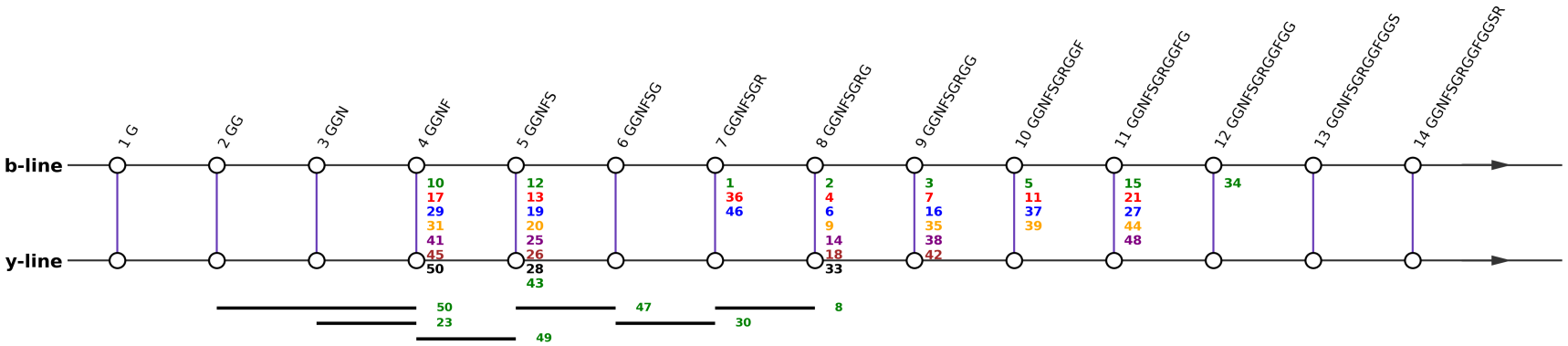
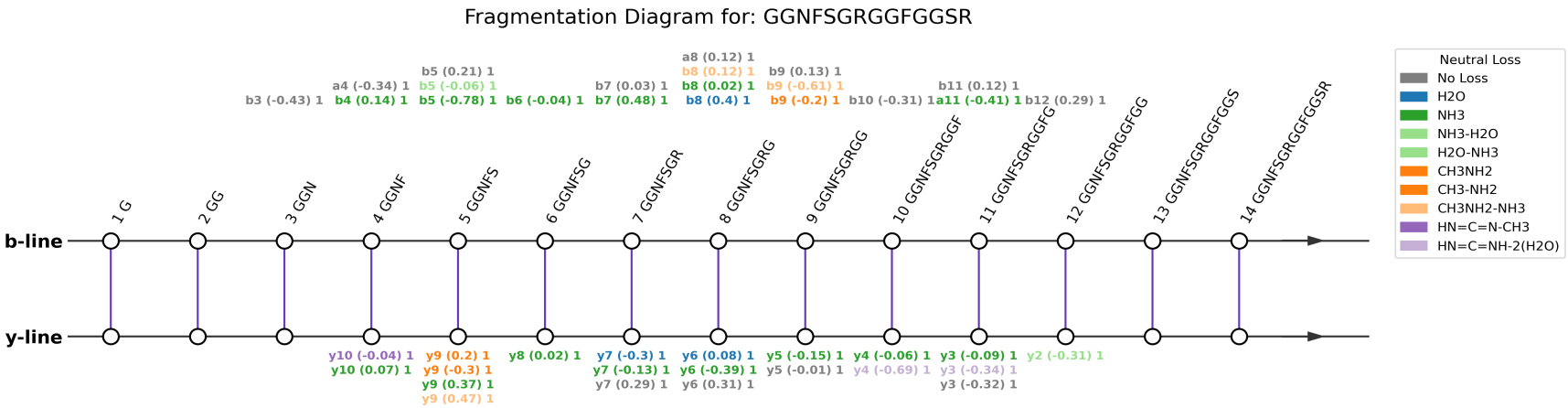
output

Fragmentation Diagram for: GGNFSGRGGFGGSR



	b1y13	b2y12	b3y11	b4y10	b5y9	b6y8	b7y7	b8y6	b9y5	b10y4	b11y3	b12y2	b13y1	Row_Count
Parent	--	--	--	--	--	--	(b7,y7) (1+ , 1+) 0.11 (1)	(b8,y6) (1+ , 1+) 0.18 (2)	(b9,y5) (1+ , 1+) -0.01 (3)	--	(b11,y3) (1+ , 1+) -0.21 (48)	--	--	4
NH3	--	--	--	--	--	--	(b7,NH3) (1+ , 1+) 0.87 (36)	(b8,NH3) (1+ , 1+) 0.03 (9)	(b9,NH3) (1+ , 1+) -0.02 (7)	(b10,NH3) (1+ , 1+) -0.37 (5)	(b11,NH3) (1+ , 1+) 0.31 (15)	--	--	5
H2O	--	--	--	--	--	--	--	--	--	--	--	--	--	0
NH3 + H2O	--	--	--	--	--	--	(NH3,H2O) (1+ , 1+) 0.18 (46)	--	--	--	--	--	--	1
H2O + NH3	--	--	--	--	--	--	--	--	--	--	--	--	--	0
a	--	--	--	--	--	--	--	(a8,y6) (1+ , 1+) 0.4 (18)	--	--	--	--	--	1
Col_Count	0	0	0	0	0	0	3	3	2	1	2	0	0	11



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

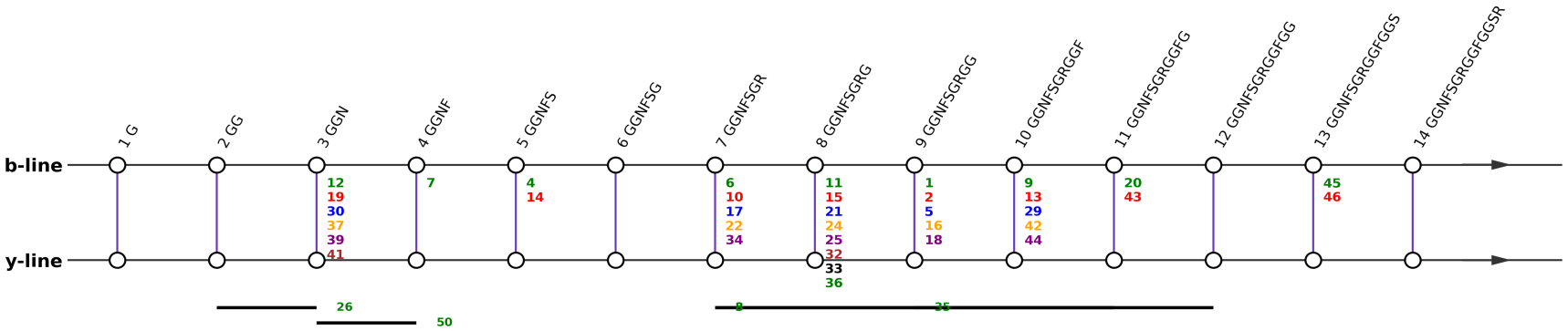
n	classification	line	mass1	correct_mass1	mass2	correct_mass2	chosen_sum	Cluster ID eps_1.0	Cluster ID eps_0.8	Cluster ID eps_0.6	Cluster ID eps_0.4
1	usable	y7 (1+) @ 637.39 & b7 (1+) @ 690.36	637.39	637.31	690.36	690.33	1327.75	0.0	0.0	0.0	0.0
2	usable	y6 (1+) @ 580.39 & b8 (1+) @ 747.43	580.39	580.28	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

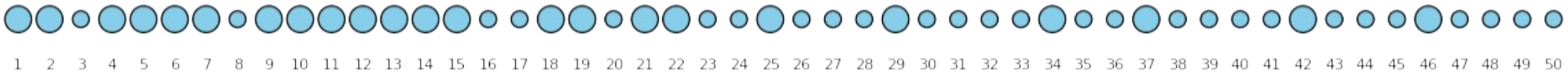
37	rare_mod	b10 (1+) @ 952.06 & [y4 - HN=C=NH -2(H2O)] (1+) @ 297.46	952.06	951.44	297.46	298.15	1249.52	5.0	5.0	5.0	4.0
38	usable	[b9 - CH3-NH2] (1+) @ 773.13 & y5 (1+) @ 523.25	773.13	773.33	523.25	523.26	1296.38	7.0	7.0	8.0	7.0
39	usable	a10 (1+) @ 924.2 & [y4 – NH3- 2(H2O)] (1+) @ 323.33	924.2	923.43	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

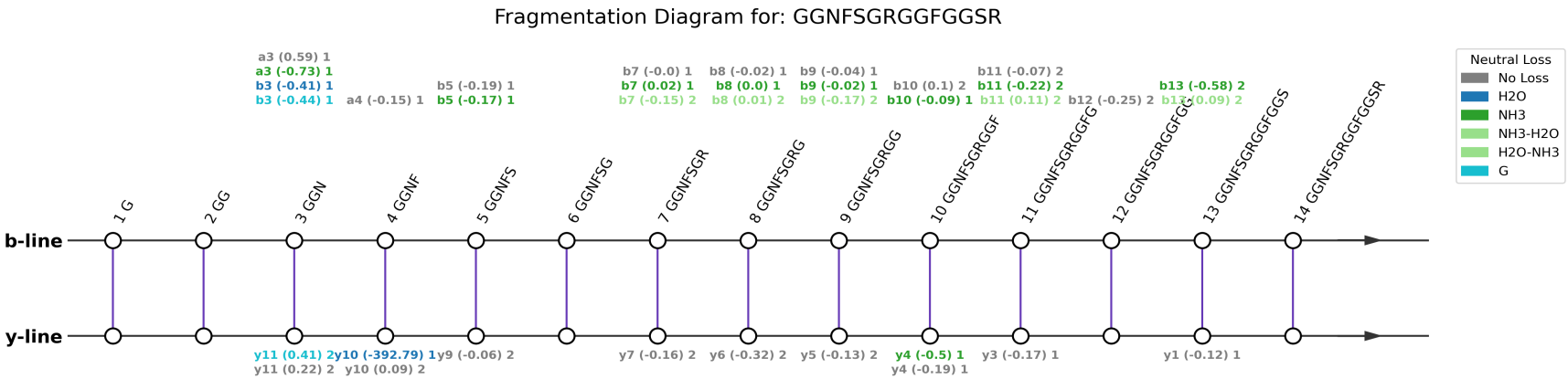
output

Fragmentation Diagram for: GGNFSGRGGFGGSR



	b1y13	b2y12	b3y11	b4y10	b5y9	b6y8	b7y7	b8y6	b9y5	b10y4	b11y3	b12y2	b13y1	Row_Count
Parent	--	--	(b3,y11) (1+ , 2+) -0.2 (19)	--	(b5,y9) (1+ , 2+) -0.25 (4)	--	(b7,y7) (1+ , 2+) -0.16 (22)	(b8,y6) (1+ , 2+) -0.34 (21)	(b9,y5) (1+ , 2+) -0.18 (5)	(b10,y4) (2+ , 1+) -0.42 (13)	--	--	--	6
NH3	--	--	--	--	(NH3,y9) (1+ , 2+) -0.22 (14)	--	(NH3,y7) (1+ , 2+) -0.13 (34)	(NH3,y6) (1+ , 2+) -0.31 (25)	(NH3,y5) (1+ , 2+) -0.15 (18)	(NH3,y4) (1+ , 2+) -0.69 (42)	--	--	(NH3,y1) (2+ , 1+) -1.03 (46)	6
H2O	--	--	(H2O,y11) (1+ , 2+) -0.19 (12)	--	--	--	--	--	--	--	--	--	--	1
NH3 + H2O	--	--	--	--	--	--	--	--	--	--	--	--	--	0
H2O + NH3	--	--	--	--	--	--	--	--	--	--	--	--	--	0
a	--	--	(a3,y11) (1+ , 2+) 0.48 (37)	(a4,y10) (1+ , 2+) -0.06 (7)	--	--	--	--	--	--	--	--	--	2
Col_Count	0	0	3	1	2	0	2	2	2	2	0	0	1	15





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)

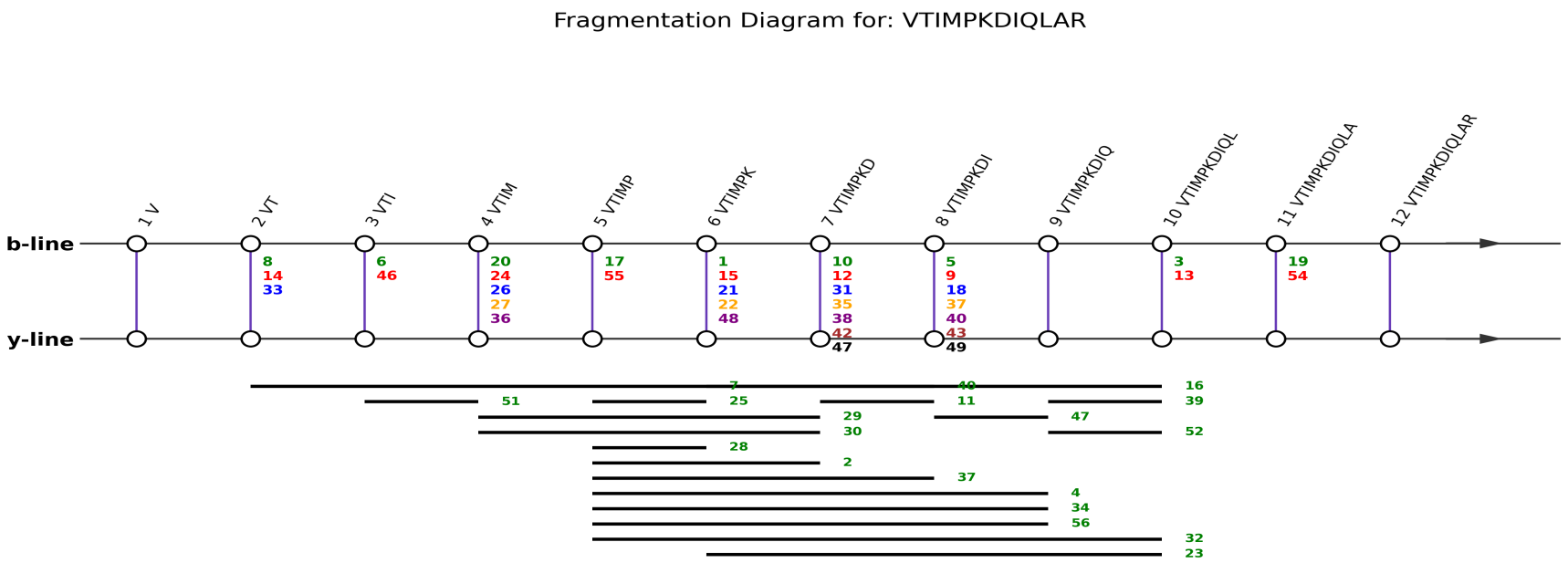
Detailed Data - Table 3

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

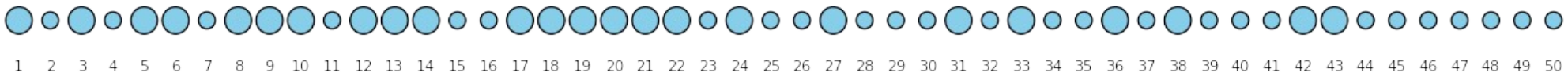
16	usable	y5 (1+) @ 523.33 & [b9 – H2O – NH3] (2+) @ 385.0	523.33	523.26	385.0	385.17	1293.33	3.0	3.0	3.0	3.0
17	usable	y7 (1+) @ 637.33 & [b7 – H2O – NH3] (2+) @ 328.0	637.33	637.31	328.0	328.15	1293.33	3.0	3.0	3.0	3.0
18	usable	y5 (2+) @ 262.0 & [b9 - NH3] (1+) @ 787.33	262.0	262.13	787.33	787.35	1311.33	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 & bi2-3 (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

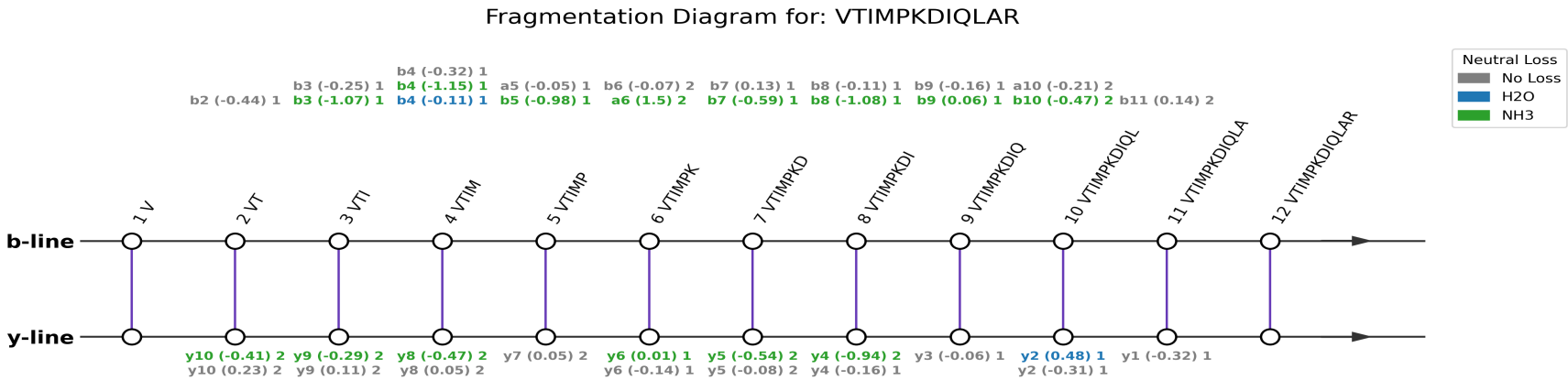
44	usable	y4 (1+) @ 376.0 & ai9-10 (1+) @ 176.67	376.0	376.19	176.67	177.09	928.67	-1.0	-1.0	-1.0	-1.0
45	usable	[b13-H2O-NH3] (2+) @ 559.33 & y1(1+) @ 175.0	559.33	559.24	175.0	175.12	1293.66	3.0	3.0	3.0	3.0
46	usable	y1 (1+) @ 174.67 & [b13-NH3] (2+) @ 567.67	174.67	175.12	567.67	568.25	1310.01	0.0	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

output



	b1y11	b2y10	b3y9	b4y8	b5y7	b6y6	b7y5	b8y4	b9y3	b10y2	b11y1	Row_Count
Parent	--	(b2,y10) (1+ , 2+) -0.18 (8)	--	(b4,y8) (1+ , 2+) -0.3 (20)	(b5,y7) (1+ , 2+) 0.11 (17)	(b6,y6) (2+ , 1+) -0.02 (1)	(b7,y5) (1+ , 2+) -0.21 (12)	(b8,y4) (1+ , 2+) -0.28 (18)	--	(b10,y2) (2+ , 1+) -0.29 (3)	(b11,y1) (2+ , 1+) -0.4 (19)	8
NH3	--	(b2,NH3) (1+ , 2+) -0.85 (33)	(NH3,y9) (1+ , 2+) -1.06 (6)	(NH3,y8) (1+ , 2+) -0.99 (36)	(NH3,y7) (1+ , 2+) -0.94 (55)	(NH3,y6) (2+ , 1+) -0.5 (22)	(NH3,y5) (1+ , 2+) -0.67 (42)	(NH3,y4) (1+ , 2+) -1.66 (43)	--	(NH3,y2) (2+ , 1+) -0.81 (13)	--	8
H2O	--	--	--	--	--	--	--	--	--	--	--	0
NH3 + H2O	--	--	--	--	--	--	--	--	--	--	--	0
H2O + NH3	--	--	--	--	--	--	--	--	--	--	--	0
a	--	(a2,y10) (1+ , 2+) -0.25 (14)	--	(a4,y8) (1+ , 2+) -0.1 (24)	--	--	--	(a8,y4) (2+ , 1+) -0.09 (5)	--	--	--	3
Col_Count	0	3	1	3	2	2	2	3	0	2	1	19





Detailed Data - Table 1

Unnamed: 0	b2	b3	b4	b5	b6	b7	b8	b9	b10	b11
H2O	nan	nan	b4-H2O (-0.11) (1 , 1)	nan	nan	nan	nan	nan	nan	nan
NH3	nan	b3-NH3 (-1.07) (1 , 2)	b4-NH3 (-1.15) (1 , 2)	b5-NH3 (-0.98) (1 , 2)	a6-NH3 (1.5) (2 , 1)	b7-NH3 (-0.59) (1 , 2)	b8-NH3 (-1.08) (1 , 2)	b9-NH3 (0.06) (1 , 1)	b10-NH3 (-0.47) (2 , 1)	nan
No Loss	b2 (-0.44) (1 , 2)	b3 (-0.25) (1 , 2)	b4 (-0.32) (1 , 1)	a5 (-0.05) (1 , 1)	b6 (-0.07) (2 , 1)	b7 (0.13) (1 , 2)	b8 (-0.11) (1 , 2)	b9 (-0.16) (1 , 1)	a10 (-0.21) (2 , 1)	b11 (0.14) (2 , 1)

Detailed Data - Table 2

Unnamed: 0	y1	y2	y3	y4	y5	y6	y7	y8	y9	y10
H2O	nan	y2-H2O (0.48) (1 , 1)	nan	nan	nan	nan	nan	nan	nan	nan
NH3	nan	nan	nan	y4-NH3 (-0.94) (2 , 1)	y5-NH3 (-0.54) (2 , 1)	y6-NH3 (0.01) (1 , 2)	nan	y8-NH3 (-0.47) (2 , 1)	y9-NH3 (-0.29) (2 , 1)	y10-NH3 (-0.41) (2 , 1)
No Loss	y1 (-0.32) (1 , 2)	y2 (-0.31) (1 , 1)	y3 (-0.06) (1 , 1)	y4 (-0.16) (1 , 1)	y5 (-0.08) (2 , 1)	y6 (-0.14) (1 , 2)	y7 (0.05) (2 , 1)	y8 (0.05) (2 , 1)	y9 (0.11) (2 , 1)	y10 (0.23) (2 , 1)

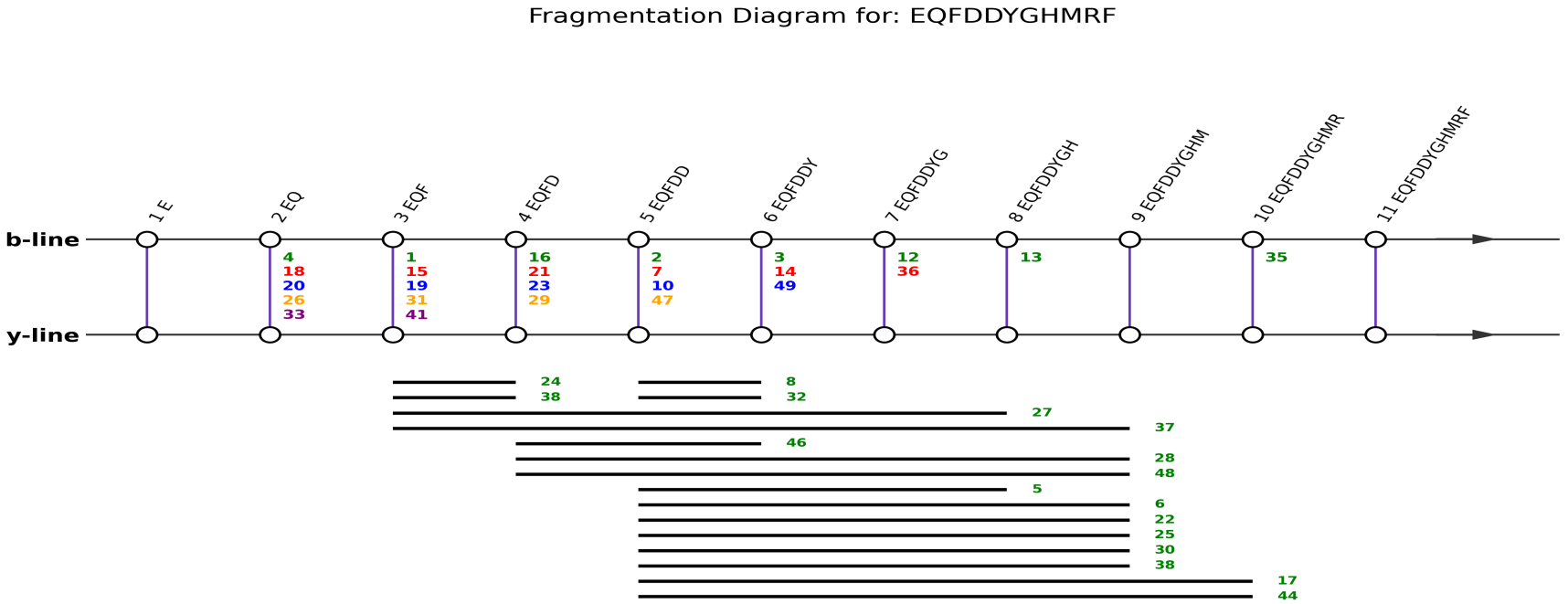
Detailed Data - Table 3

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	y6 (1+) @ 715.44 & b6 (2+) @ 356.66	715.44	715.41	356.66	356.71	1428.76	0	0	0	0
2	internal_acid	y5 (1+) @ 600.46 & bi5-7 (1+) @ 383.1	600.46	600.38	383.1	383.19	1366.66	-1	-1	-1	-1
3	usable	y2 (1+) @ 245.82 & b10 (2+) @ 591.38	245.82	246.16	591.38	591.33	1428.58	0	0	0	0
4	internal_acid	bi5-9 (1+) @ 624.4 & y3 (1+) @ 359.18	624.4	624.34	359.18	359.24	1342.76	-1	-1	-1	-1
5	usable	y4 (1+) @ 487.22 & a8(2+) @ 456.75	487.22	487.3	456.75	456.76	1431.19	-1	-1	-1	-1
6	usable	y9 (2+) @ 557.42 & [b3-NH3] (1+) @ 296.01	557.42	557.31	296.01	297.18	1410.85	1	1	1	1
7	non_complementary	y6 (2+) @ 359.14 & b9 (2+) @ 534.76	359.14	358.21	534.76	534.79	1428.66	0	0	0	0
8	usable	y10 (2+) @ 614.08 & b2 (1+) @ 200.71	614.08	613.85	200.71	201.12	1428.87	0	0	0	0
9	usable	[y4-NH3] (2+) @ 234.85 & b8 (1+) @ 940.45	234.85	235.64	940.45	940.52	1410.15	1	1	1	1
10	usable	y5 (1+) @ 600.38 & b7 (2+) @ 414.18	600.38	600.38	414.18	414.22	1428.74	0	0	0	0
11	non_complementary	y4 (1+) @ 487.33 & b7 (1+) @ 827.44	487.33	487.3	827.44	827.43	1314.77	2	2	2	-1
12	usable	y5 (2+) @ 300.5 & b7 (1+) @ 827.42	300.5	300.69	827.42	827.43	1428.42	0	0	0	0
13	usable	y2 (1+) @ 245.82 & [b10-NH3] (2+) @ 582.35	245.82	246.16	582.35	582.82	1410.52	1	1	1	1
14	usable	y10 (2+) @ 614.08 & a2 (1+) @ 172.63	614.08	613.85	172.63	173.11	1400.79	3	3	3	2
15	usable	y6 (1+) @ 715.45 & c5 (1+) @ 559.34	715.45	715.41	559.34	nan	1274.79	-1	-1	-1	-1
16	non_complementary	y2 (1+) @ 245.79 & b9 (1+) @ 1068.42	245.79	246.16	1068.42	1068.58	1314.21	2	2	2	-1
17	usable	y7 (2+) @ 443.34 & b5 (1+) @ 542.33	443.34	443.26	542.33	542.3	1429.01	0	0	0	0
18	usable	y4 (2+) @ 243.98 & b8 (1+) @ 940.41	243.98	244.15	940.41	940.52	1428.37	0	0	0	0

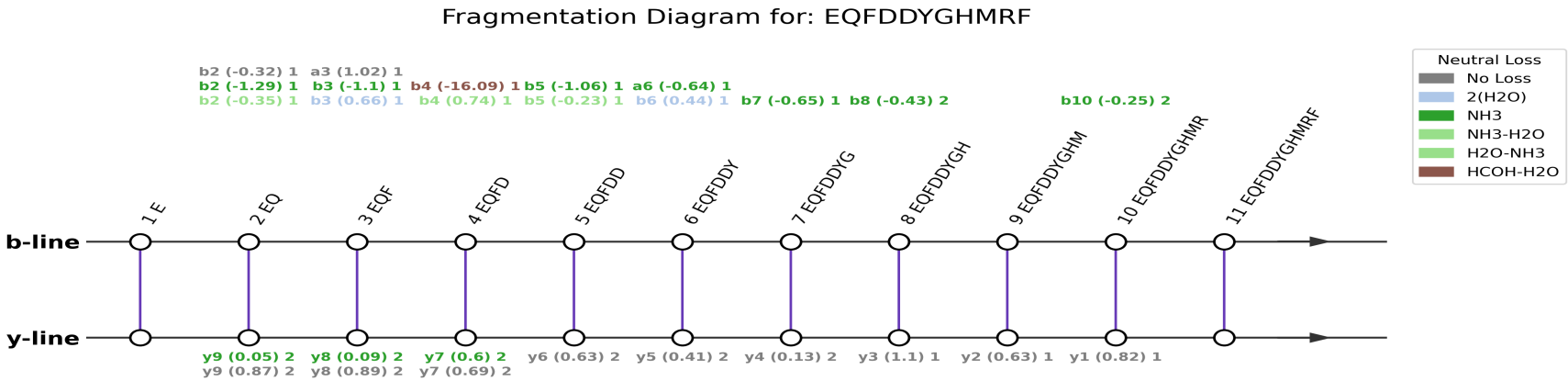
19	usable	y1 (1+) @ 174.58 & b11 (2+) @ 626.99	174.58	175.12	626.99	626.85	1428.56	0	0	0	0
20	usable	y8 (2+) @ 491.76 & b4 (1+) @ 444.98	491.76	491.79	444.98	445.25	1428.5	0	0	0	0
21	usable	[y6-NH3] (1+) @ 698.39 & b6 (2+) @ 356.64	698.39	698.38	356.64	356.71	1411.67	1	1	-1	-1
22	usable	y6 (1+) @ 715.54 & [b6-NH3] (2+) @ 347.56	715.54	715.41	347.56	348.19	1410.66	1	1	1	1
23	non_complementary	b6 (1+) @ 712.43 & [y2 – H2O] (1+) @ 228.63	712.43	712.41	228.63	228.15	1653.49	-1	-1	-1	-1
24	usable	y8 (2+) @ 491.82 & a4 (1+) @ 417.1	491.82	491.79	417.1	417.24	1400.74	3	3	3	2
25	non_complementary	y6 (2+) @ 359.14 & [b5-NH3] (1+) @ 525.62	359.14	358.21	525.62	525.27	1410.38	1	1	1	1
26	usable	y8 (2+) @ 491.96 & [b4 - CH3SH - CO] (1+) @ 369.04	491.96	491.79	369.04	369.25	1352.96	-1	-1	-1	-1
27	usable	[y8-NH3] (2+) @ 482.8 & b4 (1+) @ 445.14	482.8	483.27	445.14	445.25	1410.74	1	1	1	1
28	internal_acid	y6 (1+) @ 715.66 & bi5-6 @ 267.85	715.66	715.41	267.85	268.17	1251.36	-1	-1	-1	-1
29	internal_acid	y4 (1+) @ 487.09 & [bi4-7 – HCOOH] (1+) @ 468.09	487.09	487.3	468.09	468.23	1423.27	-1	-1	-1	-1
30	internal_acid	[bi4-7 – HCOOH] (1+) @ 468.13 & ??? @ 445.09	468.13	468.23	445.09	nan	1381.35	-1	-1	-1	-1
31	usable	y5(1+) @ 600.3 & [b7-NH3] (2+) @ 405.11	600.3	600.38	405.11	405.71	1410.52	1	1	1	1
32	internal_acid	bi5-10 (1+) @ 737.3 & y2 (1+) @ 245.92	737.3	737.42	245.92	246.16	1229.14	-1	-1	-1	-1
33	usable	[y10-NH3] (2+) @ 604.93 & b2(1+) @ 200.68	604.93	605.34	200.68	201.12	1410.54	1	1	1	1
34	internal_acid	bi5-9 (1+) @ 624.41 & b4 (1+) @ 444.93	624.41	624.34	444.93	445.25	1514.27	-1	-1	-1	-1
35	usable	y5(1+) @ 600.44 & a5 (1+) @ 514.24	600.44	600.38	514.24	514.29	1628.92	-1	-1	-1	-1
36	usable	y8(2+) @ 491.95 & [b4-NH3] (1+) @ 427.07	491.95	491.79	427.07	428.22	1410.97	1	1	1	1
37	usable	bi (5-8) (1+) @ 496.41 & y4 (1+) @ 487.01	496.41	496.28	487.01	487.3	1470.43	-1	-1	-1	-1
38	usable	[y5-NH3](2+) @ 291.64 & b7 (1+) @ 827.56	291.64	292.18	827.56	827.43	1410.84	1	1	1	1
39	non_complementary	y2(1+) @ 245.81 & [b9-NH3] (1+) @ 1051.61	245.81	246.16	1051.61	1051.55	1543.23	-1	-1	-1	-1
40	usable	bi (2-8) (1+) @ 841.49 & y4 (1+) @ 487.14	841.49	841.45	487.14	487.3	1328.63	4	4	4	-1
41	unclear	b8(1+) @ 940.89 & ??? @ 195.81	940.89	940.52	195.81	nan	1332.51	-1	-1	-1	-1
42	usable	y5(2+) @ 300.61 & [b7-NH3] (1+) @ 809.82	300.61	300.69	809.82	810.41	1411.04	1	1	1	1
43	usable	y4(2+) @ 243.81 & [b8-NH3] (1+) @ 922.17	243.81	244.15	922.17	923.49	1409.79	1	1	1	1
44	unclear	b6(1+) @ 712.31 & ??? @ 200.73	712.31	712.41	200.73	nan	1625.35	-1	-1	-1	-1
45	unclear	y9 (2+) @ 557.39 & ??? @ 250.74	557.39	557.31	250.74	nan	1365.52	-1	-1	-1	-1
46	usable	[y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.11	548.5	548.79	296.11	297.18	1393.11	-1	-1	-1	-1

47	usable	b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91	827.88	827.43	241.91	242.15	1311.7	-1	-1	-1	-1
48	usable	y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69	715.27	715.41	335.69	334.19	1386.65	-1	-1	-1	-1
49	usable	[y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.41	234.7	235.64	922.41	923.49	1391.81	-1	-1	-1	-1
50	unclear	y8 (1+) @ 983.52 & ??? @ 216.78	983.52	982.57	216.78	nan	1417.08	-1	-1	-1	-1
51	non_complementary	y8(2+) @ 491.84 & b3(1+) @ 313.96	491.84	491.79	313.96	314.21	1297.64	-1	-1	-1	-1
52	non_complementary	[b9-2(H2O)] (1+) @ 516.81 & y2 (1+) @ 245.85	516.81	1032.55	245.85	246.16	1279.47	-1	-1	-1	-1
53	unclear	??? @ 755.18 & y6(2+) @ 359.22	755.18	nan	359.22	358.21	1473.62	-1	-1	-1	-1
54	usable	y1 (1+) @ 174.8 & a10 (2+) @ 577.12	174.8	175.12	577.12	577.33	1329.04	4	4	4	-1
55	usable	y7 (2+) @ 443.31 & [b5-NH3] (1+) @ 524.29	443.31	443.26	524.29	525.27	1410.91	1	1	1	1
56	internal_acid	bi5-9 (1+) @ 624.36 & [b4- H2O] (1+) @ 427.13	624.36	624.34	427.13	427.24	1478.62	-1	-1	-1	-1

output



	b1y10	b2y9	b3y8	b4y7	b5y6	b6y5	b7y4	b8y3	b9y2	b10y1	Row_Count
Parent	--	(b2,y9) (1+ , 2+) 0.6 (20)	--	--	--	--	--	--	--	--	1
NH3	--	(NH3,y9) (1+ , 2+) -0.7 (4)	(NH3,y8) (1+ , 2+) -0.4 (1)	--	(NH3,y6) (1+ , 2+) -0.45 (2)	(NH3,y5) (1+ , 2+) -0.56 (3)	(NH3,y4) (1+ , 2+) -0.52 (36)	(NH3,y3) (2+ , 1+) 0.52 (13)	--	(NH3,y1) (2+ , 1+) 0.56 (35)	7
H2O	--	--	--	--	--	--	--	--	--	--	0
NH3 + H2O	--	--	--	--	--	--	--	--	--	--	0
H2O + NH3	--	--	--	--	--	--	--	--	--	--	0
a	--	--	--	--	--	--	--	--	--	--	0
Col_Count	0	2	1	0	1	1	1	1	0	1	8



Detailed Data - Table 1

Unnamed: 0	b2	b3	b4	b5	b6	b7	b8	b10
2(H2O)	nan	b3-2(H2O) (0.66) (1 , 2)	nan	nan	b6-2(H2O) (0.44) (1 , 2)	nan	nan	nan
H2O-NH3	b2-H2O-NH3 (-0.35) (1 , 2)	nan	b4-H2O-NH3 (0.74) (1 , 1)	b5-H2O-NH3 (-0.23) (1 , 2)	nan	nan	nan	nan
NH3	b2-NH3 (-1.29) (1 , 2)	b3-NH3 (-1.1) (1 , 2)	nan	b5-NH3 (-1.06) (1 , 2)	a6-NH3 (-0.64) (1 , 2)	b7-NH3 (-0.65) (1 , 2)	b8-NH3 (-0.43) (2 , 1)	b10-NH3 (-0.25) (2 , 1)
HCOH-H2O	nan	nan	b4-HCOH-H2O (-16.09) (1 , 1)	nan	nan	nan	nan	nan
No Loss	b2 (-0.32) (1 , 2)	a3 (1.02) (1 , 1)	nan	nan	nan	nan	nan	nan

Detailed Data - Table 2

Unnamed: 0	y1	y2	y3	y4	y5	y6	y7	y8	y9
NH3	nan	nan	nan	nan	nan	nan	y7-NH3 (0.6) (2 , 1)	y8-NH3 (0.09) (2 , 1)	y9-NH3 (0.05) (2 , 1)
No Loss	y1 (0.82) (1 , 2)	y2 (0.63) (1 , 1)	y3 (1.1) (1 , 1)	y4 (0.13) (2 , 1)	y5 (0.41) (2 , 1)	y6 (0.63) (2 , 1)	y7 (0.69) (2 , 1)	y8 (0.89) (2 , 1)	y9 (0.87) (2 , 1)

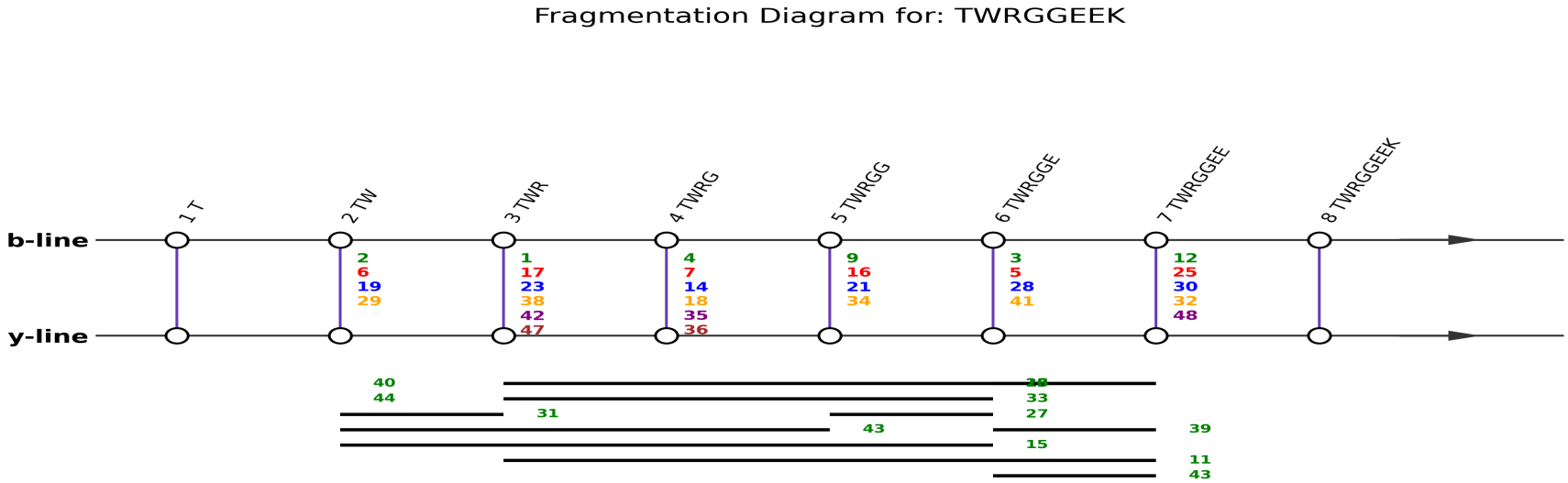
Detailed Data - Table 3

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	y8(2+) @ 560.4 & [b3-NH3] (1+) @ 387.05	560.4	559.7	387.05	388.15	1507.85	0.0	0.0	0.0	0.0
2	usable	y6(2+) @ 445.29 & [b5-NH3] (1+) @ 617.14	445.29	444.68	617.14	618.2	1507.72	0.0	0.0	0.0	0.0
3	usable	y5(2+) @ 323.67 & [b6-NH3] (1+) @ 860.17	323.67	323.16	860.17	861.23	1507.51	0.0	0.0	0.0	0.0
4	usable	y9(2+) @ 633.88 & [b2-NH3] (1+) @ 239.74	633.88	633.24	239.74	241.08	1507.5	0.0	0.0	0.0	0.0
5	internal_acid	bi5-8 (1+) @ 1553.17 & y3 (1+) @ 452.35	1553.17	553.14	452.35	451.24	2005.52	-1.0	-1.0	-1.0	-1.0
6	internal_acid	bi5-9 (1+) @ 684.16 & y2 (1+) @ 321.1	684.16	684.18	321.1	320.2	1689.42	-1.0	-1.0	-1.0	-1.0
7	usable	y6(2+) @ 445.35 & a3(1+) @ 378.1	445.35	444.68	378.1	377.17	1268.8	-1.0	-1.0	-1.0	-1.0
8	internal_acid	y5+ @ 646.41 & bi5-6 (1+) @ 359.02	646.41	nan	359.02	359.06	1651.84	-1.0	-1.0	-1.0	-1.0
9	undefined	503.73 & 498.42	503.73	nan	498.42	nan	1505.88	-1.0	-1.0	-1.0	-1.0
10	usable	[b5-H2O-NH3] (1+) @ 599.96 & y6 (2+) @ 445.31	599.96	600.19	445.31	444.68	1490.58	1.0	1.0	1.0	1.0
11	usable	y5 (1+) 646.38 & ai5-6 (1+) @ 330.84	nan	nan	330.84	331.05	nan	nan	nan	nan	nan
12	usable	y4(1+) @ 589.39 & [a6-NH3](2+) @ 416.05	589.39	588.29	416.05	417.12	1594.83	-1.0	-1.0	-1.0	-1.0
13	usable	y3(1+) @ 452.19 & [b8-NH3](2+) @ 527.73	452.19	451.24	527.73	528.16	1507.65	0.0	0.0	0.0	0.0
14	usable	[b6-2(H2O)] (1+) @ 842.68 & y5 (2+) @ 323.57	842.68	842.24	323.57	323.16	1489.82	1.0	1.0	2.0	2.0
15	usable	y8(2+) @ 560.27 & [a3-NH3](1+) @ 358.97	560.27	559.7	358.97	360.14	1479.51	2.0	2.0	3.0	3.0
16	usable	[b4-H2O-NH3] (1+) @ 485.79 & [y7- CHONH2] (2+) @ 480.35	485.79	485.17	480.35	479.68	1451.93	-1.0	-1.0	-1.0	-1.0
17	internal_acid	bi5-10 (1+) @ 840.5 & y1 (1+) 164.73	840.5	840.29	nan	nan	nan	nan	nan	nan	nan

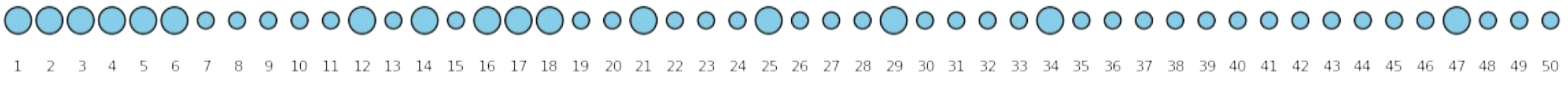
18	usable	y9(2+) @ 633.84 & [a2-NH3](1+) @ 211.71	633.84	633.24	211.71	213.07	1479.39	2.0	2.0	3.0	3.0
19	usable	[y8-NH3](2+) @ 551.2 & [b3-NH3](1+) @ 387.05	551.2	551.19	387.05	388.15	1489.45	1.0	1.0	2.0	2.0
20	usable	y9(2+) @ 634.16 & b2(1+) @ 257.79	634.16	633.24	257.79	258.11	1526.11	-1.0	-1.0	-1.0	-1.0
21	usable	[y7-NH3] (2+) @ 494.13 & [b4-HCOH – H2O] (1+) @ 456.16	494.13	493.68	456.16	472.18	1444.42	-1.0	-1.0	-1.0	-1.0
22	internal_acid	bi5-9 (1+) @ 656.39 & y2 (1+) @ 321.11	656.39	684.18	321.11	320.2	1633.89	-1.0	-1.0	-1.0	-1.0
23	usable	y7 (2+) @ 502.88 & [b4-HCOH – H2O] (1+) @ 455.94	502.88	502.19	455.94	472.18	1461.7	3.0	3.0	4.0	-1.0
24	internal_acid	[y7 – NH3] 2+ @ 494.11 & bi3-4 @ 262.78	494.11	nan	262.78	263.1	1251.0	-1.0	-1.0	-1.0	-1.0
25	internal_acid	[bi5-9 – CH3CH2SCH3] (1+) @ 608.2 & y2 (1+) @ 320.89	608.2	608.15	320.89	320.2	1537.29	-1.0	-1.0	-1.0	-1.0
26	usable	[y9-NH3] (2+) @ 624.77 & [b2-NH3] (1+) @ 239.79	624.77	624.72	239.79	241.08	1489.33	1.0	1.0	2.0	2.0
27	internal_acid	bi3-8 (1+) @ 815.6 & y3 (1+) @ 452.34	815.6	815.24	452.34	451.24	1720.28	-1.0	-1.0	-1.0	-1.0
28	non_complementary	[b4-HCOH – H2O] (1+) @ 456.12 & y2 (1+) @ 321.07	456.12	472.18	321.07	320.2	1233.31	-1.0	-1.0	-1.0	-1.0
29	usable	[y7 – NH3] (2+) @ 494.28 & [b4 - H2O – NH3] (1+) @ 484.76	494.28	493.68	484.76	485.17	1473.32	-1.0	-1.0	-1.0	-1.0
30	internal_acid	[bi5-9] (1+) @ 683.79 & [b4 - HCOH – H2O] (1+) @ 456.23	683.79	684.18	456.23	472.18	1596.25	-1.0	-1.0	-1.0	-1.0
31	usable	y8 (2+) @ 560.59 & [b3 – 2(H2O)] (1+) @ 369.82	560.59	559.7	369.82	369.16	1491.0	1.0	1.0	1.0	1.0
32	internal_acid	y5 (1+) @ 646.41 & bi5-6 (1+) @ 312.22	646.41	645.32	312.22	359.06	1605.04	-1.0	-1.0	-1.0	-1.0
33	usable	y9 (2+) @ 634.11 & [b2 – H2O – NH3] (1+) @ 222.72	634.11	633.24	222.72	223.07	1490.94	1.0	1.0	1.0	1.0
34	unclear	b8 (2+) @ 536.55 & ??? @ 454.17	536.55	536.67	454.17	nan	1527.27	-1.0	-1.0	-1.0	-1.0
35	usable	y1(1+) @ 164.91 & [b10-NH3](2+) @ 671.48	164.91	164.09	671.48	671.73	1507.87	0.0	0.0	0.0	0.0
36	usable	y4(2+) @ 294.78 & [b7-NH3](1+) @ 917.61	294.78	294.65	917.61	918.26	1507.17	0.0	0.0	0.0	0.0
37	internal_acid	bi3-9 (1+) @ 946.47 & y2 (1+) 321.09	946.47	946.28	nan	nan	nan	nan	nan	nan	nan
38	internal_acid	bi5-9 (1+) @ 683.85 & bi3-4 (1+) @ 263.1	683.85	684.18	263.1	263.1	1630.8	-1.0	-1.0	-1.0	-1.0
39	undefined	591.11 & 398.48	591.11	nan	398.48	nan	1580.7	-1.0	-1.0	-1.0	-1.0
40	unclear	y9 (2+) @ 634.11 & ??? @ 194.76	634.11	633.24	194.76	nan	1462.98	-1.0	-1.0	-1.0	-1.0
41	usable	[y8-NH3] (2+) @ 551.28 & [a3-H2O] (1+) @ 358.64	551.28	551.19	358.64	359.16	1461.2	3.0	3.0	4.0	-1.0
42	unclear	y8(2+) @ 560.81 & ??? @ 342.47	560.81	559.7	342.47	nan	1464.09	-1.0	-1.0	-1.0	-1.0
43	unclear	y4(1+) @ 589.96 & ??? @ 329.12	589.96	588.29	329.12	nan	1509.04	-1.0	-1.0	-1.0	-1.0
44	internal_acid	bi5-10 (1+) @ 840.36 & [b4 – H2O – NH3] (1+) @ 485.91	840.36	840.29	485.91	485.17	1326.27	-1.0	-1.0	-1.0	-1.0
45	undefined	518.97 & 454.06	518.97	nan	454.06	nan	1492.0	1.0	-1.0	-1.0	-1.0

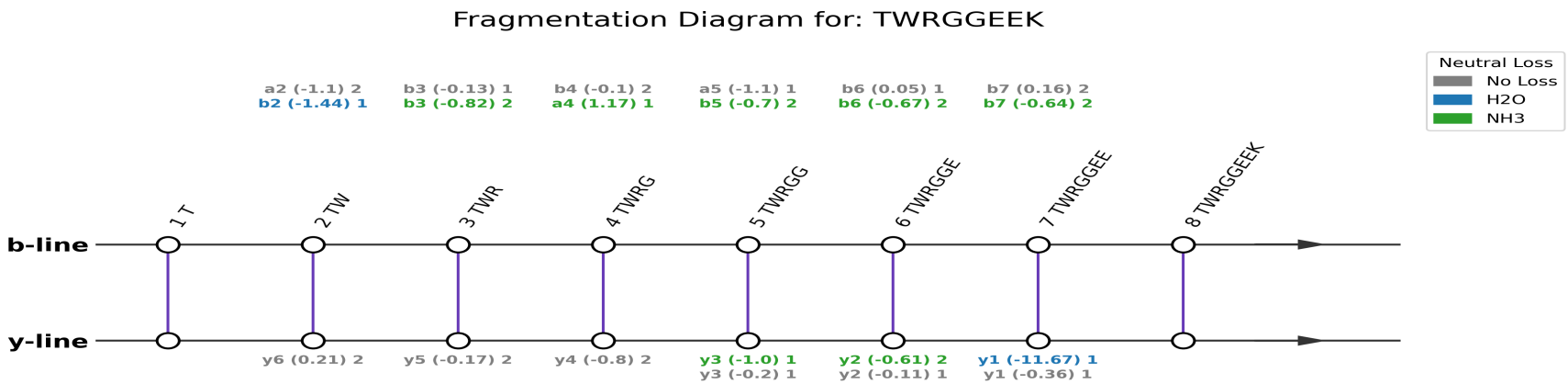
46	non_complementary	y5 (1+) @ 646.3 & [b4-HCOH – H2O] (1+) @ 456.09	646.3	645.32	456.09	472.18	1558.48	-1.0	-1.0	-1.0	-1.0
47	usable	y6 (1+) @ 889.27 & a3 (1+) @ 378.19	889.27	888.35	378.19	377.17	1645.65	-1.0	-1.0	-1.0	-1.0
48	non_complementary	[b4 – H2O – NH3] (1+) @ 484.86 & y2 (1+) @ 320.83	484.86	485.17	320.83	320.2	1290.55	-1.0	-1.0	-1.0	-1.0
49	usable	y5 (2+) @ 323.7 & [a6-NH3] (1+) @ 832.58	323.7	323.16	832.58	833.22	1479.98	2.0	2.0	3.0	-1.0
50	undefined	567.88 & 374.49	567.88	nan	374.49	nan	1510.25	-1.0	-1.0	-1.0	-1.0

output



	b1y7	b2y6	b3y5	b4y4	b5y3	b6y2	b7y1	Row_Count
Parent	--	(b2,y6) (1+ , 2+) -0.18 (2)	(b3,y5) (1+ , 2+) -0.3 (47)	(b4,y4) (2+ , 1+) -0.12 (4)	(b5,y3) (2+ , 1+) -0.31 (34)	(b6,y2) (2+ , 1+) -0.12 (3)	(b7,y1) (2+ , 1+) -0.27 (25)	6
NH3	--	--	(NH3,y5) (2+ , 1+) -0.77 (17)	(NH3,y4) (1+ , 2+) -1.11 (18)	(b5,NH3) (2+ , 1+) -1.08 (21)	(NH3,y2) (2+ , 1+) -0.87 (5)	(NH3,y1) (2+ , 1+) -0.81 (12)	5
H2O	--	(H2O,y6) (1+ , 2+) -0.61 (29)	--	--	--	--	--	1
NH3 + H2O	--	--	--	--	--	--	--	0
H2O + NH3	--	--	--	--	--	--	--	0
a	--	(a2,y6) (1+ , 2+) 0.03 (6)	--	--	--	--	--	1
Col_Count	0	3	2	2	2	2	2	13





Detailed Data - Table 1

Unnamed: 0	b2	b3	b4	b5	b6	b7
H2O	b2-H2O (-1.44) (1 , 2)	nan	nan	nan	nan	nan
NH3	nan	b3-NH3 (-0.82) (2 , 1)	a4-NH3 (1.17) (1 , 2)	b5-NH3 (-0.7) (2 , 1)	b6-NH3 (-0.67) (2 , 1)	b7-NH3 (-0.64) (2 , 2)
No Loss	a2 (-1.1) (2 , 1)	b3 (-0.13) (1 , 2)	b4 (-0.1) (2 , 1)	a5 (-1.1) (1 , 1)	b6 (0.05) (1 , 1)	b7 (0.16) (2 , 1)

Detailed Data - Table 2

Unnamed: 0	y1	y2	y3	y4	y5	y6
H2O	y1-H2O (-11.67) (1 , 2)	nan	nan	nan	nan	nan
NH3	nan	y2-NH3 (-0.61) (2 , 2)	y3-NH3 (-1.0) (1 , 2)	nan	nan	nan
No Loss	y1 (-0.36) (1 , 1)	y2 (-0.11) (1 , 1)	y3 (-0.2) (1 , 2)	y4 (-0.8) (2 , 1)	y5 (-0.17) (2 , 1)	y6 (0.21) (2 , 1)

Detailed Data - Table 3

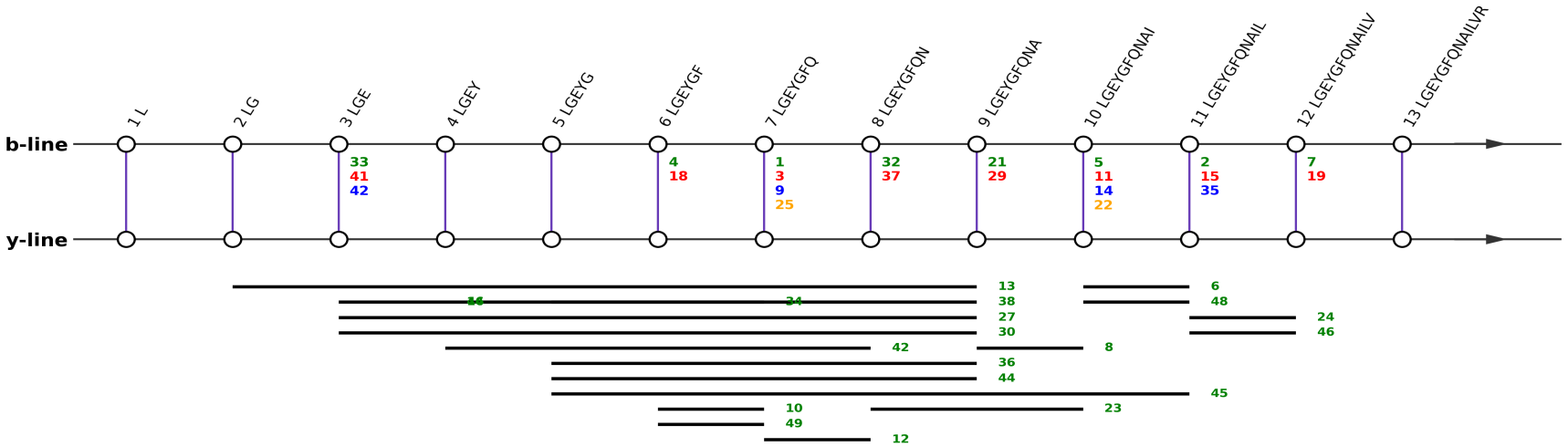
n	classification	line	mass1	correct_mass1	mass2	correct_mass2	chosen_sum	Cluster ID eps_1.0	Cluster ID eps_0.8	Cluster ID eps_0.6	Cluster ID eps_0.4
1	usable	y5 (1+) @ 519.33 & b3 (2+) @ 236.46	519.33	519.24	236.46	236.64	992.25	0.0	0.0	0.0	0.0
2	usable	y6 (2+) @ 352.17 & b2 (1+) @ 287.97	352.17	352.19	287.97	288.13	992.31	0.0	0.0	0.0	0.0
3	usable	y2 (1+) @ 276.0 & b6 (2+) @ 358.22	276.0	276.16	358.22	358.18	992.44	0.0	0.0	0.0	0.0
4	usable	y4 (1+) @ 462.2 & b4 (2+) @ 265.05	462.2	462.22	265.05	265.15	992.3	0.0	0.0	0.0	0.0
5	usable	y2 (1+) @ 275.95 & [b6-NH3] (2+) @ 349.0	275.95	276.16	349.0	349.67	973.95	1.0	1.0	1.0	1.0
6	usable	y6 (2+) @ 352.25 & a2 (1+) @ 260.09	352.25	352.19	260.09	260.12	964.59	-1.0	-1.0	-1.0	-1.0
7	usable	b4 (1+) @ 529.34 & Im(W) @ 158.68	529.34	529.29	158.68	nan	846.7	-1.0	-1.0	-1.0	-1.0
8	undefined	379.75 & 197.76	379.75	nan	197.76	nan	957.26	2.0	2.0	-1.0	-1.0
9	usable	[y3-NH3] (1+) @ 387.08 & [b5-NH3] (2+) @ 284.5	387.08	388.17	284.5	285.15	956.08	2.0	2.0	2.0	2.0
10	non_complementary	[y2-NH3] (2+) @ 129.42 & b7 (2+) @ 422.56	129.42	130.07	422.56	422.7	974.54	1.0	1.0	1.0	1.0
11	internal_acid	[bi3-7 - HCOOH] (1+) @ 511.25 & Im (W) @ 158.67	511.25	511.26	158.67	nan	828.59	-1.0	-1.0	-1.0	-1.0
12	usable	y1(1+) @ 146.68 & [b7-NH3](2+) @ 413.81	146.68	147.11	413.81	414.19	974.3	1.0	1.0	1.0	1.0
13	internal_acid	bi3-6 (1+) @ 428.14 & y2 (1+) @ 276.01	428.14	428.23	276.01	276.16	980.16	3.0	3.0	-1.0	-1.0
14	usable	y4 (1+) @ 462.16 & [b4-NH3] (2+) @ 255.92	462.16	462.22	255.92	256.63	974.0	1.0	1.0	1.0	1.0
15	internal_acid	bi2-6 (1+) @ 614.19 & y2 (1+) @ 276.05	614.19	614.3	276.05	276.16	890.24	-1.0	-1.0	-1.0	-1.0
16	usable	y3 (1+) @ 405.15 & [b5-NH3] (2+) @ 284.45	405.15	405.2	284.45	285.15	974.05	1.0	1.0	1.0	1.0
17	usable	y5 (1+) @ 519.29 & [b3-NH3] (2+) @ 227.3	519.29	519.24	227.3	228.12	973.89	1.0	1.0	1.0	1.0
18	usable	y4 (2+) @ 231.48 & [b4-NH3] (1+) @ 511.28	231.48	231.61	511.28	512.26	974.24	1.0	1.0	1.0	1.0

19	usable	[y6 - CH3NHCH3] (1+) @ 658.39 & Im(W) 158.65	658.39	658.32	nan	nan	nan	nan	nan	nan	nan
20	undefined	519.31 & 343.18	519.31	nan	343.18	nan	862.49	-1.0	-1.0	-1.0	-1.0
21	usable	[y3-NH3] (1+) @ 387.17 & b5 (2+) @ 293.58	387.17	388.17	293.58	293.66	974.33	1.0	1.0	1.0	1.0
22	undefined	583.42 & 243.89	583.42	nan	243.89	nan	1071.2	-1.0	-1.0	-1.0	-1.0
23	usable	y5 (1+) @ 519.34 & [b3-H2O-NH3] (2+) @ 218.59	519.34	519.24	218.59	219.12	956.52	2.0	2.0	2.0	2.0
24	undefined	360.8 & 257.89	360.8	nan	257.89	nan	979.49	3.0	3.0	-1.0	-1.0
25	usable	y1 (1+) @ 146.68 & b7 (2+) @ 422.86	146.68	147.11	422.86	422.7	992.4	0.0	0.0	0.0	0.0
26	non_complementary	[y2-NH3] (2+) @ 129.33 & [b7-NH3] (2+) @ 413.55	129.33	130.07	413.55	414.19	956.43	2.0	2.0	2.0	2.0
27	internal_acid	[b4-NH3] (1+) @ 511.38 & bi5-6 (1+) @ 186.59	511.38	512.26	186.59	187.07	884.56	-1.0	-1.0	-1.0	-1.0
28	usable	[y2-NH3] (2+) @ 129.46 & a6(2+) @ 342.91	129.46	130.07	342.91	344.17	815.28	-1.0	-1.0	-1.0	-1.0
29	usable	y6(2+) @ 353.02 & [b2-H2O] (1+) @ 268.68	353.02	352.19	268.68	270.12	974.72	1.0	1.0	1.0	1.0
30	usable	y6 (2+) @ 352.16 & [y1-H2O] (1+) @ 117.43	352.16	352.19	117.43	129.1	821.75	-1.0	-1.0	-1.0	-1.0
31	internal_acid	bi2-3 (1+) @ 370.7 & ??? @ 197.72	370.7	371.22	197.72	nan	939.12	-1.0	-1.0	-1.0	-1.0
32	usable	[b7+H2O] (2+) @ 431.82 & y1-H2O (1+)128.45	431.82	431.71	nan	nan	nan	nan	nan	nan	nan
33	internal_acid	bi3-6 (1+) @ 428.11 & b2 (1+) @ 287.75	428.11	428.23	287.75	288.13	1003.61	-1.0	-1.0	-1.0	-1.0
34	usable	y3 (1+) @ 405.0 & b5 (2+) @ 293.55	405.0	405.2	293.55	293.66	992.1	0.0	0.0	0.0	0.0
35	usable	y4 (1+) @ 462.22 & [a4-NH3] (2+) @ 242.05	462.22	462.22	242.05	242.63	946.32	4.0	4.0	-1.0	-1.0
36	usable	y4 (2+) @ 230.81 & [a4-NH3] (1+) @ 485.42	230.81	231.61	485.42	484.25	947.04	4.0	4.0	-1.0	-1.0
37	unclear	y7-H2O (2+) 436.23 & ??? @ 118.35	nan	nan	118.35	nan	nan	nan	nan	nan	nan
38	usable	y5 (1+) @ 519.35 & [b3 - CH3NHCH3 – H2O] (2+) @ 205.31	519.35	519.24	205.31	205.1	929.97	-1.0	-1.0	-1.0	-1.0
39	non_complementary	y1 (1+) @ 147.54 & b6 (1+) @ 715.4	147.54	147.11	715.4	715.35	1010.48	-1.0	-1.0	-1.0	-1.0
40	internal_acid	[y6 - CH3-NH-CH3] (1+) @ 658.42 & bi2-2 (1+) @ 186.66	658.42	658.32	186.66	187.09	1031.74	-1.0	-1.0	-1.0	-1.0
41	usable	[b6 – H3C-N=CH2 - NH3] (1+) @ 654.37 & y2 (1+) @ y2 (1+) 275.92	654.37	655.28	nan	nan	nan	nan	nan	nan	nan
42	usable	y5 (1+) @ 519.11 & a2 (2+) @ 129.47	519.11	519.24	129.47	130.57	1167.69	-1.0	-1.0	-1.0	-1.0
43	usable	bi 2-5 (1+) @ 485.29 & [bi 6-7 – HCOOH] (1+) @ 212.85	485.29	485.26	212.85	213.09	910.99	-1.0	-1.0	-1.0	-1.0
44	internal_acid	y6 (2+) @ 352.4 & bi2-2 (1+) @ 186.67	352.4	352.19	186.67	187.09	891.47	-1.0	-1.0	-1.0	-1.0
45	unclear	y5 (1+) @ 519.0 & ??? @ 177.74	519.0	519.24	177.74	nan	874.48	-1.0	-1.0	-1.0	-1.0
46	undefined	697.71 & 101.31	697.71	nan	101.31	nan	900.33	-1.0	-1.0	-1.0	-1.0

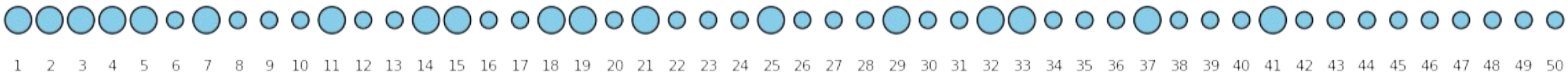
47	usable	y5 (2+) @ 259.95 & b3 (1+) @ 472.14	259.95	260.12	472.14	472.27	992.04	0.0	0.0	0.0	0.0
48	usable	y1 (1+) @ 146.75 & a5 (1+) @ 557.2	146.75	147.11	557.2	558.3	850.7	-1.0	-1.0	-1.0	-1.0
49	undefined	404.6 & 146.46	404.6	nan	146.46	nan	955.66	2.0	2.0	2.0	-1.0
50	undefined	352.05 & 131.78	352.05	nan	131.78	nan	835.88	-1.0	-1.0	-1.0	-1.0

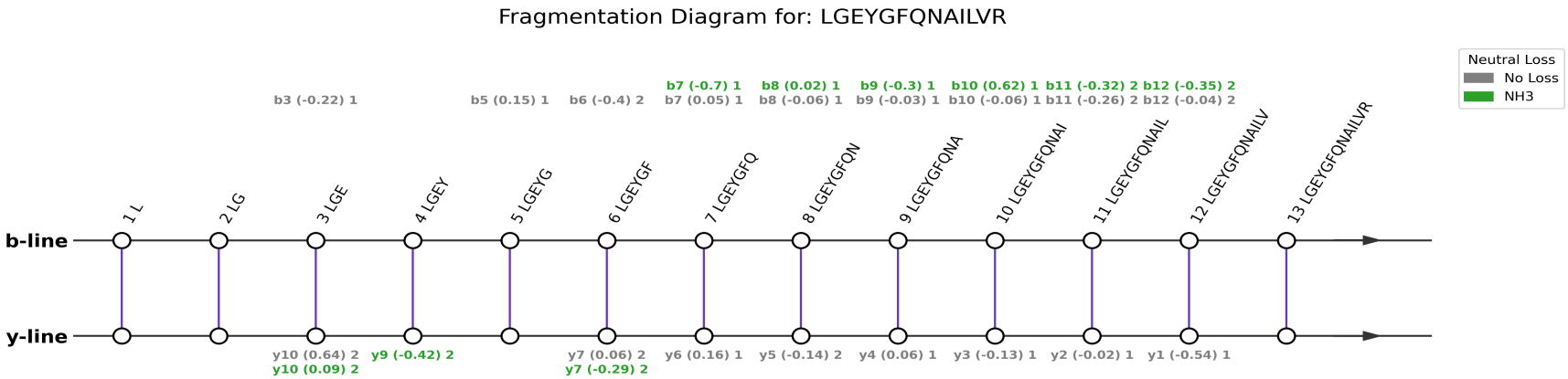
output

Fragmentation Diagram for: LGEYGFQNAILVR



	b1y12	b2y11	b3y10	b4y9	b5y8	b6y7	b7y6	b8y5	b9y4	b10y3	b11y2	b12y1	Row_Count
Parent	--	--	(b3,y10) (1+ , 2+) 0.31 (33)	--	--	(b6,y7) (1+ , 2+) 0.14 (4)	(b7,y6) (1+ , 2+) 0.01 (3)	(b8,y5) (1+ , 2+) -0.2 (32)	(b9,y4) (1+ , 2+) -0.37 (21)	(b10,y3) (2+ , 1+) -0.17 (5)	(b11,y2) (2+ , 1+) -0.11 (2)	(b12,y1) (2+ , 1+) -0.51 (7)	8
NH3	--	--	(b3,**NH3**) (1+ , 2+) -0.25 (41)	--	--	(b6,**NH3**) (1+ , 2+) -0.17 (18)	(**NH3**,y6) (1+ , 2+) -0.75 (25)	(**NH3**,y5) (1+ , 2+) -0.12 (37)	(**NH3**,y4) (1+ , 2+) -0.48 (29)	(**NH3**,y3) (2+ , 1+) -0.47 (14)	(**NH3**,y2) (2+ , 1+) -0.41 (15)	(**NH3**,y1) (2+ , 1+) -0.88 (19)	8
H2O	--	--	--	--	--	--	--	--	--	--	--	--	0
NH3 + H2O	--	--	--	--	--	--	--	--	--	--	--	--	0
H2O + NH3	--	--	--	--	--	--	--	--	--	--	--	--	0
a	--	--	--	--	--	--	--	--	--	--	--	--	0
Col_Count	0	0	2	0	0	2	2	2	2	2	2	2	16





Detailed Data - Table 1

Unnamed: 0	b3	b5	b6	b7	b8	b9	b10	b11	b12
No Loss	b3 (-0.22) (1 , 1)	b5 (0.15) (1 , 1)	b6 (-0.4) (2 , 1)	b7 (0.05) (1 , 2)	b8 (-0.06) (1 , 2)	b9 (-0.03) (1 , 2)	b10 (-0.06) (1 , 1)	b11 (-0.26) (2 , 1)	b12 (-0.04) (2 , 1)
NH3	nan	nan	nan	b7-NH3 (-0.7) (1 , 2)	b8-NH3 (0.02) (1 , 2)	b9-NH3 (-0.3) (1 , 2)	b10-NH3 (0.62) (1 , 1)	b11-NH3 (-0.32) (2 , 1)	b12-NH3 (-0.35) (2 , 1)

Detailed Data - Table 2

Unnamed: 0	y1	y2	y3	y4	y5	y6	y7	y9	y10
No Loss	y1 (-0.54) (1 , 2)	y2 (-0.02) (1 , 1)	y3 (-0.13) (1 , 2)	y4 (0.06) (1 , 1)	y5 (-0.14) (2 , 1)	y6 (0.16) (1 , 1)	y7 (0.06) (2 , 1)	nan	y10 (0.64) (2 , 1)
NH3	nan	nan	nan	nan	nan	nan	y7-NH3 (-0.29) (2 , 1)	y9-NH3 (-0.42) (2 , 1)	y10-NH3 (0.09) (2 , 1)

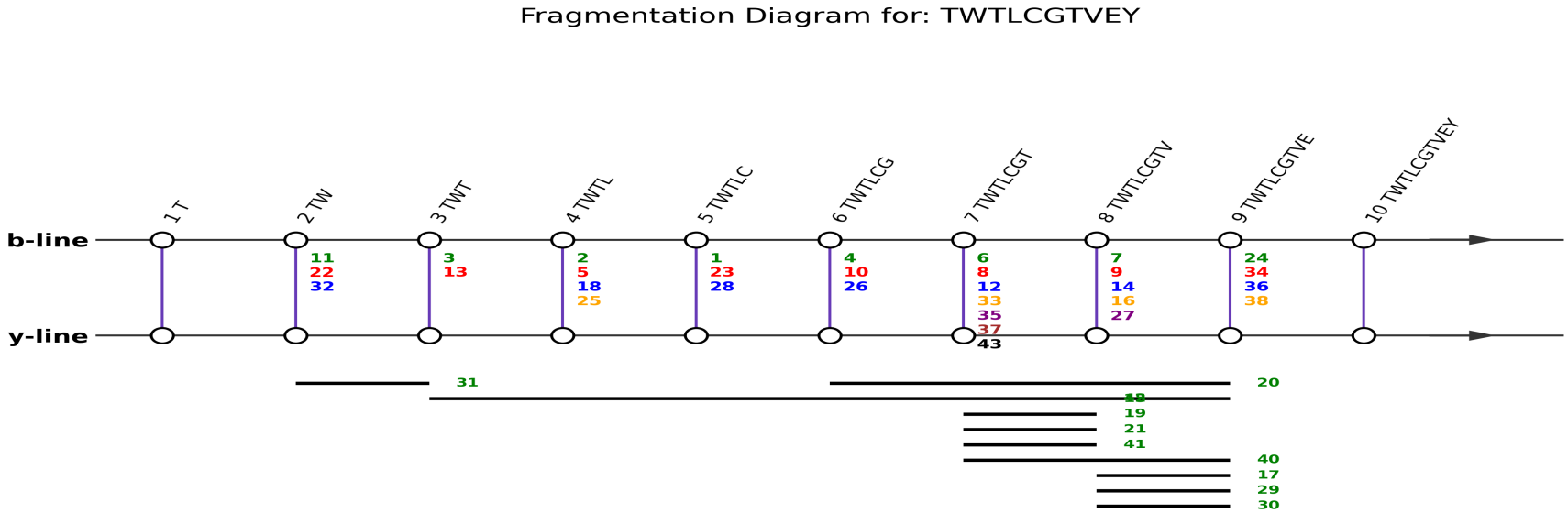
Detailed Data - Table 3

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	y6 (1+) @ 685.47 & b7 (2+) @ 420.68	685.47	685.44	420.68	420.68	1526.83	0.0	0.0	0.0	0.0
2	usable	y2 (1+) @ 274.0 & b11 (2+) @ 626.38	274.0	274.19	626.38	626.3	1526.76	0.0	0.0	0.0	0.0
3	usable	y6 (2+) @ 343.18 & b7 (1+) @ 840.4	343.18	343.22	840.4	840.35	1526.76	0.0	0.0	0.0	0.0
4	usable	y7 (2+) @ 407.31 & b6 (1+) @ 712.37	407.31	407.25	712.37	712.29	1526.99	0.0	0.0	0.0	0.0
5	usable	y3 (1+) @ 387.15 & b10 (2+) @ 569.71	387.15	387.27	569.71	569.76	1526.57	0.0	0.0	0.0	0.0
6	non_complementary	y2 (1+) @ 273.94 & b10 (1+) @ 1138.46	273.94	274.19	1138.46	1138.52	1412.4	1.0	1.0	1.0	1.0
7	usable	y1 (1+) @ 174.65 & b12 (2+) @ 675.8	174.65	175.12	675.8	675.84	1526.25	0.0	0.0	0.0	0.0
8	non_complementary	y3 (1+) @ 387.19 & b9 (1+) @ 1025.41	387.19	387.27	1025.41	1025.43	1412.6	1.0	1.0	1.0	1.0
9	usable	c6 (1+) @ 729.52 & y6 (1+) @ 685.6	729.52	nan	685.6	685.44	1415.12	-1.0	-1.0	-1.0	-1.0
10	non_complementary	y6 (1+) @ 685.52 & b6(1+) @ 712.65	685.52	685.44	712.65	712.29	1398.17	2.0	2.0	2.0	2.0
11	usable	y3 (2+) @ 193.8 & [b10-NH3] (1+) @ 1121.15	193.8	194.14	1121.15	1121.49	1508.75	3.0	3.0	3.0	3.0
12	internal_acid	b6 (1+) @ 712.35 & bi7-8 (1+) @ 242.83	712.35	712.29	242.83	243.11	1667.53	-1.0	-1.0	-1.0	-1.0
13	internal_acid	bi2-9 (1+) @ 912.43 & y4 (1+) 500.2	912.43	912.35	nan	nan	nan	nan	nan	nan	nan
14	usable	y3 (1+) @ 387.1 & [b10-NH3] (2+) @ 560.95	387.1	387.27	560.95	561.25	1509.0	3.0	3.0	3.0	3.0
15	usable	y2 (1+) @ 274.1 & [b11-NH3] (2+) @ 617.47	274.1	274.19	617.47	617.79	1509.04	3.0	3.0	3.0	3.0
16	non_complementary	[y9-NH3] (2+) @ 500.36 & b8 (1+) @ 954.34	500.36	500.78	954.34	954.4	1454.7	-1.0	-1.0	-1.0	-1.0
17	internal_acid	B6 (1+) 712.44 & [bi7-10 – HCONH2] (1+) 382.53	nan	nan	nan	nan	nan	nan	nan	nan	nan
18	usable	[y7-NH3] (2+) @ 398.45 & b6 (1+) @ 712.41	398.45	398.74	712.41	712.29	1509.31	3.0	3.0	3.0	3.0
19	usable	y1(1+) @ 174.59 & [b12-NH3] (2+) @ 666.97	174.59	175.12	666.97	667.32	1508.53	3.0	3.0	3.0	3.0

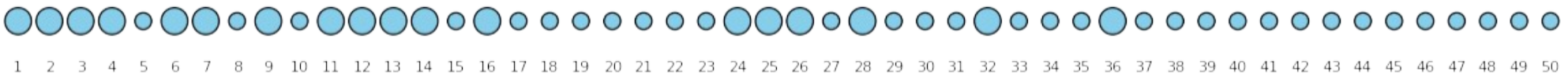
20	undefined	518.11 & 319.86	518.11	nan	319.86	nan	1356.08	-1.0	-1.0	-1.0	-1.0
21	usable	y4 (2+) @ 250.34 & b9 (1+) @ 1025.4	250.34	250.68	1025.4	1025.43	1526.08	0.0	0.0	0.0	0.0
22	usable	y3 (1+) @ 387.14 & [a10-NH3] (2+) @ 547.28	387.14	387.27	547.28	547.24	1481.7	-1.0	-1.0	-1.0	-1.0
23	internal_acid	b7 (1+) @ 840.43 & [bi8-10 – HCONH2] (1+) @ 253.8	840.43	840.35	253.8	254.15	1348.03	-1.0	-1.0	-1.0	-1.0
24	non_complementary	y1 (1+) @ 174.67 & b11 (1+) @ 1251.44	174.67	175.12	1251.44	1251.6	1600.78	-1.0	-1.0	-1.0	-1.0
25	usable	y6 (2+) @ 343.17 & [b7-NH3] (1+) @ 822.63	343.17	343.22	822.63	823.33	1508.97	3.0	3.0	3.0	3.0
26	internal_acid	b6 (1+) @ 712.2 & [bi7-8 – NH3] (1+) 225.78	712.2	712.29	nan	nan	nan	nan	nan	nan	nan
27	internal_acid	bi3-9 (1+) @ 855.2 & y4 (1+) 500.38	855.2	855.33	nan	nan	nan	nan	nan	nan	nan
28	undefined	840.47 & 298.93	840.47	nan	298.93	nan	1438.33	-1.0	-1.0	-1.0	-1.0
29	usable	y4 (2+) @ 250.5 & [b9-NH3] (1+) @ 1008.11	250.5	250.68	1008.11	1008.41	1509.11	3.0	3.0	3.0	3.0
30	internal_acid	[bi3-9 -H2O] (1+) @ 837.58 & y4 (1+) @ 500.18	837.58	837.32	500.18	500.36	1337.76	-1.0	-1.0	-1.0	-1.0
31	usable	c7 (1+) @ 857.81 & [z6 – H2O] (1+) @ 325.64	857.81	nan	325.64	nan	1509.09	3.0	3.0	3.0	3.0
32	usable	y5 (2+) @ 286.06 & b8 (1+) @ 954.34	286.06	286.2	954.34	954.4	1526.46	0.0	0.0	0.0	0.0
33	usable	y10 (2+) @ 613.96 & b3 (1+) @ 299.83	613.96	613.32	299.83	300.16	1527.75	0.0	0.0	-1.0	-1.0
34	non_complementary	y6 (1+) @ 685.7 & b5 (1+) @ 565.38	685.7	685.44	565.38	565.23	1251.08	-1.0	-1.0	-1.0	-1.0
35	usable	y2 (1+) @ 273.99 & ai10-11 (1+) @ 198.67	273.99	274.19	198.67	199.16	746.65	-1.0	-1.0	-1.0	-1.0
36	internal_acid	bi5-9 (1+) @ 518.33 & y4 (1+) @ 500.42	518.33	518.24	500.42	500.36	1519.17	-1.0	-1.0	-1.0	-1.0
37	usable	y5 (2+) @ 286.06 & [b8-NH3] (1+) @ 937.39	286.06	286.2	937.39	937.37	1509.51	3.0	3.0	3.0	3.0
38	internal_acid	b7 (1+) @ 840.79 & bi8-9 (1+) @ 185.67	840.79	840.35	185.67	186.09	1212.13	-1.0	-1.0	-1.0	-1.0
39	usable	c11 (2+) @ 634.43 & [z2-H2O] (1+) @ 239.69	634.43	nan	239.69	nan	1508.55	3.0	3.0	3.0	3.0
40	undefined	447.1 & 337.82	447.1	nan	337.82	nan	1232.02	-1.0	-1.0	-1.0	-1.0
41	usable	[y10-NH3] (2+) @ 604.9 & b3 (1+) @ 299.81	604.9	604.81	299.81	300.16	1509.61	3.0	3.0	3.0	3.0
42	usable	bi(4-8) (1+) @ 655.43 & b3 (1+) @ 299.94	655.43	655.25	299.94	300.16	1610.8	-1.0	-1.0	-1.0	-1.0
43	undefined	537.05 & 461.15	537.05	nan	461.15	nan	1535.25	-1.0	-1.0	-1.0	-1.0
44	internal_acid	bi5-9 (1+) @ 518.15 & [bi3-4 – HCOOH] (1+) @ 291.85	518.15	518.24	291.85	292.09	1328.15	-1.0	-1.0	-1.0	-1.0
45	internal_acid	bi5-11 (1+) @ 744.47 & y2 (1+) @ 274.17	744.47	744.4	274.17	274.19	1292.81	-1.0	-1.0	-1.0	-1.0
46	non_complementary	y1 (1+) @ 174.58 & b11 (2+) @ 626.04	174.58	175.12	626.04	626.3	1426.66	-1.0	-1.0	-1.0	-1.0
47	undefined	524.22 & 313.54	524.22	nan	313.54	nan	1361.98	-1.0	-1.0	-1.0	-1.0

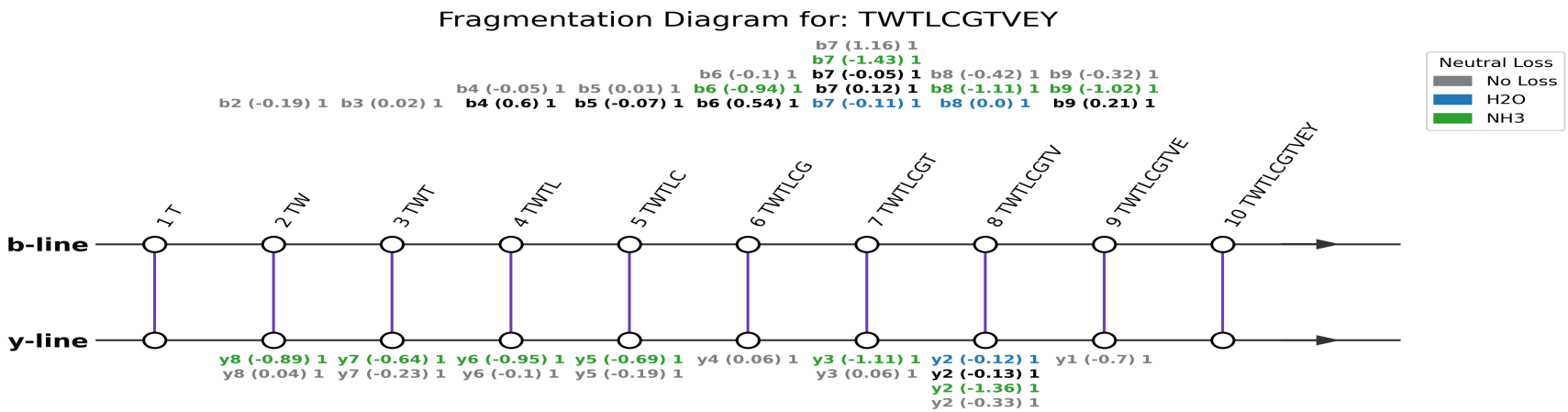
48	non_complementary	y2 (1+) @ 273.88 & [b10-NH3] (1+) @ 1122.11	273.88	274.19	1122.11	1121.49	1395.99	-1.0	-1.0	-1.0	-1.0
49	non_complementary	y6 (1+) @ 685.28 & b6 (2+) @ 356.25	685.28	685.44	356.25	356.65	1397.78	2.0	2.0	2.0	2.0
50	undefined	395.09 & 332.94	395.09	nan	332.94	nan	1123.12	-1.0	-1.0	-1.0	-1.0

output



	b1y9	b2y8	b3y7	b4y6	b5y5	b6y4	b7y3	b8y2	b9y1	Row_Count
Parent	--	(b2,y8) (1+ , 1+) -0.15 (32)	(b3,y7) (1+ , 1+) -0.02 (3)	(b4,y6) (1+ , 1+) -0.31 (2)	(b5,y5) (1+ , 1+) -0.26 (1)	(b6,y4) (1+ , 1+) -0.2 (4)	(b7,y3) (1+ , 1+) -0.37 (6)	(b8,y2) (1+ , 1+) -0.72 (14)	(b9,y1) (1+ , 1+) -1.02 (36)	8
NH3	--	(b2,**NH3**) (1+ , 1+) 0.5 (11)	(b3,**NH3**) (1+ , 1+) -0.62 (13)	(b4,**NH3**) (1+ , 1+) -1.01 (25)	(b5,**NH3**) (1+ , 1+) -0.69 (28)	(**NH3**,y4) (1+ , 1+) -0.88 (26)	(**NH3**,y3) (1+ , 1+) -1.22 (12)	(**NH3**,y2) (1+ , 1+) -1.28 (16)	(**NH3**,y1) (1+ , 1+) -1.6 (24)	8
H2O	--	--	--	--	--	--	--	--	--	0
NH3 + H2O	--	--	--	--	--	--	--	(NH3,H2O) (1+ , 1+) -0.82 (9)	--	1
H2O + NH3	--	--	--	--	--	--	--	--	--	0
a	--	--	--	--	--	--	--	--	--	0
Col_Count	0	2	2	2	2	2	2	3	2	17





Detailed Data - Table 1

Unnamed: 0	b2	b3	b4	b5	b6	b7	b8	b9
H2O	nan	nan	nan	nan	nan	b7-H2O (-0.11) (1 , 1)	b8-H2O (0.0) (1 , 1)	nan
H3PO4	nan	nan	b4-H3PO4 (0.6) (1 , 1)	b5-H3PO4 (-0.07) (1 , 1)	b6-H3PO4 (0.54) (1 , 1)	b7-H3PO4 (0.12) (1 , 1)	nan	b9-H3PO4 (0.21) (1 , 1)
H3PO4-H2O	nan	nan	nan	nan	nan	b7-H3PO4-H2O (-0.05) (1 , 1)	nan	nan
NH3	nan	nan	nan	nan	b6-NH3 (-0.94) (1 , 1)	b7-NH3 (-1.43) (1 , 1)	b8-NH3 (-1.11) (1 , 1)	b9-NH3 (-1.02) (1 , 1)
No Loss	b2 (-0.19) (1 , 1)	b3 (0.02) (1 , 1)	b4 (-0.05) (1 , 1)	b5 (0.01) (1 , 1)	b6 (-0.1) (1 , 1)	b7 (1.16) (1 , 1)	b8 (-0.42) (1 , 1)	b9 (-0.32) (1 , 1)

Detailed Data - Table 2

Unnamed: 0	y1	y2	y3	y4	y5	y6	y7	y8
H2O	nan	y2-H2O (-0.12) (1 , 1)	nan	nan	nan	nan	nan	nan
HCOOH-H2O	nan	y2-HCOOH-H2O (-0.13) (1 , 1)	nan	nan	nan	nan	nan	nan
NH3	nan	y2-NH3 (-1.36) (1 , 1)	y3-NH3 (-1.11) (1 , 1)	nan	y5-NH3 (-0.69) (1 , 1)	y6-NH3 (-0.95) (1 , 1)	y7-NH3 (-0.64) (1 , 1)	y8-NH3 (-0.89) (1 , 1)
No Loss	y1 (-0.7) (1 , 1)	y2 (-0.33) (1 , 1)	y3 (0.06) (1 , 1)	y4 (0.06) (1 , 1)	y5 (-0.19) (1 , 1)	y6 (-0.1) (1 , 1)	y7 (-0.23) (1 , 1)	y8 (0.04) (1 , 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+) @ 568.12 & b5 (1+) @ 685.12	568.12	568.26	685.12	685.24	1253.24	0.0	0.0	0.0	0.0
2	usable	y6 (1+) @ 671.16 & b4 (1+) @ 582.03	671.16	671.27	582.03	582.23	1253.19	0.0	0.0	0.0	0.0
3	usable	y7 (1+) @ 784.38 & b3 (1+) @ 469.1	784.38	784.35	469.1	469.15	1253.48	0.0	0.0	0.0	0.0
4	usable	y4 (1+) @ 511.14 & b6 (1+) @ 742.16	511.14	511.24	742.16	742.26	1253.3	0.0	0.0	0.0	0.0
5	usable	y6 (1+) @ 671.17 & [b4-H3PO4] (1+) @ 484.11	671.17	671.27	484.11	484.26	1155.28	1.0	1.0	1.0	1.0
6	usable	y3 (1+) @ 410.06 & b7 (1+) @ 843.07	410.06	410.19	843.07	843.31	1253.13	0.0	0.0	0.0	0.0
7	usable	[y2-NH3] (1+) @ 292.81 & b8 (1+) @ 942.06	292.81	294.1	942.06	942.38	1234.87	2.0	2.0	2.0	2.0
8	usable	y3 (1+) @ 410.14 & [b7-H3PO4] (1+) @ 745.45	410.14	410.19	745.45	745.33	1155.59	1.0	1.0	1.0	1.0
9	usable	[y2-H2O] (1+) @ 292.99 & [b8-NH3] (1+) @ 924.66	292.99	293.11	924.66	925.35	1217.65	3.0	3.0	3.0	3.0
10	usable	y4 (1+) @ 511.35 & [b6-H3PO4] (1+) @ 644.83	511.35	511.24	644.83	644.29	1156.18	1.0	1.0	1.0	-1.0
11	usable	[y8-NH3] (1+) @ 949.32 & b2 (1+) @ 287.66	949.32	948.34	287.66	288.13	1236.98	-1.0	-1.0	-1.0	-1.0
12	usable	y3 (1+) @ 410.08 & [b7-NH3] (1+) @ 825.18	410.08	410.19	825.18	826.28	1235.26	2.0	2.0	2.0	2.0
13	usable	[y7-NH3] (1+) @ 766.69 & b3 (1+) @ 469.17	766.69	767.33	469.17	469.15	1235.86	2.0	2.0	2.0	2.0
14	usable	y2 (1+) @ 310.82 & b8 (1+) @ 941.96	310.82	311.12	941.96	942.38	1252.78	0.0	0.0	0.0	0.0
15	non_complementary	b9 (1+) @ 942.37 & [y2 – HCOOH – H2O] (1+) @ 246.94	942.37	1071.42	246.94	247.11	1189.31	-1.0	-1.0	-1.0	-1.0

16	usable	y2 (1+) @ 310.96 & [b8-NH3] (1+) @ 924.24	310.96	311.12	924.24	925.35	1235.2	2.0	2.0	2.0	2.0
17	internal_acid	b7 (1+) @ 843.12 & bi8-9 (1+) @ 228.81	843.12	843.31	228.81	229.12	1300.74	-1.0	-1.0	-1.0	-1.0
18	usable	[y6-NH3] (1+) @ 653.25 & [b4-H3PO4] (1+) @ 484.86	653.25	654.24	484.86	484.26	1138.11	4.0	4.0	4.0	4.0
19	non_complementary	[y2-NH3] (1+) @ 292.74 & b7 (1+) @ 844.74	292.74	294.1	844.74	843.31	1137.48	4.0	4.0	4.0	4.0
20	internal_acid	b5 (1+) @ 685.65 & bi6-9 (1+) @ 387.07	685.65	685.24	387.07	387.19	1072.72	-1.0	-1.0	-1.0	-1.0
21	non_complementary	y2 (1+) @ 310.67 & b7 (1+) @ 844.47	310.67	311.12	844.47	843.31	1155.14	1.0	1.0	1.0	1.0
22	usable	[y8-NH3] (1+) @ 947.45 & a2 (1+) @ 259.8	947.45	948.34	259.8	260.12	1207.25	-1.0	-1.0	-1.0	-1.0
23	usable	y5 (1+) @ 568.07 & [b5-H3PO4] (1+) @ 587.19	568.07	568.26	587.19	587.26	1155.26	1.0	1.0	1.0	1.0
24	usable	y1 (1+) @ 181.5 & [b9-NH3] (1+) @ 1053.38	181.5	182.08	1053.38	1054.4	1234.88	2.0	2.0	2.0	2.0
25	usable	[y6-NH3] (1+) @ 653.29 & b4 (1+) @ 582.18	653.29	654.24	582.18	582.23	1235.47	2.0	2.0	2.0	2.0
26	usable	y4 (1+) @ 511.3 & [b6-NH3] (1+) @ 724.3	511.3	511.24	724.3	725.24	1235.6	2.0	2.0	2.0	2.0
27	usable	[b8-H2O] (1+) @ 924.37 & [y2 – HCOOH – H2O] (1+) @ 246.98	924.37	924.37	246.98	247.11	1171.35	-1.0	-1.0	-1.0	-1.0
28	usable	[y5-NH3] (1+) @ 550.54 & b5 (1+) @ 685.25	550.54	551.23	685.25	685.24	1235.79	2.0	2.0	2.0	2.0
29	internal_acid	[b7-H2O] (1+) @ 825.19 & bi8-9 (1+) @ 228.81	825.19	825.3	228.81	229.12	1282.81	-1.0	-1.0	-1.0	-1.0
30	internal_acid	[b7-H3PO4] (1+) 745.72 & bi8-9 (1+) @ 228.74	nan	nan	228.74	229.12	nan	nan	nan	nan	nan
31	non_complementary	y7 (1+) @ 784.12 & b2 (1+) @ 287.76	784.12	784.35	287.76	288.13	1359.64	-1.0	-1.0	-1.0	-1.0
32	usable	y8 (1+) @ 965.41 & b2 (1+) @ 287.94	965.41	965.37	287.94	288.13	1253.35	0.0	0.0	0.0	0.0
33	usable	[b7-2(H2O)]/[b7-NH3-H2O] (1+) @ 807.36 & y3 (1+) @ 410.11	807.36	nan	410.11	410.19	1217.47	3.0	3.0	3.0	3.0
34	usable	y1(1+) @ 181.74 & [b9-H3PO4] (1+) @ 973.65	181.74	182.08	973.65	973.44	1337.13	-1.0	-1.0	-1.0	-1.0
35	usable	[b7-H3PO4-H2O] (1+) @ 727.27 & y3 (1+) @ 410.25	727.27	727.32	410.25	410.19	1137.52	4.0	4.0	4.0	4.0
36	usable	y1 (1+) @ 181.38 & b9 (1+) @ 1071.1	181.38	182.08	1071.1	1071.42	1252.48	0.0	0.0	0.0	0.0
37	usable	b7 (1+) @ 843.61 & ai8-9 (1+) @ 200.62	843.61	843.31	200.62	201.11	1244.85	-1.0	-1.0	-1.0	-1.0
38	usable	[b9-H3PO4-H2O] (1+) @ 955.76 & y1 (1+) 181.5	955.76	955.43	nan	nan	nan	nan	nan	nan	nan
39	unclear	??? @ 867.7 & [y2 – H2O] (1+) @ 291.9	867.7	nan	291.9	293.11	1159.6	-1.0	-1.0	-1.0	-1.0
40	internal_acid	b6 (1+) @ 743.52 & bi7-9 (1+) @ 329.71	743.52	742.26	329.71	330.17	1402.94	-1.0	-1.0	-1.0	-1.0
41	non_complementary	y2 (1+) @ 311.27 & [b7-NH3] (1+) @ 826.46	311.27	311.12	826.46	826.28	1137.73	4.0	4.0	4.0	4.0
42	internal_acid	bi3-8 (1+) @ 627.78 & y2 (1+) @ 310.79	627.78	655.25	310.79	311.12	1249.36	-1.0	-1.0	-1.0	-1.0
43	usable	[y3-NH3] (1+) @ 392.06 & [b7-NH3] (1+) @ 824.85	392.06	393.17	824.85	826.28	1216.91	3.0	3.0	3.0	5.0

44	undefined	728.32 & 569.4	728.32	nan	569.4	nan	1297.72	-1.0	-1.0	-1.0	-1.0
45	undefined	844.84 & 274.35	844.84	nan	274.35	nan	1119.19	-1.0	-1.0	-1.0	-1.0
46	undefined	844.25 & 806.82	844.25	nan	806.82	nan	1651.07	-1.0	-1.0	-1.0	-1.0
47	undefined	587.33 & 538.42	587.33	nan	538.42	nan	1125.75	-1.0	-1.0	-1.0	-1.0
48	undefined	535.98 & 435.95	535.98	nan	435.95	nan	1407.88	-1.0	-1.0	-1.0	-1.0
49	undefined	939.22 & 609.33	939.22	nan	609.33	nan	1548.55	-1.0	-1.0	-1.0	-1.0
50	undefined	941.73 & 274.8	941.73	nan	274.8	nan	1216.53	3.0	3.0	3.0	5.0