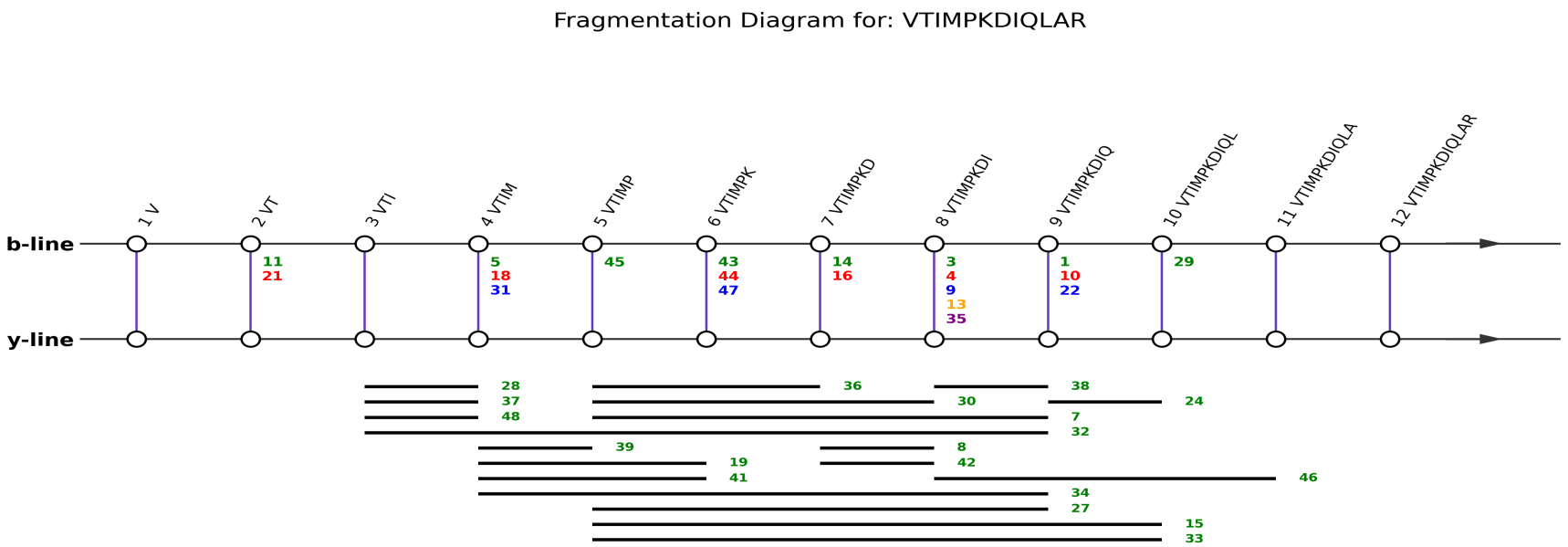
ME16_3+:[VTIMPKDIQLAR+3H]3+



	b1y11	b2y10	b3y9	b4y8	b5y7	b6y6	b7y5	b8y4	b9y3	b10y2	b11y1	Row_Count	Unexplained Count	Abs Average Mass Difference	Unexplained Pairs
Parent	--	(b2,y10) (1+ , 2+) (-0.49, 0.16) 11	--	(b4,y8) (1+ , 2+) (-0.19, 0.19) 5	(b5,y7) (1+ , 2+) (0.18, 0.01) 45	(b6,y6) (2+ , 1+) (-0.04, 0.03) 47	(b7,y5) (1+ , 2+) (-0.1, 0.19) 16	(b8,y4) (1+ , 2+) (-0.29, 0.25) 13	(b9,y3) (2+ , 1+) (-0.12, 0.18) 1	--	--	7	0	0.35	
(NH3)	--	--	--	--	--	--	--	--	--	--	--	0	0	0.0	
(H2O)	--	--	--	((H2O),y8) (1+ , 2+) (-0.07, 0.02) 31	--	((H2O),y6) (2+ , 1+) (-0.02, 0.19) 43	((H2O),y5) (2+ , 1+) (-0.04, 0.01) 14	(b8,(H2O)) (1+ , 2+) (-0.14, -0.1) 9	((H2O),y3) (2+ , 1+) (-0.06, 0.22) 10	((H2O),y2) (2+ , 1+) (-0.4, 0.15) 29	--	6	0	0.23	
(NH3)-(H2O)	--	--	--	--	--	--	--	--	--	--	--	0	0	0.0	
a	--	(a2,y10) (1+ , 2+) (-0.58, 0.4) 21	--	(a4,y8) (1+ , 2+) (-0.18, 0.22) 18	--	--	--	(a8,y4) (2+ , 1+) (0.11, 0.08) 3	--	--	--	3	0	0.52	
2(H2O)	--	--	--	--	--	--	--	(b8,2(H2O)) (1+ , 2+) (-0.23, 0.24) 35	--	--	--	1	0	0.48	
2(NH3)	--	--	--	--	--	--	--	--	(2(NH3),y3) (2+ , 1+) (-0.47, 0.07) 22	--	--	1	0	0.54	
Col_Count	0	2	0	3	1	2	2	4	3	1	0	18	0	0.3	nan
Ion Mass	(100.08, 1285.73)	(201.12, 1184.68)	(314.21, 1071.6)	(445.25, 940.56)	(542.3, 843.5)	(670.4, 715.41)	(785.42, 600.38)	(898.51, 487.3)	(1026.57, 359.24)	(1139.65, 246.16)	(1210.69, 175.12)	0	0	0.0	0

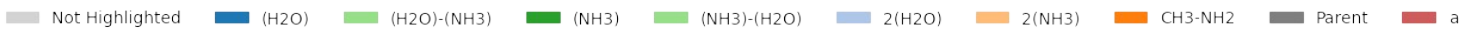


Table ME16_3+

n	classification	ion1	loss1	mass1	correct_mass1	mass_difference1	ion2	loss2	mass2	correct_mass2	mass_difference2	chosen_sum
1	usable	y3	nan	359.12	359.24	-0.12	b9	nan	513.97	513.79	0.18	1387.06
2	internal_acid	ai(5-7)	(NH3)	296.03	295.14	0.89	y5	2(NH3)-(HCOH)	536.45	536.32	0.13	1368.93
3	usable	a8	nan	435.86	435.75	0.11	y4	nan	487.38	487.3	0.08	1410.62
4	usable	b8	nan	449.78	449.76	0.02	y4	nan	487.39	487.3	0.09	1386.95
5	usable	b4	nan	445.06	445.25	-0.19	y8	nan	470.97	470.78	0.19	1387.0
6	internal_acid	ai(3-7)	2(H2O)-(HCOH)	245.99	245.63	0.36	y5	(HCOH)	570.5	570.37	0.13	1386.99
7	internal_acid	y3	nan	359.08	359.24	-0.16	bi(5-9)	nan	582.21	581.32	0.89	1300.37
8	non_complementary	y4	nan	487.4	487.3	0.1	b7	nan	785.66	785.42	0.24	1273.06
9	usable	y4	(H2O)	235.01	235.15	-0.14	b8	nan	898.41	898.51	-0.1	1368.43
10	usable	y3	nan	359.18	359.24	-0.06	b9	(H2O)	505.0	504.78	0.22	1369.18
11	usable	b2	nan	200.63	201.12	-0.49	y10	nan	593.0	592.84	0.16	1386.63
12	rare_mode	a3	2(H2O)	250.93	250.18	0.75	y5	2(NH3)-(HCOH)	536.45	536.32	0.13	1323.83
13	usable	y4	nan	243.86	244.15	-0.29	b8	nan	898.76	898.51	0.25	1386.48
14	usable	b7	(H2O)	384.17	384.21	-0.04	y5	nan	600.39	600.38	0.01	1368.73
15	internal_acid	y2	nan	246.0	246.16	-0.16	bi(5-10)	nan	695.38	694.4	0.98	1187.38
16	usable	y5	nan	300.59	300.69	-0.1	b7	nan	785.61	785.42	0.19	1386.79
17	rare_mode	a5	2(NH3)-(HCOH)	225.81	225.62	0.19	y6	nan	715.47	715.41	0.06	1167.09
18	usable	a4	nan	417.06	417.24	-0.18	y8	nan	471.0	470.78	0.22	1359.06
19	non_complementary	b4	nan	445.1	445.25	-0.15	y6	nan	715.61	715.41	0.2	1605.81
20	rare_mode	b4	(CH3CH2SCH3)	369.1	369.21	-0.11	y8	nan	470.87	470.78	0.09	1310.84
21	usable	a2	nan	172.53	173.11	-0.58	y10	nan	593.24	592.84	0.4	1359.01
22	usable	y3	nan	358.77	359.24	-0.47	b9	2(NH3)	496.83	496.76	0.07	1352.43
23	internal_acid	ai(3-4)	nan	216.79	216.11	0.68	y8	nan	470.88	470.78	0.1	1158.55
24	non_complementary	y2	nan	245.81	246.16	-0.35	b9	nan	1026.5	1026.57	-0.07	1272.31
25	internal_acid	a4	(CH2S)-(HCOH)	341.25	341.24	0.01	ai(5-10)	2(H2O)-(HCOH)	600.92	600.36	0.56	1283.42

26	rare_mode	a3	(H2O)	268.36	268.19	0.17	y5	2(NH3)-(HCOH)	536.64	536.32	0.32	1341.64
27	internal_acid	b4	nan	445.13	445.25	-0.12	bi(5-9)	nan	582.23	581.32	0.91	1472.49
28	internal_acid	bi(3-4)	nan	244.83	244.12	0.71	y8	nan	470.96	470.78	0.18	1186.75
29	usable	y2	nan	245.76	246.16	-0.4	b10	(H2O)	561.47	561.32	0.15	1368.7
30	internal_acid	b4	nan	445.05	445.25	-0.2	bi(5-8)	nan	454.11	453.26	0.85	1353.27
31	usable	b4	(H2O)	427.17	427.24	-0.07	y8	nan	470.8	470.78	0.02	1368.77
32	internal_acid	y3	nan	359.15	359.24	-0.09	bi(3-9)	nan	826.51	825.44	1.07	1544.81
33	internal_acid	b4	nan	444.9	445.25	-0.35	bi(5-10)	nan	695.16	694.4	0.76	1584.96
34	internal_acid	y3	nan	359.1	359.24	-0.14	bi(4-9)	nan	713.54	712.36	1.18	1431.74
35	usable	y4	2(H2O)	225.91	226.14	-0.23	b8	nan	898.75	898.51	0.24	1350.57
36	internal_acid	bi(5-7)	nan	340.93	340.17	0.76	b4	nan	444.88	445.25	-0.37	1230.69
37	non_complementary	b3	nan	313.87	314.21	-0.34	y8	nan	470.8	470.78	0.02	1255.47
38	non_complementary	y3	nan	359.97	359.24	0.73	b8	nan	898.28	898.51	-0.23	1258.25
39	non_complementary	b4	nan	445.53	445.25	0.28	y7	nan	843.15	843.5	-0.35	1288.68
40	internal_acid	ai(4-7)	2(NH3)-(HCOOH)	182.72	182.08	0.64	y5	2(NH3)-(HCOH)	536.47	536.32	0.15	1255.66
41	non_complementary	b4	(H2O)	427.14	427.24	-0.1	y6	nan	715.45	715.41	0.04	1569.73
42	non_complementary	b7	nan	393.49	393.21	0.28	y4	nan	487.9	487.3	0.6	1369.29
43	usable	b6	(H2O)	326.68	326.7	-0.02	y6	nan	715.6	715.41	0.19	1368.96
44	usable	y6	nan	358.51	358.21	0.3	b6	nan	670.08	670.4	-0.32	1387.1
45	usable	y7	nan	422.44	422.26	0.18	b5	nan	542.31	542.3	0.01	1387.19
46	non_complementary	y1	nan	174.88	175.12	-0.24	b8	nan	898.77	898.51	0.26	1248.53
47	usable	b6	nan	335.66	335.7	-0.04	y6	nan	715.44	715.41	0.03	1386.76
48	internal_acid	bi(3-4)	(CH3CH2SCH3)	168.77	168.09	0.68	y8	nan	471.2	470.78	0.42	1111.17
49	non_complementary	a4	nan	416.71	417.24	-0.53	y6	nan	715.32	715.41	-0.09	1548.74
50	unclear	???	nan	369.44	nan	nan	???	nan	717.0	nan	nan	1455.88