

**TM1- LFPALLEC(+125.05, NEM)FGIVLCGYIAGR**

#	b+ theoretical	b+ observed	b++ theoretical	b++ observed	Seq.	y+ theoretical	y+ observed	y+++H2O theoretical	y+++H2O observed	y++++H2O theoretical	y++++H2O observed	#
1					L	2280.1941		1131.5955		754.7327		20
2	261.1603		131.0835		F	2167.1096		1075.0532		717.0378		19
3	358.213		179.6099		P	2020.0411		1001.5189		668.015		18
4	429.2502		215.1285		A	1922.9884		952.9926		635.6641		17
5	542.3342	<b>542.3385</b>	271.6707		L	1851.9513		917.474		611.985		16
6	655.4183	<b>655.4157</b>	328.2128		L	1738.8672		860.9319		574.2903		15
7	784.4609	<b>784.4598</b>	392.7341		E	1625.7832		804.39		536.5957		14
8	1012.5201		506.7637		<b>C(+125.05, NEM)</b>	1496.7406		739.8687				13
9	1159.5885	<b>1159.5944</b>	580.2979		F	1268.6814		625.8391				12
10	1216.61	<b>1216.5897</b>	608.8087		G	1121.613		552.3049				11
11	1329.694	<b>1329.6908</b>	665.3506	<b>665.3516</b>	I	1064.5916		523.7942				10
12	1428.7625	<b>1428.7394</b>	714.8849	<b>714.8787</b>	V	951.5074		467.2521				9
13	1541.8464	<b>1541.8351</b>	771.4269	<b>771.4122</b>	L	852.4391		417.7179				8
14	1644.8556		822.9315		C	739.355		361.1758				7
15	1701.8771		851.4422		G	636.3458	<b>636.3431</b>					6
16	1864.9404		932.9739		Y	579.3243	<b>579.3212</b>					5
17	1978.0245		989.5159		I	416.261	<b>416.2581</b>					4
18	2049.0615		1025.0344		A	303.177	<b>303.1766</b>					3
19	2106.083		1053.5452		G	232.1399						2
20					R	175.1184						1

**TM1- LFPALLEC(+125.05, NEM)FGIVLC(+484.26, KK231)GYIAGR**

#	b+ theoretical	b+ observed	b++ theoretical	b++ observed	Seq.	y+ theoretical	y+ observed	y+++H2O theoretical	y+++H2O observed	y++++H2O theoretical	y++++H2O observed	#
1					L	2764.4541		1373.7255		916.1526		20
2	261.1603		131.0835		F	2651.3696		1317.1832		878.4578		19
3	358.213		179.6099		P	2504.3013		1243.649	<b>1243.6385</b>	829.4351	<b>829.4313</b>	18
4	429.2502		215.1285		A	2407.2485		1195.1227		797.0842		17
5	542.3342	<b>542.3385</b>	271.6707		L	2336.2112		1159.604		773.4050		16
6	655.4183	<b>655.4157</b>	328.2128		L	2223.1272		1103.062	<b>1103.0496</b>	735.7104		15
7	784.4609	<b>784.4598</b>	392.7341		E	2110.0432		1046.52	<b>1046.5150</b>	698.0157		14
8	1012.5201		506.7637		<b>C(+125.05, NEM)</b>	1981.0006		981.9987	<b>981.9920</b>			13
9	1159.5885	<b>1159.5944</b>	580.2979		F	1752.9414		867.9691				12
10	1216.61	<b>1216.5897</b>	608.8087		G	1605.873		794.4349				11
11	1329.694	<b>1329.6908</b>	665.3506	<b>665.3516</b>	I	1548.8516		765.9242				10
12	1428.7625	<b>1428.7394</b>	714.8849	<b>714.8787</b>	V	1435.7675		709.3821	<b>709.3759</b>			9
13	1541.8464	<b>1541.8351</b>	771.4269	<b>771.4122</b>	L	1336.6991		659.848	<b>659.8510</b>			8
14	2129.1157		1065.0615	<b>1065.0591</b>	<b>C(+484.26, KK231)</b>	1223.615		603.3059	<b>603.3077</b>			7
15	2186.1372		1093.5723		G	636.3458	<b>636.3431</b>					6
16	2349.2004		1175.1039	<b>1175.0833</b>	Y	579.3243	<b>579.3212</b>					5
17	2462.2844		1231.6459	<b>1231.6310</b>	I	416.261	<b>416.2581</b>					4
18	2533.3215		1267.1644	<b>1267.1603</b>	A	303.177	<b>303.1766</b>					3
19	2590.343		1295.6752	<b>1295.6669</b>	G	232.1399						2
20					R	175.1184						1