

<i>P. syringae</i> containing <i>mcb</i> operon	<i>P. syringae</i> that do not contain <i>mcb</i> operon
<i>P. syringae</i> pv. <i>glycinea</i> str. B076 (NZ_AEGG01000085)	<i>P. syringae</i> pv. <i>tomato</i> str. DC3000 (NC_004578)
<i>P. syringae</i> pv. <i>glycinea</i> str. race 4 (ADWY01001248)	<i>P. syringae</i> pv. <i>syringae</i> str. B728a (CP000075)
<i>P. syringae</i> pv. <i>aesculi</i> str. NCPPB 3681 (ACXS01000133)	<i>P. syringae</i> pv. <i>phaseolicola</i> str. 1448A (NC_005773)

**Table S1. *P. syringae* strains with and without *mcb* operons.** Fully or partially sequenced *P. syringae* strains that, at the time of this writing, contain an entire *mcb* operon (*mcbABCDEFG*) are listed in the left-hand side of the table along with GenBank accession numbers. Fully sequenced strains that lack *mcb* genes are listed on the right hand side.



# Mascot Search Results

## Peptide View

MS/MS Fragmentation of **LGGSCGGQGGGCGGGGCSGGNGGSGGS**

Found in **McbA\_Psg\_tev**, McbA\_Psg\_tev

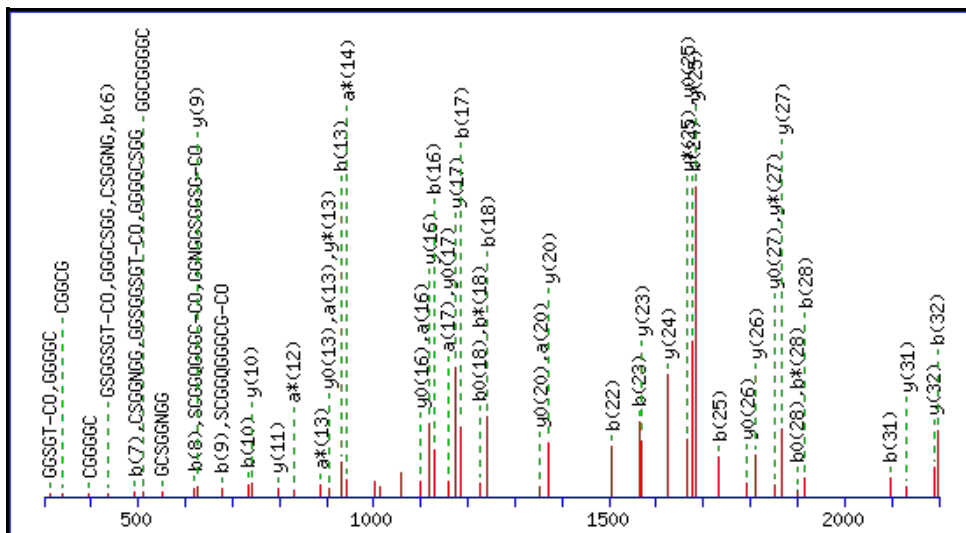
Match to Query 1: 2301.492724 from(2302.500000,1+) index(0)

Data file DATA.TXT

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

Or,   to  Da

Label all possible matches  Label matches used for scoring



Monoisotopic mass of neutral peptide  $M_r(\text{calc})$ : 2301.6605

Variable modifications:

S4 : Oxazole S (S)

C5 : Thiazole (C)

C12 : Thiazole (C)

C15 : Thiazole (C)

C20 : Thiazole (C)

S21 : Oxazole S (S)

S27 : Oxazole S (S)

S30 : Oxazole S (S)

Ions Score: 150 **Expect:** 6.9e-014

Matches : 85/767 fragment ions using 49 most intense peaks ([help](#))

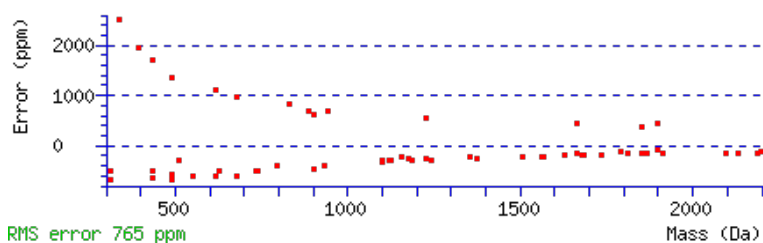
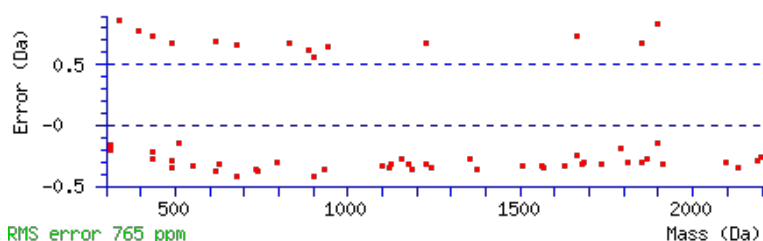
#	Immon.	a	a*	a <sup>0</sup>	b	b*	b <sup>0</sup>	Seq.	y	y*	y <sup>0</sup>	#
1	86.0964	86.0964			114.0913			L				33
2	30.0338	143.1179			171.1128			G	<b>2189.5835</b>	2172.5569	2171.5729	32
3	30.0338	200.1394			228.1343			G	<b>2132.5620</b>	2115.5355	2114.5514	31
4	40.0182	267.1452		249.1346	295.1401		277.1295	S	2075.5405	2058.5140	2057.5300	30
5	55.9953	350.1281		332.1176	378.1231		360.1125	C	2008.5347	1991.5082	1990.5242	29
6	30.0338	407.1496		389.1390	<b>435.1445</b>		417.1340	G	1925.5518	1908.5252	1907.5412	28
7	30.0338	464.1711		446.1605	<b>492.1660</b>		474.1554	G	<b>1868.5303</b>	<b>1851.5037</b>	<b>1850.5197</b>	27
8	101.0709	592.2296	575.2031	574.2191	<b>620.2246</b>	603.1980	602.2140	Q	<b>1811.5088</b>	1794.4823	<b>1793.4983</b>	26
9	30.0338	649.2511	632.2246	631.2405	<b>677.2460</b>	660.2195	659.2355	G	<b>1683.4502</b>	<b>1666.4237</b>	<b>1665.4397</b>	25
10	30.0338	706.2726	689.2460	688.2620	<b>734.2675</b>	717.2409	716.2569	G	<b>1626.4288</b>	1609.4022	1608.4182	24
11	30.0338	763.2940	746.2675	745.2835	791.2889	774.2624	773.2784	G	<b>1569.4073</b>	1552.3808	1551.3968	23
12	55.9953	846.2770	<b>829.2505</b>	828.2664	874.2719	857.2454	856.2614	C	1512.3859	1495.3593	1494.3753	22
13	30.0338	<b>893.2895</b>	<b>886.2710</b>	885.2870	<b>931.2924</b>	914.2769	913.2929	C	1420.4020	1410.2762	1411.2922	21

13	30.0338	<b>903.2985</b>	<b>886.2719</b>	885.2879	<b>951.2954</b>	914.2668	915.2828	G	1429.4029	1412.5705	1411.5925	21
14	30.0338	960.3199	<b>943.2934</b>	942.3094	988.3148	971.2883	970.3043	G	<b>1372.3814</b>	1355.3549	<b>1354.3709</b>	20
15	55.9953	1043.3029	1026.2764	1025.2923	1071.2978	1054.2713	1053.2873	C	1315.3600	1298.3334	1297.3494	19
16	30.0338	<b>1100.3244</b>	1083.2978	1082.3138	<b>1128.3193</b>	1111.2927	1110.3087	G	1232.3770	1215.3504	1214.3664	18
17	30.0338	<b>1157.3458</b>	1140.3193	1139.3353	<b>1185.3407</b>	1168.3142	1167.3302	G	<b>1175.3555</b>	1158.3290	<b>1157.3450</b>	17
18	30.0338	1214.3673	1197.3407	1196.3567	<b>1242.3622</b>	<b>1225.3357</b>	<b>1224.3516</b>	G	<b>1118.3341</b>	1101.3075	<b>1100.3235</b>	16
19	30.0338	1271.3888	1254.3622	1253.3782	1299.3837	1282.3571	1281.3731	G	1061.3126	1044.2860	1043.3020	15
20	55.9953	<b>1354.3717</b>	1337.3452	1336.3612	1382.3666	1365.3401	1364.3561	C	1004.2911	987.2646	986.2806	14
21	40.0182	1421.3775	1404.3510	1403.3670	1449.3725	1432.3459	1431.3619	S	921.3082	<b>904.2816</b>	<b>903.2976</b>	13
22	30.0338	1478.3990	1461.3725	1460.3884	<b>1506.3939</b>	1489.3674	1488.3834	G	854.3023	837.2758	836.2918	12
23	30.0338	1535.4205	1518.3939	1517.4099	<b>1563.4154</b>	1546.3888	1545.4048	G	<b>797.2809</b>	780.2543	779.2703	11
24	87.0553	1649.4634	1632.4368	1631.4528	<b>1677.4583</b>	1660.4318	1659.4477	N	<b>740.2594</b>	723.2329	722.2489	10
25	30.0338	1706.4849	1689.4583	1688.4743	<b>1734.4798</b>	1717.4532	1716.4692	G	<b>626.2165</b>		608.2059	9
26	30.0338	1763.5063	1746.4798	1745.4958	1791.5012	1774.4747	1773.4907	G	569.1950		551.1845	8
27	40.0182	1830.5121	1813.4856	1812.5016	1858.5071	1841.4805	1840.4965	S	512.1736		494.1630	7
28	30.0338	1887.5336	1870.5071	1869.5230	<b>1915.5285</b>	<b>1898.5020</b>	<b>1897.5180</b>	G	445.1678		427.1572	6
29	30.0338	1944.5551	1927.5285	1926.5445	1972.5500	1955.5234	1954.5394	G	388.1463		370.1357	5
30	40.0182	2011.5609	1994.5343	1993.5503	2039.5558	2022.5292	2021.5452	S	331.1248		313.1143	4
31	30.0338	2068.5823	2051.5558	2050.5718	<b>2096.5773</b>	2079.5507	2078.5667	G	264.1190		246.1084	3
32	74.0600	2169.6300	2152.6035	2151.6195	<b>2197.6249</b>	2180.5984	2179.6144	T	207.0975		189.0870	2
33	60.0444							S	106.0499		88.0393	1

Seq	ya	yb	Seq	ya	yb	Seq	ya	yb
GG	87.0553	115.0502	GGG	154.0611	182.0560	GGSC	237.0441	265.0390
GGSCG	294.0655	322.0605	GGSCGG	351.0870	379.0819	GGSCGGQ	479.1456	507.1405
GGSCGGQG	536.1670	564.1620	GGSCGGQGG	593.1885	621.1834	GGSCGGQGGG	650.2100	678.2049
GS	97.0396	125.0346	GSC	180.0226	208.0175	GSCG	237.0441	265.0390
GSCGG	294.0655	322.0605	GSCGGQ	422.1241	450.1190	GSCGGQG	479.1456	507.1405
GSCGGQGG	536.1670	564.1620	GSCGGQGGG	593.1885	621.1834	GSCGGQGGGC	<b>676.1715</b>	704.1664
SC	123.0011	150.9961	SCG	180.0226	208.0175	SCGG	237.0441	265.0390
SCGGQ	365.1026	393.0976	SCGGQG	422.1241	450.1190	SCGGQGG	479.1456	507.1405
SCGGQGGG	536.1670	564.1620	SCGGQGGGC	<b>619.1500</b>	647.1449	SCGGQGGGCG	<b>676.1715</b>	704.1664
CG	113.0168	141.0117	CGG	170.0383	198.0332	CGGQ	298.0968	326.0918
CGGQG	355.1183	383.1132	CGGQGG	412.1398	440.1347	CGGQGGG	469.1612	497.1561
CGGQGGGC	552.1442	580.1391	CGGQGGGCG	609.1657	637.1606	CGGQGGGCGG	666.1871	694.1820
GG	87.0553	115.0502	GGQ	215.1139	243.1088	GGQG	272.1353	300.1302
GGQGG	329.1568	357.1517	GGQGGG	386.1783	414.1732	GGQGGGC	469.1612	497.1561
GGQGGGCG	526.1827	554.1776	GGQGGGCGG	583.2042	611.1991	GGQGGGCGGC	666.1871	694.1820
GQ	158.0924	186.0873	GQG	215.1139	243.1088	GQGG	272.1353	300.1302
GQGGG	329.1568	357.1517	GQGGGC	412.1398	440.1347	GQGGGCG	469.1612	497.1561
GQGGGCGG	526.1827	554.1776	GQGGGCGGC	609.1657	637.1606	GQGGGCGGCG	666.1871	694.1820
QG	158.0924	186.0873	QGG	215.1139	243.1088	QGGG	272.1353	300.1302
QGGGC	355.1183	383.1132	QGGGCG	412.1398	440.1347	QGGGCGG	469.1612	497.1561
QGGGCGGC	552.1442	580.1391	QGGGCGGCG	609.1657	637.1606	QGGGCGGCGG	666.1871	694.1820
GG	87.0553	115.0502	GGG	144.0768	172.0717	GGGC	227.0597	255.0546
GGGCG	284.0812	<b>312.0761</b>	GGGCGG	341.1027	369.0976	GGGCGGC	424.0856	452.0805
GGGCGGCG	481.1071	<b>509.1020</b>	GGGCGGCGG	538.1285	566.1235	GGGCGGCGGG	595.1500	623.1449

GGGCGGCGGGG	652.1715	680.1664	GG	87.0553	115.0502	GGC	170.0383	198.0332
GGCG	227.0597	255.0546	GGCGG	284.0812	312.0761	GGCGGC	367.0642	395.0591
GGCGGCG	424.0856	452.0805	GGCGGCGG	481.1071	509.1020	GGCGGCGGG	538.1285	566.1235
GGCGGCGGGG	595.1500	623.1449	GGCGGCGGGGC	678.1330	706.1279	GC	113.0168	141.0117
GCG	170.0383	198.0332	GCGG	227.0597	255.0546	GCGGC	310.0427	338.0376
GCGGCG	367.0642	395.0591	GCGGCGG	424.0856	452.0805	GCGGCGGG	481.1071	509.1020
GCGGCGGGG	538.1285	566.1235	GCGGCGGGGC	621.1115	649.1064	GCGGCGGGGCS	688.1173	716.1122
CG	113.0168	141.0117	CGG	170.0383	198.0332	CGGC	253.0212	281.0161
CGGCG	310.0427	338.0376	CGGCGG	367.0642	395.0591	CGGCGGG	424.0856	452.0805
CGGCGGGG	481.1071	509.1020	CGGCGGGGC	564.0901	592.0850	CGGCGGGGCS	631.0959	659.0908
CGGCGGGGCSG	688.1173	716.1122	GG	87.0553	115.0502	GGC	170.0383	198.0332
GGCG	227.0597	255.0546	GGCGG	284.0812	312.0761	GGCGGG	341.1027	369.0976
GGCGGGG	398.1241	426.1190	GGCGGGGC	481.1071	509.1020	GGCGGGGCS	548.1129	576.1078
GGCGGGGCSG	605.1344	633.1293	GGCGGGGCSGG	662.1558	690.1507	GC	113.0168	141.0117
GCG	170.0383	198.0332	GCGG	227.0597	255.0546	GCGGG	284.0812	312.0761
GCGGGG	341.1027	369.0976	GCGGGGC	424.0856	452.0805	GCGGGGCS	491.0914	519.0863
GCGGGGCSG	548.1129	576.1078	GCGGGGCSGG	605.1344	633.1293	CG	113.0168	141.0117
CGG	170.0383	198.0332	CGGG	227.0597	255.0546	CGGGG	284.0812	312.0761
CGGGGC	367.0642	395.0591	CGGGGCS	434.0700	462.0649	CGGGGCSG	491.0914	519.0863
CGGGGCSGG	548.1129	576.1078	CGGGGCSGGN	662.1558	690.1507	GG	87.0553	115.0502
GGG	144.0768	172.0717	GGGG	201.0982	229.0931	GGGGC	284.0812	312.0761
GGGGCS	351.0870	379.0819	GGGGCSG	408.1085	436.1034	GGGGCSGG	465.1299	493.1248
GGGGCSGGN	579.1729	607.1678	GGGGCSGGNG	636.1943	664.1892	GGGGCSGGNGG	693.2158	721.2107
GG	87.0553	115.0502	GGG	144.0768	172.0717	GGGC	227.0597	255.0546
GGGCS	294.0655	322.0605	GGGCSG	351.0870	379.0819	GGGCSGG	408.1085	436.1034
GGGCSGGN	522.1514	550.1463	GGGCSGGNG	579.1729	607.1678	GGGCSGGNGG	636.1943	664.1892
GG	87.0553	115.0502	GGC	170.0383	198.0332	GGCS	237.0441	265.0390
GGCSG	294.0655	322.0605	GGCSGG	351.0870	379.0819	GGCSGGN	465.1299	493.1248
GGCSGGNG	522.1514	550.1463	GGCSGGNGG	579.1729	607.1678	GGCSGGNGGS	646.1787	674.1736
GC	113.0168	141.0117	GCS	180.0226	208.0175	GCSG	237.0441	265.0390
GCSGG	294.0655	322.0605	GCSGGN	408.1085	436.1034	GCSGGNG	465.1299	493.1248
GCSGGNGG	522.1514	550.1463	GCSGGNGGS	589.1572	617.1521	GCSGGNGGSG	646.1787	674.1736
CS	123.0011	150.9961	CSG	180.0226	208.0175	CSGG	237.0441	265.0390
CSGGN	351.0870	379.0819	CSGGNG	408.1085	436.1034	CSGGNGG	465.1299	493.1248
CSGGNGGS	532.1357	560.1307	CSGGNGGSG	589.1572	617.1521	CSGGNGGSGG	646.1787	674.1736
SG	97.0396	125.0346	SGG	154.0611	182.0560	SGGN	268.1040	296.0989
SGGNG	325.1255	353.1204	SGGNGG	382.1470	410.1419	SGGNGGS	449.1528	477.1477
SGGNGGSG	506.1742	534.1691	SGGNGGSGG	563.1957	591.1906	SGGNGGSGGS	630.2015	658.1964
SGGNGGSGGSG	687.2230	715.2179	GG	87.0553	115.0502	GGN	201.0982	229.0931
GGNG	258.1197	286.1146	GGNGG	315.1411	343.1361	GGNGGS	382.1470	410.1419
GGNGGSG	439.1684	467.1633	GGNGGSGG	496.1899	524.1848	GGNGGSGGS	563.1957	591.1906
GGNGGSGGSG	620.2172	648.2121	GN	144.0768	172.0717	GNG	201.0982	229.0931
GNGG	258.1197	286.1146	GNGGS	325.1255	353.1204	GNGGSG	382.1470	410.1419
GNGGSGG	439.1684	467.1633	GNGGSGGS	506.1742	534.1691	GNGGSGGSG	563.1957	591.1906
GNGGSGGSGT	664.2434	692.2383	NG	144.0768	172.0717	NGG	201.0982	229.0931

<b>NGGS</b>	268.1040	296.0989	<b>NGGSG</b>	325.1255	353.1204	<b>NGGSGG</b>	382.1470	410.1419
<b>NGGSGGS</b>	449.1528	477.1477	<b>NGGSGGSG</b>	506.1742	534.1691	<b>NGGSGGSGT</b>	607.2219	635.2168
<b>GG</b>	87.0553	115.0502	<b>GGS</b>	154.0611	182.0560	<b>GGSG</b>	211.0826	239.0775
<b>GGSGG</b>	268.1040	296.0989	<b>GGSGGS</b>	335.1098	363.1048	<b>GGSGGSG</b>	392.1313	420.1262
<b>GGSGGSGT</b>	493.1790	521.1739	<b>GS</b>	97.0396	125.0346	<b>GSG</b>	154.0611	182.0560
<b>GSGG</b>	211.0826	239.0775	<b>GSGGS</b>	278.0884	306.0833	<b>GSGGSG</b>	335.1098	363.1048
<b>GSGGSGT</b>	436.1575	464.1524	<b>SG</b>	97.0396	125.0346	<b>SGG</b>	154.0611	182.0560
<b>SGGS</b>	221.0669	249.0618	<b>SGGSG</b>	278.0884	306.0833	<b>SGGSGT</b>	379.1361	407.1310
<b>GG</b>	87.0553	115.0502	<b>GGS</b>	154.0611	182.0560	<b>GGSG</b>	211.0826	239.0775
<b>GGSGT</b>	312.1302	340.1252	<b>GS</b>	97.0396	125.0346	<b>GSG</b>	154.0611	182.0560
<b>GSGT</b>	255.1088	283.1037	<b>SG</b>	97.0396	125.0346	<b>SGT</b>	198.0873	226.0822
<b>GT</b>	131.0815	159.0764						



NCBI **BLAST** search of [LGGSCGGQGGGCGGC GGGGCSGGNNGGSGGSGTS](#)

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

Other BLAST [web gateways](#)

#### All matches to this query

Score	Mr(calc):	Delta	Sequence
150.5	2301.6605	-0.1678	<a href="#">LGGSCGGQGGGCGGC GGGGCSGGNNGGSGGSGTS</a>
125.3	2301.6605	-0.1678	<a href="#">LGGSCGGQGGGCGGC GGGGCSGGNNGGSGGSGTS</a>
118.0	2301.6605	-0.1678	<a href="#">LGGSCGGQGGGCGGC GGGGCSGGNNGGSGGSGTS</a>
81.5	2301.6605	-0.1678	<a href="#">LGGSCGGQGGGCGGC GGGGCSGGNNGGSGGSGTS</a>
81.5	2301.6605	-0.1678	<a href="#">LGGSCGGQGGGCGGC GGGGCSGGNNGGSGGSGTS</a>
46.1	2301.6605	-0.1678	<a href="#">LGGSCGGQGGGCGGC GGGGCSGGNNGGSGGSGTS</a>
30.3	2301.6605	-0.1678	<a href="#">LGGSCGGQGGGCGGC GGGGCSGGNNGGSGGSGTS</a>
16.1	2301.6605	-0.1678	<a href="#">TSLGGSCGGQGGGCGGC GGGGCSGGNNGGSGGSG</a>
14.9	2301.6605	-0.1678	<a href="#">TSLGGSCGGQGGGCGGC GGGGCSGGNNGGSGGSG</a>
12.9	2301.6605	-0.1678	<a href="#">TSLGGSCGGQGGGCGGC GGGGCSGGNNGGSGGSG</a>

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

Table S2. Mascot MS/MS Ion search file for peptide with m/z 2302.8

# MASCOT SCIENCE Mascot Search Results

## Peptide View

MS/MS Fragmentation of **LGGSCGGQGGGCGGGCGGGGCSGGNGGSGGSGTSAPDHV**

Found in **McbA\_Psg\_tev**, McbA\_Psg\_tev

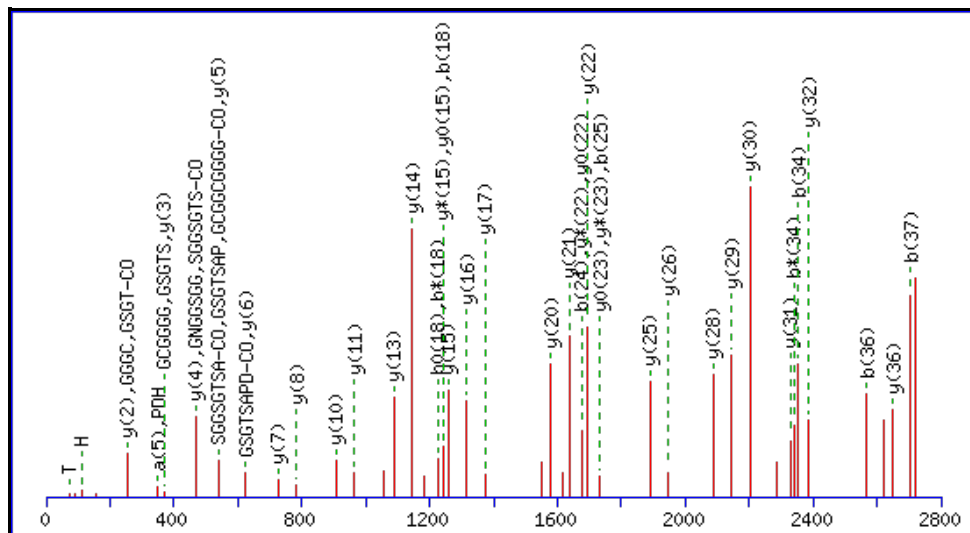
Match to Query 1: 2821.092824 from(2822.100100,1+) index(0)

Data file DATA.TXT

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

Or,   to  Da

Label all possible matches  Label matches used for scoring



Monoisotopic mass of neutral peptide  $M_r(\text{calc})$ : 2820.9046

### Variable modifications:

S4 : Oxazole S (S)

C5 : Thiazole (C)

C12 : Thiazole (C)

C15 : Thiazole (C)

C20 : Thiazole (C)

S21 : Oxazole S (S)

S27 : Oxazole S (S)

S30 : Oxazole S (S)

Ions Score: 234 **Expect:** 2.4e-021

Matches : 65/889 fragment ions using 42 most intense peaks ([help](#))

#	Immon.	a	a*	a <sup>0</sup>	b	b*	b <sup>0</sup>	Seq.	y	y*	y <sup>0</sup>	#
1	86.0964	86.0964			114.0913			L				38
2	30.0338	143.1179			171.1128			G	2708.8276	2691.8011	2690.8170	37
3	30.0338	200.1394			228.1343			G	<b>2651.8061</b>	2634.7796	2633.7956	36
4	40.0182	267.1452		249.1346	295.1401		277.1295	S	2594.7847	2577.7581	2576.7741	35
5	55.9953	<b>350.1281</b>		332.1176	378.1231		360.1125	C	2527.7789	2510.7523	2509.7683	34
6	30.0338	407.1496		389.1390	435.1445		417.1340	G	2444.7959	2427.7694	2426.7853	33
7	30.0338	464.1711		446.1605	492.1660		474.1554	G	<b>2387.7744</b>	2370.7479	2369.7639	32
8	101.0709	592.2296	575.2031	574.2191	620.2246	603.1980	602.2140	Q	<b>2330.7530</b>	2313.7264	2312.7424	31
9	30.0338	649.2511	632.2246	631.2405	677.2460	660.2195	659.2355	G	<b>2202.6944</b>	2185.6678	2184.6838	30
10	30.0338	706.2726	689.2460	688.2620	734.2675	717.2409	716.2569	G	<b>2145.6729</b>	2128.6464	2127.6624	29
11	30.0338	763.2940	746.2675	745.2835	791.2889	774.2624	773.2784	G	<b>2088.6515</b>	2071.6249	2070.6409	28
12	55.9953	846.2770	829.2505	828.2664	874.2719	857.2454	856.2614	C	2031.6300	2014.6035	2013.6194	27
13	30.0338	903.2985	886.2710	885.2870	931.2934	914.2669	913.2829	C	<b>1978.6170</b>	1961.5905	1960.6065	26

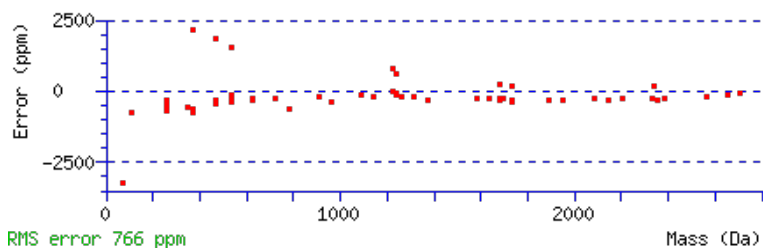
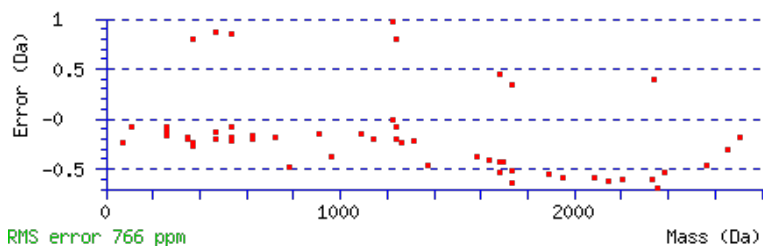
13	30.0338	903.2983	880.2719	883.2879	931.2934	914.2008	913.2828	G	1948.0470	1931.0203	1930.0303	20
14	30.0338	960.3199	943.2934	942.3094	988.3148	971.2883	970.3043	G	1891.6256	1874.5990	1873.6150	25
15	55.9953	1043.3029	1026.2764	1025.2923	1071.2978	1054.2713	1053.2873	C	1834.6041	1817.5776	1816.5935	24
16	30.0338	1100.3244	1083.2978	1082.3138	1128.3193	1111.2927	1110.3087	G	1751.6211	1734.5946	1733.6106	23
17	30.0338	1157.3458	1140.3193	1139.3353	1185.3407	1168.3142	1167.3302	G	1694.5997	1677.5731	1676.5891	22
18	30.0338	1214.3673	1197.3407	1196.3567	1242.3622	1225.3357	1224.3516	G	1637.5782	1620.5517	1619.5676	21
19	30.0338	1271.3888	1254.3622	1253.3782	1299.3837	1282.3571	1281.3731	G	1580.5567	1563.5302	1562.5462	20
20	55.9953	1354.3717	1337.3452	1336.3612	1382.3666	1365.3401	1364.3561	C	1523.5353	1506.5087	1505.5247	19
21	40.0182	1421.3775	1404.3510	1403.3670	1449.3725	1432.3459	1431.3619	S	1440.5523	1423.5258	1422.5417	18
22	30.0338	1478.3990	1461.3725	1460.3884	1506.3939	1489.3674	1488.3834	G	1373.5465	1356.5199	1355.5359	17
23	30.0338	1535.4205	1518.3939	1517.4099	1563.4154	1546.3888	1545.4048	G	1316.5250	1299.4985	1298.5145	16
24	87.0553	1649.4634	1632.4368	1631.4528	1677.4583	1660.4318	1659.4477	N	1259.5036	1242.4770	1241.4930	15
25	30.0338	1706.4849	1689.4583	1688.4743	1734.4798	1717.4532	1716.4692	G	1145.4606		1127.4501	14
26	30.0338	1763.5063	1746.4798	1745.4958	1791.5012	1774.4747	1773.4907	G	1088.4392		1070.4286	13
27	40.0182	1830.5121	1813.4856	1812.5016	1858.5071	1841.4805	1840.4965	S	1031.4177		1013.4071	12
28	30.0338	1887.5336	1870.5071	1869.5230	1915.5285	1898.5020	1897.5180	G	964.4119		946.4013	11
29	30.0338	1944.5551	1927.5285	1926.5445	1972.5500	1955.5234	1954.5394	G	907.3904		889.3799	10
30	40.0182	2011.5609	1994.5343	1993.5503	2039.5558	2022.5292	2021.5452	S	850.3690		832.3584	9
31	30.0338	2068.5823	2051.5558	2050.5718	2096.5773	2079.5507	2078.5667	G	783.3632		765.3526	8
32	74.0600	2169.6300	2152.6035	2151.6195	2197.6249	2180.5984	2179.6144	T	726.3417		708.3311	7
33	60.0444	2256.6620	2239.6355	2238.6515	2284.6570	2267.6304	2266.6464	S	625.2940		607.2835	6
34	44.0495	2327.6992	2310.6726	2309.6886	2355.6941	2338.6675	2337.6835	A	538.2620		520.2514	5
35	70.0651	2424.7519	2407.7254	2406.7414	2452.7468	2435.7203	2434.7363	P	467.2249		449.2143	4
36	88.0393	2539.7789	2522.7523	2521.7683	2567.7738	2550.7472	2549.7632	D	370.1721		352.1615	3
37	110.0713	2676.8378	2659.8112	2658.8272	2704.8327	2687.8061	2686.8221	H	255.1452			2
38	72.0808							V	118.0863			1

Seq	ya	yb	Seq	ya	yb	Seq	ya	yb
GG	87.0553	115.0502	GGG	154.0611	182.0560	GGSC	237.0441	265.0390
GGSCG	294.0655	322.0605	GGSCGG	351.0870	379.0819	GGSCGGQ	479.1456	507.1405
GGSCGGQG	536.1670	564.1620	GGSCGGQGG	593.1885	621.1834	GGSCGGQGGG	650.2100	678.2049
GS	97.0396	125.0346	GSC	180.0226	208.0175	GSCG	237.0441	265.0390
GSCGG	294.0655	322.0605	GSCGGQ	422.1241	450.1190	GSCGGQG	479.1456	507.1405
GSCGGQGG	536.1670	564.1620	GSCGGQGGG	593.1885	621.1834	GSCGGQGGGC	676.1715	704.1664
SC	123.0011	150.9961	SCG	180.0226	208.0175	SCGG	237.0441	265.0390
SCGGQ	365.1026	393.0976	SCGGQG	422.1241	450.1190	SCGGQGG	479.1456	507.1405
SCGGQGGG	536.1670	564.1620	SCGGQGGGC	619.1500	647.1449	SCGGQGGGCG	676.1715	704.1664
CG	113.0168	141.0117	CGG	170.0383	198.0332	CGGQ	298.0968	326.0918
CGGQG	355.1183	383.1132	CGGQGG	412.1398	440.1347	CGGQGGG	469.1612	497.1561
CGGQGGGC	552.1442	580.1391	CGGQGGGCG	609.1657	637.1606	CGGQGGGCGG	666.1871	694.1820
GG	87.0553	115.0502	GGQ	215.1139	243.1088	GGQG	272.1353	300.1302
GGQGG	329.1568	357.1517	GGQGGG	386.1783	414.1732	GGQGGGC	469.1612	497.1561
GGQGGGCG	526.1827	554.1776	GGQGGGCGG	583.2042	611.1991	GGQGGGCGGC	666.1871	694.1820
GQ	158.0924	186.0873	GQG	215.1139	243.1088	GQGG	272.1353	300.1302
GQGGG	329.1568	357.1517	GQGGGC	412.1398	440.1347	GQGGGCG	469.1612	497.1561
GQGGGCGG	526.1827	554.1776	GQGGGCGGC	609.1657	637.1606	GQGGGCGGCG	666.1871	694.1820
OG	158.0924	186.0873	OGG	215.1139	243.1088	OGGG	272.1353	300.1302

QGGGC	355.1183	383.1132	QGGGCG	412.1398	440.1347	QGGGCGG	469.1612	497.1561
QGGGCGGC	552.1442	580.1391	QGGGCGGCG	609.1657	637.1606	QGGGCGGCGG	666.1871	694.1820
GG	87.0553	115.0502	GGG	144.0768	172.0717	GGGC	227.0597	255.0546
GGGCG	284.0812	312.0761	GGGCGG	341.1027	369.0976	GGGCGGC	424.0856	452.0805
GGGCGGCG	481.1071	509.1020	GGGCGGCGG	538.1285	566.1235	GGGCGGCGGG	595.1500	623.1449
GGGCGGCGGGG	652.1715	680.1664	GG	87.0553	115.0502	GGC	170.0383	198.0332
GGCG	227.0597	255.0546	GGCGG	284.0812	312.0761	GGCGGC	367.0642	395.0591
GGCGGCG	424.0856	452.0805	GGCGGCGG	481.1071	509.1020	GGCGGCGGG	538.1285	566.1235
GGCGGCGGGG	595.1500	623.1449	GGCGGCGGGGC	678.1330	706.1279	GC	113.0168	141.0117
GCG	170.0383	198.0332	GCGG	227.0597	255.0546	GCGGC	310.0427	338.0376
GCGGCG	367.0642	395.0591	GCGGCGG	424.0856	452.0805	GCGGCGGG	481.1071	509.1020
GCGGCGGGG	538.1285	566.1235	GCGGCGGGGC	621.1115	649.1064	GCGGCGGGGCS	688.1173	716.1122
CG	113.0168	141.0117	CGG	170.0383	198.0332	CGGC	253.0212	281.0161
CGGCG	310.0427	338.0376	CGGCGG	367.0642	395.0591	CGGCGGG	424.0856	452.0805
CGGCGGGG	481.1071	509.1020	CGGCGGGGC	564.0901	592.0850	CGGCGGGGCS	631.0959	659.0908
CGGCGGGGCSG	688.1173	716.1122	GG	87.0553	115.0502	GGC	170.0383	198.0332
GGCG	227.0597	255.0546	GGCGG	284.0812	312.0761	GGCGGG	341.1027	369.0976
GGCGGGG	398.1241	426.1190	GGCGGGGC	481.1071	509.1020	GGCGGGGCS	548.1129	576.1078
GGCGGGGCSG	605.1344	633.1293	GGCGGGGCSGG	662.1558	690.1507	GC	113.0168	141.0117
GCG	170.0383	198.0332	GCGG	227.0597	255.0546	GCGGG	284.0812	312.0761
GCGGGG	341.1027	369.0976	GCGGGGC	424.0856	452.0805	GCGGGGCS	491.0914	519.0863
GCGGGGCSG	548.1129	576.1078	GCGGGGCSGG	605.1344	633.1293	CG	113.0168	141.0117
CGG	170.0383	198.0332	CGGG	227.0597	255.0546	CGGGG	284.0812	312.0761
CGGGGC	367.0642	395.0591	CGGGGCS	434.0700	462.0649	CGGGGCSG	491.0914	519.0863
CGGGGCSGG	548.1129	576.1078	CGGGGCSGGN	662.1558	690.1507	GG	87.0553	115.0502
GGG	144.0768	172.0717	GGGG	201.0982	229.0931	GGGGC	284.0812	312.0761
GGGGCS	351.0870	379.0819	GGGGCSG	408.1085	436.1034	GGGGCSGG	465.1299	493.1248
GGGGCSGGN	579.1729	607.1678	GGGGCSGGNG	636.1943	664.1892	GGGGCSGGNGG	693.2158	721.2107
GG	87.0553	115.0502	GGG	144.0768	172.0717	GGGC	227.0597	255.0546
GGGCS	294.0655	322.0605	GGGCSG	351.0870	379.0819	GGGCSGG	408.1085	436.1034
GGGCSGGN	522.1514	550.1463	GGGCSGGNG	579.1729	607.1678	GGGCSGGNGG	636.1943	664.1892
GG	87.0553	115.0502	GGC	170.0383	198.0332	GGCS	237.0441	265.0390
GGCSG	294.0655	322.0605	GGCSGG	351.0870	379.0819	GGCSGGN	465.1299	493.1248
GGCSGGNG	522.1514	550.1463	GGCSGGNGG	579.1729	607.1678	GGCSGGNGGS	646.1787	674.1736
GC	113.0168	141.0117	GCS	180.0226	208.0175	GCSG	237.0441	265.0390
GCSGG	294.0655	322.0605	GCSGGN	408.1085	436.1034	GCSGGNG	465.1299	493.1248
GCSGGNGG	522.1514	550.1463	GCSGGNGGS	589.1572	617.1521	GCSGGNGGSG	646.1787	674.1736
CS	123.0011	150.9961	CSG	180.0226	208.0175	CSGG	237.0441	265.0390
CSGGN	351.0870	379.0819	CSGGNG	408.1085	436.1034	CSGGNGG	465.1299	493.1248
CSGGNGGS	532.1357	560.1307	CSGGNGGSG	589.1572	617.1521	CSGGNGGSGG	646.1787	674.1736
SG	97.0396	125.0346	SGG	154.0611	182.0560	SGGN	268.1040	296.0989
SGGNG	325.1255	353.1204	SGGNGG	382.1470	410.1419	SGGNGGS	449.1528	477.1477
SGGNGGSG	506.1742	534.1691	SGGNGGSGG	563.1957	591.1906	SGGNGGSGGS	630.2015	658.1964
SGGNGGSGGSG	687.2230	715.2179	GG	87.0553	115.0502	GGN	201.0982	229.0931
GGNG	258.1197	286.1146	GGNGG	315.1411	343.1361	GGNGGS	382.1470	410.1419



<b>GGNGGSG</b>	439.1684	<b>467.1633</b>	<b>GGNGGSGG</b>	496.1899	524.1848	<b>GGNGGSGGS</b>	563.1957	591.1906
<b>GGNGGSGGSG</b>	620.2172	648.2121	<b>GN</b>	144.0768	172.0717	<b>GNG</b>	201.0982	229.0931
<b>GNGG</b>	258.1197	286.1146	<b>GNGGS</b>	325.1255	353.1204	<b>GNGGSG</b>	382.1470	410.1419
<b>GNGGSGG</b>	439.1684	<b>467.1633</b>	<b>GNGGSGGS</b>	506.1742	534.1691	<b>GNGGSGGSG</b>	563.1957	591.1906
<b>GNGGSGGSGT</b>	664.2434	692.2383	<b>NG</b>	144.0768	172.0717	<b>NGG</b>	201.0982	229.0931
<b>NGGS</b>	268.1040	296.0989	<b>NGGSG</b>	325.1255	353.1204	<b>NGGSGG</b>	382.1470	410.1419
<b>NGGSGGS</b>	449.1528	477.1477	<b>NGGSGGSG</b>	506.1742	534.1691	<b>NGGSGGSGT</b>	607.2219	635.2168
<b>NGGSGGSGTS</b>	694.2539	722.2489	<b>GG</b>	87.0553	115.0502	<b>GGG</b>	154.0611	182.0560
<b>GGSG</b>	211.0826	239.0775	<b>GGSGG</b>	268.1040	296.0989	<b>GGSGGS</b>	335.1098	363.1048
<b>GGSGGSG</b>	392.1313	420.1262	<b>GGSGGSGT</b>	493.1790	521.1739	<b>GGSGGSGTS</b>	580.2110	608.2059
<b>GGSGGSGTSA</b>	651.2481	679.2430	<b>GS</b>	97.0396	125.0346	<b>GSG</b>	154.0611	182.0560
<b>GSGG</b>	211.0826	239.0775	<b>GSGGS</b>	278.0884	306.0833	<b>GSGGSG</b>	335.1098	363.1048
<b>GSGGSGT</b>	436.1575	464.1524	<b>GSGGSGTS</b>	523.1895	551.1845	<b>GSGGSGTSA</b>	594.2267	622.2216
<b>GSGGSGTSAP</b>	691.2794	719.2743	<b>SG</b>	97.0396	125.0346	<b>SGG</b>	154.0611	182.0560
<b>SGGS</b>	221.0669	249.0618	<b>SGGSG</b>	278.0884	306.0833	<b>SGGSGT</b>	379.1361	407.1310
<b>SGGSGTS</b>	<b>466.1681</b>	494.1630	<b>SGGSGTSA</b>	<b>537.2052</b>	565.2001	<b>SGGSGTSAP</b>	634.2580	662.2529
<b>GG</b>	87.0553	115.0502	<b>GGS</b>	154.0611	182.0560	<b>GGSG</b>	211.0826	239.0775
<b>GGSGT</b>	312.1302	340.1252	<b>GGSGTS</b>	399.1623	427.1572	<b>GGSGTSA</b>	470.1994	498.1943
<b>GGSGTSAP</b>	567.2522	595.2471	<b>GGSGTSAPD</b>	682.2791	710.2740	<b>GS</b>	97.0396	125.0346
<b>GSG</b>	154.0611	182.0560	<b>GSGT</b>	<b>255.1088</b>	283.1037	<b>GSGTS</b>	342.1408	<b>370.1357</b>
<b>GSGTSA</b>	413.1779	441.1728	<b>GSGTSAP</b>	510.2307	<b>538.2256</b>	<b>GSGTSAPD</b>	<b>625.2576</b>	653.2525
<b>SG</b>	97.0396	125.0346	<b>SGT</b>	198.0873	226.0822	<b>SGTS</b>	285.1193	313.1143
<b>SGTSA</b>	356.1565	384.1514	<b>SGTSAP</b>	453.2092	481.2041	<b>SGTSAPD</b>	568.2362	596.2311
<b>GT</b>	131.0815	159.0764	<b>GTS</b>	218.1135	246.1084	<b>G TSA</b>	289.1506	317.1456
<b>GTSAP</b>	386.2034	414.1983	<b>GTSAPD</b>	501.2304	529.2253	<b>GTSAPDH</b>	638.2893	666.2842
<b>TS</b>	161.0921	189.0870	<b>TSA</b>	232.1292	260.1241	<b>TSAP</b>	329.1819	357.1769
<b>TSAPD</b>	444.2089	472.2038	<b>TSAPDH</b>	581.2678	609.2627	<b>SA</b>	131.0815	159.0764
<b>SAP</b>	228.1343	256.1292	<b>SAPD</b>	343.1612	371.1561	<b>SAPDH</b>	480.2201	508.2150
<b>AP</b>	141.1022	169.0972	<b>APD</b>	256.1292	284.1241	<b>APDH</b>	393.1881	421.1830
<b>PD</b>	185.0921	213.0870	<b>PDH</b>	322.1510	<b>350.1459</b>	<b>DH</b>	225.0982	253.0931



NCBI **BLAST** search of [LGGSCGGQGGGCGGCGGGGCSGGNGGSGGSGTSAPDHV](#)  
 (Parameters: blastp, nr protein database, expect=20000, no filter, PAM30)

Other BLAST [web gateways](#)**All matches to this query**

Score	Mr(calc):	Delta	Sequence
234.1	2820.9046	0.1882	<a href="#">LGGSCGGQGGGCGGC GGGGCSGGNGGSGGSGTSAPDHV</a>
187.4	2820.9046	0.1882	<a href="#">LGGSCGGQGGGCGGC GGGGCSGGNGGSGGSGTSAPDHV</a>
152.9	2820.9046	0.1882	<a href="#">LGGSCGGQGGGCGGC GGGGCSGGNGGSGGSGTSAPDHV</a>
89.2	2820.9046	0.1882	<a href="#">LGGSCGGQGGGCGGC GGGGCSGGNGGSGGSGTSAPDHV</a>
89.2	2820.9046	0.1882	<a href="#">LGGSCGGQGGGCGGC GGGGCSGGNGGSGGSGTSAPDHV</a>
58.1	2820.9046	0.1882	<a href="#">LGGSCGGQGGGCGGC GGGGCSGGNGGSGGSGTSAPDHV</a>
38.5	2820.9046	0.1882	<a href="#">LGGSCGGQGGGCGGC GGGGCSGGNGGSGGSGTSAPDHV</a>
30.2	2821.2611	-0.1683	<a href="#">LGMVNYFHNAGSICLGSMVQHHCKVH</a>
20.9	2820.9886	0.1042	<a href="#">RQSPLGVGIGGGGGGGGGSCGGQGGGCGGCSNGCSSG</a>
19.3	2821.2611	-0.1683	<a href="#">LGMVNYFHNAGSICLGSMVQHHCKVH</a>

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

Table S3. Mascot MS/MS Ion search file for peptide with m/z 2822.0