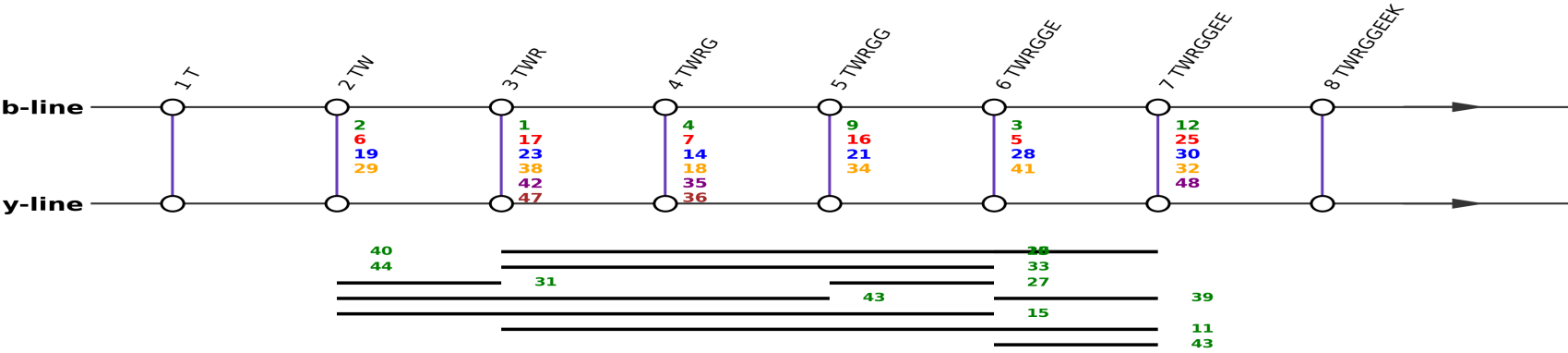
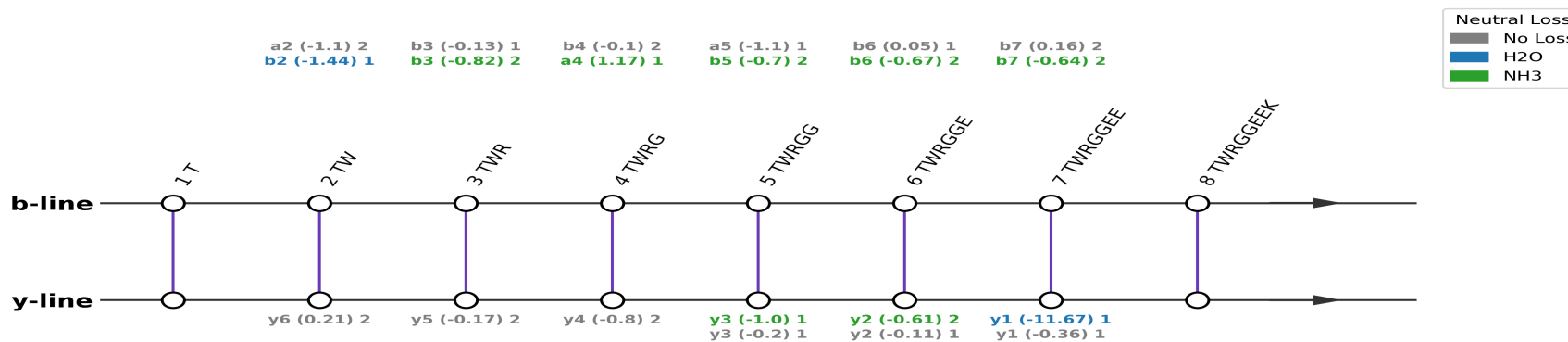


output

Fragmentation Diagram for: TWRGGEEK



Fragmentation Diagram for: TWRGGEEK



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 & lm(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 & lm (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