

DEP- LVQGGVIQHITNEYEFRDEYLFYR

#	b+ theoretical	b+ observed	b++ theoretical	b++ observed	Seq.	y+ theoretical	y+ observed	y++ theoretical	y++ observed	#
1					L	2989.4841		1495.2457		24
2	213.1603	213.1567	107.0835		V	2876.3997		1438.7035		23
3	341.2189	341.2133	171.1128		Q	2777.3313		1389.1693		22
4	398.2403		199.6235		G	2649.2727		1325.1400		21
5	455.2618	455.2554	228.1343		G	2592.2512		1296.6293		20
6	554.3302		277.6687		V	2535.2297		1268.1185		19
7	667.4142		334.2108		I	2436.1614		1218.5844	1218.5699	18
8	795.4728		398.2401		Q	2323.0771		1162.0422	1162.0262	17
9	932.5317		466.7695		H	2195.0186		1098.0129	1097.9976	16
10	1045.6158		523.3116		I	2057.9597		1029.4835	1029.4696	15
11	1146.6635		573.8354		T	1944.8757		972.9415	972.9282	14
12	1260.7064		630.8569		N	1843.8280		922.4177	922.4059	13
13	1389.749		695.3782		E	1729.7850		865.3962	865.3854	12
14	1552.8124		776.9099		Y	1600.7424		800.8749	800.8638	11
15	1681.8549		841.4311		E	1437.6792		719.3433		10
16	1828.9233		914.9653		F	1308.6366		654.8220	654.8132	9
17	1985.0244		993.0159		R	1161.5681	1161.5575	581.2877		8
18	2100.0513		1050.5293		D	1005.4670	1005.4548	503.2372		7
19	2229.094		1115.0507		E	890.4401	890.4286	445.7237		6
20	2392.1572		1196.5823		Y	761.3975	761.3877	381.2024		5
21	2505.2415		1253.1244		L	598.3342		299.6707		4
22	2652.3098		1326.6586		F	485.2501	485.2443			3
23	2815.373		1408.1902		Y	338.1817				2
24					R	175.1184				1

DEP- LVQGGVIQHITNEYEF(+396.34,LKM38)RDEYLFYR

#	b+ theoretical	b+ observed	b++ theoretical	b++ observed	Seq.	y+ theoretical	y+ observed	y++ theoretical	y++ observed	#
1					L	3385.8242		1693.4158		24
2	213.1603	213.1567	107.0835		V	3272.7395		1636.8734		23
3	341.2189	341.2133	171.1128		Q	3173.6711		1587.3392		22
4	398.2403		199.6235		G	3045.6125		1523.3099		21
5	455.2618	455.2554	228.1343		G	2988.5911		1494.7992		20
6	554.3302		277.6687		V	2931.5696		1466.2885		19
7	667.4142		334.2108		I	2832.5012		1416.7543	1416.7375	18
8	795.4728		398.2401		Q	2719.4172		1360.2123	1360.1942	17
9	932.5317		466.7695		H	2591.3586		1296.183	1296.1643	16
10	1045.6158		523.3116		I	2454.2998		1227.6536	1227.6373	15
11	1146.6635		573.8354		T	2341.2156		1171.1115	1171.0946	14
12	1260.7064		630.8569		N	2240.168		1120.5876	1120.5732	13
13	1389.749		695.3782		E	2126.125		1063.5662		12
14	1552.8124		776.9099		Y	1997.0825		999.0449	999.0314	11
15	1681.8549		841.4311		E	1834.0192		917.5132	917.5009	10
16	2225.2634		1113.1354		F(+396.34,LKM38)	1704.9766		852.9919	852.9801	9
17	2381.3645		1191.1859		R	1161.5681	1161.5575	581.2877		8
18	2496.3914		1248.6993		D	1005.467	1005.4548	503.2372		7
19	2625.4341		1313.2207		E	890.4401	890.4286	445.7237		6
20	2788.4973		1394.7523		Y	761.3975	761.3877	381.2024		5
21	2901.5813		1451.2943		L	598.3342		299.6707		4
22	3048.6497		1524.8285		F	485.2501	485.2443			3
23	3211.7131		1606.3602		Y	338.1817				2
24					R	175.1184				1