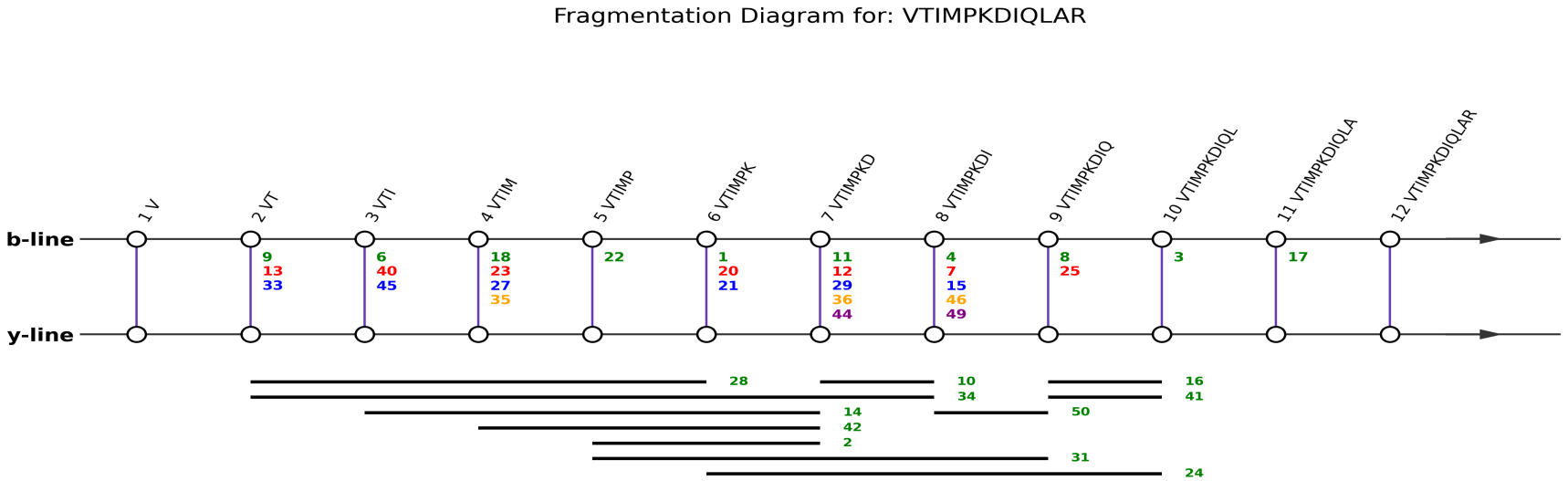
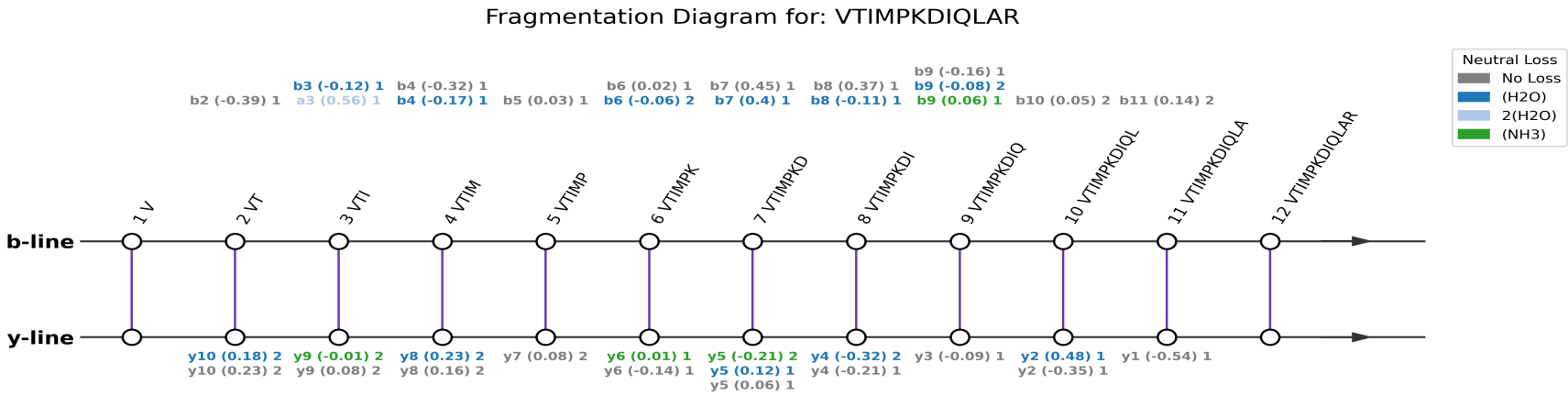
[VTIMPK(Ac)DIQLAR+3H]3+



	b1y11	b2y10	b3y9	b4y8	b5y7	b6y6	b7y5	b8y4	b9y3	b10y2	b11y1	Row_Count	Unexplained_Count	abs average mass difference	unxplained pairs
Parent	--	(b2,y10) (1+ , 2+) (-0.41, 0.23) 9	--	(b4,y8) (1+ , 2+) (-0.27, -0.03) 18	(b5,y7) (1+ , 2+) (0.03, 0.08) 22	(b6,y6) (2+ , 1+) (-0.05, 0.03) 1	(b7,y5) (1+ , 2+) (-0.01, -0.19) 12	(b8,y4) (1+ , 2+) (-0.12, -0.18) 15	(b9,y3) (2+ , 1+) (-0.03, -0.1) 8	(b10,y2) (2+ , 1+) (0.05, -0.34) 3	(b11,y1) (2+ , 1+) (0.14, -0.54) 17	9	0	0.29	
(NH3)	--	--	--	--	--	(b6,(NH3)) (2+ , 1+) (-0.07, 0.01) 21	(b7,(NH3)) (1+ , 2+) (0.17, -0.21) 36	--	--	--	--	2	0	0.23	
(H2O)	--	(b2,(H2O)) (1+ , 2+) (-0.43, 0.18) 33	((H2O),y9) (1+ , 2+) (-0.19, 0.11) 6	((H2O),y8) (1+ , 2+) (-0.17, 0.16) 35	--	((H2O),y6) (2+ , 1+) (-0.06, 0.13) 20	((H2O),y5) (1+ , 2+) (0.4, -0.08) 44	((H2O),y4) (1+ , 2+) (-0.34, -0.34) 46	((H2O),y3) (2+ , 1+) (-0.08, -0.09) 25	--	--	7	0	0.36	
(NH3)-(H2O)	--	--	((H2O),(NH3)) (1+ , 2+) (-0.12, -0.01) 45	--	--	--	--	--	--	--	--	0	0	0.0	
a	--	(a2,y10) (1+ , 2+) (-0.48, 0.23) 13	--	(a4,y8) (1+ , 2+) (-0.14, 0.03) 23	--	--	--	(a8,y4) (2+ , 1+) (-0.01, -0.08) 4	--	--	--	3	0	0.32	
2(H2O)	--	--	--	--	--	--	--	--	--	--	--	0	0	0.0	
2(NH3)	--	--	--	--	--	--	--	--	--	--	--	0	0	0.0	
Col_Count	0	3	2	3	1	3	3	3	2	1	1	22	0	0.17	nan

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50

Not Highlighted (H2O) (H2O)-(NH3) (NH3) (NH3)-(H2O) 2(H2O) 2(NH3) CH3-NH2 Parent a



Detailed Data - Table 1

b2	b3	b4	b5	b6	b7	b8	b9	b10	b11
nan	nan	nan	nan	nan	nan	nan	b9-(NH3) (0.06) (1 , 1)	nan	nan
nan	a3-2(H2O) (0.56) (1 , 2)	nan	nan	nan	nan	nan	nan	nan	nan
nan	b3-(H2O) (-0.12) (1 , 2)	b4-(H2O) (-0.17) (1 , 2)	nan	b6-(H2O) (-0.06) (2 , 1)	b7-(H2O) (0.4) (1 , 2)	b8-(H2O) (-0.11) (1 , 2)	b9-(H2O) (-0.08) (2 , 1)	nan	nan
b2 (-0.39) (1 , 1)	nan	b4 (-0.32) (1 , 1)	b5 (0.03) (1 , 2)	b6 (0.02) (1 , 1)	b7 (0.45) (1 , 1)	b8 (0.37) (1 , 1)	b9 (-0.16) (1 , 1)	b10 (0.05) (2 , 1)	b11 (0.14) (2 , 1)

Detailed Data - Table 2

y1	y2	y3	y4	y5	y6	y7	y8	y9	y10
nan	nan	nan	nan	y5-(NH3) (-0.21) (2 , 1)	y6-(NH3) (0.01) (1 , 2)	nan	nan	y9-(NH3) (-0.01) (2 , 1)	nan
nan	y2-(H2O) (0.48) (1 , 1)	nan	y4-(H2O) (-0.32) (2 , 1)	y5-(H2O) (0.12) (1 , 2)	nan	nan	y8-(H2O) (0.23) (2 , 1)	nan	y10-(H2O) (0.18) (2 , 1)
y1 (-0.54) (1 , 2)	y2 (-0.35) (1 , 1)	y3 (-0.09) (1 , 2)	y4 (-0.21) (1 , 1)	y5 (0.06) (1 , 1)	y6 (-0.14) (1 , 1)	y7 (0.08) (2 , 1)	y8 (0.16) (2 , 1)	y9 (0.08) (2 , 1)	y10 (0.23) (2 , 1)

Detailed Data - Table 3

n	classification	ion1	loss1	mass1	correct_mass1	mass_difference1	ion2	loss2	mass2	correct_mass2	mass_difference2	chosen_sum
1	usable	b6	nan	356.66	356.71	-0.05	y6	nan	715.44	715.41	0.03	1428.76
2	internal_acid	bi(5-7)	nan	383.1	382.19	0.91	y5	nan	600.46	600.38	0.08	1366.66
3	usable	y2	nan	245.82	246.16	-0.34	b10	nan	591.38	591.33	0.05	1428.58
4	usable	a8	nan	456.75	456.76	-0.01	y4	nan	487.22	487.3	-0.08	1431.19
5	rare_mode	y3	nan	359.18	359.24	-0.06	a6	(CH3COOH)	624.4	624.37	0.03	1342.76
6	usable	b3	(H2O)	296.01	296.2	-0.19	y9	nan	557.42	557.31	0.11	1410.85
7	usable	y4	(H2O)	234.85	235.15	-0.3	b8	nan	940.45	940.52	-0.07	1410.15
8	usable	y3	nan	359.14	359.24	-0.1	b9	nan	534.76	534.79	-0.03	1428.66
9	usable	b2	nan	200.71	201.12	-0.41	y10	nan	614.08	613.85	0.23	1428.87
10	non_complementary	y4	nan	487.33	487.3	0.03	b7	nan	827.44	827.43	0.01	1314.77
11	usable	b7	nan	414.18	414.22	-0.04	y5	nan	600.38	600.38	-0.0	1428.74
12	usable	y5	nan	300.5	300.69	-0.19	b7	nan	827.42	827.43	-0.01	1428.42
13	usable	a2	nan	172.63	173.11	-0.48	y10	nan	614.08	613.85	0.23	1400.79
14	internal_acid	bi(3-7)	(CH3CH2SCH3)-(CH3COOH)	245.81	245.63	0.18	y5	(H2O)	582.49	582.37	0.12	1410.79
15	usable	y4	nan	243.97	244.15	-0.18	b8	nan	940.4	940.52	-0.12	1428.34
16	non_complementary	y2	nan	245.79	246.16	-0.37	b9	nan	1068.42	1068.58	-0.16	1314.21
17	usable	y1	nan	174.58	175.12	-0.54	b11	nan	626.99	626.85	0.14	1428.56
18	usable	b4	nan	444.98	445.25	-0.27	y8	nan	491.76	491.79	-0.03	1428.5

19	unclear	???	nan	559.34	nan	nan	???	nan	715.45	nan	nan	1274.79
20	usable	b6	(H2O)	347.64	347.7	-0.06	y6	nan	715.54	715.41	0.13	1410.82
21	usable	b6	nan	356.64	356.71	-0.07	y6	(NH3)	698.39	698.38	0.01	1411.67
22	usable	y7	nan	443.34	443.26	0.08	b5	nan	542.33	542.3	0.03	1429.01
23	usable	a4	nan	417.1	417.24	-0.14	y8	nan	491.82	491.79	0.03	1400.74
24	non_complementary	y2	(H2O)	228.63	228.15	0.48	b6	nan	712.43	712.41	0.02	1653.49
25	usable	y3	nan	359.15	359.24	-0.09	b9	(H2O)	525.71	525.79	-0.08	1410.57
26	rare_mode	b4	(CH3CH2SCH3)	369.04	369.21	-0.17	y8	nan	491.96	491.79	0.17	1352.96
27	usable	b4	nan	445.11	445.25	-0.14	y8	(H2O)	483.01	482.78	0.23	1411.13
28	internal_acid	bi(2-6)	(CH3SH)-(HCOH)	267.85	267.66	0.19	y6	nan	715.66	715.41	0.25	1251.36
29	usable	b7	(H2O)	405.31	405.21	0.1	y5	nan	600.32	600.38	-0.06	1410.94
30	rare_mode	b4	nan	445.09	445.25	-0.16	y8	(NH3)-(HCOH)	468.13	468.27	-0.14	1381.35
31	internal_acid	b4	nan	444.93	445.25	-0.32	bi(5-9)	nan	624.41	623.33	1.08	1514.27
32	internal_acid	ai(5-8)	nan	468.09	467.26	0.83	y4	nan	487.09	487.3	-0.21	1423.27
33	usable	b2	nan	200.69	201.12	-0.43	y10	(H2O)	605.02	604.84	0.18	1410.73
34	internal_acid	y4	nan	487.14	487.3	-0.16	bi(2-8)	nan	841.49	840.44	1.05	1328.63
35	usable	b4	(H2O)	427.07	427.24	-0.17	y8	nan	491.95	491.79	0.16	1410.97
36	usable	y5	(NH3)	291.97	292.18	-0.21	b7	nan	827.6	827.43	0.17	1411.54
37	rare_mode	y2	nan	245.92	246.16	-0.24	b7	(CH3COOH)-(HCOH)	737.3	737.4	-0.1	1229.14
38	internal_acid	ai(9-10)	(H2O)	195.81	195.12	0.69	b8	nan	940.89	940.52	0.37	1332.51
39	internal_acid	b2	nan	200.73	201.12	-0.39	ai(3-8)	nan	712.31	711.38	0.93	1625.35
40	usable	a3	2(H2O)	250.74	250.18	0.56	y9	nan	557.39	557.31	0.08	1365.52
41	non_complementary	y2	nan	245.81	246.16	-0.35	b9	(NH3)	1051.61	1051.55	0.06	1543.23
42	internal_acid	bi(4-7)	nan	514.24	513.23	1.01	y5	nan	600.44	600.38	0.06	1628.92
43	internal_acid	ai(4-6)	2(H2O)	335.69	334.17	1.52	y6	nan	715.27	715.41	-0.14	1386.65
44	usable	y5	nan	300.61	300.69	-0.08	b7	(H2O)	809.82	809.42	0.4	1411.04
45	usable	b3	(H2O)	296.08	296.2	-0.12	y9	(NH3)	548.78	548.79	-0.01	1393.64
46	usable	y4	nan	243.81	244.15	-0.34	b8	(H2O)	922.17	922.51	-0.34	1409.79

47	rare_mode	y4	nan	487.01	487.3	-0.29	b5	(CH2S)	496.41	496.31	0.1	1470.43
48	unclear	???	nan	216.78	nan	nan	???	nan	983.52	nan	nan	1417.08
49	usable	y4	(H2O)	234.83	235.15	-0.32	b8	(H2O)	922.4	922.51	-0.11	1392.06
50	internal_acid	bi(8-9)	nan	241.91	241.14	0.77	b7	nan	827.88	827.43	0.45	1311.7