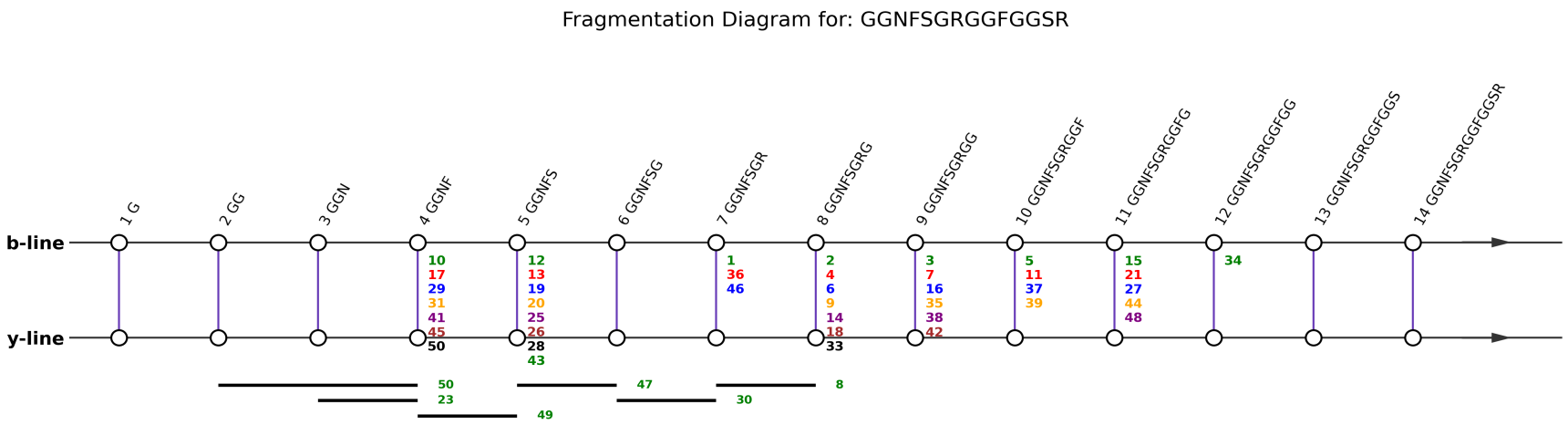
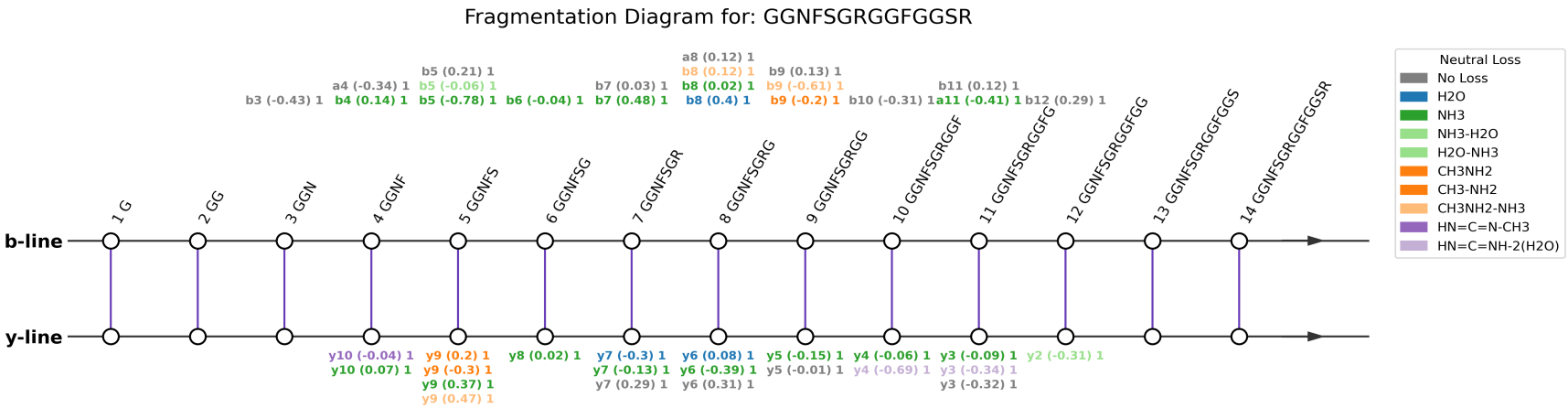
output


Fragmentation Diagram for: GGNFSGRGGFGGSR
b-line
y-line
1 G
2 GG
3 GGN
4 GGNF
5 GGNFS
6 GGNFSG
7 GGNFSGR
8 GGNFSGRG
9 GGNFSGRGG
10 GGNFSGRGGF
11 GGNFSGRGGFG
12 GGNFSGRGGFGG
13 GGNFSGRGGFGGS
14 GGNFSGRGGFGGSR
10 17 29 31 41 45 50
12 13 19 20 25 26 28 43
1 36 46
2 4 6 9 14 18 33
3 7 16 35 38 42
5 11 37 39
15 21 27 44 48
34
50 23 49
47 30
8



Detailed Data - Table 1

Unnamed: 0	b3	b4	b5	b6	b7	b8	b9	b10	b11	b12
CH3-NH2	nan	nan	nan	nan	nan	nan	b9-CH3-NH2 (-0.2) (1 , 1)	nan	nan	nan
H2O	nan	nan	nan	nan	nan	b8-H2O (0.4) (1 , 1)	nan	nan	nan	nan
NH3	nan	b4-NH3 (0.14) (1 , 1)	b5-NH3 (-0.78) (1 , 1)	b6-NH3 (-0.04) (1 , 1)	b7-NH3 (0.48) (1 , 1)	b8-NH3 (0.02) (1 , 1)	nan	nan	a11-NH3 (-0.41) (1 , 1)	nan
NH3-H2O	nan	nan	b5-NH3-H2O (-0.06) (1 , 1)	nan	nan	nan	nan	nan	nan	nan
CH3NH2-NH3	nan	nan	nan	nan	nan	b8-CH3NH2-NH3 (0.12) (1 , 1)	b9-CH3NH2-NH3 (-0.61) (1 , 1)	nan	nan	nan
No Loss	b3 (-0.43) (1 , 1)	a4 (-0.34) (1 , 1)	b5 (0.21) (1 , 1)	nan	b7 (0.03) (1 , 1)	a8 (0.12) (1 , 1)	b9 (0.13) (1 , 1)	b10 (-0.31) (1 , 1)	b11 (0.12) (1 , 1)	b12 (0.29) (1 , 1)

Detailed Data - Table 2

Unnamed: 0	y2	y3	y4	y5	y6	y7	y8	y9	y10
CH3NH2	nan	nan	nan	nan	nan	nan	nan	y9-CH3NH2 (0.2) (1 , 1)	nan
HN=C=N-CH3	nan	nan	nan	nan	nan	nan	nan	nan	y10-HN=C=N-CH3 (-0.04) (1 , 1)
CH3-NH2	nan	nan	nan	nan	nan	nan	nan	y9-CH3-NH2 (-0.3) (1 , 1)	nan
H2O-NH3	y2-H2O-NH3 (-0.31) (1 , 1)	nan	nan	nan	nan	nan	nan	nan	nan
H2O	nan	nan	nan	nan	y6-H2O (0.08) (1 , 1)	y7-H2O (-0.3) (1 , 1)	nan	nan	nan
NH3	nan	y3-NH3 (-0.09) (1 , 1)	y4-NH3 (-0.06) (1 , 1)	y5-NH3 (-0.15) (1 , 1)	y6-NH3 (-0.39) (1 , 1)	y7-NH3 (-0.13) (1 , 1)	y8-NH3 (0.02) (1 , 1)	y9-NH3 (0.37) (1 , 1)	y10-NH3 (0.07) (1 , 1)
HN=C=NH-2(H2O)	nan	y3-HN=C=NH-2(H2O) (-0.34) (1 , 1)	y4-HN=C=NH-2(H2O) (-0.69) (1 , 1)	nan	nan	nan	nan	nan	nan
CH3NH2-NH3	nan	nan	nan	nan	nan	nan	nan	y9-CH3NH2-NH3 (0.47) (1 , 1)	nan
No Loss	nan	y3 (-0.32) (1 , 1)	nan	y5 (-0.01) (1 , 1)	y6 (0.31) (1 , 1)	y7 (0.29) (1 , 1)	nan	nan	nan

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	y7 (1+) @ 637.39 & b7 (1+) @ 690.36	637.39	637.31	690.36	690.33	1327.75	0.0	0.0	0.0	0.0
2	usable	y6 (1+) @ 580.39 & b8 (1+) @ 747.43	580.39	580.28	747.43	747.35	1327.82	0.0	0.0	0.0	0.0
3	usable	y5 (1+) @ 523.26 & b9 (1+) @ 804.37	523.26	523.26	804.37	804.37	1327.63	0.0	0.0	0.0	0.0
4	usable	y6 (1+) @ 580.37 & [b8-NH3] (1+) @ 730.35	580.37	580.28	730.35	730.33	1310.72	1.0	1.0	1.0	1.0
5	usable	[y4-NH3] (1+) @ 359.11 & b10 (1+) @ 951.13	359.11	359.17	951.13	951.44	1310.24	1.0	1.0	1.0	1.0
6	usable	[b8-CH3NH2-NH3] (1+) @ 699.38 & y6 (1+) @ 580.59	699.38	699.28	580.59	580.28	1279.97	2.0	2.0	2.0	2.0
7	usable	[y5-NH3] (1+) @ 506.09 & b9 (1+) @ 804.5	506.09	506.24	804.5	804.37	1310.59	1.0	1.0	1.0	1.0
8	non_complementary	y6(1+) @ 580.43 & [b7-NH3] (1+) @ 673.04	580.43	580.28	673.04	673.31	1253.47	-1.0	-1.0	-1.0	-1.0

9	usable	[y6-NH3] (1+) @ 562.87 & b8 (1+) @ 747.77	562.87	563.26	747.77	747.35	1310.64	1.0	1.0	1.0	1.0
10	usable	[y10-CH3NH2] (1+) @ 921.04 & a4 (1+) @	921.04	920.43	nan	nan	nan	nan	nan	nan	nan
11	usable	b10 (1+) @ 951.13 & [y4-2(H2O)-NH3] (1+) @ 323.13	951.13	951.44	323.13	323.15	1274.26	-1.0	-1.0	-1.0	-1.0
12	usable	[y9-NH3] (1+) @ 847.45 & [b5-NH3] (1+) @ 446.02	847.45	847.42	446.02	446.17	1293.47	3.0	3.0	3.0	-1.0
13	usable	[y9-CH3NH2] (1+) @ 833.18 & [b5-NH3-H2O] (1+) @ 427.77	833.18	833.4	427.77	428.16	1260.95	4.0	-1.0	-1.0	-1.0
14	usable	[b8+H2O] (1+) @ 765.76 & [y6-H2O] (1+) @ 562.31	765.76	765.36	562.31	562.27	1328.07	0.0	0.0	0.0	0.0
15	usable	[y3-NH3] (1+) @ 301.75 & b11(1+) @ 1009.17	301.75	302.15	1009.17	1008.46	1310.92	1.0	1.0	1.0	1.0
16	usable	b9 (1+) @ 804.33 & [y5-2(NH3)](1+) @ 490.22	804.33	804.37	490.22	489.21	1294.55	3.0	3.0	-1.0	-1.0
17	rare_mod	[y10 - HN=C=N-CH3] (1+) @ 895.4 & a4 (1+) @ 347.81	895.4	895.44	347.81	348.15	1243.21	-1.0	-1.0	-1.0	-1.0
18	usable	y6(1+) @ 580.57 & a8(1+) @ 719.46	580.57	580.28	719.46	719.34	1300.03	-1.0	-1.0	-1.0	-1.0
19	usable	[y9-NH3] (1+) @ 847.25 & [b5-NH3-H2O] (1+) @ 428.27	847.25	847.42	428.27	428.16	1275.52	-1.0	-1.0	-1.0	-1.0
20	usable	[y9- CH3NH2] (1+) @ 833.18 & [a5-NH3-H2O] (1+) @ 400.18	833.18	833.4	400.18	400.15	1233.36	-1.0	-1.0	-1.0	-1.0
21	usable	[y3-NH3] (1+) @ 301.89 & [b11-NH3] (1+) @ 992.02	301.89	302.15	992.02	991.44	1293.91	3.0	3.0	3.0	-1.0
22	unclear	a9 (1+) @ 776.68 & ??? @ 485.61	776.68	776.36	485.61	nan	1262.29	4.0	4.0	4.0	3.0
23	non_complementary	[y10-NH3] (1+) @ 934.85 & b3(1+) @ 228.71	934.85	934.45	228.71	229.09	1392.27	-1.0	-1.0	-1.0	-1.0
24	unclear	??? @ 682.12 & y6 (1+) @ 580.14	682.12	nan	580.14	580.28	1262.26	4.0	4.0	4.0	3.0
25	usable	[y9- CH3NH2 – NH3] (1+) @ 816.84 & [b5-NH3-H2O] (1+) @ 428.1	816.84	816.37	428.1	428.16	1244.94	-1.0	-1.0	-1.0	-1.0
26	usable	[y9- CH3NH2] (1+) @ 833.6 & [b5-NH3] (1+) @ 446.11	833.6	833.4	446.11	446.17	1279.71	2.0	2.0	2.0	2.0
27	rare_mod	b11 (1+) @ 1008.62 & [y3 - HN=C=NH - 2(H2O)] (1+) @ 240.79	1008.62	1008.46	240.79	241.13	1249.41	5.0	5.0	5.0	4.0
28	usable	[y9-NH3] (1+) @ 847.79 & [a5-NH3] (1+) @ 418.1	847.79	847.42	418.1	418.16	1265.89	6.0	6.0	-1.0	-1.0
29	usable	[y10-NH3] (1+) @ 934.52 & [a4-NH3] (1+) @ 330.69	934.52	934.45	330.69	331.12	1265.21	6.0	6.0	6.0	5.0
30	non_complementary	y7(1+) @ 637.6 & [b6-NH3] (1+) @ 503.15	637.6	637.31	503.15	503.19	1140.75	-1.0	-1.0	-1.0	-1.0
31	rare_mod	[y10- HN=C=NH - NH3] (1+) @ 891.57 & b3 (1+) @ 228.66	891.57	892.43	228.66	229.09	1348.89	-1.0	-1.0	-1.0	-1.0
32	ambiguous	y10/b10 (1+) @ 51.14 & [b4/y4 -NH3-H2O] (1+) @ 341.21	51.14	951.48	341.21	341.12	733.56	-1.0	-1.0	-1.0	-1.0
33	usable	[b8- CH3NH2 - NH3] (1+) @ 699.4 & [y6 - H2O] (1+) @ 562.35	699.4	699.28	562.35	562.27	1261.75	4.0	4.0	4.0	-1.0
34	usable	b12 (1+) @ 1065.78 & [y2-H2O-NH3] (1+) @ 226.8	1065.78	1065.49	226.8	227.11	1292.58	3.0	3.0	7.0	6.0
35	usable	[b9- CH3NH2 - NH3] (1+) @ 755.7 & y5 (1+) @ 523.15	755.7	756.31	523.15	523.26	1278.85	2.0	-1.0	-1.0	-1.0
36	usable	b7 (1+) @ 691.33 & [y7-NH3] (1+) @ 620.15	691.33	690.33	620.15	620.28	1311.48	1.0	1.0	1.0	-1.0

37	rare_mod	b10 (1+) @ 952.06 & [y4 - HN=C=NH -2(H2O)] (1+) @ 297.46	952.06	951.44	297.46	298.15	1249.52	5.0	5.0	5.0	4.0
38	usable	[b9 - CH3-NH2] (1+) @ 773.13 & y5 (1+) @ 523.25	773.13	773.33	523.25	523.26	1296.38	7.0	7.0	8.0	7.0
39	usable	a10 (1+) @ 924.2 & [y4 – NH3- 2(H2O)] (1+) @ 323.33	924.2	923.43	323.33	323.15	1247.53	-1.0	-1.0	-1.0	-1.0
40	unclear	??? @ 921.76 & y4 (1+) @ 376.36	921.76	nan	376.36	376.19	1298.12	-1.0	-1.0	-1.0	-1.0
41	rare_mod	[y10 – HN=C=NH – H2O] (1+) @ 891.45 & [b4-HCONH2] (1+) @ 330.79	891.45	891.44	330.79	331.14	1222.24	-1.0	-1.0	-1.0	-1.0
42	usable	[b9 + H2O] (1+) @ 822.35 & [y5-H2O] @ 505.13	822.35	822.39	505.13	505.25	1327.48	0.0	0.0	0.0	0.0
43	usable	[y9 - CH3-NH2] (1+) @ 833.1 & b5 (1+) @ 463.4	833.1	833.4	463.4	463.19	1296.5	7.0	7.0	8.0	7.0
44	usable	[y3-NH3] (1+) @ 302.06 & [a11-NH3](1+) @ 963.02	302.06	302.15	963.02	963.43	1265.08	6.0	6.0	6.0	5.0
45	rare_mod	[y10 - HN=C=N-CH3– H2O] @ 877.52 & a4 (1+) @ 348.45	877.52	877.43	348.45	348.15	1225.97	-1.0	-1.0	-1.0	-1.0
46	usable	[y7 - H2O] (1+) @ 618.99 & [b7-NH3] (1+) @ 673.79	618.99	619.29	673.79	673.31	1292.78	3.0	3.0	7.0	6.0
47	non_complementary	[y8-NH3] (1+) @ 790.42 & [b5-NH3] (1+) @ 445.39	790.42	790.4	445.39	446.17	1235.81	-1.0	-1.0	-1.0	-1.0
48	usable	y3 (1+) @ 318.85 & b11 (1+) @ 1008.58	318.85	319.17	1008.58	1008.46	1327.43	0.0	0.0	0.0	0.0
49	non_complementary	[y9 - CH3-NH2 – NH3] (1+) @ 816.74 & [b4-NH3] (1+) @ 359.27	816.74	816.37	359.27	359.13	1176.01	-1.0	-1.0	-1.0	-1.0
50	rare_mod	[y10 - HN=C=N-CH3] @ 895.4 & [bi(2-4) – H2O – NH3] (1+) @ 284.64	895.4	895.44	284.64	284.1	1464.68	-1.0	-1.0	-1.0	-1.0