PEAKPLOT: Visualizing Fragmented Peptide Mass Spectra in Proteomics

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· · · f·g·c·z
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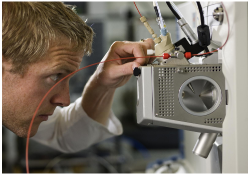
July 8, useR-2009, Agrocampus-Ouest, Rennes, France

goals of shotgun proteomics

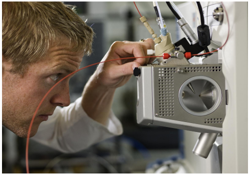
- **identification**
- quantification
- detection and discovery of post translational modifications

method of choice: mass spectrometry



ion source

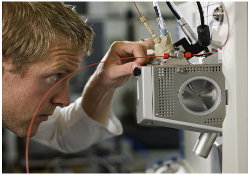
method of choice: mass spectrometry



ion source

mass analyzer

method of choice: mass spectrometry


ion source

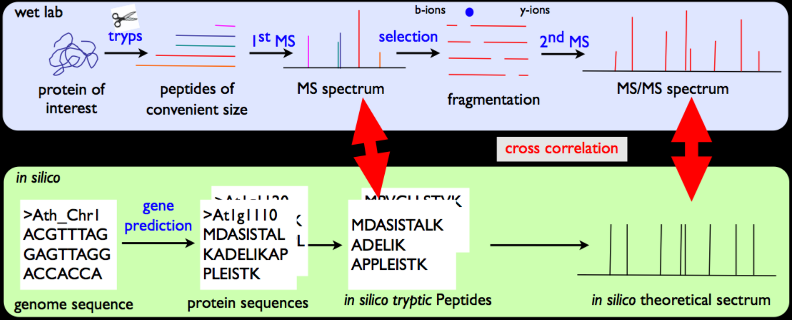

mass analyzer


detector

source: FGCZ, http://en.wikipedia.org/wiki/Mass_spectrometry

Protein Identification with Database Search

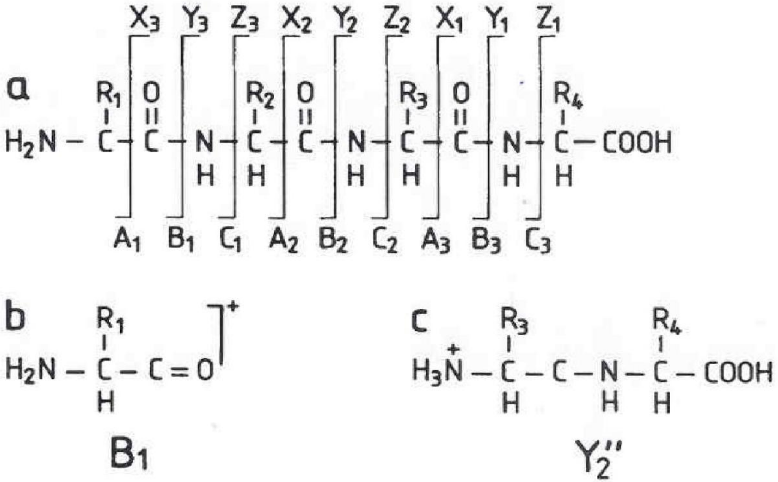
(using protein sequence databases)



peptide identification → **protein inference**

slide by Jonas Grossmann `jg@fgcz.ethz.ch`

peptide fragmentation into b and y ions



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- no manual annotation/validation of individual spectra is feasible
- existing software has limitations

  not open, not scalable, too complex to install

peakplot input

file containing:

- mass spectrum
- peptide sequence

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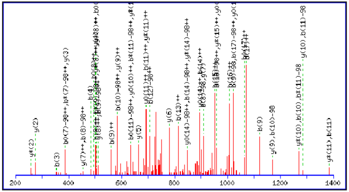
Mascot Search Results

Peptide View

MS/MS Fragmentation of **LIQQLSKDDFDEDYLLQK**
Found in **FBpp0078892**, CG31638-PA

Match to Query 1181: 2290.078452 from(764.366760,3+) intensity(758083.
Title: 2006: Scan 3229 (rt=66.4117) [S:\p215\Proteomics\ORBI_1\gerritsb_
Data file 20061106_03_i_B5_3.mgf

Click mouse within plot area to zoom in by factor of two about that point
Or, Plot from 200 to 1400 Da Full range



Monoisotopic mass of neutral peptide Mr(calc): 2290.0770
Fixed modifications: Carbamidomethyl (C)
Variable modifications:
S6 : Phospho (S), with neutral losses 0.0000(shown in table), 97.9769
Ions Score: 81 **Expect:** 2.7e-07
Matches (Bold Red): 61/282 fragment ions using 36 most intense peaks

step 0: parsing the input data

reqired attributes:

- peptide query# and peptide hit#
- MS/MS
- assigned peptide sequence
- score or e-value
- peptide modification

step 1: computing b- and y-ion matrix

of LIQQL*SKDDFDEDYLLQK

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letter	a	a*	a_0	b	b*	b_0	y	y*	y_0	z+1	z+2	b-98	b*-98	b_0-98	y-98	y*-98	y_0-98	letter
L[1]	86.10			114.09			2291.08	2274.06	2273.07	2276.07			-0.91	-1.90	2193.11	2176.08	2175.10	L[18]
I[2]	199.18			227.18			2178.00	2160.97	2159.99	2162.99			112.17	111.19	2080.02	2063.00	2062.01	I[17]
Q[3]	327.24	310.21		355.23	338.21		2064.92	2047.89	2046.91	2049.91	2050.91		240.23	239.25	1966.94	1949.91	1948.93	Q[16]
Q[4]	455.30	438.27		483.29	466.27		1936.86	1919.83	1918.85	1921.85	1922.85		368.29	367.31	1838.88	1821.85	1820.87	Q[15]
L[5]	568.38	551.36		596.38	579.35		1808.80	1791.77	1790.79	1793.79	1794.80		481.37	480.39	1710.82	1693.80	1692.81	L[14]
S[6]	735.38	718.35	717.37	763.37	746.35	745.36	1695.71	1678.69	1677.70	1680.70	1681.71	665.40	648.37	647.39	1597.74	1580.71	1579.73	S[13]
K[7]	863.48	846.45	845.46	891.47	874.44	873.46	1528.72	1511.69	1510.71	1513.71	1514.71	793.49	776.47	775.48	1430.74	1413.71	1412.73	K[12]
D[8]	978.50	961.48	960.49	1006.50	989.47	988.49	1400.62	1383.60	1382.61	1385.61	1386.62	908.52	891.49	890.51	1302.64	1285.62	1284.63	D[11]
D[9]	1093.53	1076.50	1075.52	1121.52	1104.50	1103.51	1285.59	1268.57	1267.58	1270.58	1271.59	1023.55	1006.52	1005.54	1187.62	1170.59	1169.61	D[10]
F[10]	1240.60	1223.57	1222.59	1268.59	1251.57	1250.58	1170.57	1153.54	1152.56	1155.56	1156.56	1170.62	1153.59	1152.60	1072.59	1055.56	1054.58	F[9]
D[11]	1355.62	1338.60	1337.61	1383.62	1366.59	1365.61	1023.50	1006.47	1005.49	1008.49	1009.50	1285.64	1268.62	1267.63	925.52	908.50	907.51	D[8]
E[12]	1484.67	1467.64	1466.66	1512.66	1495.64	1494.65	908.47	891.45	890.46	893.46	894.47	1414.68	1397.66	1396.67	810.50	793.47	792.48	E[7]
D[13]	1599.69	1582.67	1581.68	1627.69	1610.66	1609.68	779.43	762.40	761.42	764.42	765.43	1529.71	1512.69	1511.70	681.45	664.43	663.44	D[6]
Y[14]	1762.76	1745.73	1744.75	1790.75	1773.73	1772.74	664.40	647.38		649.39	650.40	1692.78	1675.75	1674.76		549.40	548.42	Y[5]
L[15]	1875.84	1858.81	1857.83	1903.84	1886.81	1885.83	501.34	484.31		486.33	487.34	1805.86	1788.83	1787.85		386.34	385.35	L[4]
L[16]	1988.93	1971.90	1970.91	2016.92	1999.89	1998.91	388.26	371.23		373.24	374.25	1918.94	1901.92	1900.93		273.25	272.27	L[3]
Q[17]	2116.98	2099.96	2098.97	2144.98	2127.95	2126.97	275.17	258.14		260.16	261.17	2047.00	2029.98	2028.99		160.17	159.18	Q[2]
K[18]	2245.08	2228.05	2227.07	2273.07	2256.05	2255.06	147.11	130.09		132.10	133.11	2175.10	2158.07	2157.09		32.11	31.13	K[1]

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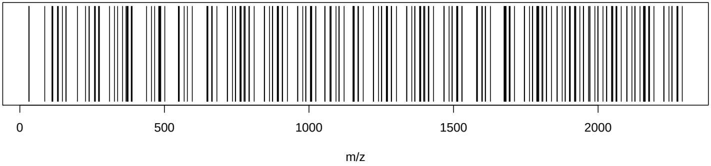

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F[10]	1240.60	1223.57	1222.59	1268.59	1251.57	1250.58	1170.57	1153.54	1152.56	1155.56	1156.56	1170.62	1153.59	1152.60	1072.59	1055.56	1054.58	F[9]
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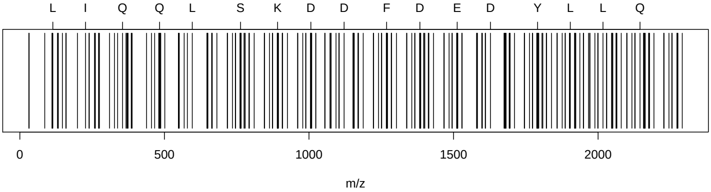

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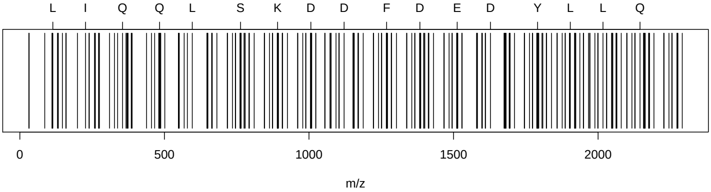
K[7]	863.48	846.45	845.46	891.47	874.44	873.46	1528.72	1511.69	1510.71	1513.71	1514.71	793.49	776.47	775.48	1430.74	1413.71	1412.73	K[12]
D[8]	978.50	961.48	960.49	1006.50	989.47	988.49	1400.62	1383.60	1382.61	1385.61	1386.62	908.52	891.49	890.51	1302.64	1285.62	1284.63	D[11]
D[9]	1093.53	1076.50	1075.52	1121.52	1104.50	1103.51	1285.59	1268.57	1267.58	1270.58	1271.59	1023.55	1006.52	1005.54	1187.62	1170.59	1169.61	D[10]
F[10]	1240.60	1223.57	1222.59	1268.59	1251.57	1250.58	1170.57	1153.54	1152.56	1155.56	1156.56	1170.62	1153.59	1152.60	1072.59	1055.56	1054.58	F[9]
D[11]	1355.62	1338.60	1337.61	1383.62	1366.59	1365.61	1023.50	1006.47	1005.49	1008.49	1009.50	1285.64	1268.62	1267.63	925.52	908.50	907.51	D[8]
E[12]	1484.67	1467.64	1466.66	1512.66	1495.64	1494.65	908.47	891.45	890.46	893.46	894.47	1414.68	1397.66	1396.67	810.50	793.47	792.48	E[7]
D[13]	1599.69	1582.67	1581.68	1627.69	1610.66	1609.68	779.43	762.40	761.42	764.42	765.43	1529.71	1512.69	1511.70	681.45	664.43	663.44	D[6]
Y[14]	1762.76	1745.73	1744.75	1790.75	1773.73	1772.74	664.40	647.38		649.39	650.40	1692.78	1675.75	1674.76		549.40	548.42	Y[5]
L[15]	1875.84	1858.81	1857.83	1903.84	1886.81	1885.83	501.34	484.31		486.33	487.34	1805.86	1788.83	1787.85		386.34	385.35	L[4]
L[16]	1988.93	1971.90	1970.91	2016.92	1999.89	1998.91	388.26	371.23		373.24	374.25	1918.94	1901.92	1900.93		273.25	272.27	L[3]
Q[17]	2116.98	2099.96	2098.97	2144.98	2127.95	2126.97	275.17	258.14		260.16	261.17	2047.00	2029.98	2028.99		160.17	159.18	Q[2]
K[18]	2245.08	2228.05	2227.07	2273.07	2256.05	2255.06	147.11	130.09		132.10	133.11	2175.10	2158.07	2157.09		32.11	31.13	K[1]

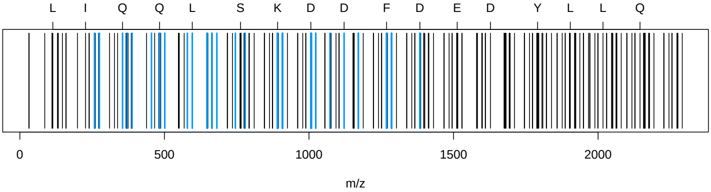


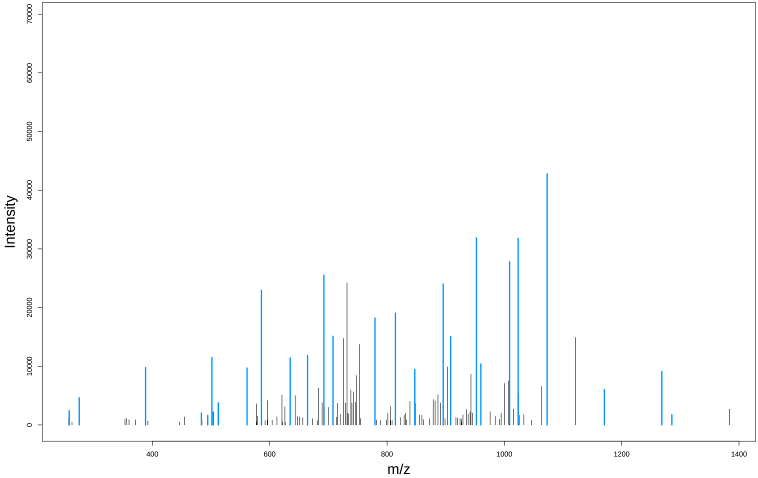
step 1: computing b- and y-ion matrix

of LIQQL*SKDDFDEDYLLQK

A	71.037114
B	114.534940
C	160.030649
D	115.026943
E	129.042593
F	147.068414
G	57.021464
H	137.058912
I	113.084064
J	0.000000
K	128.094963
L	113.084064
M	131.040485
N	114.042927
O	0.000000
P	97.052764
Q	128.058578
R	156.101111
S	87.032028
T	101.047679
U	150.953630
V	99.068414
W	186.079313
X	111.000000
Y	163.063329
Z	128.550590

letter	a	a*	a_0	b	b*	b_0	y	y*	y_0	z+1	z+2	b-98	b*-98	b_0-98	y-98	y*-98	y_0-98	letter
L[1]	86.10			114.09			2291.08	2274.06	2273.07	2276.07			-0.91	-1.90	2193.11	2176.08	2175.10	L[18]
I[2]	199.18			227.18			2178.00	2160.97	2159.99	2162.99			112.17	111.19	2080.02	2063.00	2062.01	I[17]
Q[3]	327.24	310.21		355.23	338.21		2064.92	2047.89	2046.91	2049.91	2050.91		240.23	239.25	1966.94	1949.91	1948.93	Q[16]
Q[4]	455.30	438.27		483.29	466.27		1936.86	1919.83	1918.85	1921.85	1922.85		368.29	367.31	1838.88	1821.85	1820.87	Q[15]
L[5]	568.38	551.36		596.38	579.35		1808.80	1791.77	1790.79	1793.79	1794.80		481.37	480.39	1710.82	1693.80	1692.81	L[14]
S[6]	735.38	718.35	717.37	763.37	746.35	745.36	1695.71	1678.69	1677.70	1680.70	1681.71	665.40	648.37	647.39	1597.74	1580.71	1579.73	S[13]
K[7]	863.48	846.45	845.46	891.47	874.44	873.46	1528.72	1511.69	1510.71	1513.71	1514.71	793.49	776.47	775.48	1430.74	1413.71	1412.73	K[12]
D[8]	978.50	961.48	960.49	1006.50	989.47	988.49	1400.62	1383.60	1382.61	1385.61	1386.62	908.52	891.49	890.51	1302.64	1285.62	1284.63	D[11]
D[9]	1093.53	1076.50	1075.52	1121.52	1104.50	1103.51	1285.59	1268.57	1267.58	1270.58	1271.59	1023.55	1006.52	1005.54	1187.62	1170.59	1169.61	D[10]
F[10]	1240.60	1223.57	1222.59	1268.59	1251.57	1250.58	1170.57	1153.54	1152.56	1155.56	1156.56	1170.62	1153.59	1152.60	1072.59	1055.56	1054.58	F[9]
D[11]	1355.62	1338.60	1337.61	1383.62	1366.59	1365.61	1023.50	1006.47	1005.49	1008.49	1009.50	1285.64	1268.62	1267.63	925.52	908.50	907.51	D[8]
E[12]	1484.67	1467.64	1466.66	1512.66	1495.64	1494.65	908.47	891.45	890.46	893.46	894.47	1414.68	1397.66	1396.67	810.50	793.47	792.48	E[7]
D[13]	1599.69	1582.67	1581.68	1627.69	1610.66	1609.68	779.43	762.40	761.42	764.42	765.43	1529.71	1512.69	1511.70	681.45	664.43	663.44	D[6]
Y[14]	1762.76	1745.73	1744.75	1790.75	1773.73	1772.74	664.40	647.38		649.39	650.40	1692.78	1675.75	1674.76		549.40	548.42	Y[5]
L[15]	1875.84	1858.81	1857.83	1903.84	1886.81	1885.83	501.34	484.31		486.33	487.34	1805.86	1788.83	1787.85		386.34	385.35	L[4]
L[16]	1988.93	1971.90	1970.91	2016.92	1999.89	1998.91	388.26	371.23		373.24	374.25	1918.94	1901.92	1900.93		273.25	272.27	L[3]
Q[17]	2116.98	2099.96	2098.97	2144.98	2127.95	2126.97	275.17	258.14		260.16	261.17	2047.00	2029.98	2028.99		160.17	159.18	Q[2]
K[18]	2245.08	2228.05	2227.07	2273.07	2256.05	2255.06	147.11	130.09		132.10	133.11	2175.10	2158.07	2157.09		32.11	31.13	K[1]





Intensity
0
10000
20000
30000
40000
50000
60000
70000
400
600
800
1000
1200
1400
m/z

step 2: setting the ion labels

objectives

- avoidance of overlapping labels

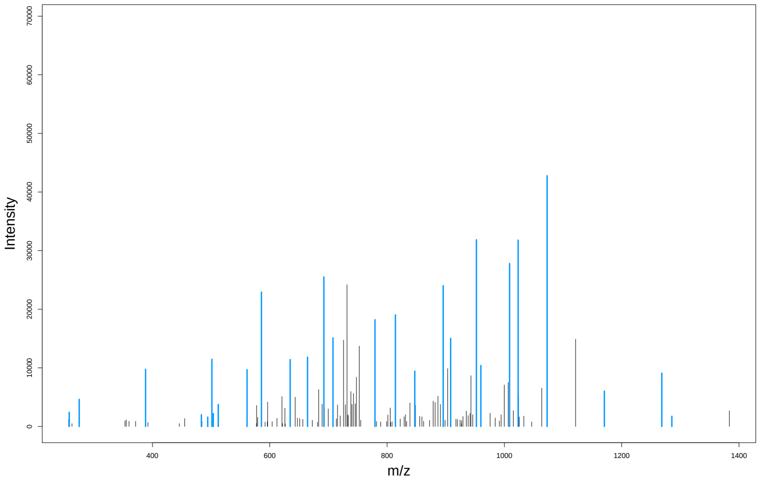
step 2: setting the ion labels

objectives

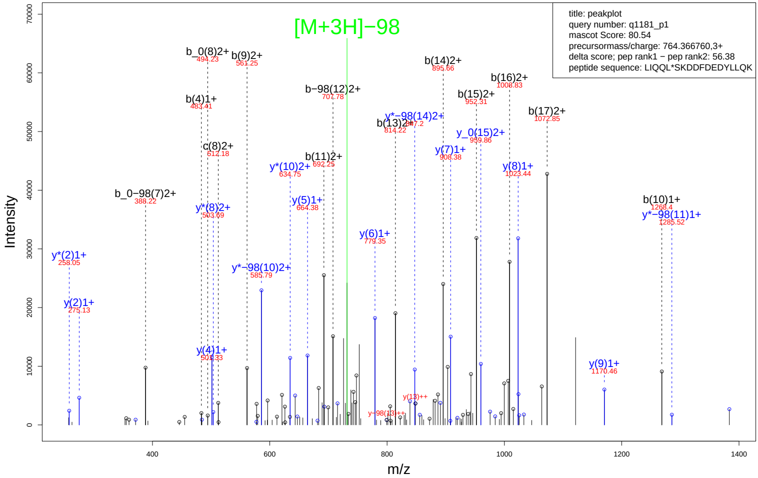
- avoidance of overlapping labels

solution heuristic

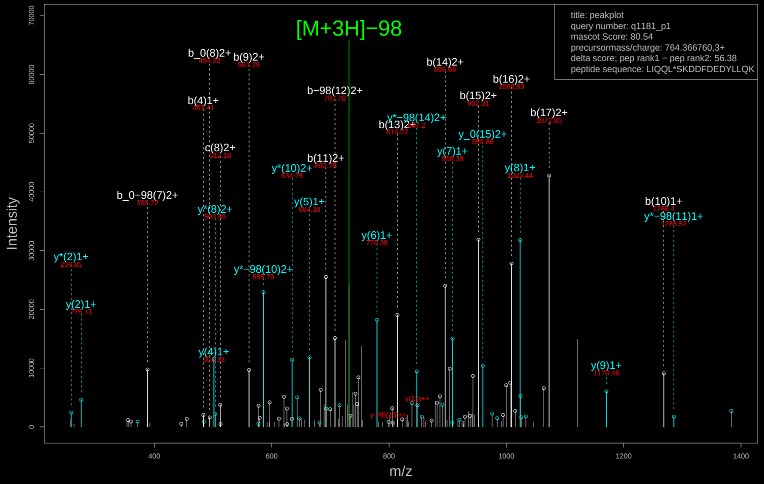
- bins depending on the peptide sequence along the m/z axis
- label is only drawn if the corresponding ion count of the m/z peak is higher than a given threshold

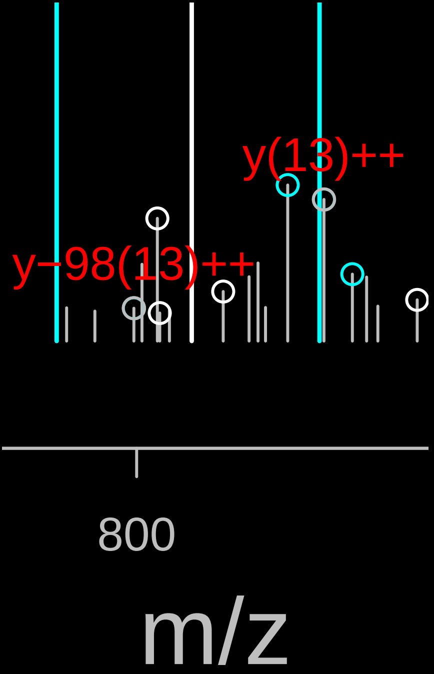


Intensity
0
10000
20000
30000
40000
50000
60000
70000
400
600
800
1000
1200
1400
m/z

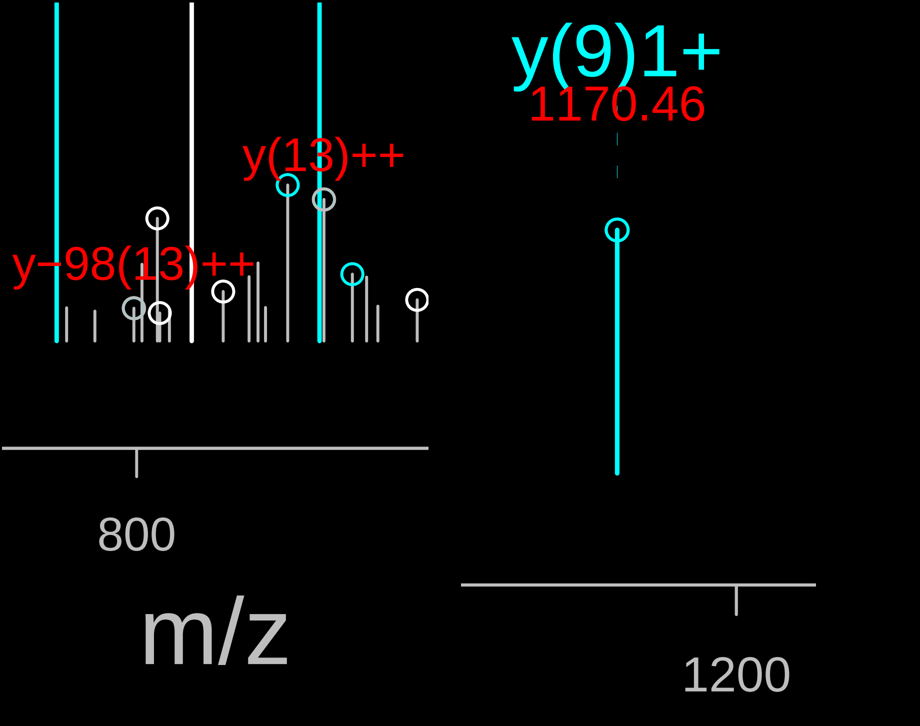


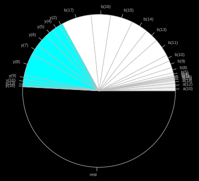
title: peakplot
query number: q1181_p1
mascot Score: 80.54
precursormass/charge: 764.366760,3+
delta score; pep rank1 − pep rank2: 56.38
peptide sequence: LIQQL*SKDDFDEDYLLQK
[M+3H]−98
Intensity
m/z
y*(2)1+ 258.05
y(2)1+ 275.13
b_0−98(7)2+ 388.22
b(4)1+ 483.41
b_0(8)2+ 494.23
y*(8)2+ 503.69
y(4)1+ 503.33
c(8)2+ 512.18
b(9)2+ 561.25
y*−98(10)2+ 585.79
y*(10)2+ 634.75
y(5)1+ 664.38
b(11)2+ 692.25
b−98(12)2+ 707.78
y(6)1+ 779.35
b(13)2+ 814.22
y*−98(14)2+ 847.2
y(13)++
y−98(13)++
b(14)2+ 895.66
y(7)1+ 908.38
b(15)2+ 952.31
y_0(15)2+ 959.86
b(16)2+ 1008.83
y(8)1+ 1023.44
b(17)2+ 1072.85
y(9)1+ 1170.46
b(10)1+ 1268.4
y*−98(11)1+ 1285.52
0
10000
20000
30000
40000
50000
60000
70000
400
600
800
1000
1200
1400

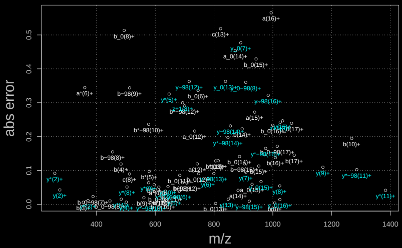

title: peakplot
query number: q1181_p1
mascot Score: 80.54
precursormass/charge: 764.366760,3+
delta score; pep rank1 − pep rank2: 56.38
peptide sequence: LIQQL*SKDDFDEDYLLQK
[M+3H]−98
b_0(8)2+
494.23
b(9)2+
561.25
b(4)1+
483.41
c(8)2+
512.18
b_0−98(7)2+
388.22
y*(8)2+
503.69
y*(2)1+
258.05
y(2)1+
275.13
y(4)1+
y*(10)2+
634.75
y*−98(10)2+
585.79
y(5)1+
664.38
b(11)2+
692.25
b−98(12)2+
707.78
y(6)1+
779.35
b(13)2+
814.22
y*−98(14)2+
b(14)2+
895.66
y(7)1+
908.38
b(15)2+
952.31
y_0(15)2+
959.86
b(16)2+
1008.83
y(8)1+
1023.44
b(17)2+
1072.85
y(9)1+
1170.46
b(10)1+
1268.4
y*−98(11)1+
1285.52
Intensity
m/z
0
10000
20000
30000
40000
50000
60000
70000
400
600
800
1000
1200
1400

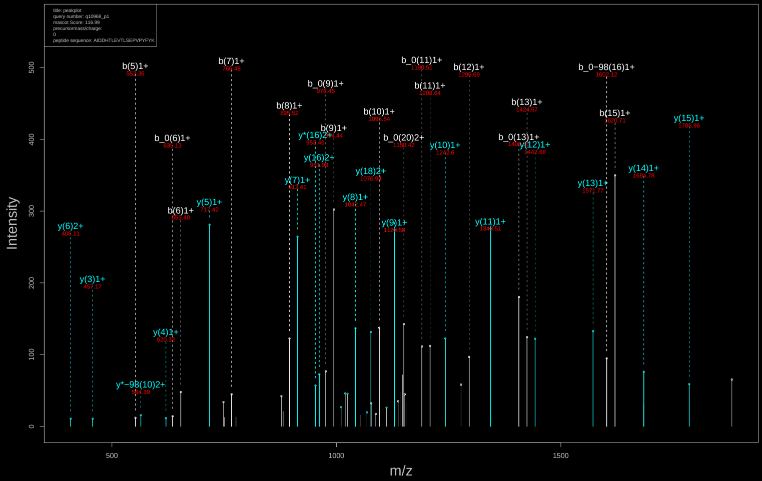


y(13)++
y−98(13)++
800
m/z

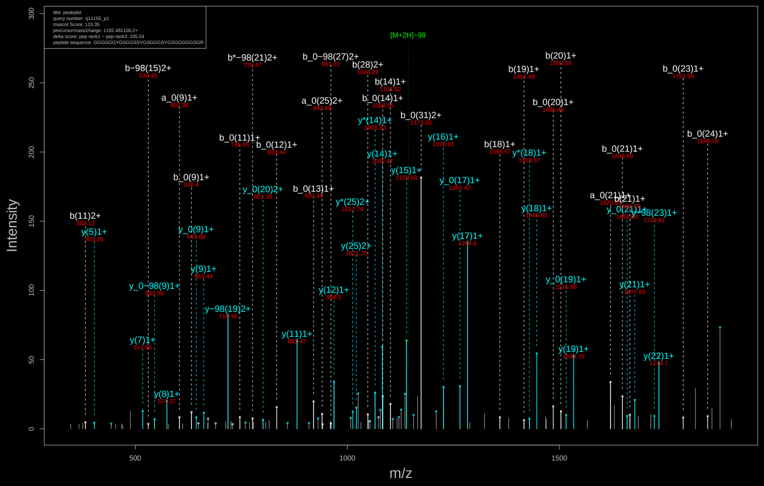

y(9)1+
1170.46
y(13)++
y−98(13)++
800
1200
m/z

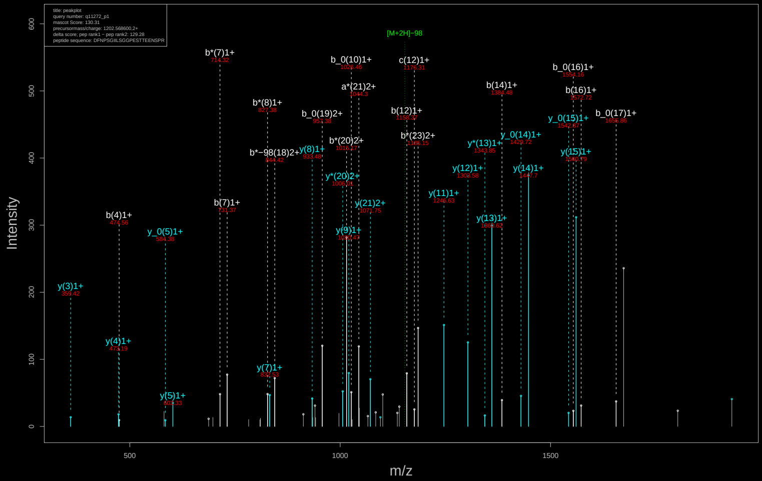

b(17)
b(16)
b(15)
b(14)
b(13)
b(11)
b(10)
b(9)
b(8)
y(2)
y(4)
y(5)
y(6)
y(7)
y(8)
y(9)
a(12)
a(10)
rest


abs error
m/z
0.0
0.1
0.2
0.3
0.4
0.5
400
600
800
1000
1200
1400
a(16)+
b_0(8)+
c(13)+
a*(6)+
b−98(9)+
b(10)+
y*−98(11)+
y*(11)+
y(9)+

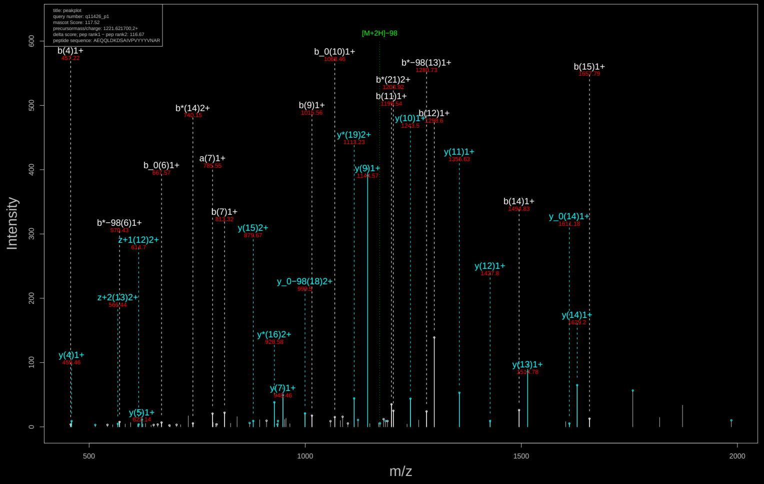


title: peakplot
query number: q10968_p1
mascot Score: 116.99
precursormass/charge:
0
peptide sequence: AIDDHTLEVTLSEPVPYFYK
Intensity
m/z
0
100
200
300
400
500
500
1000
1500
y(6)2+
408.11
y(3)1+
457.17
b(5)1+
y*−98(10)2+
564.39
y(4)1+
620.32
b_0(6)1+
635.13
b(6)1+
653.48
y(5)1+
717.42
b(7)1+
766.48
b(8)1+
895.52
y(7)1+
913.41
y*(16)2+
953.46
y(16)2+
b_0(9)1+
976.45
b(9)1+
y(8)1+
1042.47
y(18)2+
b(10)1+
1096.54
y(9)1+
b_0(20)2+
1150.42
b_0(11)1+
1190.51
b(11)1+
1208.64
y(10)1+
1242.6
b(12)1+
y(11)1+
b_0(13)1+
b(13)1+
1424.67
y(12)1+
1442.68
y(13)1+
1571.77
b_0−98(16)1+
1602.12
b(15)1+
1620.71
y(14)1+
1684.78
y(15)1+
1785.96

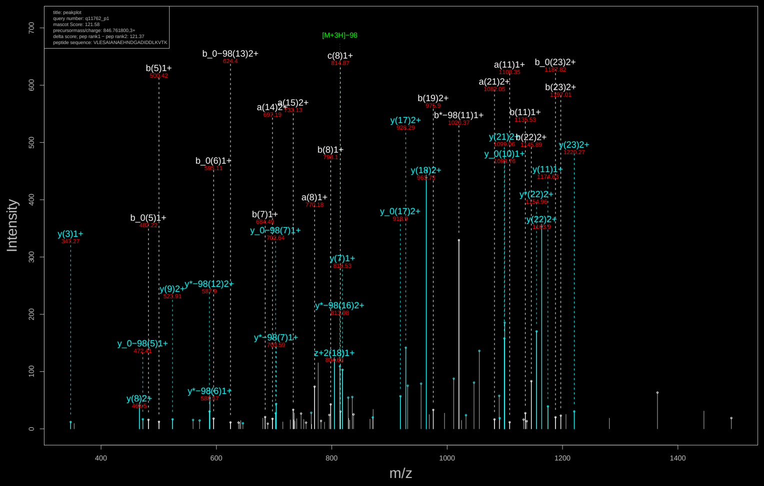

title: peakplot
query number: q11155_p1
mascot Score: 115.35
precursormass/charge: 1192.481100,2+
delta score; pep rank1 − pep rank2: 105.54
peptide sequence: GGGGGGYGSGGSSYGSGGGSYGSGGGGGGGR
[M+2H]−98
b−98(15)2+
b*−98(21)2+
b_0−98(27)2+
b(28)2+
b(14)1+
b_0(14)1+
a_0(9)1+
a_0(25)2+
b_0(31)2+
b(20)1+
b(19)1+
b_0(20)1+
b_0(23)1+
b_0(24)1+
b_0(11)1+
b_0(12)1+
b(18)1+
b_0(21)1+
b_0(9)1+
b_0(13)1+
y*(14)1+
y(14)1+
y(15)1+
y(16)1+
y_0(17)1+
y*(18)1+
y(18)1+
y_0(20)2+
y*(25)2+
y(25)2+
y(17)1+
b(11)2+
y(5)1+
y_0(9)1+
y(9)1+
y_0−98(9)1+
y−98(19)2+
y(12)1+
y(11)1+
y(7)1+
y(8)1+
y_0(19)1+
y(19)1+
y(21)1+
y(22)1+
y−98(23)1+
Intensity
m/z
0
50
100
150
200
250
300
500
1000
1500



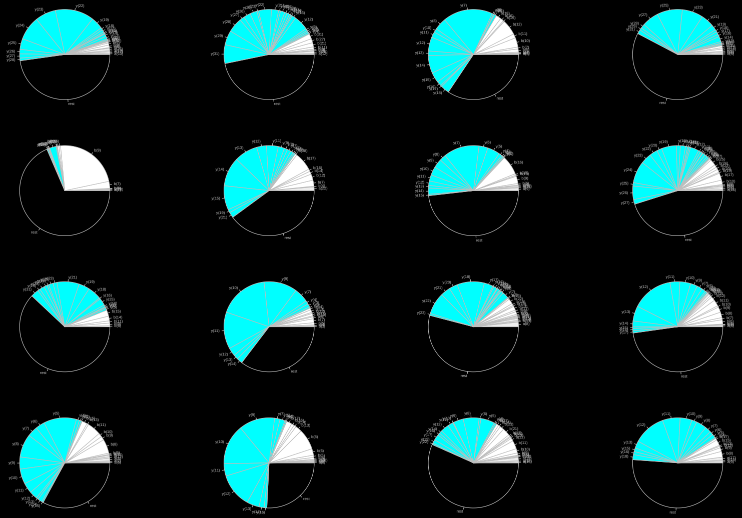
title: peakplot
query number: q11272_p1
mascot Score: 130.31
precursormass/charge: 1202.568600,2+
delta score; pep rank1 − pep rank2: 129.28
peptide sequence: DFNPSGIILSGGPESTTEENSPR
Intensity
m/z
0
100
200
300
400
500
600
500
1000
1500
[M+2H]−98
y(3)1+
b(4)1+
y(4)1+
y_0(5)1+
y(5)1+
b*(7)1+
b(7)1+
b*(8)1+
b*−98(18)2+
y(7)1+
y(8)1+
b_0(19)2+
b*(20)2+
y*(20)2+
y(9)1+
b_0(10)1+
a*(21)2+
y(21)2+
c(12)1+
b(12)1+
b*(23)2+
y(11)1+
y(12)1+
y*(13)1+
y(13)1+
b(14)1+
y_0(14)1+
y(14)1+
b_0(16)1+
b(16)1+
y_0(15)1+
y(15)1+
b_0(17)1+

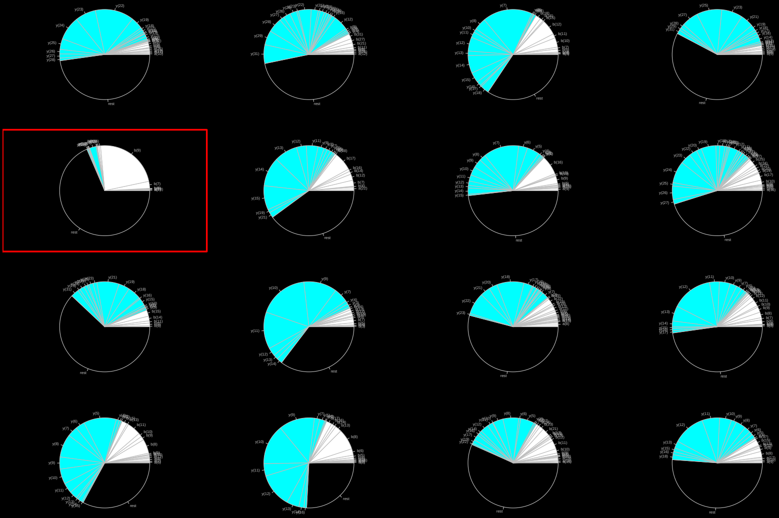


title: peakplot
query number: q11426_p1
mascot Score: 117.52
precursormass/charge: 1221.621700,2+
delta score; pep rank1 − pep rank2: 116.67
peptide sequence: AEQQLDKDSAIVPVYYYVNAR
[M+2H]−98
b(4)1+
457.22
b_0(10)1+
b*−98(13)1+
b(15)1+
b*(21)2+
b(11)1+
b*(14)2+
740.15
b(9)1+
1015.56
y(10)1+
1243.5
b(12)1+
y*(19)2+
1113.23
y(11)1+
1356.63
b_0(6)1+
667.57
a(7)1+
785.55
y(9)1+
b(14)1+
y_0(14)1+
b(7)1+
813.32
b*−98(6)1+
570.43
y(15)2+
879.67
z+1(12)2+
y(12)1+
y_0−98(18)2+
z+2(13)2+
y(14)1+
y*(16)2+
928.58
y(4)1+
y(13)1+
y(7)1+
y(5)1+
Intensity
m/z
0
100
200
300
400
500
600
500
1000
1500
2000

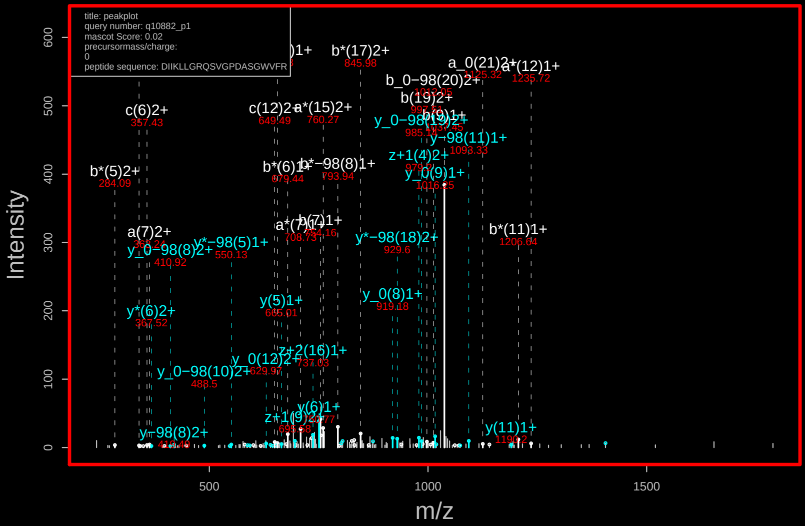


title: peakplot
query number: q11762_p1
mascot Score: 121.58
precursormass/charge: 846.761800,3+
delta score; pep rank1 − pep rank2: 121.37
peptide sequence: VLESAIANAEHNDGADIDDLKVTK
[M+3H]−98
b_0−98(13)2+
c(8)1+
b(5)1+
a(11)1+
b_0(23)2+
a(21)2+
b(23)2+
a(14)2+
a(15)2+
b(19)2+
b*−98(11)1+
y(17)2+
b(11)1+
y(21)2+
b(22)2+
y(23)2+
y_0(10)1+
b_0(6)1+
b(8)1+
y(18)2+
y(11)1+
y*(22)2+
a(8)1+
y_0(17)2+
b_0(5)1+
b(7)1+
y(22)2+
y(3)1+
y_0−98(7)1+
y(7)1+
y(9)2+
y*−98(12)2+
y*−98(16)2+
y*−98(7)1+
y_0−98(5)1+
z+2(18)1+
y*−98(6)1+
y(8)2+
Intensity
m/z






Intensity
m/z


title: peakplot
query number: q10882_p1
mascot Score: 0.02
precursormass/charge:
0
peptide sequence: DIIKLLGRQSVGPDASGWVFR
Intensity
m/z
0
100
200
300
400
500
600
500
1000
1500
b*(17)2+
845.98
a_0(21)2+
1125.32
a*(12)1+
1235.72
b_0−98(20)2+
1012.05
b(19)2+
997.51
c(6)2+
357.43
c(12)2+
649.49
a*(15)2+
760.27
y_0−98(19)2+
985.14
y−98(11)1+
1093.33
z+1(4)2+
979.2
b*(5)2+
284.09
b*(6)1+
679.44
b*−98(8)1+
793.94
y_0(9)1+
1016.25
a(7)2+
y_0−98(8)2+
410.92
y*−98(5)1+
550.13
b(7)1+
754.16
a*(7)1+
708.73
y*−98(18)2+
929.6
b*(11)1+
1206.64
y*(6)2+
367.52
y(5)1+
665.01
y_0(8)1+
919.18
z+2(16)1+
737.03
y_0(12)2+
629.97
y_0−98(10)2+
488.5
y(6)1+
y−98(8)2+
y(11)1+
1190.2

summary

contribution

- peakplot enables large scale high throughput labeling of tandem mass spectra
- easy to adapt and to plugin into existing software, e.g., LIMS
- open source code
- no commercial libraries nessesary

availability

- source: `svn co https://peakplot.svn.sourceforge.net/svnroot/peakplot peakplot`
- CGI: `http://fgcz-peakplot.uzh.ch`
- LIMS: `http://fgcz-bfabric.uzh.ch`

thanks

special thanks to:

- Ralph Schlapbach (general support)
- Bertran Gerrits (peakplot)
- Jonas Grossmann (discussion and slides)