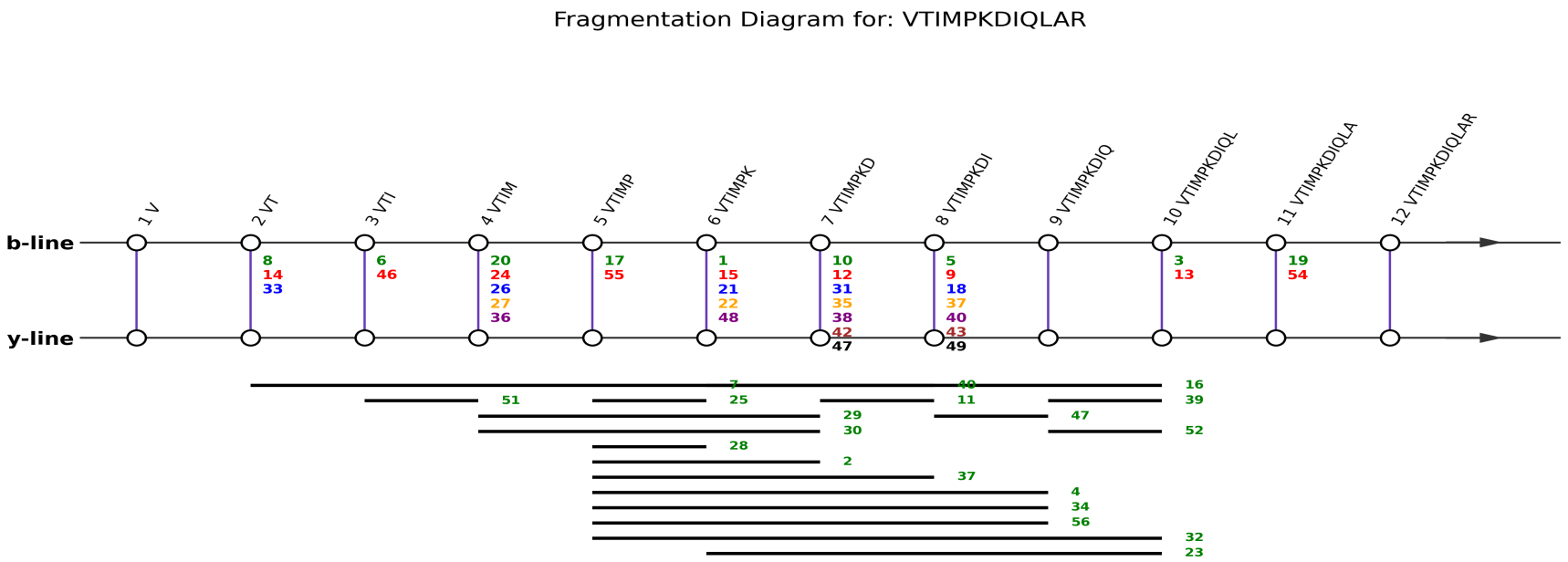
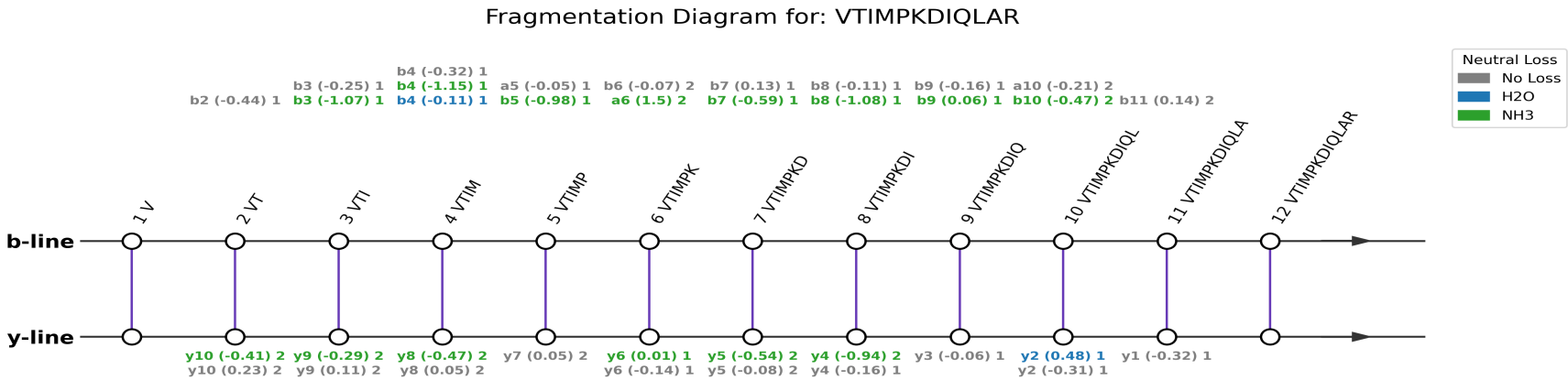
output


Fragmentation Diagram for: VTIMPKDIQLAR
b-line
y-line
1 V
2 VT
3 VTI
4 VTIM
5 VTIMP
6 VTIMPK
7 VTIMPKD
8 VTIMPKDI
9 VTIMPKDIQ
10 VTIMPKDIQL
11 VTIMPKDIQLA
12 VTIMPKDIQLAR
8 14 33
6 46
20 24 26 27 36
17 55
1 15 21 22 48
10 12 31 35 38 42 47
5 9 18 37 40 43 49
3 13
19 54
7
40
16
51
25
11
39
29
47
30
52
28
2
37
4
34
56
32
23



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

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

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