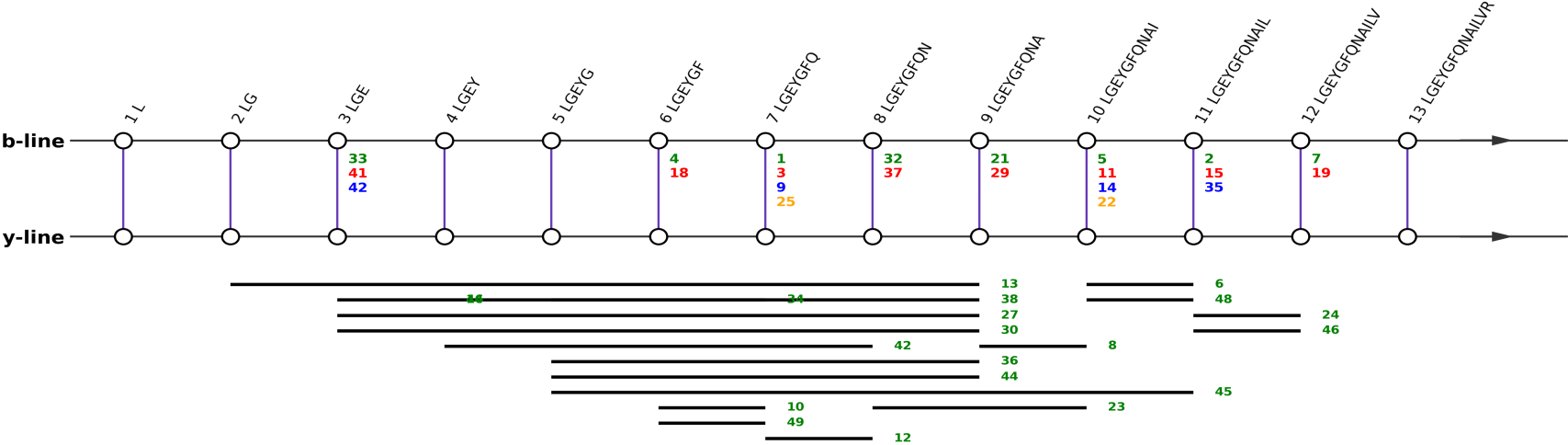
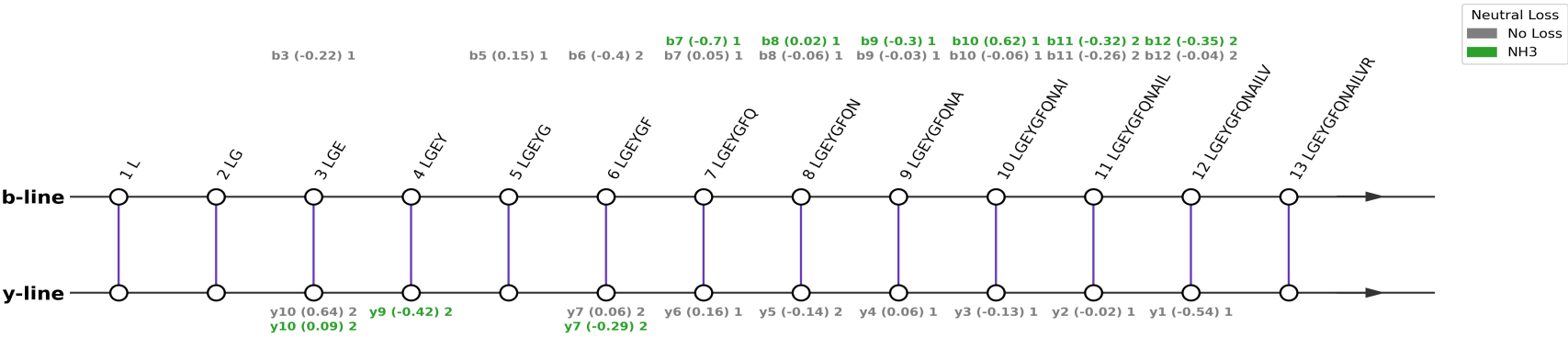


output

Fragmentation Diagram for: LGEYGFQNAILVR



Fragmentation Diagram for: LGEYGFQNAILVR



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