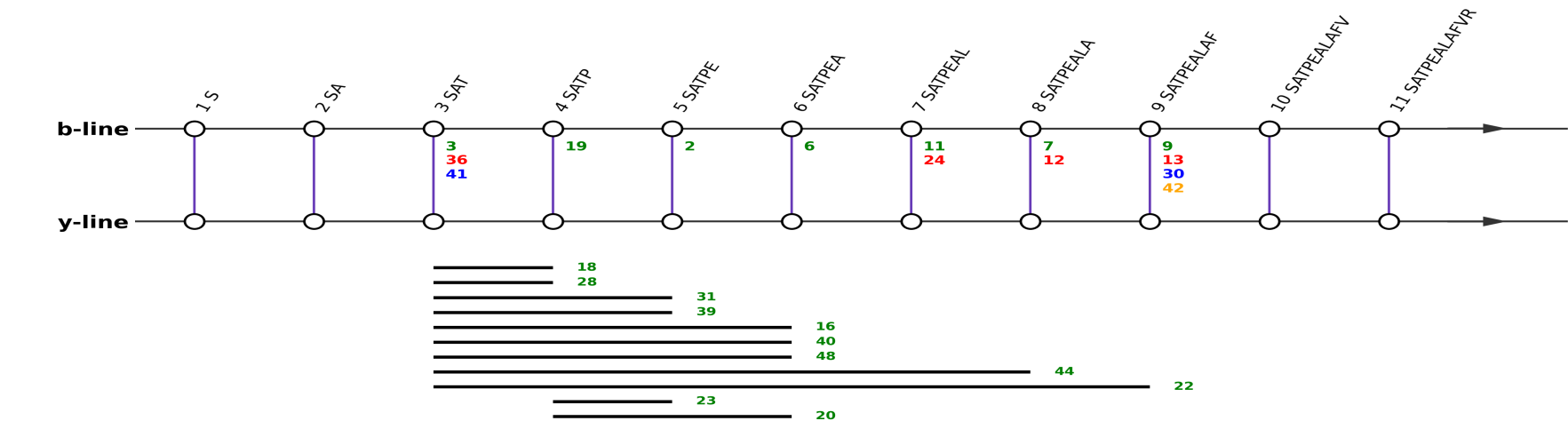


PH15_2+: [SapTPEALAFVR+2H]2+

Fragmentation Diagram for: SATPEALAFVR



| | b1y10 | b2y9 | b3y8 | b4y7 | b5y6 | b6y5 | b7y4 | b8y3 | b9y2 | b10y1 | Row_Count | Unexplained Count | Abs Average Mass Difference | Unexplained Pairs |
|-------------|------------------|-------------------|---|---|--|--|--|--|--|-------------------|-----------|-------------------|-----------------------------|-------------------|
| Parent | -- | -- | (b3,y8) (1+ , 1+) (-0.23, 0.23) 3 | (b4,y7) (1+ , 1+) (-0.08, 0.22) 19 | (b5,y6) (1+ , 1+) (-0.04, 0.12) 2 | (b6,y5) (1+ , 1+) (0.04, -0.03) 6 | (b7,y4) (1+ , 1+) (-0.06, 0.07) 11 | (b8,y3) (1+ , 1+) (-0.09, 0.06) 7 | (b9,y2) (1+ , 1+) (-0.26, 0.03) 9 | -- | 7 | 0 | 0.22 | |
| (NH3) | -- | -- | -- | -- | -- | -- | -- | -- | -- | -- | 0 | 0 | 0.0 | |
| (H2O) | -- | -- | ((H2O),y8) (1+ , 1+) (-0.42, -0.34) 41 | -- | -- | -- | ((H2O),y4) (1+ , 1+) (-0.22, 0.02) 24 | ((H2O),y3) (1+ , 1+) (-0.07, 0.04) 12 | (b9,(H2O)) (1+ , 1+) (0.4, 0.12) 30 | -- | 4 | 0 | 0.41 | |
| (NH3)-(H2O) | -- | -- | -- | -- | -- | -- | -- | -- | -- | -- | 0 | 0 | 0.0 | |
| a | -- | -- | (a3,y8) (1+ , 1+) (-0.47, -0.1) 36 | -- | -- | -- | -- | -- | (a9,y2) (1+ , 1+) (-0.47, 0.04) 42 | -- | 2 | 0 | 0.54 | |
| 2(H2O) | -- | -- | -- | -- | -- | -- | -- | -- | -- | -- | 0 | 0 | 0.0 | |
| 2(NH3) | -- | -- | -- | -- | -- | -- | -- | -- | -- | -- | 0 | 0 | 0.0 | |
| Col_Count | 0 | 0 | 3 | 1 | 1 | 1 | 2 | 2 | 3 | 0 | 13 | 0 | 0.17 | nan |
| Ion Mass | (88.04, 1154.56) | (239.04, 1003.56) | (340.09, 902.51) | (437.14, 805.46) | (566.19, 676.41) | (637.22, 605.38) | (750.31, 492.29) | (821.34, 421.26) | (968.41, 274.19) | (1067.48, 175.12) | 0 | 0 | 0.0 | 0 |

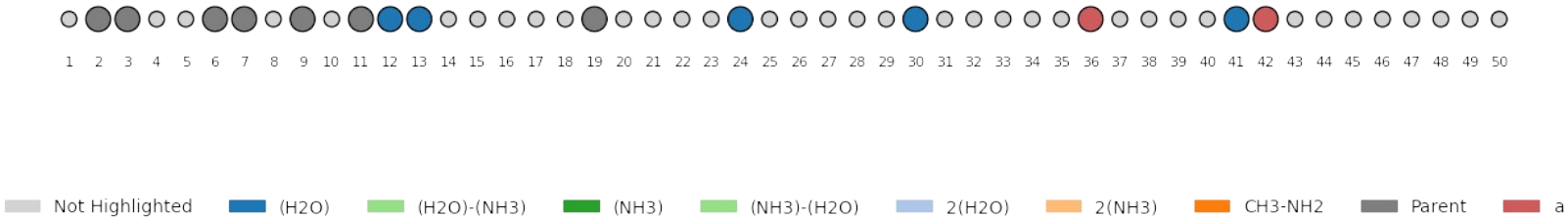


Table PH15_2+

| 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(H2O) | 238.81 | 238.17 | 0.64 | b9 | (H3PO4) | 870.26 | 870.44 | -0.18 | 1347.88 |
| 46 | rare_mode | y2 | 2(NH3)-(HN=C=NH) | 197.62 | 198.11 | -0.49 | b9 | 2(H2O)-(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(H2O)-(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 | (H3PO4)-(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 |