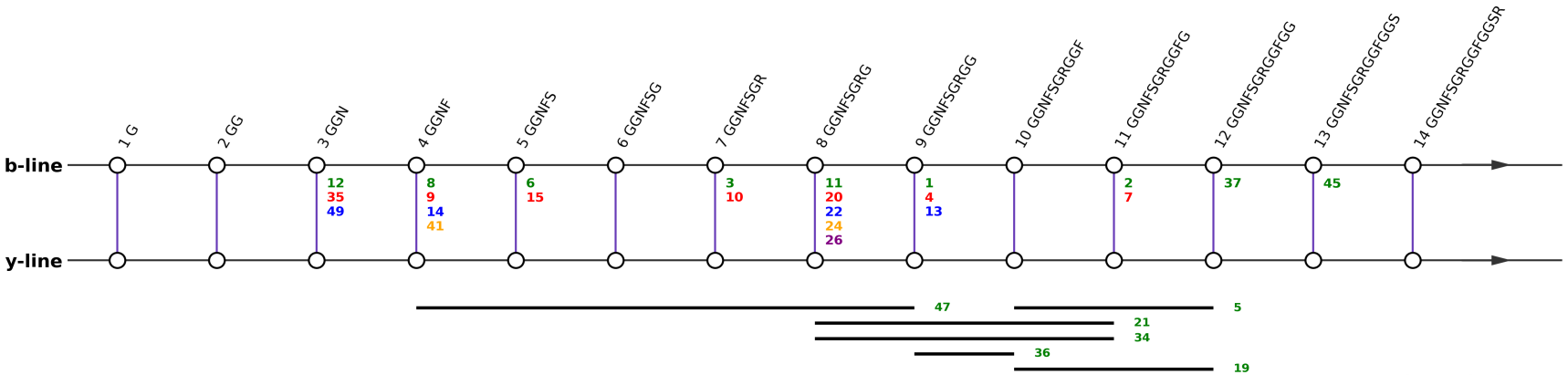
ME8_3+:[GGNFSGR(Me)GGFGGSR+3H]3+

Fragmentation Diagram for: GGNFSGRGGFGGSR



	b1y13	b2y12	b3y11	b4y10	b5y9	b6y8	b7y7	b8y6	b9y5	b10y4	b11y3	b12y2	b13y1	Row_Count	Unexplained Count	Abs Average Mass Difference	Unexplained Pairs
Parent	--	--	--	(b4,y10) (1+, 2+) (-0.29, 0.1) 14	(b5,y9) (1+, 2+) (0.04, -0.03) 6	--	(b7,y7) (2+, 1+) (-0.04, 0.07) 10	(b8,y6) (1+, 2+) (-0.16, 0.1) 22	(b9,y5) (2+, 1+) (0.02, 0.1) 4	--	(b11,y3) (2+, 1+) (-0.14, 0.08) 7	(b12,y2) (2+, 1+) (-0.28, 0.01) 37	--	7	2	0.21	-0.13(25) 0.09(31)
(NH3)	--	--	--	(b4,(NH3)) (2+, 1+) (-0.48, 0.02) 41	((NH3),y9) (1+, 2+) (0.07, -0.03) 15	--	((NH3),y7) (2+, 1+) (-0.15, 0.09) 3	((NH3),y6) (1+, 2+) (-0.18, 0.04) 26	((NH3),y5) (2+, 1+) (-0.06, 0.11) 1	--	((NH3),y3) (2+, 1+) (-0.11, -0.06) 2	--	--	6	0	0.23	
(H2O)	--	--	((H2O),y11) (1+, 2+) (-0.3, 0.16) 12	--	--	--	--	--	--	--	--	--	((H2O),y1) (2+, 1+) (-0.42, 0.08) 45	2	1	0.48	-0.34(50)
(NH3)-(H2O)	--	--	--	--	--	--	--	--	--	--	--	--	--	0	0	0.0	
a	--	--	(a3,y11) (1+, 2+) (0.19, -0.07) 35	(a4,y10) (1+, 2+) (-0.12, 0.14) 8	--	--	--	--	--	--	--	--	--	2	0	0.26	
2(H2O)	--	--	--	--	--	--	--	--	--	--	--	--	--	0	0	0.0	
2(NH3)	--	--	--	--	--	--	--	(2(NH3),y6) (2+, 1+) (-0.46, 0.09) 24	(2(NH3),y5) (2+, 1+) (-0.46, 0.13) 13	--	--	--	--	2	0	0.57	
Col_Count	0	0	2	3	2	0	2	3	3	0	2	1	1	19	3	0.25	nan
Ion Mass	(58.03, 1269.61)	(115.05, 1212.59)	(229.09, 1098.54)	(376.16, 951.48)	(463.19, 864.44)	(520.22, 807.42)	(690.33, 637.31)	(747.35, 580.28)	(804.37, 523.26)	(951.44, 376.19)	(1008.46, 319.17)	(1065.49, 262.15)	(1152.52, 175.12)	0	0	0.0	0

Not Highlighted (H2O) (H2O)-(NH3) (NH3) (NH3)-(H2O) 2(H2O) 2(NH3) CH3-NH2 Parent a

Table ME8_3+

n	classification	ion1	loss1	mass1	correct_mass1	mass_difference1	ion2	loss2	mass2	correct_mass2	mass_difference2	chosen_sum
1	usable	b9	(NH3)	394.12	394.18	-0.06	y5	nan	523.37	523.26	0.11	1311.61
2	usable	y3	nan	319.06	319.17	-0.11	b11	(NH3)	496.16	496.22	-0.06	1311.38
3	usable	b7	(NH3)	337.01	337.16	-0.15	y7	nan	637.4	637.31	0.09	1311.42
4	usable	b9	nan	402.71	402.69	0.02	y5	nan	523.36	523.26	0.1	1328.78
5	internal_acid	bi(10-12)	nan	262.01	261.11	0.9	b9	nan	804.43	804.37	0.06	1328.45
6	usable	y9	nan	432.77	432.73	0.04	b5	nan	463.16	463.19	-0.03	1328.7
7	usable	y3	nan	319.03	319.17	-0.14	b11	nan	504.82	504.74	0.08	1328.67
8	usable	a4	nan	348.03	348.15	-0.12	y10	nan	476.38	476.24	0.14	1300.79
9	usable	b4	nan	376.1	376.16	-0.06	y10	(NH3)	467.68	467.73	-0.05	1311.46
10	usable	b7	nan	345.63	345.67	-0.04	y7	nan	637.38	637.31	0.07	1328.64
11	usable	b8	(NH3)	365.48	365.67	-0.19	y6	nan	580.38	580.28	0.1	1311.34
12	usable	b3	(H2O)	210.78	211.08	-0.3	y11	nan	549.94	549.78	0.16	1310.66
13	usable	b9	2(NH3)	385.2	385.66	-0.46	y5	nan	523.39	523.26	0.13	1293.79
14	usable	b4	nan	375.87	376.16	-0.29	y10	nan	476.34	476.24	0.1	1328.55
15	usable	y9	nan	432.8	432.73	0.07	b5	(NH3)	446.14	446.17	-0.03	1325.08
16	rare_mode	b4	(H2O)-(HCOH)	328.11	328.14	-0.03	y7	nan	637.42	637.31	0.11	1293.64
17	internal_acid	y7	nan	319.11	319.16	-0.05	ai(3-7)	(CH3NH2)-(HCOH)	487.37	486.22	1.15	1293.85
18	rare_mode	a6	2(H2O)	228.75	228.6	0.15	y6	(HCOH)	549.99	550.27	-0.28	1328.73
19	internal_acid	bi(10-12)	nan	262.01	261.11	0.9	b9	(NH3)	787.4	787.35	0.05	1311.42
20	usable	b8	nan	374.08	374.18	-0.1	y6	nan	580.37	580.28	0.09	1328.53
21	internal_acid	bi(8-11)	nan	319.1	318.13	0.97	b7	nan	690.45	690.33	0.12	1328.65
22	usable	y6	nan	290.49	290.65	-0.16	b8	nan	747.45	747.35	0.1	1328.43
23	rare_mode	b4	nan	376.12	376.16	-0.04	y5	2(NH3)-(HCOH)	458.79	459.2	-0.41	1293.7
24	usable	b8	2(NH3)	356.69	357.15	-0.46	y6	nan	580.37	580.28	0.09	1293.75
25	unclear	???	nan	171.69	nan	nan	???	nan	578.41	nan	nan	1328.51

26	usable	y6	nan	290.47	290.65	-0.18	b8	(NH3)	730.37	730.33	0.04	1311.31
27	rare_mode	y8	(HN=C=NH)	383.03	383.2	-0.17	b5	(HCOH)	432.81	433.18	-0.37	1248.65
28	unclear	???	nan	376.09	nan	nan	???	nan	450.06	nan	nan	1276.21
29	rare_mode	a9	(HCOH)-(HCOH)	358.7	358.68	0.02	y5	(NH3)-(HCOH)	476.38	476.23	0.15	1311.46
30	internal_acid	ai(9-10)	nan	176.75	176.08	0.67	b8	(NH3)	730.48	730.33	0.15	1083.98
31	unclear	???	nan	285.75	nan	nan	???	nan	521.49	nan	nan	1328.73
32	internal_acid	ai(9-10)	nan	176.71	176.08	0.63	b8	nan	747.42	747.35	0.07	1100.84
33	unclear	???	nan	366.07	nan	nan	???	nan	595.38	nan	nan	1327.52
34	internal_acid	bi(8-11)	nan	319.08	318.13	0.95	b7	(NH3)	673.36	673.31	0.05	1311.52
35	usable	a3	nan	201.27	201.08	0.19	y11	nan	549.71	549.78	-0.07	1300.69
36	internal_acid	bi(9-10)	nan	204.8	204.09	0.71	b8	nan	747.98	747.35	0.63	1157.58
37	usable	y2	nan	261.87	262.15	-0.28	b12	nan	533.26	533.25	0.01	1328.39
38	internal_acid	ai(7-8)	(NH3)	183.55	182.1	1.45	y6	(HCOH)	550.02	550.27	-0.25	1283.59
39	rare_mode	b3	2(H2O)	193.53	193.07	0.46	y6	(HCOH)	550.08	550.27	-0.19	1293.69
40	unclear	???	nan	402.58	nan	nan	???	nan	504.37	nan	nan	1309.53
41	usable	b4	nan	188.1	188.58	-0.48	y10	(NH3)	934.47	934.45	0.02	1310.67
42	internal_acid	ai(5-9)	(H2O)-(HCOH)	176.6	176.59	0.01	b4	nan	375.98	376.16	-0.18	928.56
43	rare_mode	y4	2(H2O)-(HCOH)	310.27	310.16	0.11	b7	nan	690.44	690.33	0.11	1310.98
44	rare_mode	y8	(HCOH)	388.96	389.21	-0.25	a6	(HCOH)	461.47	462.19	-0.72	1311.9
45	usable	y1	nan	174.7	175.12	-0.42	b13	(H2O)	567.84	567.76	0.08	1310.38
46	non_complementary	a4	2(NH3)	314.32	314.1	0.22	y7	nan	637.17	637.31	-0.14	1265.81
47	internal_acid	bi(4-9)	(HCOH)	273.97	273.14	0.83	y5	(H2O)	504.69	505.25	-0.56	1283.35
48	rare_mode	b9	2(NH3)-(HCOH)	370.46	370.66	-0.2	y5	nan	523.56	523.26	0.3	1264.48
49	usable	a3	2(H2O)	165.32	165.06	0.26	y11	nan	549.8	549.78	0.02	1264.92
50	unclear	???	nan	131.57	nan	nan	???	nan	589.36	nan	nan	1310.29