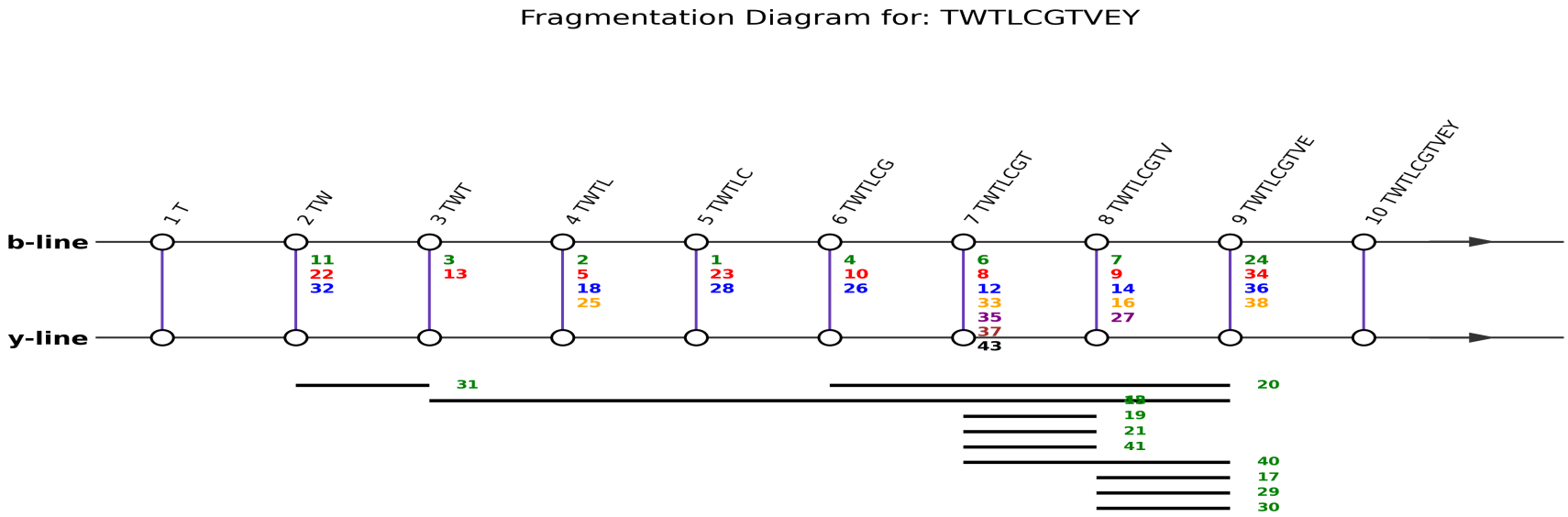
output


Fragmentation Diagram for: TWTLCGTVEY
b-line
y-line
1 T
2 TW
3 TWT
4 TWTL
5 TWTLC
6 TWTLCG
7 TWTLCGT
8 TWTLCGTV
9 TWTLCGTVE
10 TWTLCGTVEY
11
22
32
3
13
2
5
18
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10
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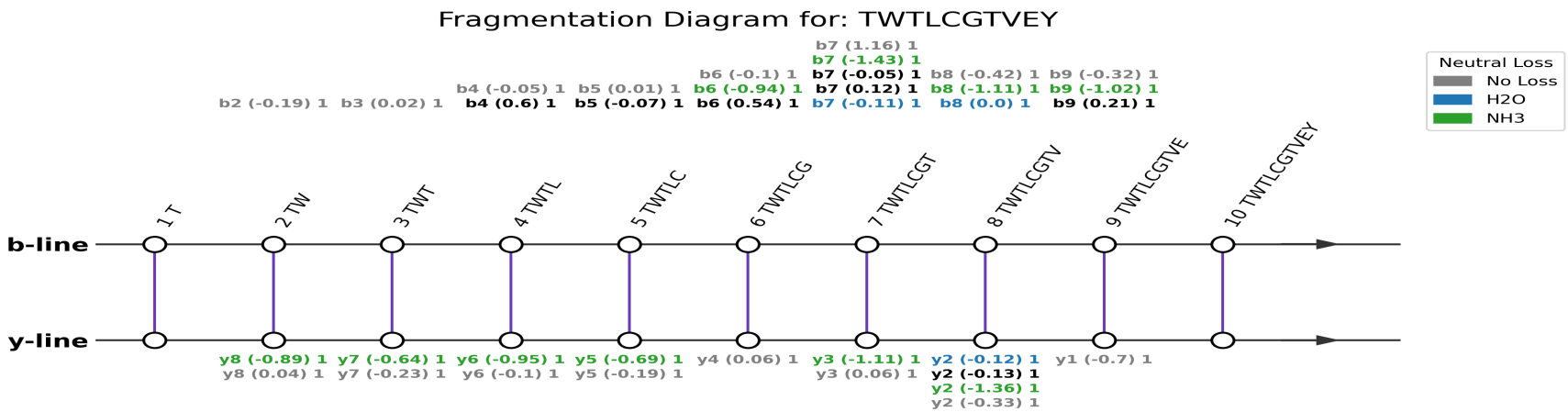

Detailed Data - Table 1

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