

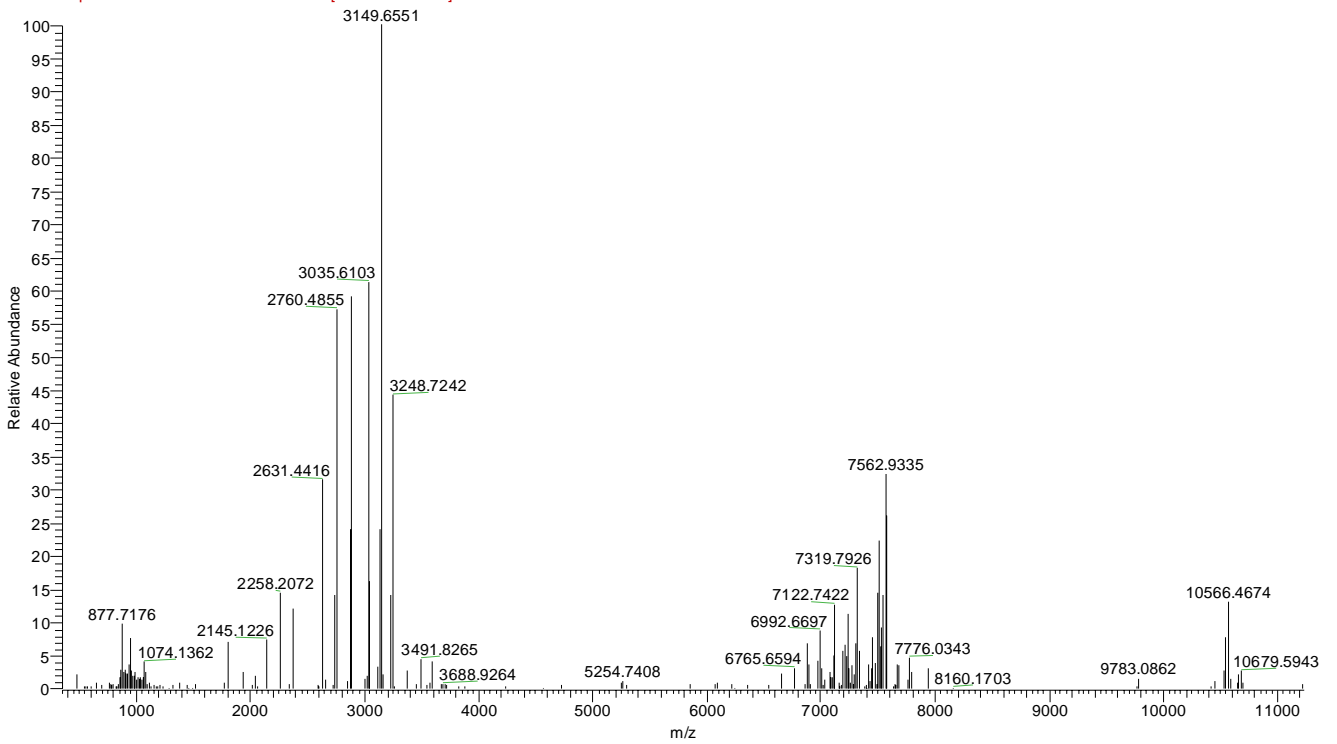
S100A8 MS/MS spectrum

Exp mass	%	Theor mass	Aa res	Exp mass	%	Thor mass
			M			
		10697.62 (y92)	L			245.14 (b2)
10584.4993 10566.4674	1.48 13.00	10584.53 (y91) 10566.52 (y91-H ₂ O)	T			346.18 (b3)
		10483.48 (y90)	E			475.22 (b4)
		10354.44 (y89)	L			588.31 (b5)
		10241.36 (y88)	E			717.35 (b6)
		10112.32 (y87)	K			845.44 (b7)
		9984.22 (y86)	A			916.48 (b8)
		9913.18 (y85)	L			1029.56 (b9)
		9800.10 (y84)	N			1143.61 (b10)
		9686.06 (y83)	S			1230.64 (b11)
		9599.02 (y82)	I			1343.72 (b12)
		9485.94 (y81)	I			1456.81(b13)
		9372.86 (y80)	D			1571.83 (b14)
		9257.83 (y79)	V			1670.90 (b15)
		9158.76 (y78)	Y			1833.97 (b16)
		8995.70 (y77)	H			1971.03 (b17)
		8858.64 (y76)	K			2099.12 (b18)
		8730.54 (y75)	Y			2262.18 (b19)
		8567.48 (y74)	S			2349.22 (b20)
		8480.45 (y73)	L			2462.30 (b21)
		8367.36 (y72)	I			2575.38 (b22)
		8254.28 (y71)	K			2703.48 (b23)
		8126.18 (y70)	G			2760.50 (b24)
		8069.16 (y69)	N			2874.54 (b25)
		7955.12 (y68)	F			3021.61 (b26)
		7808.05 (y67)	H			3158.67 (b27)
		7670.99 (y66)	A			3229.71 (b28)
		7599.96 (y65)	V			3328.78 (b29)
		7500.89 (y64)	Y			3491.84 (b30)
		7337.82 (y63)	R			3647.94 (b31)
		7181.72 (y62)	D			3762.97 (b32)
		7066.70 (y61)	D			3877.99 (b33)
		6951.70 (y60)	L			3991.08 (b34)
		6838.59 (y59)	K			4119.17 (b35)
		6710.49 (y58)	K			4247.27 (b36)
		6582.40 (y57)	L			4360.35 (b37)
		6469.31 (y56)	L			4473.44 (b38)
		6356.23 (y55)	E			4602.48 (b39)
		6227.18 (y54)	T			4703.53 (b40)
		6126.14 (y53)	E			4832.57 (b41)
		5997.09 (y52)	C			4935.58 (b42)
		5894.08 (y51)	P			5032.63 (b43)
		5797.03 (y50)	Q			5160.69 (b44)
		5668.97 (y49)	Y			5323.75 (b45)
		5505.91 (y48)	I			5436.84 (b46)

		5392.83 (y47)	R			5592.94 (b47)
		5236.73 (y46)	K			5721.03 (b48)
		5108.63 (y45)	K			5849.13 (b49)
		4980.54 (y44)	G			5906.15 (b50)
		4923.51 (y43)	A			5977.19 (b51)
		4852.48 (y42)	D			6092.21 (b52)
		4737.45 (y41)	V			6191.28 (b53)
		4638.38 (y40)	W			6377.36 (b54)
		4452.30 (y39)	F			6524.43 b55
		4305.23 (y38)	K			6652.53 b56
		4177.14 (y37)	E			6781.57 b57
		4048.10 (y36)	L	6894.6557 6877.5951	3.64 6.70	6894.65 (b58) 6877.62 (b58-NH ₃)
		3935.01 (y35)	D	7009.6714 6992.6697	3.00 8.72	7009.68 (b59) 6992.65 (b59-NH ₃)
		3819.99 (y34)	I	7122.7422	12.57	7122.76 (b60)
		3706.90 (y33)	N	7237.7874 7208.7820	11.36 6.61	7236.81 (b61) 7208.81 (a61)
3592.8535	4.02	3592.86 (y32)	T	7337.7927 7319.7926	5.57 18.14	7337.85 (b62) 7319.84 (b62-H ₂ O)
3491.8265	4.45	3491.81 (y31)	D	7452.8700 7434.8654	7.77 3.06	7452.88 (b63) 7434.87 (b63-H ₂ O)
3376.7745	2.59	3376.78 (y30)	G	7510.8956 7492.8909	22.18 14.38	7509.90 (b64) 7492.87 (b64-NH ₃)
		3319.76 (y29)	A	7581.9328 7562.9335 7545.9229	26.05 32.21 13.95	7580.94 (b65) 7562.92 (b65-H ₂ O) 7545.90 (b65-H ₂ O-NH ₃)
3248.7242	44.17	3248.72 (y28)	V	7680.0056	3.33	7680.01 (b66)
3231.6967	14.03	3231.69 (y28-NH ₃)		7662.9787	3.55	7662.98 (b66-NH ₃)
3149.6551	100.00	3149.66 (y27)	N	-----		7794.05 (b67)
3132.6293	24.03	3132.63 (y27-NH ₃)		7776.0343	4.54	7776.04 (b67-H ₂ O)
3035.6103	61.36	3035.61 (y26)	F	7941.1281	3.01	7941.12 (b68)
2888.5443	59.07	2888.55 (y25)	Q			8069.18 (b69)
2871.5310	24.02	2871.52 (y25-NH ₃)				
2760.4855	57.17	2760.49 (y24-H ₂ O)	E			8198.22 (b70)
2742.4735	14.08					
2631.4416	31.50	2631.44 (y23)	F			8345.29 (b71)
		2484.38 (y22)	L			8458.37 (b72)
2371.2917	12.03	2371.29 (y21)	I			8571.46 (b73)
2258.2072	14.49	2258.21 (y20)	L			8684.54 (b74)
2145.1226	7.34	2145.12 (y19)	V			8783.61 (b75)
2046.0525	1.81	2046.05 (y18)	I			8896.69 (b76)
1932.9700	2.35	1932.97 (y17)	K			9024.79 (b77)
1804.8754	6.93	1804.88 (y16)	M			9155.83 (b78)
		1673.84 (y15)	G			9212.85 (b79)
		1616.81 (y14)	V			9311.92 (b80)
		1517.75 (y13)	A			9382.96 (b81)
		1446.71 (y12)	A			9453.99 (b82)
		1375.67(y11)	H			9591.05 (b83)
		1238.61(y10)	K			9719.15 (b84)
		1110.52 (y9)	K			9847.24 (b85)

		982.42 (y8)	S			9934.27 (b86)
		895.39 (y7)	H			10071.33 (b87)
		758.33 (y6)	E			10200.37 (b88)
		629.29 (y5)	E			10329.42 (b89)
		500.25 (y4)	S			10416.45 (b90)
		413.21 (y3)	H			10553.51 (b91)
		276.18 (y2)	K			10681.60 (b92)
		148.06(y1)	E			-----
3045.5971	16.13	3045.58	KYSLIKGNFHAVYRDDLLKKLLETECP-NH₃			

Lelli_XT_00001_MHp_#2 RT: 2.00 AV: 1 NL: 3.56E5
F: FTMS + p ESI d Full ms2 834.44@cid35.00 [215.00-2000.00]



S100A9* MS/MS

Exp mass	%	Theor mass	Aa res	Exp mass	%	Theor mass
		12682.29 (y109)	S(Acetyl)			
		12553.25 (y108)	Q			258.11 (b2)
12407.02	13.05	12425.19 (y107) 12407.18 (y107-H ₂ O)	L			371.19 (b3)
12311.05		12312.11 (y106)	E			500.23 (b4)
12181.03		12183.06 (y105)	R			656.34 (b5)
		12026.96 (y104)	N	770.37891	95.83	770.38 (b6)
		11912.92 (y103)	I	883.4632	74.72	883.46 (b7)
11799.83	9.37	11799.84 (y102)	E	1012.51 995.38	58.48 20.10	1012.51 (b8) 995.48 (b8-NH ₃)
11669.78	36.95	11670.79 (y101)	T	1113.55	59.16	1113.55 (b9)
11651.75	14.81	11652.78 (y10-H ₂ O)		1095.54	94.32	1095.54 (b9-H ₂ O)
11569.71		11569.75 (y100)	I	1226.64	46.71	1226.64 (b10)
11456.68	45.28	11456.66 (y99)	I			1339.72 (b11)
11438.63	25.96	11438.65 (y99-H ₂ O)				
11325.60	17.60	11343.58 (y98) 11325.57 (y98-H ₂ O)	N			1453.76 (b12)
11229.53	10.07	11229.54 (y97)	T			1554.81 (b13)
		11128.49 (y96)	F			1701.88 (b14)
		10981.42 (y95)	H			1838.94 (b15)
		10844.36 (y94)	Q			1967.00 (b16)
		10716.30 (y93)	Y			2130.06 (b17)
		10553.24 (y92)	S			2217.09 (b18)
		10466.21 (y91)	V			2316.16 (b19)
		10367.14 (y90)	K			2444.26 (b20)
		10239.04 (y89)	L			2557.34 (b21)
		10125.96 (y88)	G			2614.36 (b22)
		10068.94 (y87)	H	2751.42	96.57	2751.42 (b23)
		9931.88 (y86)	P			2848.47 (b24)
		9834.83 (y85)	D			2963.50 (b25)
		9719.78 (y84)	T			3064.55 (b26)
		9618.75 (y83)	L			3177.63 (b27)
9505.65	4.77	9505.67 (y82)	N			3291.68 (b28)
		9391.62 (y81)	Q			3419.73 (b29)
		9263.57 (y80)	G			3476.76 (b30)
		9206.55 (y79)	E			3605.80 (b31)
		9077.50 (y78)	F			3752.87 (b32)
		8930.43 (y77)	K			3880.96 (b33)
		8802.34 (y76)	E			4010.00 (b34)
		8673.30 (y75)	L			4123.09 (b35)
		8560.21 (y74)	V			4222.16 (b36)
		8461.14 (y73)	R			4378.26 (b37)
		8305.04 (y72)	K			4506.35 (b38)
		8176.95 (y71)	D			4621.38 (b39)
		8061.92 (y70)	L			4734.46 (b40)
		7948.84 (y69)	Q			4862.52 (b41)
		7820.78 (y68)	N			4976.56 (b42)
		7706.74 (y67)	F			5123.63 (b43)
		7559.67 (y66)	L			5236.72 (b44)
		7446.58 (y65)	K			5364.81 (b45)
		7318.49 (y64)	K			5492.91 (b46)
		7190.39 (y63)	E			5621.95 (b47)
		7061.35 (y62)	N			5735.99 (b48)
		6947.31 (y61)	K			5864.09 (b49)
		6819.21 (y60)	N			5978.13 (b50)

		6705.17 (y59)	E			6107.17 (b51)
		6576.13 (y58)	K			6235.27 (b52)
		6448.03 (y57)	V			6334.34 (b53)
		6348.96 (y56)	I			6447.42 (b54)
		6235.88 (y55)	E			6576.46 (b55)
		6106.84 (y54)	H	6713.50	16.59	6713.52 (b56)
		5969.78 (y53)	I			6826.61 (b57)
5856.70	26.74	5856.69 (y52)	M			6957.65 (b58)
5724.63	14.68	5725.65 (y51)	E			7086.69 (b59)
5709.65	4.53	5708.63 (y51-NH ₃)				
		5596.61 (y50)	D			7201.72 (b60)
		5481.58 (y49)	L			7314.81 (b61)
		5368.50 (y48)	D	7429.83	9.71	7429.83 (b62)
5253.54	3.40	5253.47 (y47)	T	7530.85	4.75	7530.87 (b63)
		5152.42 (y46)	N	7643.92	9.05	7644.92 (b64)
		5038.38 (y45)	A	7715.95	8.53	7715.95 (b65)
		4967.34 (y44)	D	7830.96	36.73	7830.98 (b66)
				7813.87	13.08	7812.97 (b66-H ₂ O)
4852.31		4852.32 (y43)	K			7959.08 (b67)
		4724.22 (y42)	Q			8087.14 (b68)
4707.20	6.19	4707.20 (y42- NH ₃)				
4596.17	8.43	4596.17 (y41)	L			8200.22 (b69)
4483.09	19.62	4483.08 (y40)	S			8287.25 (b70)
		4396.05 (y39)	F			8434.32 (b71)
		4248.98 (y38)	E			8563.36 (b72)
4120.96		4119.94 (y37)	E	8692.40	43.14	8692.41 (b73)
		3990.89 (y36)	F			8839.47 (b74)
3843.82	2..72	3843.83 (y35)	I			8952.56 (b75)
3825.84	15.22	3826.80 (y35-H ₂ O)				
3730.75	96.16	3730.74 (y34)	M			9083.60 (b76)
3599.68	27.84	3599.70 (y33)	L			9196.68 (b77)
3485.64	16.42	3486.62 (y32)	M			9327.72 (b78)
		3355.58 (y31)	A			9398.76 (b79)
		3284.54 (y30)	R			9554.86 (b80)
		3128.44 (y29)	L			9667.94 (b81)
		3015.35 (y28)	T			9768.99 (b82)
		2914.31 (y27)	W			9955.07 (b83)
		2728.23 (y26)	A			10026.11 (b84)
		2657.19 (y25)	S			10113.14 (b85)
		2570.16 (y24)	H			10250.20 (b86)
		2433.10 (y23)	E			10379.24 (b87)
		2304.06 (22)	K			10507.34 (b88)
		2175.96 (y21)	M			10638.38 (b89)
		2044.92 (y20)	H	10775.44	14.28	10775.44 (b90)
		1907.86 (y19)	E			10904.48 (b91)
1778.82	10.29	1778.82 (y18)	G			10961.50 (b92)
		1721.80 (y17)	D			11076.53 (b93)
1606.77	14.17	1606.77 (y16)	E			11205.57 (b94)
1588.76	14.47	1588.76 (y16-H ₂ O)				
1477.73	19.44	1477.73 (y15)	G			11262.59 (b95)
		1420.71 (y14)	P	11341.46	38.67	11359.64 (b96)
						11341.63 (b96-H ₂ O)
		1323.65 (y13)	G			11416.67 (b97)
		1266.63 (y12)	H	11554.62	19.91	11553.73 (b98)
1129.57	10.04	1129.57 (y11)	H			11690.78 (b99)
		992.52 (y10)	H			11827.84 (b100)
855.4555	12.86	855.46 (y9)	K			11955.94 (b101)
727.3617	33.56	727.36 (y8)	P			12052.99 (b102)
		630.31 (y7)	G			12110.01 (b103)

	573.29 (y6)	L			12223.10 (b104)
	460.20 (y5)	G			12280.12 (b105)
	403.18 (y4)	E			12409.17 (b106)
	274.14 (y3)	G			12466.18 (b107)
	217.12 (y2)	T	12567.22	100.00	12567.23 (b108)
			12549.25	56.83	12549.22 (b108-H ₂ O)
	116.07 (y1)	P			---

Lelli_XT_00001_MHp_100128094433 #2 RT: 2.00 AV: 1 NL: 2.07E4
 F: FTMS + p ESI d Full ms2 977.02@cid35.00 [255.00-2000.00]

