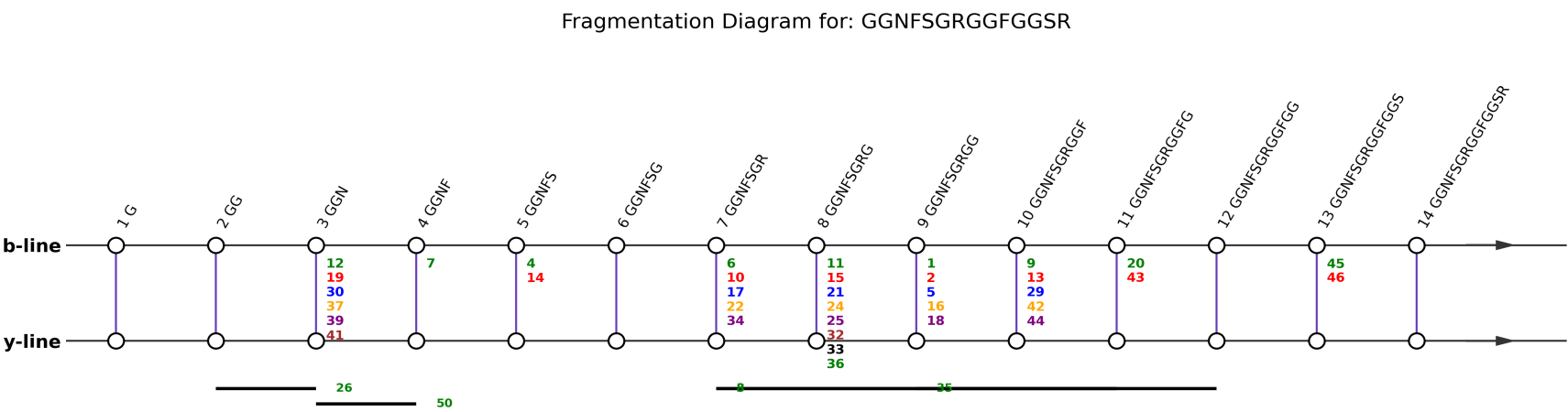
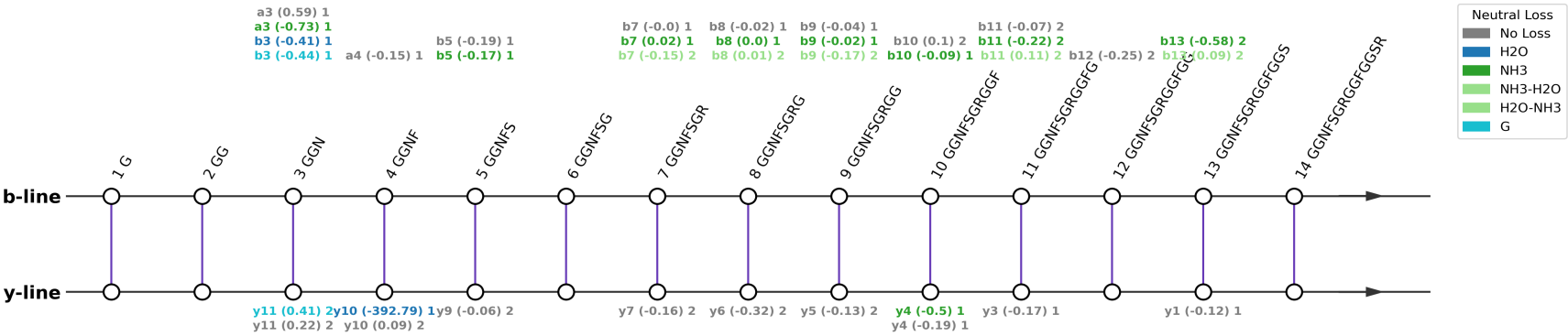


output



Fragmentation Diagram for: GGNFSGRGGFGGSR



Detailed Data - Table 1

Unnamed: 0	b3	b4	b5	b7	b8	b9	b10	b11	b12	b13
H2O-NH3	nan	nan	nan	b7-H2O-NH3 (-0.15) (2 , 1)	b8-H2O-NH3 (0.01) (2 , 1)	b9-H2O-NH3 (-0.17) (2 , 1)	nan	b11-H2O-NH3 (0.11) (2 , 1)	nan	b13-H2O-NH3 (0.09) (2 , 1)
G	b3-G (-0.44) (1 , 2)	nan	nan	nan	nan	nan	nan	nan	nan	nan
H2O	b3-H2O (-0.41) (1 , 2)	nan	nan	nan	nan	nan	nan	nan	nan	nan
NH3	a3-NH3 (-0.73) (1 , 2)	nan	b5-NH3 (-0.17) (1 , 2)	b7-NH3 (0.02) (1 , 2)	b8-NH3 (0.0) (1 , 2)	b9-NH3 (-0.02) (1 , 2)	b10-NH3 (-0.09) (1 , 2)	b11-NH3 (-0.22) (2 , 2)	nan	b13-NH3 (-0.58) (2 , 1)
No Loss	a3 (0.59) (1 , 2)	a4 (-0.15) (1 , 2)	b5 (-0.19) (1 , 2)	b7 (-0.0) (1 , 2)	b8 (-0.02) (1 , 2)	b9 (-0.04) (1 , 2)	b10 (0.1) (2 , 1)	b11 (-0.07) (2 , 2)	b12 (-0.25) (2 , 2)	nan

Detailed Data - Table 2

Unnamed: 0	y1	y3	y4	y5	y6	y7	y9	y10	y11
G	nan	nan	nan	nan	nan	nan	nan	nan	y11-G (0.41) (2 , 1)
H2O	nan	nan	nan	nan	nan	nan	nan	y10-H2O (-392.79) (1 , 1)	nan
NH3	nan	nan	y4-NH3 (-0.5) (1 , 2)	nan	nan	nan	nan	nan	nan
No Loss	y1 (-0.12) (1 , 2)	y3 (-0.17) (1 , 2)	y4 (-0.19) (1 , 1)	y5 (-0.13) (2 , 2)	y6 (-0.32) (2 , 1)	y7 (-0.16) (2 , 1)	y9 (-0.06) (2 , 1)	y10 (0.09) (2 , 1)	y11 (0.22) (2 , 1)

Detailed Data - Table 3

n	classification	line	mass1	correct_mass1	mass2	correct_mass2	chosen_sum	Cluster ID eps_1.0	Cluster ID eps_0.8	Cluster ID eps_0.6	Cluster ID eps_0.4
1	usable	y5 (1+) @ 523.33 & [b9 - NH3] (2+) @ 394.0	523.33	523.26	394.0	394.18	1311.33	0.0	0.0	0.0	0.0
2	usable	y5 (1+) @ 523.33 & b9 (2+) @ 402.67	523.33	523.26	402.67	402.69	1328.67	1.0	1.0	1.0	1.0
3	non_complementary	y7 (2+) @ 319.0 & [b11 - NH3] (2+) @ 496.0	319.0	319.16	496.0	496.22	1311.0	0.0	0.0	0.0	0.0
4	usable	y9 (2+) @ 432.67 & b5 (1+) @ 463.0	432.67	432.73	463.0	463.19	1328.34	1.0	1.0	1.0	1.0
5	usable	y5 (2+) @ 262.0 & b9 (1+) @ 804.33	262.0	262.13	804.33	804.37	1328.33	1.0	1.0	1.0	1.0
6	usable	y7 (1+) @ 637.33 & [b7 - NH3] (2+) @ 337.0	637.33	637.31	337.0	337.16	1311.33	0.0	0.0	0.0	0.0
7	usable	y10 (2+) @ 476.33 & a4 (1+) @ 348.0	476.33	476.24	348.0	348.15	1300.66	2.0	2.0	2.0	2.0
8	non_complementary	y7 (2+) @ 319.0 & b11 (2+) @ 504.67	319.0	319.16	504.67	504.74	1328.34	1.0	1.0	1.0	1.0
9	usable	y4 (1+) @ 376.0 & [b10 - NH3] (2+) @ 467.67	376.0	376.19	467.67	467.71	1311.34	0.0	0.0	0.0	0.0
10	usable	y7 (1+) @ 637.33 & b7 (2+) @ 345.67	637.33	637.31	345.67	345.67	1328.67	1.0	1.0	1.0	1.0
11	usable	y6 (1+) @ 580.33 & [b8 - NH3] (2+) @ 365.33	580.33	580.28	365.33	365.67	1310.99	0.0	0.0	0.0	0.0
12	usable	y11 (2+) @ 550.0 & [b3 - H2O] (1+) @ 210.67	550.0	549.78	210.67	211.08	1310.67	0.0	0.0	0.0	0.0
13	usable	y4 (1+) @ 375.67 & b10 (2+) @ 476.33	375.67	376.19	476.33	476.23	1328.33	1.0	1.0	1.0	1.0
14	usable	y9 (2+) @ 432.67 & [b5 - NH3] (1+) @ 446.0	432.67	432.73	446.0	446.17	1324.67	-1.0	-1.0	-1.0	-1.0
15	usable	y6 (1+) @ 580.33 & b8 (2+) @ 374.0	580.33	580.28	374.0	374.18	1328.33	1.0	1.0	1.0	1.0

16	usable	y5 (1+) @ 523.33 & [b9 – H2O – NH3] (2+) @ 385.0	523.33	523.26	385.0	385.17	1293.33	3.0	3.0	3.0	3.0
17	usable	y7 (1+) @ 637.33 & [b7 – H2O – NH3] (2+) @ 328.0	637.33	637.31	328.0	328.15	1293.33	3.0	3.0	3.0	3.0
18	usable	y5 (2+) @ 262.0 & [b9 - NH3] (1+) @ 787.33	262.0	262.13	787.33	787.35	1311.33	0.0	0.0	0.0	0.0
19	usable	y11 (2+) @ 550.0 & b3 (1+) @ 228.67	550.0	549.78	228.67	229.09	1328.67	1.0	1.0	1.0	1.0
20	usable	[b11 – H2O – NH3] (2+) @ 487.33 & y3 (1+) @ 319.0	487.33	487.22	319.0	319.17	1293.66	3.0	3.0	3.0	3.0
21	usable	y6 (2+) @ 290.33 & b8 (1+) @ 747.33	290.33	290.65	747.33	747.35	1327.99	1.0	1.0	1.0	1.0
22	usable	y7 (2+) @ 319.0 & b7(1+) @ 690.33	319.0	319.16	690.33	690.33	1328.33	1.0	1.0	1.0	1.0
23	ambiguous	[y10 – NH3 – H2O] (2+) @ 458.67 & b4/y4 (1+) @ 376.0	458.67	458.72	376.0	376.16	1293.34	3.0	3.0	3.0	3.0
24	usable	y6 (1+) @ 580.33 & [b8 – H2O - NH3] (2+) @ 356.67	580.33	580.28	356.67	356.66	1293.67	3.0	3.0	3.0	3.0
25	usable	y6 (2+) @ 290.33 & [b8-NH3] (1+) @ 730.33	290.33	290.65	730.33	730.33	1310.99	0.0	0.0	0.0	0.0
26	internal_acid	[y11 + G] (2+) @ 578.33 & b12-3 (1+) @ 171.67	578.33	578.29	171.67	172.07	1328.33	1.0	1.0	1.0	1.0
27	unclear	y9 (2+) @ 432.67 & ??? @ 383.0	432.67	432.73	383.0	nan	1248.34	-1.0	-1.0	-1.0	-1.0
28	unclear	??? @ 595.33 & [b8 - NH3] (2+) @ 366.0	595.33	nan	366.0	365.67	1327.33	1.0	1.0	-1.0	-1.0
29	usable	[y4-NH3] (1+) @ 358.67 & b10 (2+) @ 476.33	358.67	359.17	476.33	476.23	1311.33	0.0	0.0	0.0	0.0
30	usable	[y11 - G] (2+) @ 521.67 & [b3 + G] (1+) @ 285.67	521.67	521.26	285.67	286.11	1329.01	1.0	1.0	1.0	1.0
31	ambiguous	[b10/y10 – H2O – 2(NH3)] (2+) @ 450.0 & y4/b4 @ 376.0	450.0	450.19	376.0	376.19	1276.0	-1.0	-1.0	-1.0	-1.0
32	usable	[b8 – NH3] (1+) @ 730.33 & ai9-10 (1+) @ 176.67	730.33	730.33	176.67	177.09	1083.67	-1.0	-1.0	-1.0	-1.0
33	usable	b8 (1+) @ 747.33 & ai9-10 (1+) 176.67	747.33	747.35	nan	nan	nan	nan	nan	nan	nan
34	usable	y7 (2+) @ 319.0 & [b7-NH3] (1+) @ 673.33	319.0	319.16	673.33	673.31	1311.33	0.0	0.0	0.0	0.0
35	non_complementary	y5 (2+) @ 262.0 & b12 (2+) @ 533.0	262.0	262.13	533.0	533.25	1328.0	1.0	1.0	1.0	1.0
36	usable	b8 (1+) @ 748.0 & ai9-10 (1+) @ 204.67	748.0	747.35	204.67	177.09	1157.34	-1.0	-1.0	-1.0	-1.0
37	usable	y11(2+) @ 549.67 & a3(1+) @ 201.67	549.67	549.78	201.67	201.08	1301.01	2.0	2.0	2.0	2.0
38	undefined	549.67 & 165.33	549.67	nan	165.33	nan	1264.67	4.0	4.0	4.0	4.0
39	usable	y11 (2+) @ 550.0 & [a3 – 2(H2O)] (1+) @ 193.33	550.0	549.78	193.33	165.06	1293.33	3.0	3.0	3.0	3.0
40	undefined	461.67 & 389.0	461.67	nan	389.0	nan	1312.34	0.0	-1.0	-1.0	-1.0
41	usable	y11 (2+) @ 550.0 & [a3-NH3] (1+) @ 183.33	550.0	549.78	183.33	184.06	1283.33	5.0	5.0	5.0	5.0
42	usable	y4 (2+) @ 188.0 & [b10-NH3] (1+) @ 934.33	188.0	188.6	934.33	934.42	1310.33	0.0	0.0	0.0	0.0
43	usable	b11 (1+) @ 504.67 & [y3 – CO2] (1+) @ 274.0	504.67	1008.46	274.0	275.18	1283.34	5.0	5.0	5.0	5.0

44	usable	y4 (1+) @ 376.0 & ai9-10 (1+) @ 176.67	376.0	376.19	176.67	177.09	928.67	-1.0	-1.0	-1.0	-1.0
45	usable	[b13-H2O-NH3] (2+) @ 559.33 & y1(1+) @ 175.0	559.33	559.24	175.0	175.12	1293.66	3.0	3.0	3.0	3.0
46	usable	y1 (1+) @ 174.67 & [b13-NH3] (2+) @ 567.67	174.67	175.12	567.67	568.25	1310.01	0.0	0.0	0.0	0.0
47	unclear	y5 (1+) @ 523.67 & ??? @ 370.33	523.67	523.26	370.33	nan	1264.33	4.0	4.0	4.0	4.0
48	undefined	637.0 & 314.33	637.0	nan	314.33	nan	1265.66	4.0	-1.0	-1.0	-1.0
49	undefined	589.33 & 131.67	589.33	nan	131.67	nan	1310.33	0.0	0.0	0.0	0.0
50	internal_acid	[y10-H2O] (1+) @ 540.67 & [bi3-4 - 2(NH3)] (1+) @ 228.0	540.67	933.46	228.0	228.07	1309.34	0.0	0.0	-1.0	-1.0