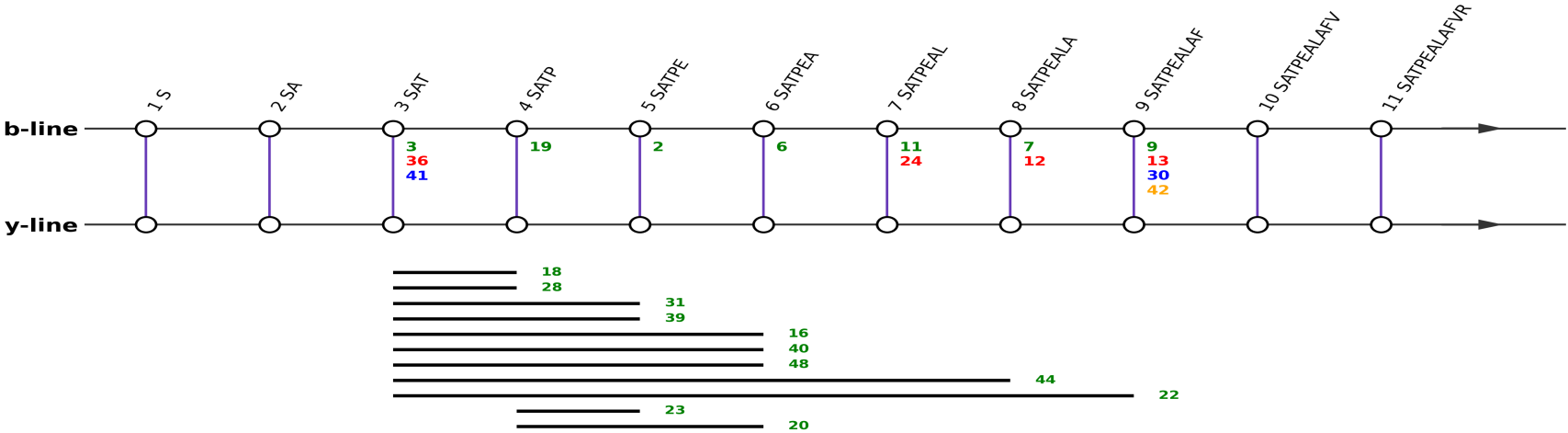
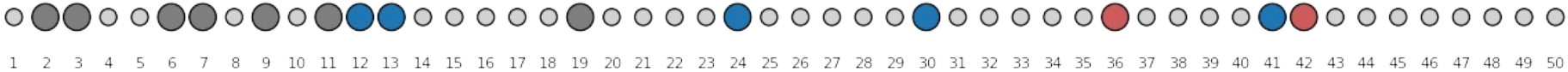


[SApTPEALAFVR+2H]2+

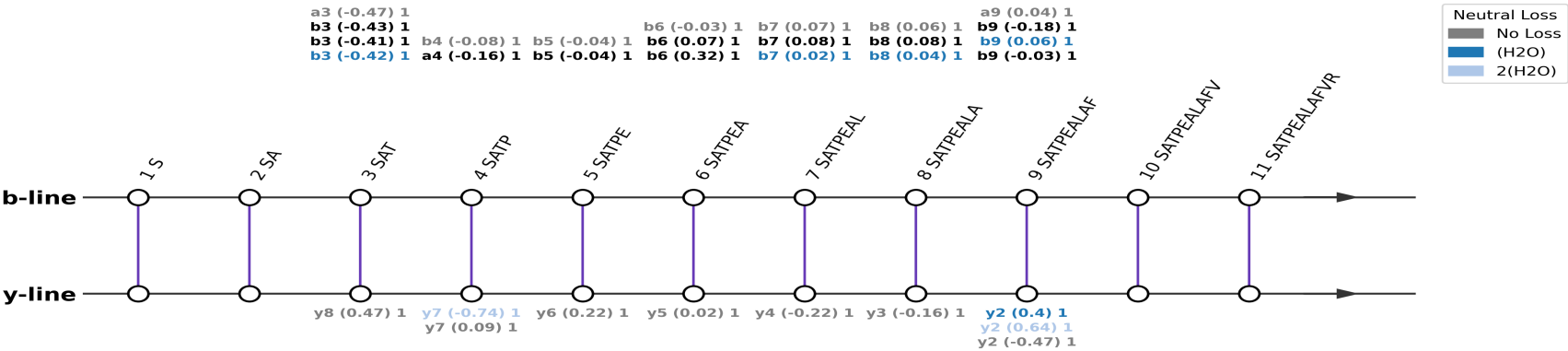
Fragmentation Diagram for: SATPEALAFVR



	b1y10 b2y9		b3y8	b4y7	b5y6	b6y5	b7y4	b8y3	b9y2	b10y1	Row_Count
Parent	--	--	(b3,y8) (1+ , 1+) 0.0 (3.0)	(b4,y7) (1+ , 1+) 0.14 (19.0)	(b5,y6) (1+ , 1+) 0.08 (2.0)	(b6,y5) (1+ , 1+) 0.01 (6.0)	(b7,y4) (1+ , 1+) 0.01 (11.0)	(b8,y3) (1+ , 1+) -0.03 (7.0)	(b9,y2) (1+ , 1+) -0.23 (9.0)	--	7
(NH3)	--	--	--	--	--	--	--	--	--	--	0
(H2O)	--	--	((H2O),y8) (1+ , 1+) -0.76 (41.0)	--	--	--	((H2O),y4) (1+ , 1+) -0.2 (24.0)	((H2O),y3) (1+ , 1+) -0.03 (12.0)	(b9,(H2O)) (1+ , 1+) 0.52 (30.0)	--	4
(NH3) + (H2O)	--	--	--	--	--	--	--	--	--	--	0
a	--	--	(a3,y8) (1+ , 1+) -0.57 (36.0)	--	--	--	--	--	(a9,y2) (1+ , 1+) -0.43 (42.0)	--	2
2(H2O)	--	--	--	--	--	--	--	--	--	--	0
2(NH3)	--	--	--	--	--	--	--	--	--	--	0
Col_Count	0	0	3	1	1	1	2	2	3	0	13



Fragmentation Diagram for: SATPEALAFVR



Detailed Data - Table 1

b3	b4	b5	b6	b7	b8	b9
nan	nan	nan	b6-2(H2O)-(HCOH) (0.32) (1 , 1)	nan	nan	b9-2(H2O)-(HCOH) (-0.03) (1 , 1)
b3-(H2O) (-0.42) (1 , 1)	nan	nan	nan	b7-(H2O) (0.02) (1 , 1)	b8-(H2O) (0.04) (1 , 1)	b9-(H2O) (0.06) (1 , 1)
b3-(H3PO4) (-0.41) (1 , 1)	a4-(H3PO4) (-0.16) (1 , 1)	b5-(H3PO4) (-0.04) (1 , 1)	b6-(H3PO4) (0.07) (1 , 1)	b7-(H3PO4) (0.08) (1 , 1)	b8-(H3PO4) (0.08) (1 , 1)	b9-(H3PO4) (-0.18) (1 , 1)
b3-(HCOH) (-0.43) (1 , 1)	nan	nan	nan	nan	nan	nan
a3 (-0.47) (1 , 1)	b4 (-0.08) (1 , 1)	b5 (-0.04) (1 , 1)	b6 (-0.03) (1 , 1)	b7 (0.07) (1 , 1)	b8 (0.06) (1 , 1)	a9 (0.04) (1 , 1)

Detailed Data - Table 2

y2	y3	y4	y5	y6	y7	y8
y2-(H2O) (0.4) (1 , 1)	nan	nan	nan	nan	nan	nan
y2-2(H2O) (0.64) (1 , 1)	nan	nan	nan	nan	y7-2(H2O) (-0.74) (1 , 1)	nan
y2 (-0.47) (1 , 1)	y3 (-0.16) (1 , 1)	y4 (-0.22) (1 , 1)	y5 (0.02) (1 , 1)	y6 (0.22) (1 , 1)	y7 (0.09) (1 , 1)	y8 (0.47) (1 , 1)

Detailed Data - Table 3

n	classification	ion1	loss1	mass1	correct_mass1	mass_difference1	ion2	loss2	mass2	correct_mass2	mass_difference2	chosen_sum
1	rare_mode	y3	nan	421.15	421.26	-0.11	b8	(H3PO4)	723.45	723.37	0.08	1144.6
2	usable	b5	nan	566.15	566.19	-0.04	y6	nan	676.53	676.41	0.12	1242.68
3	usable	b3	nan	339.86	340.09	-0.23	y8	nan	902.74	902.51	0.23	1242.6
4	rare_mode	b6	(H3PO4)	539.32	539.25	0.07	y5	nan	605.48	605.38	0.1	1144.8
5	rare_mode	y4	nan	492.13	492.29	-0.16	b7	(H3PO4)	652.41	652.33	0.08	1144.54
6	usable	y5	nan	605.42	605.38	0.04	b6	nan	637.19	637.22	-0.03	1242.61
7	usable	y3	nan	421.17	421.26	-0.09	b8	nan	821.4	821.34	0.06	1242.57
8	rare_mode	y2	nan	273.87	274.19	-0.32	b9	(H3PO4)	870.5	870.44	0.06	1144.37
9	usable	y2	nan	273.93	274.19	-0.26	b9	nan	968.44	968.41	0.03	1242.37
10	rare_mode	b5	(H3PO4)	468.17	468.21	-0.04	y6	nan	676.64	676.41	0.23	1144.81
11	usable	y4	nan	492.23	492.29	-0.06	b7	nan	750.38	750.31	0.07	1242.61
12	usable	y3	nan	421.19	421.26	-0.07	b8	(H2O)	803.37	803.33	0.04	1224.56
13	usable	y2	nan	273.83	274.19	-0.36	b9	(H2O)	950.46	950.4	0.06	1224.29
14	internal_acid	y3	nan	421.13	421.26	-0.13	ai(2-8)	nan	705.85	705.29	0.56	1126.98
15	rare_mode	b3	(H3PO4)	241.7	242.11	-0.41	y8	nan	902.95	902.51	0.44	1144.65
16	internal_acid	bi(3-6)	(H3PO4)	380.98	300.2	80.78	y5	nan	605.44	605.38	0.06	1367.4

17	non_complementary	a5	(NH3)	521.16	521.15	0.01	y5	nan	605.48	605.38	0.1	1126.64
18	internal_acid	bi(3-4)	nan	278.81	198.1	80.71	y7	nan	805.49	805.46	0.03	1363.11
19	usable	b4	nan	437.06	437.14	-0.08	y7	nan	805.68	805.46	0.22	1242.74
20	internal_acid	bi(4-6)	nan	297.85	297.13	0.72	y5	nan	605.48	605.38	0.1	1201.18
21	internal_acid	y2	nan	273.91	274.19	-0.28	ai(2-9)	nan	852.72	852.36	0.36	1126.63
22	internal_acid	y2	nan	273.8	274.19	-0.39	bi(3-9)	(H3PO4)	712.59	631.39	81.2	1260.19
23	internal_acid	bi(4-5)	nan	226.66	226.1	0.56	y6	nan	676.49	676.41	0.08	1129.81
24	usable	y4	nan	492.07	492.29	-0.22	b7	(H2O)	732.32	732.3	0.02	1224.39
25	rare_mode	a5	(HCOOH)	492.17	492.17	0.0	y6	(HN=C=NH)	634.36	634.39	-0.03	1126.53
26	rare_mode	b3	(HCOH)	309.86	310.08	-0.22	y6	nan	676.51	676.41	0.1	1296.23
27	rare_mode	b4	(H3PO4)	338.82	339.17	-0.35	y7	nan	805.7	805.46	0.24	1144.52
28	internal_acid	bi(3-4)	(H3PO4)	180.41	100.12	80.29	y7	nan	805.55	805.46	0.09	1166.37
29	rare_mode	y2	(H2O)	256.56	256.18	0.38	b9	(H3PO4)	870.49	870.44	0.05	1127.05
30	usable	y2	(H2O)	256.58	256.18	0.4	b9	nan	968.53	968.41	0.12	1225.11
31	internal_acid	bi(3-5)	nan	407.82	327.14	80.68	y6	nan	676.5	676.41	0.09	1084.32
32	rare_mode	y5	2(NH3)-(HCOH)	541.56	541.31	0.25	b6	2(H2O)-(HCOH)	571.53	571.19	0.34	1113.09
33	unclear	???	nan	223.82	nan	nan	???	nan	903.26	nan	nan	1350.9
34	unclear	???	nan	571.54	nan	nan	???	nan	901.55	nan	nan	1473.09
35	rare_mode	a4	(H3PO4)	311.0	311.16	-0.16	y7	2(H2O)	768.7	769.44	-0.74	1390.7
36	usable	a3	nan	311.61	312.08	-0.47	y8	nan	902.41	902.51	-0.1	1214.02
37	rare_mode	y2	(H2O)-(HN=C=NH)	214.1	214.15	-0.05	b9	nan	968.09	968.41	-0.32	1182.19
38	unclear	???	nan	274.53	nan	nan	???	nan	879.45	nan	nan	1153.98
39	internal_acid	bi(3-5)	(H2O)	389.91	309.13	80.78	y6	nan	676.63	676.41	0.22	1066.54
40	internal_acid	bi(3-6)	(H2O)	460.77	380.17	80.6	y5	nan	606.05	605.38	0.67	1066.82
41	usable	b3	(H2O)	321.66	322.08	-0.42	y8	nan	902.17	902.51	-0.34	1223.83
42	usable	y2	nan	273.72	274.19	-0.47	a9	nan	940.44	940.4	0.04	1214.16
43	unclear	???	nan	491.56	nan	nan	???	nan	901.93	nan	nan	1393.49
44	internal_acid	y3	nan	421.1	421.26	-0.16	bi(3-8)	nan	663.51	582.3	81.21	1084.61

45	rare_mode	y2	2(H ₂ O)	238.81	238.17	0.64	b9	(H ₃ PO ₄)	870.26	870.44	-0.18	1347.88
46	rare_mode	y2	2(NH ₃)-(HN=C=NH)	197.62	198.11	-0.49	b9	2(H ₂ O)-(HCOH)	902.35	902.38	-0.03	1297.59
47	rare_mode	y4	(HN=C=NH)-(HCOH)	420.57	420.26	0.31	b6	2(H ₂ O)-(HCOH)	571.51	571.19	0.32	1412.65
48	internal_acid	bi(3-6)	nan	478.72	398.18	80.54	y5	nan	605.19	605.38	-0.19	1083.91
49	rare_mode	b3	(H ₃ PO ₄)-(HCOH)	211.72	212.1	-0.38	y8	nan	902.98	902.51	0.47	1326.42
50	rare_mode	b3	(HCOH)	309.65	310.08	-0.43	y5	nan	605.4	605.38	0.02	1224.7