS/MS of m/z 766.91 (PepSeq score = 313)



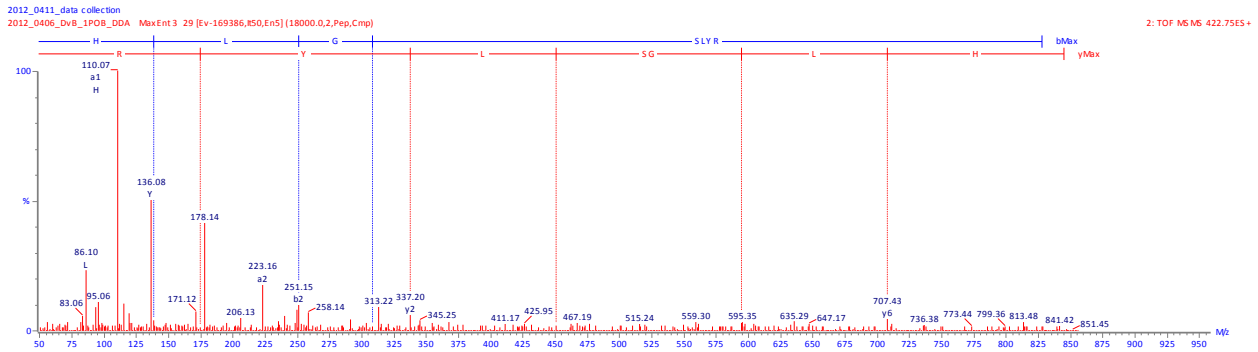
Orcokinin NFDEIDRSSFGFN (m/z 1547.6815)

MS/MS of m/z 774.37 (PepSeq score = 555)



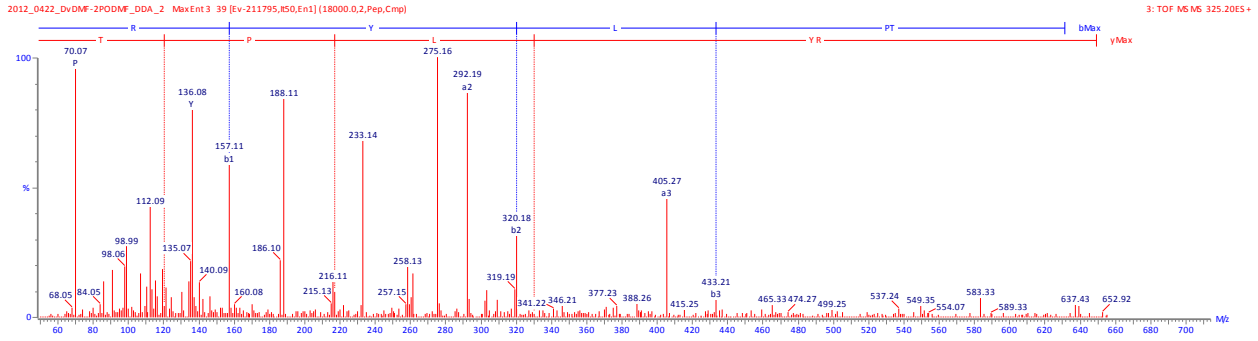
Other peptide: HLGSLKYRa (m/z 844.4788)

MS/MS of m/z 422.75 (PepSeq score = 11)



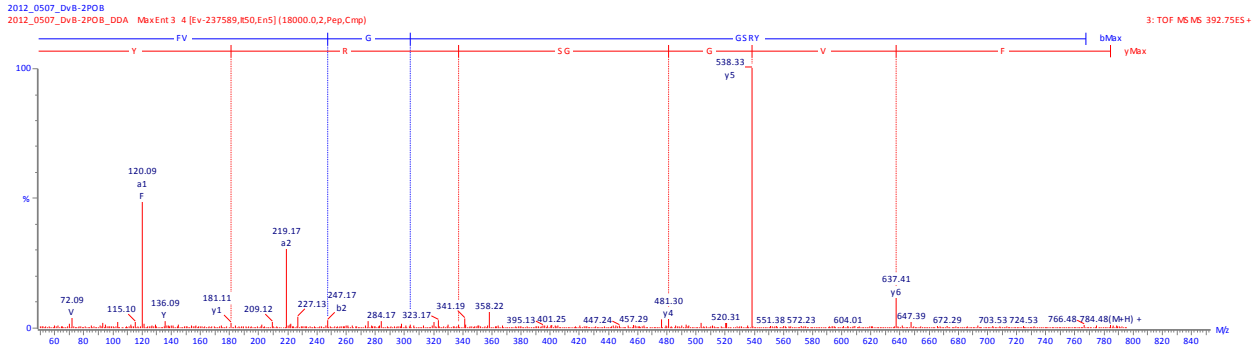
Proctolin RYLPT (m/z 649.3668)

MS/MS of m/z 325.20 (PepSeq score = 36)



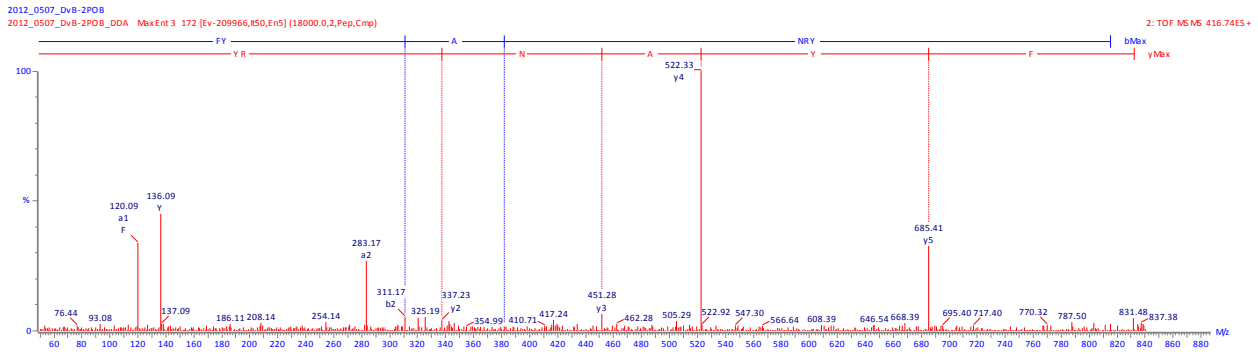
RYamide FVGGSRYa (m/z 784.4101)

MS/MS of m/z 392.75 (PepSeq score = 28)



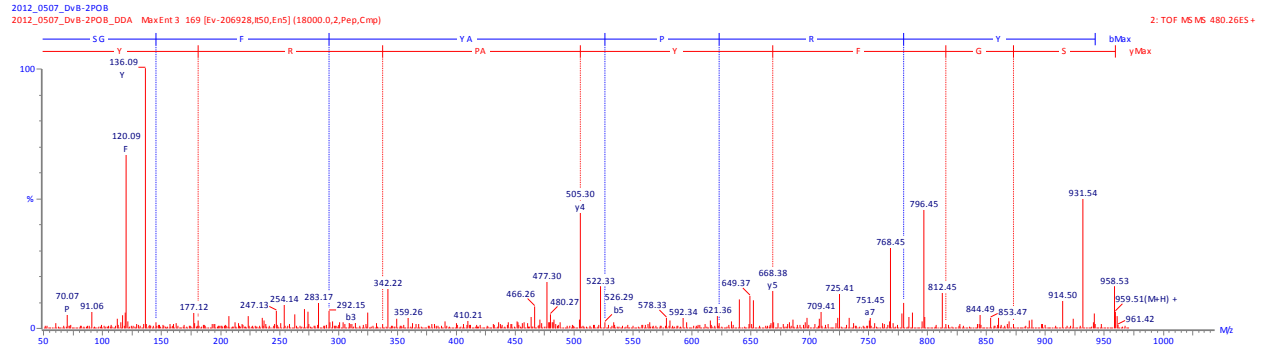
RYamide FVGGSRYa (m/z 832.4101)

MS/MS of m/z 416.74 (PepSeq score = 48)



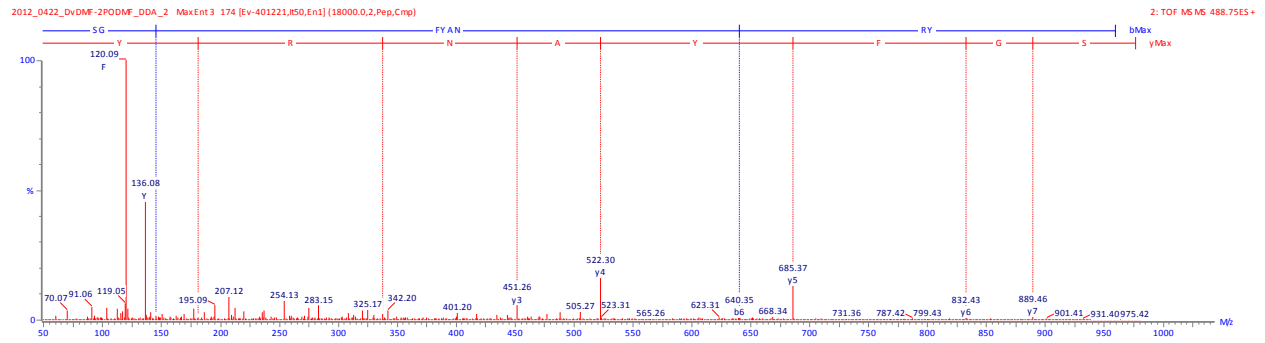
RYamide SGFYAPRYa (m/z 959.4734)

MS/MS of m/z 480.26 (PepSeq score = 47)



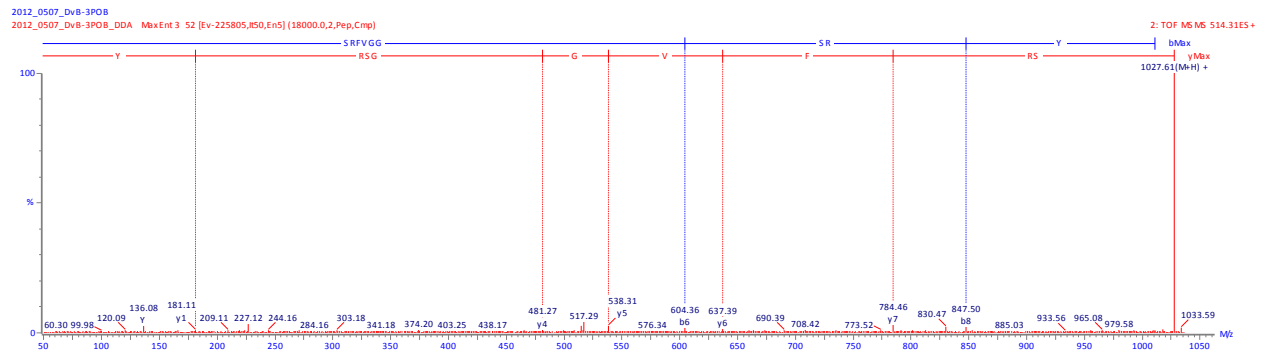
RYamide SGFYANRYa (m/z 976.4734)

MS/MS of m/z 488.75 (PepSeq score = 17)



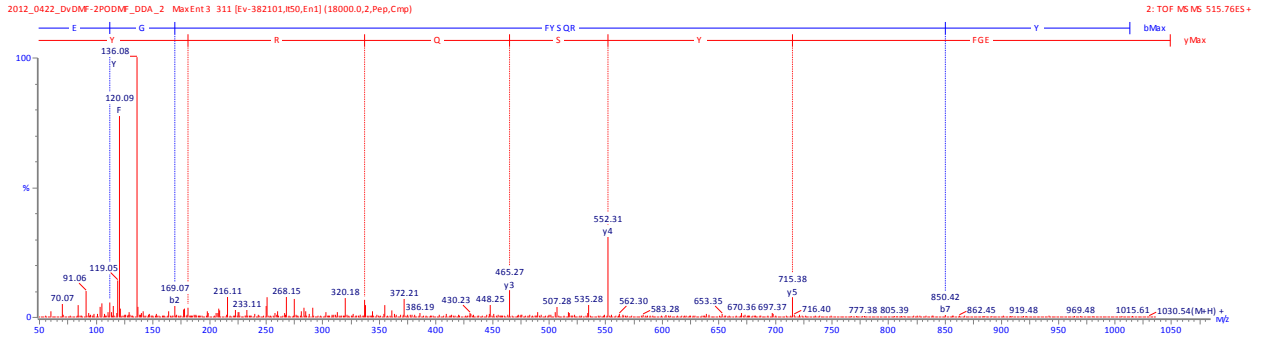
RYamide SRFVGGSRYa (m/z 1027.5432)

MS/MS of m/z 514.31 (PepSeq score = 26)



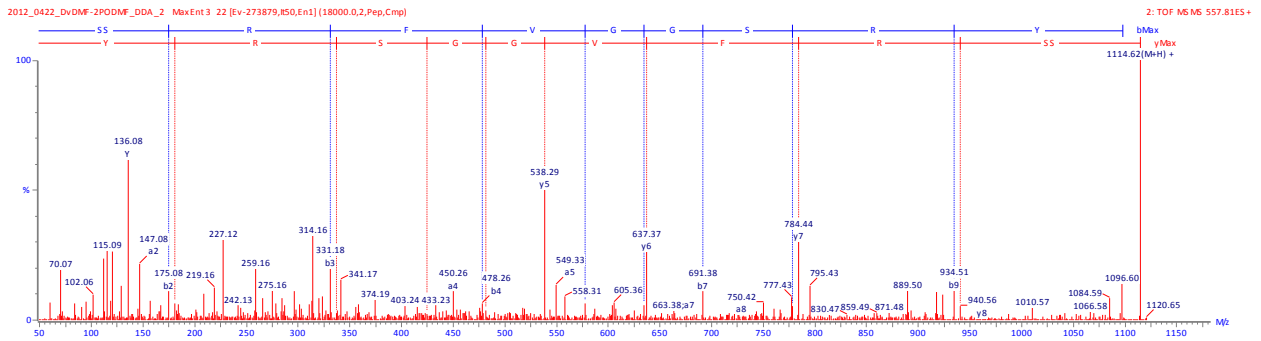
RYamide pEGFYSQRYa (m/z 1030.4741)

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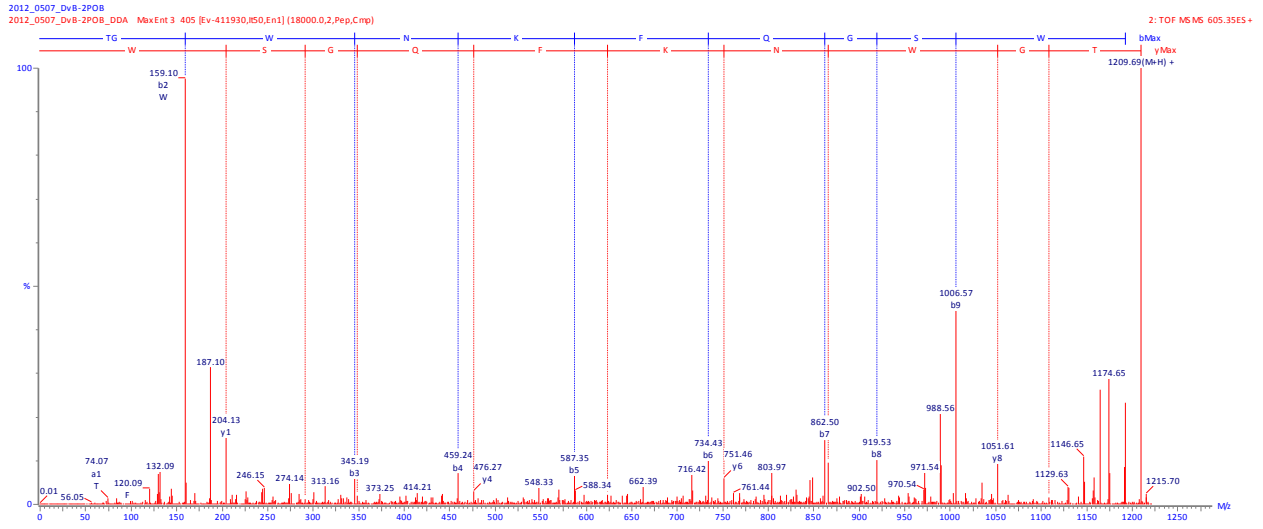
RYamide SSRFVGGSRYa (m/z 1114.5752)

MS/MS of m/z 557.81 (PepSeq score = 593)



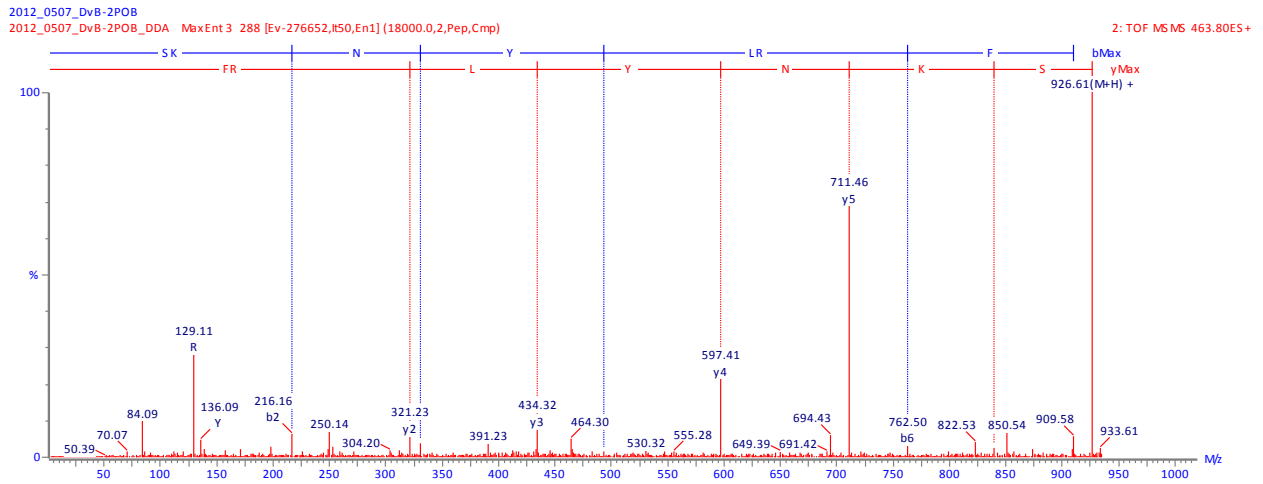
AST-B TGWNKFQGSWa (m/z 1209.5800)

MS/MS of m/z 605.35⁺² (PepSeq score = 278)



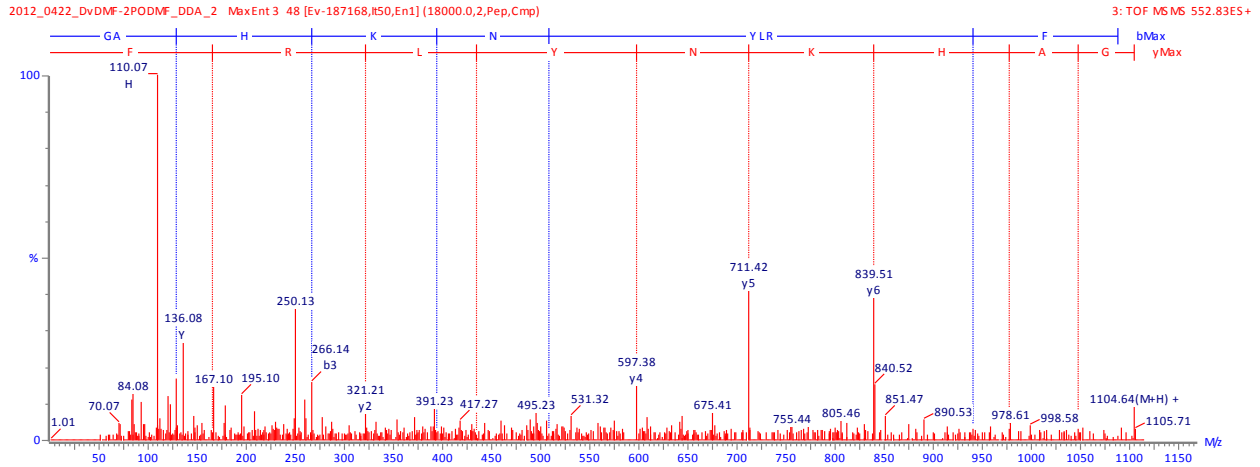
FLP-SKNYLRF (m/z 926.5207)

MS/MS of m/z 463.80⁺² (PepSeq score = 62)



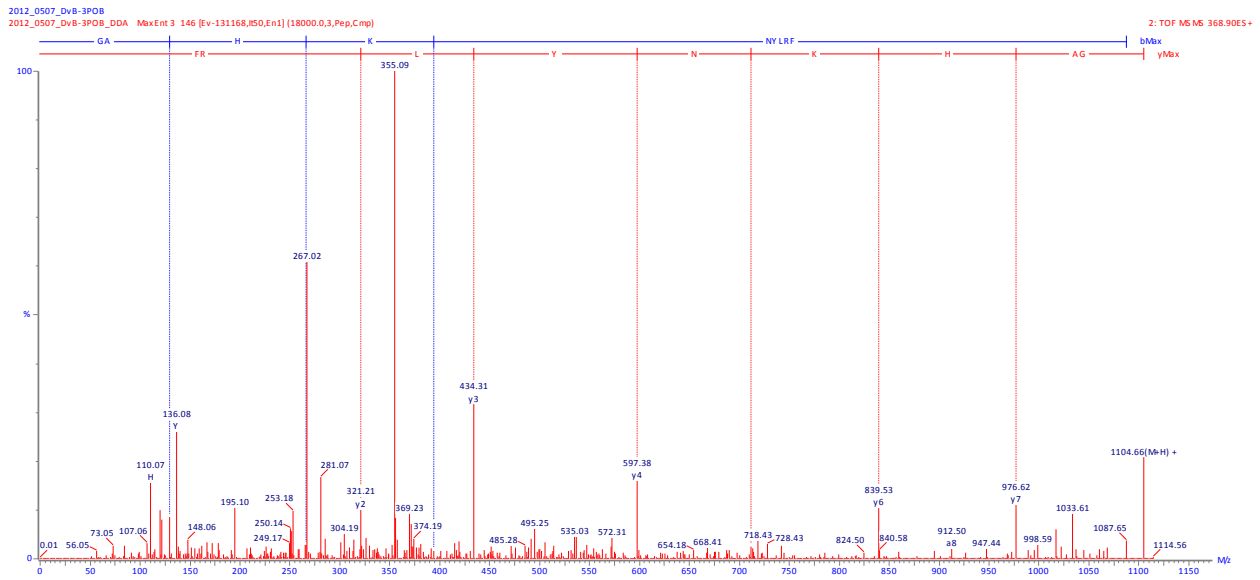
FLP-GAHKNYLRFa (m/z 1104.6061)

MS/MS of m/z 552.83²⁺ (PepSeq score = 132)



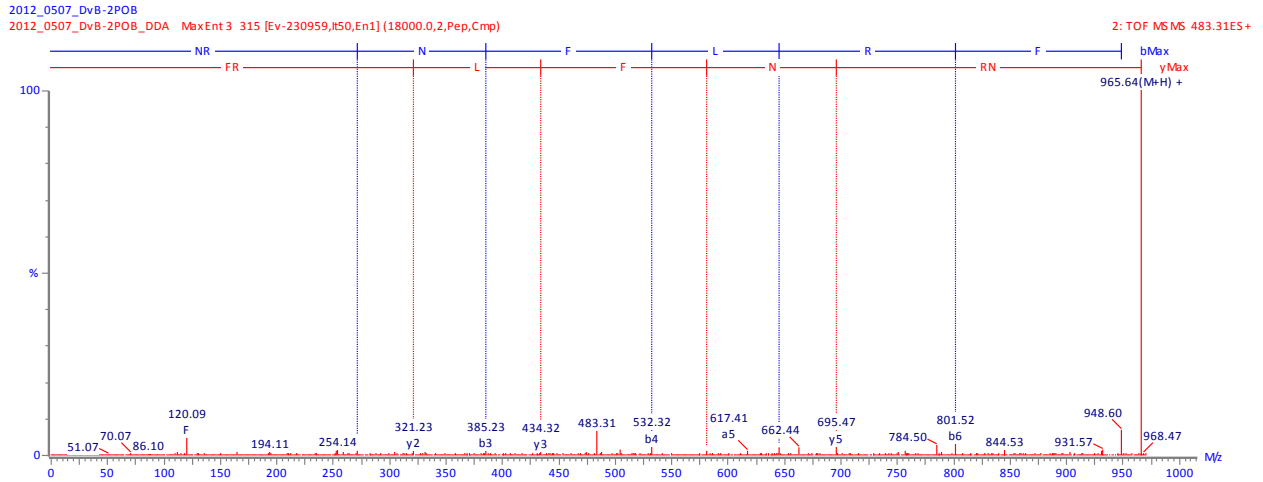
FLP-GAHKNYLRFa (m/z 1104.6061)

MS/MS of m/z 368.90³⁺ (PepSeq score = 27)



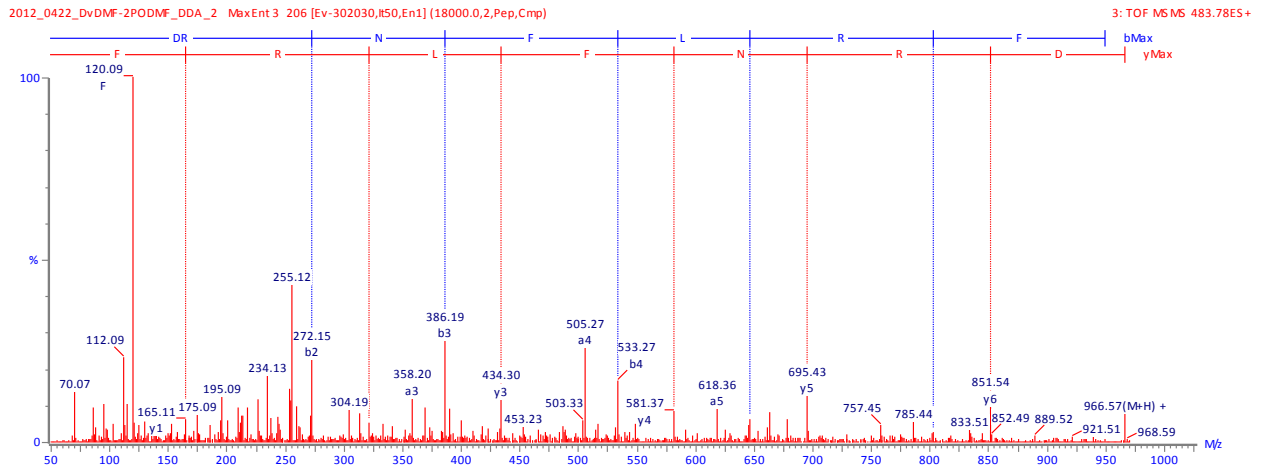
FLP-NRNFLRFa (m/z 965.5428)

MS/MS of m/z 483.31²⁺ (PepSeq score = 53)



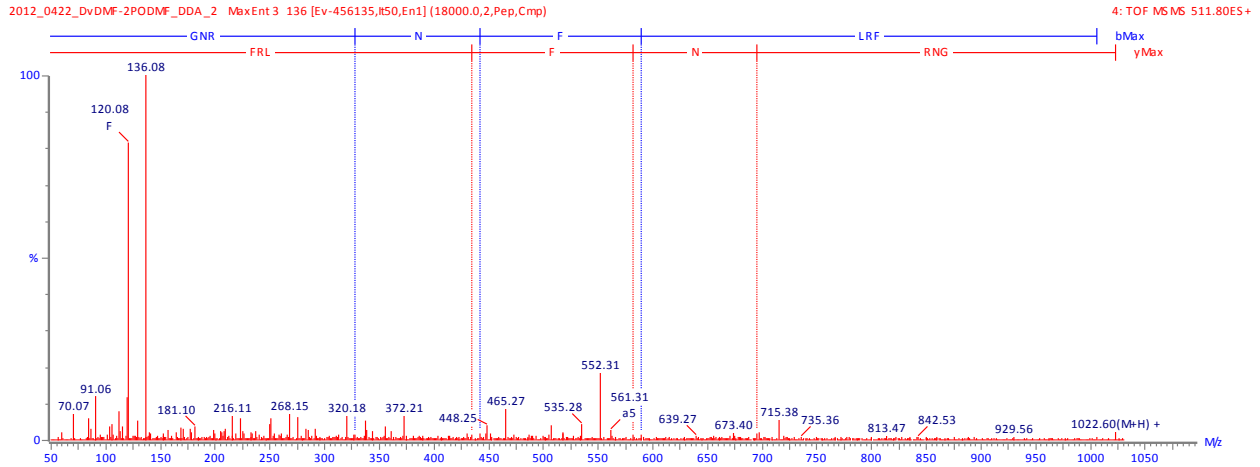
FLP-DRNFLRFa (m/z 966.5268)

MS/MS of m/z 483.78²⁺ (PepSeq score = 135)



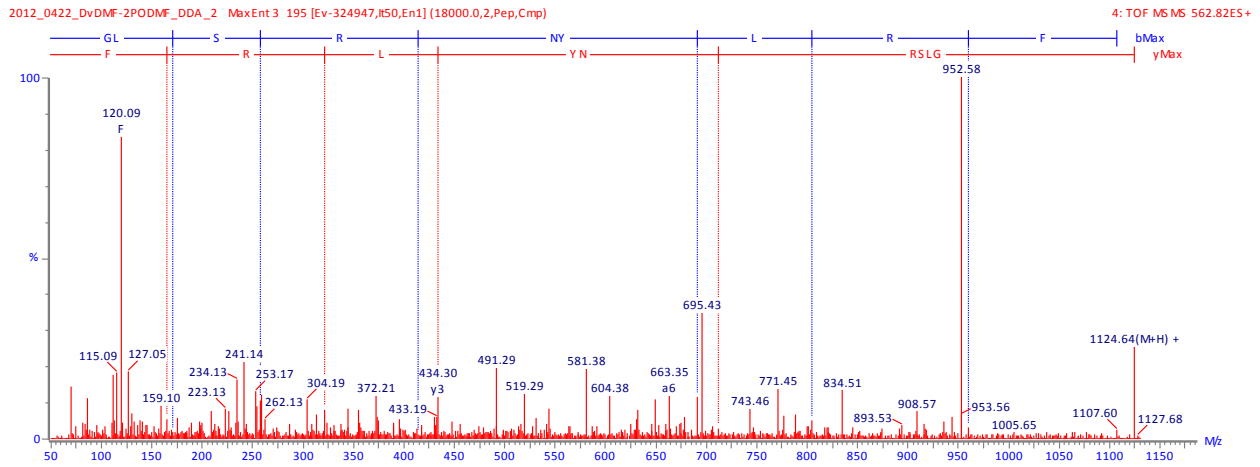
FLP-GNRRNFLRFa (m/z 1022.5646)

MS/MS of m/z 511.80²⁺ (PepSeq score = 2)



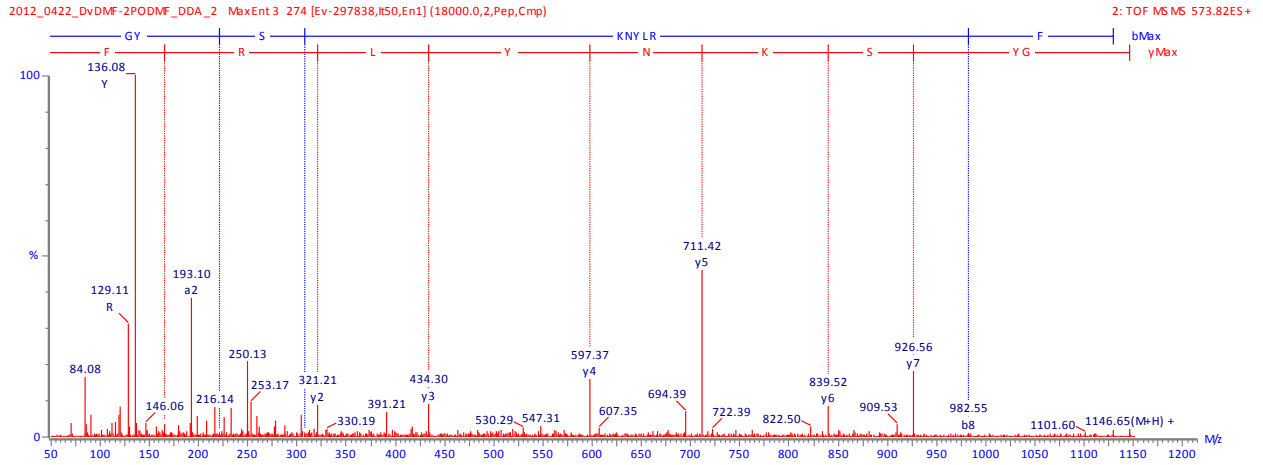
FLP-GLSRNYLRFa (m/z 1124.6323)

MS/MS of m/z 562.82²⁺ (PepSeq score = 47)



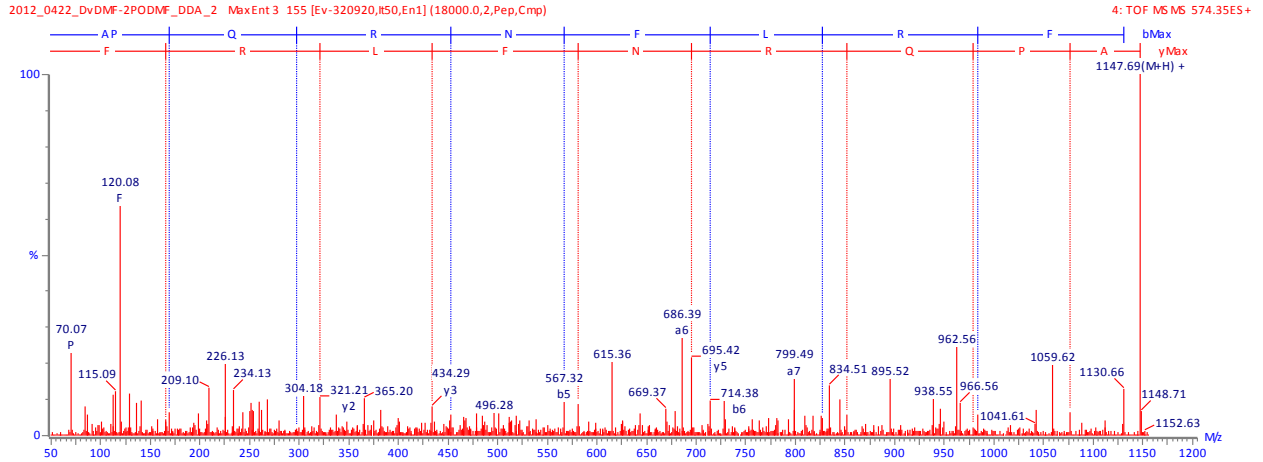
FLP-GYSKNYLRFa (m/z 1146.6055)

MS/MS of m/z 573.82²⁺ (PepSeq score = 73)



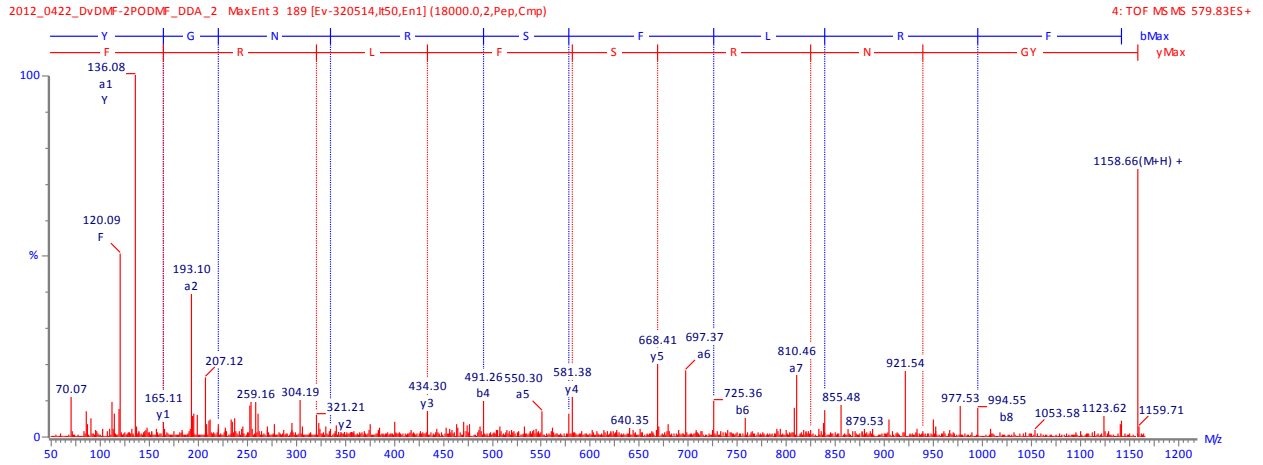
FLP-APQRNFLRFa (m/z 1147.6483)

MS/MS of m/z 574.3242²⁺ (PepSeq score = 259)



FLP-YGNRSFLRFa (m/z 1158.6167)

MS/MS of m/z 579.82²⁺ (PepSeq score = 142)



MATRIX SCIENCE Mascot Search Results

Peptide View

MS/MS Fragmentation of **RSAEGLGRMGRLASLKSDVTPLRGFEGETGHPLE**

Found in **LL380**, CPRP_(CHH_precursor-related_peptide)

_Casap_CPRP_RSAEGLGRMGRLASLKSDVTPLRGFEGETGHPLE_3838.00280_Csap_SG

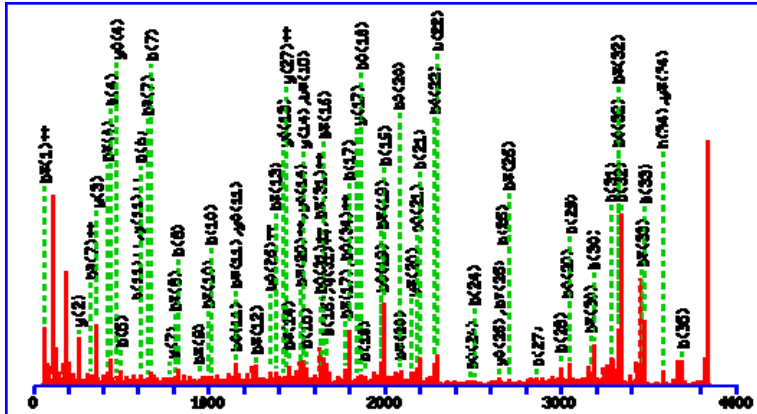
Match to Query 1093: 3837.030120 from(768.413300,5+) intensity(2450831.2000) index(309)

Data file C:\Users\llilabadmin\Desktop\fast dvdmf\2012_0422_DvDMF-2PODMF_DDA_2_CID.pkl

Click mouse within plot area to zoom in by factor of two about that point

Or, Plot from 0 to 4000 Da Full range

Label all possible matches Label matches used for scoring



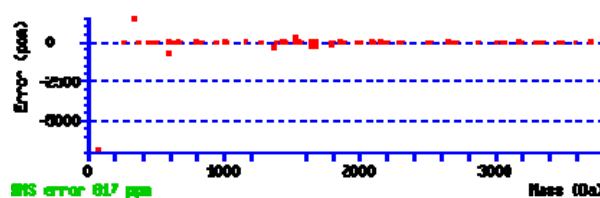
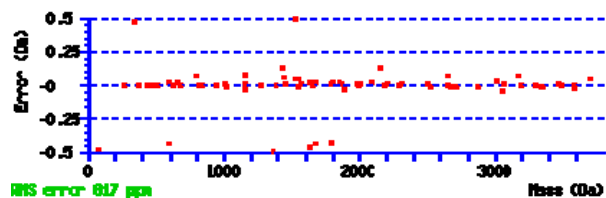
Monoisotopic mass of neutral peptide Mr(calc): 3836.9955

Ions Score: 109 Expect: 5.8e-011

Matches : 75/396 fragment ions using 152 most intense peaks (help)

#	b	b ⁺⁺	b*	b ⁺⁺ *	b ⁰	b ⁰⁺⁺	Seq.	y	y ⁺⁺	y*	y ⁺⁺ *	y ⁰	y ⁰⁺⁺	#
1	157.1084	79.0578	140.0818	70.5446			R							36
2	244.1404	122.5738	227.1139	114.0606	226.1298	113.5686	S	3681.9017	1841.4545	3664.8752	1832.9412	3663.8912	1832.4492	35
3	315.1775	158.0924	298.1510	149.5791	297.1670	149.0871	A	3594.8697	1797.9385	3577.8431	1789.4252	3576.8591	1788.9332	34
4	444.2201	222.6137	427.1936	214.1004	426.2096	213.6084	E	3523.8326	1762.4199	3506.8060	1753.9067	3505.8220	1753.4146	33
5	501.2416	251.1244	484.2150	242.6112	483.2310	242.1191	G	3394.7900	1697.8986	3377.7634	1689.3854	3376.7794	1688.8933	32
6	614.3257	307.6665	597.2991	299.1532	596.3151	298.6612	L	3337.7685	1669.3879	3320.7420	1660.8746	3319.7580	1660.3826	31
7	671.3471	336.1772	654.3206	327.6639	653.3365	327.1719	G	3224.6845	1612.8459	3207.6579	1604.3326	3206.6739	1603.8406	30
8	827.4482	414.2278	810.4217	405.7145	809.4377	405.2225	R	3167.6630	1584.3351	3150.6364	1575.8219	3149.6524	1575.3299	29
9	958.4887	479.7480	941.4622	471.2347	940.4781	470.7427	M	3011.5619	1506.2846	2994.5353	1497.7713	2993.5513	1497.2793	28
10	1015.5102	508.2587	998.4836	499.7455	997.4996	499.2534	G	2880.5214	1440.7643	2863.4948	1432.2511	2862.5108	1431.7591	27
11	1171.6113	586.3093	1154.5847	577.7960	1153.6007	577.3040	R	2823.4999	1412.2536	2806.4734	1403.7403	2805.4894	1403.2483	26
12	1284.6953	642.8513	1267.6688	634.3380	1266.6848	633.8460	L	2667.3988	1334.2030	2650.3723	1325.6898	2649.3883	1325.1978	25
13	1397.7794	699.3933	1380.7529	690.8801	1379.7688	690.3881	L	2554.3148	1277.6610	2537.2882	1269.1477	2536.3042	1268.6557	24
14	1468.8165	734.9119	1451.7900	726.3986	1450.8060	725.9066	A	2441.2307	1221.1190	2424.2041	1212.6057	2423.2201	1212.1137	23
15	1555.8486	778.4279	1538.8220	769.9146	1537.8380	769.4226	S	2370.1936	1185.6004	2353.1670	1177.0872	2352.1830	1176.5951	22
16	1668.9326	834.9699	1651.9061	826.4567	1650.9221	825.9647	L	2283.1616	1142.0844	2266.1350	1133.5711	2265.1510	1133.0791	21
17	1797.0276	899.0174	1780.0010	890.5042	1779.0170	890.0121	K	2170.0775	1085.5424	2153.0509	1077.0291	2152.0669	1076.5371	20
18	1884.0596	942.5334	1867.0331	934.0202	1866.0490	933.5282	S	2041.9825	1021.4949	2024.9560	1012.9816	2023.9720	1012.4896	19
19	1999.0866	1000.0469	1982.0600	991.5336	1981.0760	991.0416	D	1954.9505	977.9789	1937.9239	969.4656	1936.9399	968.9736	18
20	2100.1342	1050.5708	2083.1077	1042.0575	2082.1237	1041.5655	T	1839.9236	920.4654	1822.8970	911.9521	1821.9130	911.4601	17
21	2199.2026	1100.1050	2182.1761	1091.5917	2181.1921	1091.0997	V	1738.8759	869.9416	1721.8493	861.4283	1720.8653	860.9363	16
22	2300.2503	1150.6288	2283.2238	1142.1155	2282.2398	1141.6235	T	1639.8075	820.4074	1622.7809	811.8941	1621.7969	811.4021	15
23	2397.3031	1199.1552	2380.2765	1190.6419	2379.2925	1190.1499	P	1538.7598	769.8835	1521.7332	761.3703	1520.7492	760.8782	14
24	2510.3872	1255.6972	2493.3606	1247.1839	2492.3766	1246.6919	L	1441.7070	721.3571	1424.6805	712.8439	1423.6965	712.3519	13
25	2666.4883	1333.7478	2649.4617	1325.2345	2648.4777	1324.7425	R	1328.6230	664.8151	1311.5964	656.3018	1310.6124	655.8098	12

26	2723.5097	1362.2585	2706.4832	1353.7452	2705.4992	1353.2532	G	1172.5218	586.7646			1154.5113	577.7593	11
27	2870.5781	1435.7927	2853.5516	1427.2794	2852.5676	1426.7874	F	1115.5004	558.2538			1097.4898	549.2485	10
28	2999.6207	1500.3140	2982.5942	1491.8007	2981.6102	1491.3087	E	968.4320	484.7196			950.4214	475.7143	9
29	3056.6422	1528.8247	3039.6156	1520.3115	3038.6316	1519.8195	G	839.3894	420.1983			821.3788	411.1930	8
30	3185.6848	1593.3460	3168.6582	1584.8328	3167.6742	1584.3408	E	782.3679	391.6876			764.3573	382.6823	7
31	3286.7325	1643.8699	3269.7059	1635.3566	3268.7219	1634.8646	T	653.3253	327.1663			635.3148	318.1610	6
32	3343.7539	1672.3806	3326.7274	1663.8673	3325.7434	1663.3753	G	552.2776	276.6425			534.2671	267.6372	5
33	3480.8128	1740.9101	3463.7863	1732.3968	3462.8023	1731.9048	H	495.2562	248.1317			477.2456	239.1264	4
34	3577.8656	1789.4364	3560.8391	1780.9232	3559.8550	1780.4312	P	358.1973	179.6023			340.1867	170.5970	3
35	3690.9497	1845.9785	3673.9231	1837.4652	3672.9391	1836.9732	L	261.1445	131.0759			243.1339	122.0706	2
36							E	148.0604	74.5339			130.0499	65.5286	1



NCBI BLAST search of [RSAEGLGRMGRLASLKS DVTVPLRGFEGETGHPLE](#)

(Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)

Other BLAST [web gateways](#)

All matches to this query

Score	Mr(calc):	Delta	Sequence
109.1	3836.9955	0.0346	RSAEGLGRMGRLASLKS DVTVPLRGFEGETGHPLE

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