

Peaklist used for CAD on Cystatin

SPECTRUM - MS

#59_1024_CAD_Xtract.raw

FTMS + p NSI Full ms2 1024.45@cid25.00 [621.82-14122.02]

Scan #: 1

RT: 116.69

Data points: 160

Mass	Intensity
626.821228	246.765823
683.362976	324.490295
756.345825	608.746155
871.373291	272.855957
1001.500366	529.361023
1008.505371	276.250824
1009.014709	251.648651
1043.526245	181.194122
1058.442505	621.803223
1059.691162	1352.483887
1061.443359	322.828064
1069.542969	198.654678
1078.527222	345.672363
1080.36145	342.606964
1081.543335	439.615295
1084.544434	213.779419
1085.538696	338.207947
1087.543091	631.589111
1088.621948	175.153595
1094.234619	497.056305
1097.366821	255.288086
1101.543335	822.320679
1102.751953	345.800354
1109.826416	189.635757
1114.888306	536.438538
1119.738281	183.80986
1120.922729	270.477753
1122.376587	1079.546021
1125.379395	380.562378
1128.567871	185.383698
1133.567017	274.010803
1140.932739	381.389618
1151.58667	209.581482
1154.573364	212.486343
1155.482056	339.919159

1156.210571	353.39917
1156.940186	253.514008
1192.598145	295.618195
1207.658447	210.889175
1209.60791	332.039368
1223.557495	166.298645
1225.612183	194.020279
1244.117432	218.168991
1316.441528	434.839569
1320.742432	1363.124146
1445.732666	139.261429
1462.76062	534.479919
1480.770874	1387.053955
1483.80603	414.904999

1547.785767	385.913849
1558.816528	272.867493
1565.860107	427.562378
1575.84375	2337.327393
1593.855103	5015.767578
1738.90918	564.349182
1756.919067	1424.15686
1852.953735	531.667053
1870.96167	1250.506348
1923.987305	156.977402
1941.997559	423.123169
2021.990845	379.895844
2057.027344	875.800293
2177.088379	495.315857
3172.574463	560.00061
3177.574463	1782.387817
3181.580078	1118.032471
3223.088623	231.06456
3316.6521	492.296692
3440.736572	207.408615
3567.786865	243.403244
3680.864746	1317.627808
3906.964355	2619.792236
3947.965576	177.573746
3966.994873	229.115219
4018.013428	198.326996
4146.081543	216.10582
4164.068359	350.304016

4301.134277	359.667023
4768.39209	191.40921
4786.388672	283.911591
4901.403809	299.258545
6234.05127	525.501404
6345.072754	169.368866
6363.095703	951.296448
6462.162109	2723.109863
6560.199707	269.422546
6577.195801	2175.161621
6707.248535	504.507874
6724.255859	4601.110352
6740.226563	172.25415
6871.333008	940.171997
7429.813477	80.992088
7447.831543	84.004707
7594.905273	125.980171
7820.964355	151.159103
7838.987793	297.908478
7856.993164	271.882172
9417.745117	956.711304
9532.75	136.350784
9877.930664	148.081024
9947.9375	71.160042
10336.16406	72.804604
10353.19824	274.599579
10620.29785	130.332397
10638.30273	162.942032
10753.38672	86.028114
10881.44727	85.946373
10900.44238	376.340363
11604.82324	117.835686
11790.93359	338.930878
11902.97852	245.077606
11919.98145	412.264038
11999.95996	130.050812
12018	480.753876
12035.00586	680.351379
12048.98242	141.467896
12098.04297	119.330452
12114.01563	514.845398
12131.02734	1411.181763
12149.03613	2375.741455
12153.03418	211.920761
12163.06543	519.27655
12227.09668	315.656464
12244.1084	855.285522
12247.10742	131.123276
12262.13086	1702.199097
12268.12598	95.688507
12276.1377	344.2883
12342.14551	601.174988
12359.14844	68.183769
12360.15332	2051.268799

12366.05762	67.900322
12371.1582	163.281845
12377.16113	4297.828613
12382.16895	304.382538
12391.17676	880.963074
12413.1709	366.337158
12426.15039	120.512634
12431.19531	1205.118042
12442.23438	118.141365
12448.20801	2429.655762
12453.21289	254.363632
12462.24023	431.980713
12510.21094	172.978699
12527.21582	563.125488
12540.23145	138.968735
12545.22852	1558.04834
12563.25586	2799.923096
12576.23535	550.233582
12673.2207	78.154678
12674.26172	136.92012
12690.23633	284.384674
12708.29199	734.070862
12725.3125	1558.026978
12738.31934	161.292709
13047.19531	154.907761
13562.82715	241.028488
14029.03027	641.26355
14046.06934	904.211792
14117.01856	189.042603

Prosight Output for Original Cystatin SN sequence (CAD)

User Specified Sequence

WSPKEEDRIIPGGIYNADLNDEWVQRALHFAISEYNKATKDDYYRRPLRVLRLARQQTVGGVNYFFDVEVGRTI[-1.007825]C
TKSQPNLDT[-1.007825]CAFHEQPELQKKQL[-1.007825]CSFEIYVWPENRRSLVKSR[-1.007825]CQES

Number of Amino Acids: 121

Theoretical Mass: 14303.1 Da

Mass Difference: 15.9108 Da

B Ions: 2 Y Ions: 27

Ion	Observed Mass (Da)	Theoretical Mass (Da)	Mass Error (Da)	Mass Error (PPM)	Delta M
B6	756.346	756.344	0.002	2.1	--
B7	871.373	871.371	0.002	2.4	--
Y29	3567.79	3567.77	0.013	3.8	--
Y30	3680.87	3680.86	0.007	2	--
Y32	3906.96	3906.95	0.012	3	--
Y34	4164.07	4164.05	0.014	3.5	--
Y35	4301.13	4301.11	0.021	5	--
Y53	6234.05	6234.03	0.02	3.2	--
Y54	6363.1	6363.07	0.022	3.4	--
Y55	6462.16	6462.14	0.02	3	--
Y56	6577.2	6577.17	0.026	4	--
Y57	6724.26	6724.24	0.018	2.7	--
Y58	6871.33	6871.31	0.027	3.9	--
Y79	9417.75	9417.72	0.029	3.1	--
Y80	9532.75	9532.74	0.007	0.8	--
Y84	9947.94	9947.95	-0.012	-1.2	--
Y87	10353.2	10353.2	0.048	4.6	--
Y91	10753.4	10753.3	0.04	3.8	--
Y92	10900.4	10900.4	0.028	2.5	--
Y98	11604.8	11604.8	0	0	--
Y99	11790.9	11790.9	0.031	2.7	--
Y100	11920	11919.9	0.037	3.1	--
Y101	12035	12035	0.034	2.8	--
Y102	12149	12149	0.021	1.8	--
Y103	12262.1	12262.1	0.032	2.6	--
Y104	12377.2	12377.1	0.035	2.9	--
Y105	12448.2	12448.2	0.045	3.6	--
Y107	12725.3	12725.3	0.043	3.4	--
Y120	14117	14117	0.009	0.6	--

Crude PScore: 1.24837e-34

McLucky Score: 40.625

Graphic
al
Fragme
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Mapper

W S P K E E D R I I P G G I Y N A D L N D E W V Q R A L H F
A I S E Y N K A T K D D Y Y R R P L R V L R A R Q Q T V G G
V N Y F F D V E V G R T I T K S Q P N L D T A F H E Q P
E L Q K K Q L S F E I Y E V P W E N R R S L V K S R Q E
S

Prosight Output for Modified Cystatin SN (CAD)

User Specified Sequence
 WSPKEEDRIILGGIYNADLNDEWVQRALHFAISEYKATKDDYRRPLRVLRARQQT VGGVNYFFDVEVGRTI[-1.007825]C
 TKSQPNLDT[-1.007825]CAFHEQPQLKKQL[-1.007825]CSFEIYVWPENRRSLVKSR[-1.007825]CQES
 Number of Amino Acids: 121
 Theoretical Mass: 14319.1 Da
 Mass Difference: -0.12051 Da
 B Ions: 15 Y Ions: 28

Ion	Observed Mass (Da)	Theoretical Mass (Da)	Mass Error (Da)	Mass Error (PPM)	Delta M
B6	756.346	756.344	0.002	2.1	--
B7	871.373	871.371	0.002	2.4	--
B13	1480.77	1480.77	0.003	2.4	--
B14	1593.86	1593.85	0.004	2.3	--
B15	1756.92	1756.92	0.004	2.4	--
B16	1870.96	1870.96	0.004	2.1	--
B17	1942	1942	0.003	1.4	--
B18	2057.03	2057.02	0.006	2.7	--
B41	4786.39	4786.38	0.011	2.3	--
B42	4901.4	4901.41	-0.001	-0.2	--
B63	7447.83	7447.81	0.017	2.3	--
B64	7594.91	7594.88	0.023	3	--
B66	7856.99	7856.98	0.015	1.9	--
B91	10638.3	10638.3	0.04	3.7	--
B104	12247.1	12247.1	0.035	2.8	--
Y29	3567.79	3567.77	0.013	3.8	--
Y30	3680.87	3680.86	0.007	2	--
Y32	3906.96	3906.95	0.012	3	--
Y34	4164.07	4164.05	0.014	3.5	--
Y35	4301.13	4301.11	0.021	5	--
Y53	6234.05	6234.03	0.02	3.2	--
Y54	6363.1	6363.07	0.022	3.4	--
Y55	6462.16	6462.14	0.02	3	--
Y56	6577.2	6577.17	0.026	4	--
Y57	6724.26	6724.24	0.018	2.7	--
Y58	6871.33	6871.31	0.027	3.9	--
Y79	9417.75	9417.72	0.029	3.1	--
Y80	9532.75	9532.74	0.007	0.8	--
Y84	9947.94	9947.95	-0.012	-1.2	--
Y87	10353.2	10353.2	0.048	4.6	--
Y91	10753.4	10753.3	0.04	3.8	--
Y92	10900.4	10900.4	0.028	2.5	--
Y98	11604.8	11604.8	0	0	--
Y99	11790.9	11790.9	0.031	2.7	--
Y100	11920	11919.9	0.037	3.1	--
Y101	12035	12035	0.034	2.8	--
Y102	12149	12149	0.021	1.8	--
Y103	12262.1	12262.1	0.032	2.6	--
Y104	12377.2	12377.1	0.035	2.9	--
Y105	12448.2	12448.2	0.045	3.6	--
Y107	12725.3	12725.3	0.043	3.4	--
Y115	13562.8	13562.8	0.051	3.8	--
Y119	14046.1	14046	0.06	4.3	--

Crude PScore: 1.01078e-57
 McLuckey Score: 63.75

Graphical Fragment Mapper

W S P K E E D R I I L G G I Y N A D L N D E W V Q R A L H F
 A I S E Y N K A T K D D Y Y R R P L R V L R A R Q Q T V G G
 V N Y F F D V E V G R T I T K S Q P N L D T C A F H E Q I P
 E L Q K K Q L C S F E I Y E V P W E N R R S L V K S R C Q E
 S

SPECTRUM - MS

#59_1024_ECD_1200MSC_Xtract.raw

FTMS + p NSI Full ms2 1024.45@cid0.00 ecd@5.00 [382.19-15658.13]

Scan #: 1

RT: 318.92

Data points: 345

Mass	Intensity
387.191698	119.64193
408.592333	20.565166
477.54503	19.912844
481.780504	18.955458
484.140764	20.843714
487.814806	20.516405
489.257463	21.53627
512.89403	20.545259
515.286974	290.610718
534.293322	19.703785
536.384996	20.343197
594.31859	21.21764
610.849474	26.2721
625.311266	22.277037
633.108019	19.000952
644.33037	497.227539
665.626512	21.329721
693.277574	37.205589
704.256517	20.803867
773.379568	512.764771
779.195737	23.920237
836.916979	37.759571
847.973728	10.578156
853.017443	26.929956
856.722521	21.347658
874.861545	11.796202
888.402147	414.284485
929.95952	36.14819
939.706713	22.13542
949.12755	23.613382
951.567919	30.187183
970.504869	46.4767
993.463949	8.890681

995.011705	26.653376
996.262499	47.478676
1009.434801	22.210598
1020.867723	38.048206
1021.421068	58.680645
1023.520677	304.804565
1033.52849	53.558735
1035.266405	31.30945
1044.50493	179.717407
1063.543552	12.264289
1065.437181	26.576084
1084.689212	91.248161
1097.632738	24.285799
1099.898363	60.267097
1119.544969	48.707024
1121.566332	42.951939
1125.569139	31.453875
1139.571215	46.579914
1144.578295	26.972485
1157.590013	177.707458
1176.282762	26.781864
1181.577806	69.212456
1183.009691	29.692621
1185.525043	78.528595
1190.47368	117.325554
1192.10222	32.067318
1192.849413	31.704742
1193.596117	63.603333
1206.982714	31.47731
1226.468431	28.505878
1231.616869	34.426788
1238.62517	32.734966
1243.11577	24.528168
1243.802904	40.296551
1247.009691	25.719482
1261.636522	23.99427
1263.9489	24.270161

1266.220507	24.025057
1266.884447	31.076925
1270.676927	148.62088
1272.272386	36.432457
1286.831713	33.333881
1290.692016	130.669373
1292.64934	118.093834
1295.289598	49.099754
1303.653951	9.637797

1304.697679	42.3591
1336.558519	27.861082
1339.151537	36.45018
1340.675951	73.543396
1344.689257	26.404844
1351.682665	30.10614
1352.248094	38.272694
1355.676439	48.54071
1357.684618	69.798004
1360.79326	29.694845
1361.685106	67.807846

1365.332567	26.686863
1370.149584	35.806301
1370.683153	78.294365
1373.6989	43.691719
1376.688036	67.893257
1378.028978	32.876175
1378.692064	54.594704
1383.758715	257.752716
1386.815111	26.511875
1387.568024	89.352409
1393.70476	27.329285
1400.699633	69.023232
1408.204793	55.414909
1409.710741	49.529606
1414.206224	37.600948
1414.714159	60.599789
1416.723558	98.185097
1418.214037	29.327572
1419.908983	43.549683
1420.846322	117.972649
1422.304098	11.130554
1423.680834	56.019783
1428.685839	41.494698
1430.683397	65.191551
1432.761814	15.908261
1433.429735	26.597467
1434.756931	12.933965
1435.271776	25.729767
1438.164476	28.327839
1440.777805	596.041504
1446.301561	42.053444
1452.315111	34.861118
1472.753588	84.927933
1475.225145	32.969635
1476.968798	206.173843
1478.064379	100.683151
1478.727709	240.147415

1483.719652	30.564003
1493.750048	45.457741
1497.744513	264.297485
1499.748461	33.98037
1505.779344	50.463303
1510.023702	9.361143
1512.808567	25.619593

1514.762377	70.380348
1524.176317	32.383572
1527.340502	29.380081
1539.742357	29.30908
1549.75571	13.047528
1552.753099	37.552032
1555.269091	35.146305
1557.297411	191.061066
1561.961718	36.950417
1564.80913	37.839317
1566.03142	28.984997
1571.460741	89.58828
1576.036425	76.63781
1577.916307	42.554943
1583.03142	88.029099
1584.760057	41.469593
1587.138597	112.039192
1588.027513	77.793732
1589.777391	63.562107
1596.811327	42.029221
1599.808763	35.435818
1603.801683	32.694988
1606.415453	32.347576
1609.448324	11.573897
1610.889818	160.558502
1619.813036	27.700544
1624.807176	69.59407
1635.140428	29.358438
1645.798387	93.184624
1662.836962	27.49559
1665.022115	9.123872
1673.81682	36.143154
1674.84116	24.767643
1680.858202	47.361282
1689.854662	44.197639
1710.865526	73.011246
1714.5833	34.011982
1734.875658	45.282375
1745.621874	38.461163
1747.23369	46.155624
1747.858202	63.32299

1751.097216	51.802067
1756.974413	34.476719
1758.843676	63.753815
1772.799242	39.519058
1773.949802	386.539825
1776.111864	61.488644
1776.61516	67.736443
1777.51494	38.44228
1780.091967	47.882057
1795.242723	32.833569
1824.514818	50.144325
1887.993625	158.849701
1959.031711	160.470825
2040.003879	197.551865
2057.046726	39.542278
2075.061863	67.336319
2187.144382	165.926453
2271.144871	19.646784
2301.190281	109.509865
2348.147312	21.157408
2399.195652	65.612427
2416.212742	282.993225
2441.226658	23.450983
2450.223484	26.703411
2503.256443	47.357231
2545.262546	148.520676
2705.363132	19.908833
2736.310642	136.643448
2841.433201	47.30463
2853.447605	58.438885
2921.283054	32.715549
2953.415623	27.31439
2963.500828	30.225533
3139.152683	19.073656
3151.802585	36.025593
3154.510349	51.844482
3265.649265	21.857277
3296.618015	76.829903
3298.747898	55.934109
3313.639988	27.658859
3324.332662	15.527793
3372.676609	61.309628
3424.712039	29.123997
3435.776462	257.570801
3551.683445	83.407654
3556.039083	36.855743
3574.711092	25.428295
3581.820955	29.369934
3585.806539	33.190994
3665.864279	196.904449
3766.950886	25.060026
3773.346102	56.234303
3774.916188	22.039635
3792.896198	44.376251

3794.901998	340.842621
3811.027882	21.132072
3837.346516	24.898308
3851.906178	14.889924
3853.985738	40.819366
3984.027698	31.054895
4019.033346	181.686554
4081.501393	16.117352
4128.062261	17.503517
4129.072408	106.539742
4146.084079	525.061096
4150.086691	131.858429
4163.013433	9.661422
4190.350207	18.633755
4260.144001	154.681717
4278.665548	65.312805
4388.220405	70.540543
4389.210866	35.136604
4401.210651	15.633807
4460.275778	248.101257
4460.777058	71.241928
4503.216511	51.265549
4543.317707	22.934046
4560.364156	145.816742
4670.36156	24.532209
4688.416403	303.655365
4702.366628	44.317661
4703.394781	59.841328
4720.457233	27.382715
4729.406027	43.454666
4734.051475	18.511452
4736.368429	58.332859
4743.39858	112.278702
4749.083942	68.836296
4751.433981	65.98661
4758.737584	99.639336
4759.416694	294.622772
4786.399116	130.412842
4803.414694	517.91449
4818.405952	55.027924
4918.483234	16.950758
4919.472358	72.875946
5031.996174	14.160384
5243.586628	24.841581
5290.43775	12.08982
5316.918171	20.561703
5382.66729	27.394575
5383.67019	28.836582
5400.68769	212.106537
5415.690879	16.721357
5489.649768	31.075508
5653.864707	25.4776
5692.892051	56.690769
5693.646838	19.147976

5766.921348	29.573593
5805.818609	83.603889
5923.033089	25.196442
6022.107505	29.10005
6219.070622	120.468849
6348.098454	250.047058
6448.18485	25.844187
6517.428521	17.047813
6518.431421	11.535551
6562.2132	105.182922
6645.454095	12.762131
6709.283024	265.82251
6774.550209	33.191628
6856.364626	134.245316
7019.39501	377.905762
7083.424137	18.612627
7133.44042	585.259583
7172.766384	15.305471
7187.762995	110.05352
7281.351797	8.582774
7289.622897	29.288012
7301.828773	40.40099
7546.685659	125.757607
7611.952844	17.100536
7674.756856	72.737793
7802.812461	95.714462
7957.953529	20.279022
7958.910391	39.225113
8300.138326	38.024899
8920.537835	76.851967
9403.800164	28.561422
9474.802177	19.241764
9499.780773	18.0856
9517.797112	67.534676
9518.755219	8.769422
9761.926966	21.262594
10062.13683	33.259583
10130.15554	12.300148
10177.17797	61.454865
12770.52673	22.487932
13309.80777	32.611935
14219.2082	82.166939
14232.26255	27.123806
14236.27415	28.955776
14243.17708	12.055311
14245.209	89.266495
14250.22897	18.891823
14257.24927	17.632208
14258.22388	22.183731
14260.32112	67.715034
14263.32982	157.711212
14273.17581	16.185795
14277.20831	159.98439
14286.25318	16.323587

14289.17942	124.56311
14302.18718	65.194199
14305.1722	171.472992
14307.26588	36.423809
14316.18035	18.874645
14321.26629	508.790039
14334.21126	45.706882
15653.12558	24.621447

ProSight output for ECD of unmodified Cystatin SN sequence

User Specified Sequence

WSPKEEDRIIPGGIYNADLNDEWVQRALHFAISEYNKATKDDYRRPLRV
TKSQPNLDT[-1.007825]CAFHEQPELQKKQL[-1.007825]CSFEIYE'

Number of Amino Acids: 121

Theoretical Mass: 14303.1 Da

Mass Difference: 15.9108 Da

C Ions: 7 Z Ions: 3

Ion	Observed Mass (Da)	Theoretical Mass (Da)	Mass Error (Da)	Mass Error (PPM)	Delta M
C3	387.192	387.19	0.001	3.2	--
C4	515.287	515.285	0.002	3	--
C5	644.33	644.328	0.002	3.7	--
C7	888.402	888.398	0.005	5.2	--
C8	1044.51	1044.5	0.006	6	--
C9	1157.59	1157.58	0.007	6.3	--
C10	1270.68	1270.67	0.01	8	--
Z14	1673.82	1673.83	-0.01	-5.9	--
Z19	2348.15	2348.13	0.014	6	--
Z37	4503.22	4503.2	0.019	4.2	--

Crude PScore: 1.45213e-05

McLucky Score: 6.39535

ProSight output for ECD of modified Cystatin SN sequence

User Specified Sequence
 WSPKEEDRIILGGIYNADLNDEWVQRALHFAISEYNKATKDDYYRRLRVLRLARQQTVGGVNYFFDVEVGRTI[-1.007825]
 TKSQPNLDT[-1.007825]CAFHEQPELQKKQL[-1.007825]CSFEIYVWPWENRRSLVKSRLVKS[-1.007825]CQES
 Number of Amino Acids: 121
 Theoretical Mass: 14319.1 Da
 Mass Difference: -0.12051 Da
 C Ions: 34 Z Ions: 3

Ion	Observed Mass (Da)	Theoretical Mass (Da)	Mass Error (Da)	Mass Error (PPM)	Delta M
C3	387.192	387.19	0.001	3.2	--
C4	515.287	515.285	0.002	3	--
C5	644.33	644.328	0.002	3.7	--
C7	888.402	888.398	0.005	5.2	--
C8	1044.51	1044.5	0.006	6	--
C9	1157.59	1157.58	0.007	6.3	--
C10	1270.68	1270.67	0.01	8	--
C11	1383.76	1383.75	0.008	5.7	--
C12	1440.78	1440.77	0.006	3.8	--
C14	1610.89	1610.88	0.012	7.5	--
C15	1773.95	1773.94	0.009	4.9	--
C16	1887.99	1887.98	0.01	5.1	--
C17	1959.03	1959.02	0.011	5.4	--
C19	2187.14	2187.13	0.012	5.6	--
C20	2301.19	2301.18	0.015	6.6	--
C21	2416.21	2416.2	0.011	4.4	--
C22	2545.26	2545.25	0.018	7	--
C32	3766.95	3766.92	0.029	7.7	--
C33	3853.99	3853.95	0.032	8.3	--
C35	4146.08	4146.06	0.024	5.9	--
C36	4260.14	4260.1	0.041	9.7	--
C37	4388.22	4388.2	0.023	5.2	--
C40	4688.42	4688.38	0.039	8.3	--
C41	4803.42	4803.4	0.01	2.2	--
C45	5400.69	5400.66	0.029	5.3	--
C47	5653.87	5653.81	0.052	9.2	--
C48	5766.92	5766.9	0.024	4.2	--
C49	5923.03	5923	0.035	5.9	--
C50	6022.11	6022.07	0.041	6.8	--
C54	6518.43	6518.39	0.042	6.4	--
C56	6774.55	6774.51	0.043	6.4	--
C61	7187.76	7187.73	0.029	4	--
C62	7301.83	7301.78	0.051	7.1	--
C64	7611.95	7611.91	0.044	5.8	--
Z14	1673.82	1673.83	-0.01	-5.9	--
Z19	2348.15	2348.13	0.014	6	--
Z37	4503.22	4503.2	0.019	4.2	--

Crude PScore: 2.05845e-35
 McLuckey Score: 17.4419

Graphic Fragment Mapper

W S P K E E D R I I L G G I Y N A D L N D E W V Q R A L H F
 A I S E Y N K A T K D D Y Y R R P L R V L R A R Q Q T V G G
 V N Y F F D V E V G R T I T K S Q P N L D T A F H E Q P
 E L Q K K Q L S F E I Y E V P W E N R R S L V K S R Q E
 S

ProSight output for ECD of modified Cystatin SN sequence with disulfides reduced

User Specified Sequence -no disulfides
 WSPKEEDRIILGGIYNADLNDEWVQRALHFAISEYNKATKDDYYRRPLRVLRARQQTVGGVNYFFDVEVGRITCKSQPNLDT
 FHEQPQLKKQLCSFEIYVWPENRRSLVKSRQES
 Number of Amino Acids: 121
 Theoretical Mass: 14323.2 Da
 Mass Difference: -4.15181 Da
 C Ions: 35 Z Ions: 4

Ion	Observed Mass (Da)	Theoretical Mass (Da)	Mass Error (Da)	Mass Error (PPM)	Delta M
C3	387.192	387.19	0.001	3.2	--
C4	515.287	515.285	0.002	3	--
C5	644.33	644.328	0.002	3.7	--
C7	888.402	888.398	0.005	5.2	--
C8	1044.51	1044.5	0.006	6	--
C9	1157.59	1157.58	0.007	6.3	--
C10	1270.68	1270.67	0.01	8	--
C11	1383.76	1383.75	0.008	5.7	--
C12	1440.78	1440.77	0.006	3.8	--
C14	1610.89	1610.88	0.012	7.5	--
C15	1773.95	1773.94	0.009	4.9	--
C16	1887.99	1887.98	0.01	5.1	--
C17	1959.03	1959.02	0.011	5.4	--
C19	2187.14	2187.13	0.012	5.6	--
C20	2301.19	2301.18	0.015	6.6	--
C21	2416.21	2416.2	0.011	4.4	--
C22	2545.26	2545.25	0.018	7	--
C32	3766.95	3766.92	0.029	7.7	--
C33	3853.99	3853.95	0.032	8.3	--
C35	4146.08	4146.06	0.024	5.9	--
C36	4260.14	4260.1	0.041	9.7	--
C37	4388.22	4388.2	0.023	5.2	--
C40	4688.42	4688.38	0.039	8.3	--
C41	4803.42	4803.4	0.01	2.2	--
C45	5400.69	5400.66	0.029	5.3	--
C47	5653.87	5653.81	0.052	9.2	--
C48	5766.92	5766.9	0.024	4.2	--
C49	5923.03	5923	0.035	5.9	--
C50	6022.11	6022.07	0.041	6.8	--
C54	6518.43	6518.39	0.042	6.4	--
C56	6774.55	6774.51	0.043	6.4	--
C61	7187.76	7187.73	0.029	4	--
C62	7301.83	7301.78	0.051	7.1	--
C64	7611.95	7611.91	0.044	5.8	--
C81	9499.78	9499.86	-0.08	-8.4	--
Z10	1119.55	1119.55	-0.002	-1.7	--
Z14	1674.84	1674.84	0.007	3.9	--
Z17	2057.05	2057.04	0.012	5.7	--
Z34	4150.09	4150.05	0.038	9.1	--

Crude PScore: 4.37773e-38
 McLuckey Score: 18.314

Graphical Fragment Mapper

W S P K E E D R I I L G G I Y N A D L N D E W V Q R A L H F
 A I S E Y N K A T K D D Y Y R R P L R V L R A R Q Q T V G G
 V N Y F F D V E V G R T I C T K S Q P N L D T C A F H E Q P
 E L Q K K Q L C S F E I Y E V P W E N R R S L V K S R C Q E
 S

Test of CH4 modification

User Specified Sequence

WSPKEEDRIIIGGIYNADLNDEWVQRALHFAISEYNKATKDDYYRRPLRVLRARQQ

TKSQPNLDT[-1.007825]CAFHEQPQLQKKQL[-1.007825]CSFEIYVWPWENRRSLV

Number of Amino Acids: 121

Theoretical Mass: 14319.1 Da

Mass Difference: 0.05049 Da

C Ions: 37 Z Ions: 5

Ion	Observed M	Theoretical Mass	Mass Error	Mass Error Delta M	
C3	387.192	387.19	0.001	3.2 --	10.24
C4	515.287	515.285	0.002	3 --	9
C5	644.33	644.328	0.002	3.7 --	13.69
C6	773.38	773.371	0.009	11.6 --	134.56
C7	888.402	888.398	0.005	5.2 --	27.04
C8	1044.505	1044.499	0.006	6 --	36
C9	1157.59	1157.583	0.007	6.3 --	39.69
C10	1270.677	1270.667	0.01	8 --	64
C11	1383.759	1383.751	0.008	5.7 --	32.49
C12	1440.778	1440.772	0.006	3.8 --	14.44
C14	1610.89	1610.878	0.012	7.5 --	56.25
C15	1773.95	1773.941	0.009	4.9 --	24.01
C16	1887.994	1887.984	0.01	5.1 --	26.01
C17	1959.032	1959.021	0.011	5.4 --	29.16
C19	2187.144	2187.132	0.012	5.6 --	31.36
C20	2301.19	2301.175	0.015	6.6 --	43.56
C21	2416.213	2416.202	0.011	4.4 --	19.36
C22	2545.263	2545.245	0.018	7 --	49
C29	3435.776	3435.732	0.044	12.9 --	166.41
C32	3766.951	3766.922	0.029	7.7 --	59.29
C33	3853.986	3853.954	0.032	8.3 --	68.89
C35	4146.084	4146.06	0.024	5.9 --	34.81
C36	4260.144	4260.103	0.041	9.7 --	94.09
C37	4388.22	4388.198	0.023	5.2 --	27.04
C40	4688.416	4688.377	0.039	8.3 --	68.89
C41	4803.415	4803.404	0.01	2.2 --	4.84
C42	4918.483	4918.431	0.052	10.6 --	112.36
C45	5400.688	5400.659	0.029	5.3 --	28.09
C47	5653.865	5653.813	0.052	9.2 --	84.64
C48	5766.921	5766.897	0.024	4.2 --	17.64
C49	5923.033	5922.998	0.035	5.9 --	34.81
C50	6022.108	6022.066	0.041	6.8 --	46.24
C54	6518.431	6518.39	0.042	6.4 --	40.96
C56	6774.55	6774.507	0.043	6.4 --	40.96
C61	7187.763	7187.734	0.029	4 --	16
C62	7301.829	7301.777	0.051	7.1 --	50.41
C64	7611.953	7611.909	0.044	5.8 --	33.64
Z14	1673.817	1673.827	-0.01	-5.9 --	34.81
Z19	2348.147	2348.133	0.014	6 --	36
Z33	4019.033	4018.991	0.043	10.6 --	112.36
Z37	4503.217	4503.198	0.019	4.2 --	17.64
Z68	7957.954	7957.838	0.116	14.6 --	213.16

Crude PScore: 3.6418e-35

50.09143

McLucky Score: 20.6395

RMS=

7.07753

Test of O modification

User Specified Sequence

WSPKEEDRII[15.994915]PGGIYNADLNDEWVQRALHFAISEYNKATKDDYYRRPI
-1.007825]CTKSQPNLDT[-1.007825]CAFHEQPELQKKQL[-1.007825]CSFEIYEVF
5]CQES

Number of Amino Acids: 121

Theoretical Mass: 14319.1 Da

Mass Difference: 0.086875 Da

C Ions: 21 Z Ions: 5

Ion	Observed M	Theoretical Mass	Mass Error	Mass Error	Delta M
C3	387.192	387.19	0.001	3.2 --	10.24
C4	515.287	515.285	0.002	3 --	9
C5	644.33	644.328	0.002	3.7 --	13.69
C6	773.38	773.371	0.009	11.6 --	134.56
C7	888.402	888.398	0.005	5.2 --	27.04
C8	1044.505	1044.499	0.006	6 --	36
C9	1157.59	1157.583	0.007	6.3 --	39.69
C10	1270.677	1270.667	0.01	8 --	64
C13	1497.745	1497.757	-0.013	-8.6 --	73.96
C35	4146.084	4146.023	0.061	14.7 --	216.09
C37	4388.22	4388.161	0.059	13.5 --	182.25
C41	4803.415	4803.368	0.047	9.8 --	96.04
C45	5400.688	5400.623	0.065	12.1 --	146.41
C48	5766.921	5766.86	0.061	10.6 --	112.36
C49	5923.033	5922.962	0.071	12.1 --	146.41
C50	6022.108	6022.03	0.078	12.9 --	166.41
C54	6518.431	6518.353	0.078	12 --	144
C56	6774.55	6774.471	0.08	11.8 --	139.24
C61	7187.763	7187.698	0.065	9 --	81
C62	7301.829	7301.741	0.088	12 --	144
C64	7611.953	7611.873	0.08	10.5 --	110.25
Z14	1673.817	1673.827	-0.01	-5.9 --	34.81
Z19	2348.147	2348.133	0.014	6 --	36
Z33	4019.033	4018.991	0.043	10.6 --	112.36
Z37	4503.217	4503.198	0.019	4.2 --	17.64
Z68	7957.954	7957.838	0.116	14.6 --	213.16
Crude PScore:	1.98365e-17				96.40808
McLucky Score:	13.6628			RMS=	9.818761

Test of NH2 modification

User Specified Sequence

WSPKEEDRII[16.01872]PGGIYNADLNDEWVQRALHFAISEYNKATKDDYYRRPLF
 1.007825]CTKSQPNLDT[-1.007825]CAFHEQPELQKKQL[-1.007825]CSFEIYEVPI
]CQES

Number of Amino Acids: 121

Theoretical Mass: 14319.1 Da

Mass Difference: 0.06307 Da

C Ions: 35 Z Ions: 5

Ion	Observed M	Theoretical	Mass Error	Mass Error	Delta M
C3	387.192	387.19	0.001	3.2 --	10.24
C4	515.287	515.285	0.002	3 --	9
C5	644.33	644.328	0.002	3.7 --	13.69
C6	773.38	773.371	0.009	11.6 --	134.56
C7	888.402	888.398	0.005	5.2 --	27.04
C8	1044.505	1044.499	0.006	6 --	36
C9	1157.59	1157.583	0.007	6.3 --	39.69
C10	1270.677	1270.667	0.01	8 --	64
C11	1383.759	1383.738	0.02	14.8 --	219.04
C12	1440.778	1440.76	0.018	12.6 --	158.76
C15	1773.95	1773.929	0.021	12 --	144
C16	1887.994	1887.971	0.022	11.7 --	136.89
C17	1959.032	1959.009	0.023	11.8 --	139.24
C19	2187.144	2187.12	0.025	11.3 --	127.69
C20	2301.19	2301.163	0.028	12.1 --	146.41
C21	2416.213	2416.189	0.023	9.6 --	92.16
C22	2545.263	2545.232	0.03	12 --	144
C32	3766.951	3766.909	0.042	11.1 --	123.21
C33	3853.986	3853.941	0.045	11.6 --	134.56
C35	4146.084	4146.047	0.037	8.9 --	79.21
C36	4260.144	4260.09	0.054	12.7 --	161.29
C37	4388.22	4388.185	0.035	8.1 --	65.61
C40	4688.416	4688.365	0.052	11 --	121
C41	4803.415	4803.392	0.023	4.8 --	23.04
C42	4918.483	4918.419	0.065	13.1 --	171.61
C45	5400.688	5400.646	0.041	7.7 --	59.29
C47	5653.865	5653.8	0.064	11.4 --	129.96
C48	5766.921	5766.884	0.037	6.4 --	40.96
C49	5923.033	5922.985	0.048	8.1 --	65.61
C50	6022.108	6022.054	0.054	8.9 --	79.21
C54	6518.431	6518.377	0.054	8.3 --	68.89
C56	6774.55	6774.494	0.056	8.2 --	67.24
C61	7187.763	7187.722	0.041	5.7 --	32.49
C62	7301.829	7301.765	0.064	8.8 --	77.44
C64	7611.953	7611.896	0.056	7.4 --	54.76
Z14	1673.817	1673.827	-0.01	-5.9 --	34.81
Z19	2348.147	2348.133	0.014	6 --	36
Z33	4019.033	4018.991	0.043	10.6 --	112.36
Z37	4503.217	4503.198	0.019	4.2 --	17.64
Z68	7957.954	7957.838	0.116	14.6 --	213.16

Crude PScore: 8.84323e-33

90.294

McLucky Score: 21.2209

RMS=

9.502316

Prosight output for PRP3, CAD, D4N

User Specified Sequence

[-17.0265]QDLNEDV[79.96633]SQEDVPLVISDGGD[79.96633]SEQFIDEERQGPPGGQSQPSAGDGNQDDGPPQ
 GPPQGGQQGPPPPQKPKQGGHPPPPQGRPPQGGHPPPP

Number of Amino Acids: 105

Theoretical Mass: 10999 Da

Mass Difference: 0.0314 Da

B Ions: 9 Y Ions: 25

Ion	Observed Mass (Da)	Theoretical Mass (Da)	Mass Error (Da)	Mass Error (PPM)	Delta M
B5	582.228	582.229	0	-0.7	--
B11	1335.45	1335.45	-0.005	-3.9	--
B12	1434.52	1434.52	-0.004	-2.5	--
B15	1743.72	1743.72	0	-0.1	--
B16	1856.81	1856.81	0.003	1.6	--
B19	2115.89	2115.89	-0.001	-0.7	--
B41	4578.91	4578.92	-0.009	-2	--
B56	6002.45	6002.48	-0.036	-6	--
B66	7078.95	7078.98	-0.029	-4.1	--
Y21	2178.12	2178.12	-0.006	-2.6	--
Y31	3161.58	3161.58	0.001	0.3	--
Y37	3765.91	3765.91	-0.005	-1.3	--
Y38	3862.96	3862.97	-0.004	-1	--
Y39	3919.98	3919.99	-0.004	-1.1	--
Y40	4048.04	4048.05	-0.003	-0.6	--
Y41	4176.1	4176.1	-0.002	-0.4	--
Y42	4304.16	4304.16	-0.005	-1.2	--
Y45	4546.25	4546.26	-0.014	-3.2	--
Y46	4674.32	4674.32	-0.002	-0.4	--
Y48	4899.43	4899.43	0	0	--
Y49	4996.48	4996.49	-0.005	-0.9	--
Y50	5053.5	5053.51	-0.005	-0.9	--
Y51	5181.56	5181.57	-0.007	-1.4	--
Y53	5406.67	5406.68	-0.003	-0.6	--
Y54	5463.69	5463.7	-0.013	-2.4	--
Y55	5578.71	5578.73	-0.012	-2.1	--
Y56	5693.75	5693.75	-0.003	-0.5	--
Y61	6164.95	6164.92	0.026	4.2	--
Y64	6420.05	6420.05	0.006	0.9	--
Y65	6548.11	6548.11	0	0	--
Y66	6635.14	6635.14	0.004	0.6	--
Y93	9564.43	9564.45	-0.018	-1.9	--
Y98	10202.6	10202.6	-0.037	-3.6	--
Y100	10416.7	10416.7	-0.038	-3.6	--

-0.7	0.49
-3.9	15.21
-2.5	6.25
-0.1	0.01
1.6	2.56
-0.7	0.49
-2	4
-6	36
-4.1	16.81
-2.6	6.76
0.3	0.09
-1.3	1.69
-1	1
-1.1	1.21
-0.6	0.36
-0.4	0.16
-1.2	1.44
-3.2	10.24
-0.4	0.16
0	0
-0.9	0.81
-0.9	0.81
-1.4	1.96
-0.6	0.36
-2.4	5.76
-2.1	4.41
-0.5	0.25
4.2	17.64
0.9	0.81
0	0
0.6	0.36
-1.9	3.61
-3.6	12.96
-3.6	12.96

Crude PScore: 2.33315e-44

McLucky Score: 78.125

RMS

4.930294

2.220427

Graphical Fragment Mapper

Q D L N E D V S Q E D V P L V I S D G G D S E Q F I D E E R
 Q G P P L G G Q S Q P S A G D G N Q D D G P Q Q G P P Q Q
G G Q Q Q G P P P P Q G K P Q G P P Q Q G G H P P P Q G
 R P Q G P P Q Q G G H P R P P

Prosight output for PRP3, ECD, WT

User Specified Sequence

[-17.0265]QDLDEDV[79.96633]SQEDVPLVISDGGD[79.96633]SEQFIDEERQGPLGGQSQPSAGDGNQDDGPPQ
GPPQGGGQQQGGPPQGGKQGGPPQGGHPPPPQGRPPQGGHPPPP

Number of Amino Acids: 105

Theoretical Mass: 11000 Da

Mass Difference: -0.95261 Da

C Ions: 18 Z Ions: 24

Ion	Observed Mass (Da)	Theoretical Mass (Da)	Mass Error (Da)	Mass Error (PPM)	Delta M
C3	356.169	356.169	0	0	--
C5	600.239	600.239	0	0	--
C6	715.266	715.266	0	-0.5	--
C7	814.332	814.334	-0.002	-2.7	--
C8	981.329	981.333	-0.004	-3.7	--
C9	1109.39	1109.39	-0.001	-1.2	--
C10	1238.44	1238.43	0.005	3.9	--
C14	1662.67	1662.67	0.001	0.6	--
C15	1761.74	1761.73	0.003	1.7	--
C17	1961.85	1961.85	0	-0.2	--
C22	2472.95	2472.95	0.008	3.1	--
C23	2601.99	2601.99	0.004	1.6	--
C31	3647.49	3647.47	0.016	4.4	--
C35	4011.71	4011.68	0.023	5.7	--
C38	4253.79	4253.78	0.004	0.9	--
C44	4852.09	4852.06	0.036	7.5	--
C49	5323.17	5323.23	-0.054	-10.2	--
C50	5438.28	5438.25	0.029	5.3	--
Z3	352.198	352.198	0	-0.5	--
Z5	586.31	586.31	0	-0.6	--
Z8	828.411	828.412	-0.001	-1	--
Z9	956.468	956.47	-0.003	-2.6	--
Z12	1207.6	1207.6	0.001	0.8	--
Z13	1335.66	1335.66	0.005	3.9	--
Z15	1588.81	1588.81	-0.002	-1.1	--
Z16	1645.83	1645.83	0	0.1	--
Z17	1773.89	1773.89	-0.002	-1.1	--
Z22	2299.16	2299.16	0.004	1.8	--
Z23	2356.18	2356.18	-0.001	-0.4	--
Z30	3048.47	3048.51	-0.031	-10.2	--
Z33	3330.66	3330.67	-0.013	-3.8	--
Z38	3846.93	3846.94	-0.015	-3.9	--
Z40	4032	4032.02	-0.02	-4.9	--
Z41	4160.09	4160.08	0.009	2.2	--
Z44	4473.23	4473.22	0.012	2.6	--
Z45	4530.26	4530.24	0.014	3.1	--
Z50	5037.48	5037.49	-0.01	-2	--
Z51	5165.55	5165.55	0.005	1	--
Z58	5919.83	5919.83	-0.007	-1.2	--
Z59	5976.86	5976.86	0.001	0.3	--
Z60	6091.86	6091.88	-0.021	-3.4	--
Z67	6747.18	6747.18	0.008	1.1	--

0	0
0	0
-0.5	0.25
-2.7	7.29
-3.7	13.69
-1.2	1.44
3.9	15.21
0.6	0.36
1.7	2.89
-0.2	0.04
3.1	9.61
1.6	2.56
4.4	19.36
5.7	32.49
0.9	0.81
7.5	56.25
-10.2	104.04
5.3	28.09
-0.5	0.25
-0.6	0.36
-1	1
-2.6	6.76
0.8	0.64
3.9	15.21
-1.1	1.21
0.1	0.01
-1.1	1.21
1.8	3.24
-0.4	0.16
-10.2	104.04
-3.8	14.44
-3.9	15.21
-4.9	24.01
2.2	4.84
2.6	6.76
3.1	9.61
-2	4
1	1
-1.2	1.44
0.3	0.09
-3.4	11.56
1.1	1.21

Crude PScore: 1.2169e-32
McLucky Score: 11.7308

RMS 3.527578

Graphic Fragment Mapper

Prosight output for PRP3, ECD, D4N

User Specified Sequence

[-17.0265]QDLDEDV[79.96633]SQEDVPLVISDGGD[79.96633]SEQFIDEERQGPPLGGQQSQPSAGDGNQDDGPPQQ
GPPQQGGQQQGGPPPPQGGKPPQGGHPPPPQGRPQGGPPQQGGHPPPP

Number of Amino Acids: 105

Theoretical Mass: 11000 Da

Mass Difference: -0.95261 Da

C Ions: 18 Z Ions: 24

Ion	Observed Mass (Da)	Theoretical Mass (Da)	Mass Error (Da)	Mass Error (PPM)	Delta M
C3	356.169	356.169	0	0	--
C5	600.239	600.239	0	0	--
C6	715.266	715.266	0	-0.5	--
C7	814.332	814.334	-0.002	-2.7	--
C8	981.329	981.333	-0.004	-3.7	--
C9	1109.39	1109.39	-0.001	-1.2	--
C10	1238.44	1238.43	0.005	3.9	--
C14	1662.67	1662.67	0.001	0.6	--
C15	1761.74	1761.73	0.003	1.7	--
C17	1961.85	1961.85	0	-0.2	--
C22	2472.95	2472.95	0.008	3.1	--
C23	2601.99	2601.99	0.004	1.6	--
C31	3647.49	3647.47	0.016	4.4	--
C35	4011.71	4011.68	0.023	5.7	--
C38	4253.79	4253.78	0.004	0.9	--
C44	4852.09	4852.06	0.036	7.5	--
C49	5323.17	5323.23	-0.054	-10.2	--
C50	5438.28	5438.25	0.029	5.3	--
Z3	352.198	352.198	0	-0.5	--
Z5	586.31	586.31	0	-0.6	--
Z8	828.411	828.412	-0.001	-1	--
Z9	956.468	956.47	-0.003	-2.6	--
Z12	1207.6	1207.6	0.001	0.8	--
Z13	1335.66	1335.66	0.005	3.9	--
Z15	1588.81	1588.81	-0.002	-1.1	--
Z16	1645.83	1645.83	0	0.1	--
Z17	1773.89	1773.89	-0.002	-1.1	--
Z22	2299.16	2299.16	0.004	1.8	--
Z23	2356.18	2356.18	-0.001	-0.4	--
Z30	3048.47	3048.51	-0.031	-10.2	--
Z33	3330.66	3330.67	-0.013	-3.8	--
Z38	3846.93	3846.94	-0.015	-3.9	--
Z40	4032	4032.02	-0.02	-4.9	--
Z41	4160.09	4160.08	0.009	2.2	--
Z44	4473.23	4473.22	0.012	2.6	--
Z45	4530.26	4530.24	0.014	3.1	--
Z50	5037.48	5037.49	-0.01	-2	--
Z51	5165.55	5165.55	0.005	1	--
Z58	5919.83	5919.83	-0.007	-1.2	--
Z59	5976.86	5976.86	0.001	0.3	--
Z60	6091.86	6091.88	-0.021	-3.4	--
Z67	6747.18	6747.18	0.008	1.1	--

0	0
0	0
-0.5	0.25
-2.7	7.29
-3.7	13.69
-1.2	1.44
3.9	15.21
0.6	0.36
1.7	2.89
-0.2	0.04
3.1	9.61
1.6	2.56
4.4	19.36
5.7	32.49
0.9	0.81
7.5	56.25
-10.2	104.04
5.3	28.09
-0.5	0.25
-0.6	0.36
-1	1
-2.6	6.76
0.8	0.64
3.9	15.21
-1.1	1.21
0.1	0.01
-1.1	1.21
1.8	3.24
-0.4	0.16
-10.2	104.04
-3.8	14.44
-3.9	15.21
-4.9	24.01
2.2	4.84
2.6	6.76
3.1	9.61
-2	4
1	1
-1.2	1.44
0.3	0.09
-3.4	11.56
1.1	1.21

Crude PScore: 1.2169e-32

McLucky Score: 11.7308

RMS 12.44381 3.527578

Graphical Fragment Mapper

Q D L D E D V S Q E D V P L V I S D G G D S E Q F I D E E R
 Q G P P L G G Q Q S Q P S A G D G N Q D D G P Q Q G P P Q Q
 G G Q Q Q G G P P P P Q G K P Q G P P Q Q G H P P P P Q G
 R P Q G P P Q Q G G H P R P P