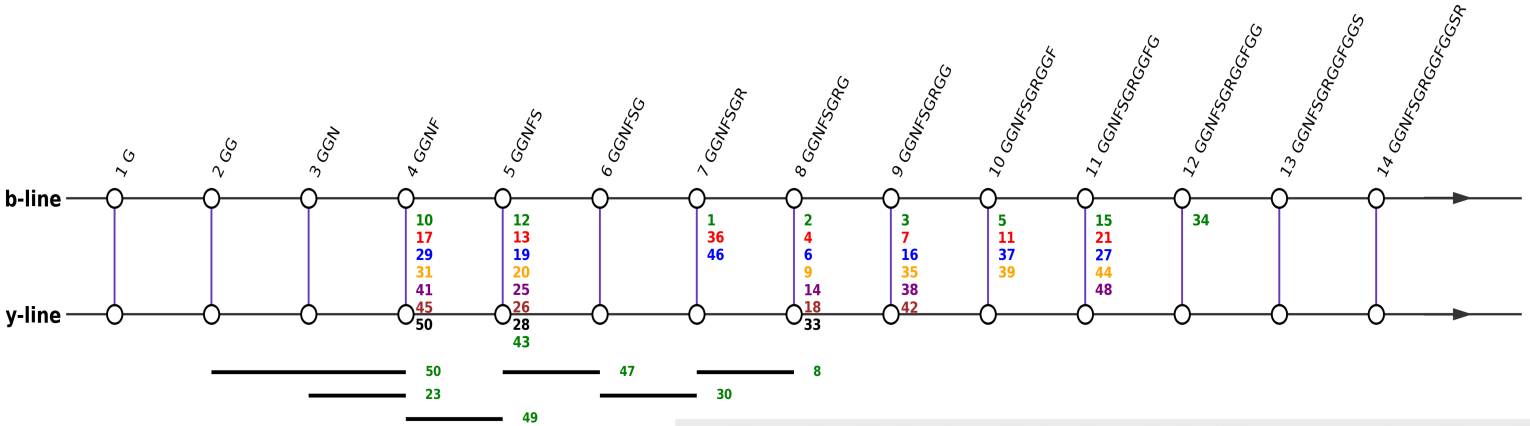
# [GGNFSGRMeGGFGGSR+2H]2+

Fragmentation Diagram for: GGNFSGRGGFGGSR




| | Cluster ID | Cluster Size | Median Mass (Da) | Difference from Actual Mass (Da) | |
|---|---|---|---|---|---|
| 0 | 0 | 6 | 1327.690 | | 0.06754 |
| 1 | 1 | 5 | 1310.640 | NH3, H2O | -16.98246 |
| 2 | 2 | 2 | 1279.840 | $HCONH_2$ | -47.78246 |
| 3 | 3 | 2 | 1293.690 | 2*NH3 | -33.93246 |
| 4 | 4 | 2 | 1262.275 | | -65.34746 |
| 5 | 5 | 2 | 1249.465 | | -78.15746 |
| 6 | 6 | 2 | 1265.145 | | -62.47746 |
| 7 | 7 | 2 | 1292.680 | 2*NH3 | -34.94246 |
| 8 | 8 | 2 | 1296.440 | $CH_3NH_2$ | -31.18246 |

## Detailed Data

| n | classification | line | mass1 | correct_mass1 | mass2 | correct_mass2 | m1+m2 | 2m1+m2 | m1+2m2 | chosen_sum |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | usable | y7 (1+) @ 637.39 & b7 (1+) @ 690.36 | 637.39 | 637.31 | 690.36 | 690.33 | 1327.75 | 1965.14 | 2018.11 | 1327.75 |
| 2 | usable | y6 (1+) @ 580.39 & b8 (1+) @ 747.43 | 580.39 | 580.28 | 747.43 | 747.35 | 1327.82 | 1908.21 | 2075.25 | 1327.82 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | usable | y5 (1+) @ 523.26 & b9 (1+) @ 804.37 | 523.26 | 523.26 | 804.37 | 804.37 | 1327.63 | 1850.89 | 2132.0 | 1327.63 |
| 4 | usable | y6 (1+) @ 580.37 & [b8-NH3] (1+) @ 730.35 | 580.37 | 580.28 | 730.35 | 730.33 | 1310.72 | 1891.09 | 2041.07 | 1310.72 |
| 5 | usable | [y4-NH3] (1+) @ 359.11 & b10 (1+) @ 951.13 | 359.11 | 359.17 | 951.13 | 951.44 | 1310.24 | 1669.35 | 2261.37 | 1310.24 |
| 6 | usable | [b8-CH3NH2-NH3] (1+) @ 699.38 & y6 (1+) @ 580.59 | 699.38 | 699.28 | 580.59 | 580.28 | 1279.97 | 1979.35 | 1860.56 | 1279.97 |
| 7 | usable | [y5-NH3] (1+) @ 506.09 & b9 (1+) @ 804.5 | 506.09 | 506.24 | 804.5 | 804.37 | 1310.59 | 1816.68 | 2115.09 | 1310.59 |
| 8 | non_complementary | y6(1+) @ 580.43 & [b7-NH3] (1+) @ 673.04 | 580.43 | 580.28 | 673.04 | 673.31 | 1253.47 | 1833.9 | 1926.51 | 1253.47 |
| 9 | usable | [y6-NH3] (1+) @ 562.87 & b8 (1+) @ 747.77 | 562.87 | 563.26 | 747.77 | 747.35 | 1310.64 | 1873.51 | 2058.41 | 1310.64 |
| 10 | usable | [y10-CH3NH2] (1+) @ 921.04 & a4 (1+) @ | 921.04 | 920.43 | nan | nan | nan | nan | nan | nan |
| 11 | usable | b10 (1+) @ 951.13 & [y4-2(H2O)-NH3] (1+) @ 323.13 | 951.13 | 951.44 | 323.13 | 323.15 | 1274.26 | 2225.39 | 1597.39 | 1274.26 |
| 12 | usable | [y9-NH3] (1+) @ 847.45 & [b5-NH3] (1+) @ 446.02 | 847.45 | 847.42 | 446.02 | 446.17 | 1293.47 | 2140.92 | 1739.49 | 1293.47 |
| 13 | usable | [y9-CH3NH2] (1+) @ 833.18 & [b5-NH3-H2O] (1+) @ 427.77 | 833.18 | 833.4 | 427.77 | 428.16 | 1260.95 | 2094.13 | 1688.72 | 1260.95 |
| 14 | usable | [b8+H2O] (1+) @ 765.76 & [y6-H2O] (1+) @ 562.31 | 765.76 | 765.36 | 562.31 | 562.27 | 1328.07 | 2093.83 | 1890.38 | 1328.07 |
| 15 | usable | [y3-NH3] (1+) @ 301.75 & b11(1+) @ 1009.17 | 301.75 | 302.15 | 1009.17 | 1008.46 | 1310.92 | 1612.67 | 2320.09 | 1310.92 |
| 16 | usable | b9 (1+) @ 804.33 & [y5-2(NH3)](1+) @ 490.22 | 804.33 | 804.37 | 490.22 | 489.21 | 1294.55 | 2098.88 | 1784.77 | 1294.55 |
| 17 | rare_mod | [y10 - HN=C=N-CH3] (1+) @ 895.4 & a4 (1+) @ 347.81 | 895.4 | 895.44 | 347.81 | 348.15 | 1243.21 | 2138.61 | 1591.02 | 1243.21 |
| 18 | usable | y6(1+) @ 580.57 & a8(1+) @ 719.46 | 580.57 | 580.28 | 719.46 | 719.34 | 1300.03 | 1880.6 | 2019.49 | 1300.03 |
| 19 | usable | [y9-NH3] (1+) @ 847.25 & [b5-NH3-H2O] (1+) @ 428.27 | 847.25 | 847.42 | 428.27 | 428.16 | 1275.52 | 2122.77 | 1703.79 | 1275.52 |
| 20 | usable | [y9- CH3NH2] (1+) @ 833.18 & [a5-NH3-H2O] (1+) @ 400.18 | 833.18 | 833.4 | 400.18 | 400.15 | 1233.36 | 2066.54 | 1633.54 | 1233.36 |
| 21 | usable | [y3-NH3] (1+) @ 301.89 & [b11-NH3] (1+) @ 992.02 | 301.89 | 302.15 | 992.02 | 991.44 | 1293.91 | 1595.8 | 2285.93 | 1293.91 |
| 22 | unclear | a9 (1+) @ 776.68 & ??? @ 485.61 | 776.68 | 776.36 | 485.61 | nan | 1262.29 | 2038.97 | 1747.9 | 1262.29 |
| 23 | non_complementary | [y10-NH3] (1+) @ 934.85 & b3(1+) @ 228.71 | 934.85 | 934.45 | 228.71 | 229.09 | 1163.56 | 2098.41 | 1392.27 | 1392.27 |
| 24 | unclear | ??? @ 682.12 & y6 (1+) @ 580.14 | 682.12 | nan | 580.14 | 580.28 | 1262.26 | 1944.38 | 1842.4 | 1262.26 |
| 25 | usable | [y9- CH3NH2 – NH3] (1+) @ 816.84 & [b5-NH3-H2O] (1+) @ 428.1 | 816.84 | 816.37 | 428.1 | 428.16 | 1244.94 | 2061.78 | 1673.04 | 1244.94 |
| 26 | usable | [y9- CH3NH2] (1+) @ 833.6 & [b5-NH3] (1+) @ 446.11 | 833.6 | 833.4 | 446.11 | 446.17 | 1279.71 | 2113.31 | 1725.82 | 1279.71 |
| 27 | rare_mod | b11 (1+) @ 1008.62 & [y3 - HN=C=NH - 2(H2O)] (1+) @ 240.79 | 1008.62 | 1008.46 | 240.79 | 241.13 | 1249.41 | 2258.03 | 1490.2 | 1249.41 |
| 28 | usable | [y9-NH3] (1+) @ 847.79 & [a5-NH3] (1+) @ 418.1 | 847.79 | 847.42 | 418.1 | 418.16 | 1265.89 | 2113.68 | 1683.99 | 1265.89 |
| 29 | usable | [y10-NH3] (1+) @ 934.52 & [a4-NH3] (1+) @ 330.69 | 934.52 | 934.45 | 330.69 | 331.12 | 1265.21 | 2199.73 | 1595.9 | 1265.21 |
| 30 | non_complementary | y7(1+) @ 637.6 & [b6-NH3] (1+) @ 503.15 | 637.6 | 637.31 | 503.15 | 503.19 | 1140.75 | 1778.35 | 1643.9 | 1140.75 |

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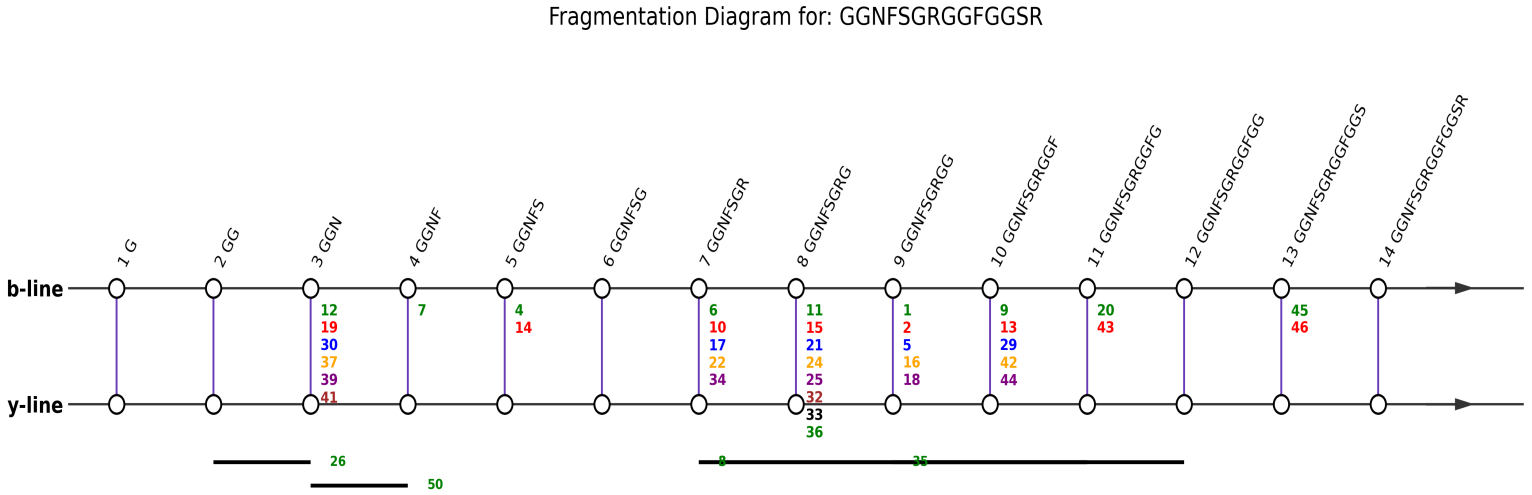
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | rare_mod | [y10- HN=C=NH - NH3] (1+) @ 891.57 & b3 (1+) @ 228.66 | 891.57 | 892.43 | 228.66 | 229.09 | 1120.23 | 2011.8 | 1348.89 | 1348.89 |
| 32 | ambiguous | y10/b10 (1+) @ 51.14 & [b4/y4 -NH3-H2O] (1+) @ 341.21 | 51.14 | 951.48 | 341.21 | 341.12 | 392.35 | 443.49 | 733.56 | 733.56 |
| 33 | usable | [b8- CH3NH2 - NH3] (1+) @ 699.4 & [y6 - H2O] (1+) @ 562.35 | 699.4 | 699.28 | 562.35 | 562.27 | 1261.75 | 1961.15 | 1824.1 | 1261.75 |
| 34 | usable | b12 (1+) @ 1065.78 & [y2-H2O-NH3] (1+) @ 226.8 | 1065.78 | 1065.49 | 226.8 | 227.11 | 1292.58 | 2358.36 | 1519.38 | 1292.58 |
| 35 | usable | [b9- CH3NH2 - NH3] (1+) @ 755.7 & y5 (1+) @ 523.15 | 755.7 | 756.31 | 523.15 | 523.26 | 1278.85 | 2034.55 | 1802.0 | 1278.85 |
| 36 | usable | b7 (1+) @ 691.33 & [y7-NH3] (1+) @ 620.15 | 691.33 | 690.33 | 620.15 | 620.28 | 1311.48 | 2002.81 | 1931.63 | 1311.48 |
| 37 | rare_mod | b10 (1+) @ 952.06 & [y4 - HN=C=NH -2(H2O)] (1+) @ 297.46 | 952.06 | 951.44 | 297.46 | 298.15 | 1249.52 | 2201.58 | 1546.98 | 1249.52 |
| 38 | usable | [b9 - CH3-NH2] (1+) @ 773.13 & y5 (1+) @ 523.25 | 773.13 | 773.33 | 523.25 | 523.26 | 1296.38 | 2069.51 | 1819.63 | 1296.38 |
| 39 | usable | a10 (1+) @ 924.2 & [y4 – NH3- 2(H2O)] (1+) @ 323.33 | 924.2 | 923.43 | 323.33 | 323.15 | 1247.53 | 2171.73 | 1570.86 | 1247.53 |
| 40 | unclear | ??? @ 921.76 & y4 (1+) @ 376.36 | 921.76 | nan | 376.36 | 376.19 | 1298.12 | 2219.88 | 1674.48 | 1298.12 |
| 41 | rare_mod | [y10 – HN=C=NH – H2O] (1+) @ 891.45 & [b4-HCONH2] (1+) @ 330.79 | 891.45 | 891.44 | 330.79 | 331.14 | 1222.24 | 2113.69 | 1553.03 | 1222.24 |
| 42 | usable | [b9 + H2O] (1+) @ 822.35 & [y5-H2O] @ 505.13 | 822.35 | 822.39 | 505.13 | 505.25 | 1327.48 | 2149.83 | 1832.61 | 1327.48 |
| 43 | usable | [y9 - CH3-NH2] (1+) @ 833.1 & b5 (1+) @ 463.4 | 833.1 | 833.4 | 463.4 | 463.19 | 1296.5 | 2129.6 | 1759.9 | 1296.5 |
| 44 | usable | [y3-NH3] (1+) @ 302.06 & [a11-NH3](1+) @ 963.02 | 302.06 | 302.15 | 963.02 | 963.43 | 1265.08 | 1567.14 | 2228.1 | 1265.08 |
| 45 | rare_mod | [y10 - HN=C=N-CH3– H2O] @ 877.52 & a4 (1+) @ 348.45 | 877.52 | 877.43 | 348.45 | 348.15 | 1225.97 | 2103.49 | 1574.42 | 1225.97 |
| 46 | usable | [y7 - H2O] (1+) @ 618.99 & [b7-NH3] (1+) @ 673.79 | 618.99 | 619.29 | 673.79 | 673.31 | 1292.78 | 1911.77 | 1966.57 | 1292.78 |
| 47 | non_complementary | [y8-NH3] (1+) @ 790.42 & [b5-NH3] (1+) @ 445.39 | 790.42 | 790.4 | 445.39 | 446.17 | 1235.81 | 2026.23 | 1681.2 | 1235.81 |
| 48 | usable | y3 (1+) @ 318.85 & b11 (1+) @ 1008.58 | 318.85 | 319.17 | 1008.58 | 1008.46 | 1327.43 | 1646.28 | 2336.01 | 1327.43 |
| 49 | non_complementary | [y9 - CH3-NH2 – NH3] (1+) @ 816.74 & [b4-NH3] (1+) @ 359.27 | 816.74 | 816.37 | 359.27 | 359.13 | 1176.01 | 1992.75 | 1535.28 | 1176.01 |
| 50 | rare_mod | [y10 - HN=C=N-CH3] @ 895.4 & [bi(2-4) – H2O – NH3] (1+) @ 284.64 | 895.4 | 895.44 | 284.64 | 284.1 | 1180.04 | 2075.44 | 1464.68 | 1464.68 |

# [GGNFSGRMeGGFGGSR+3H]3+




| | Cluster ID | Cluster Size | Median Mass (Da) | Difference from Actual Mass (Da) | |
|---|---|---|---|---|---|
| 0 | 0 | 13 | 1311.000 | NH3 | -16.62246 |
| 1 | 1 | 13 | 1328.330 | | 0.70754 |
| 2 | 2 | 2 | 1300.835 | CO? | -26.78746 |
| 3 | 3 | 7 | 1293.340 | 2NH3/H2O+NH3 | -34.28246 |
| 4 | 4 | 2 | 1264.500 | | -63.12246 |
| 5 | 5 | 2 | 1283.335 | $HCONH_2$ | -44.28746 |

## Detailed Data

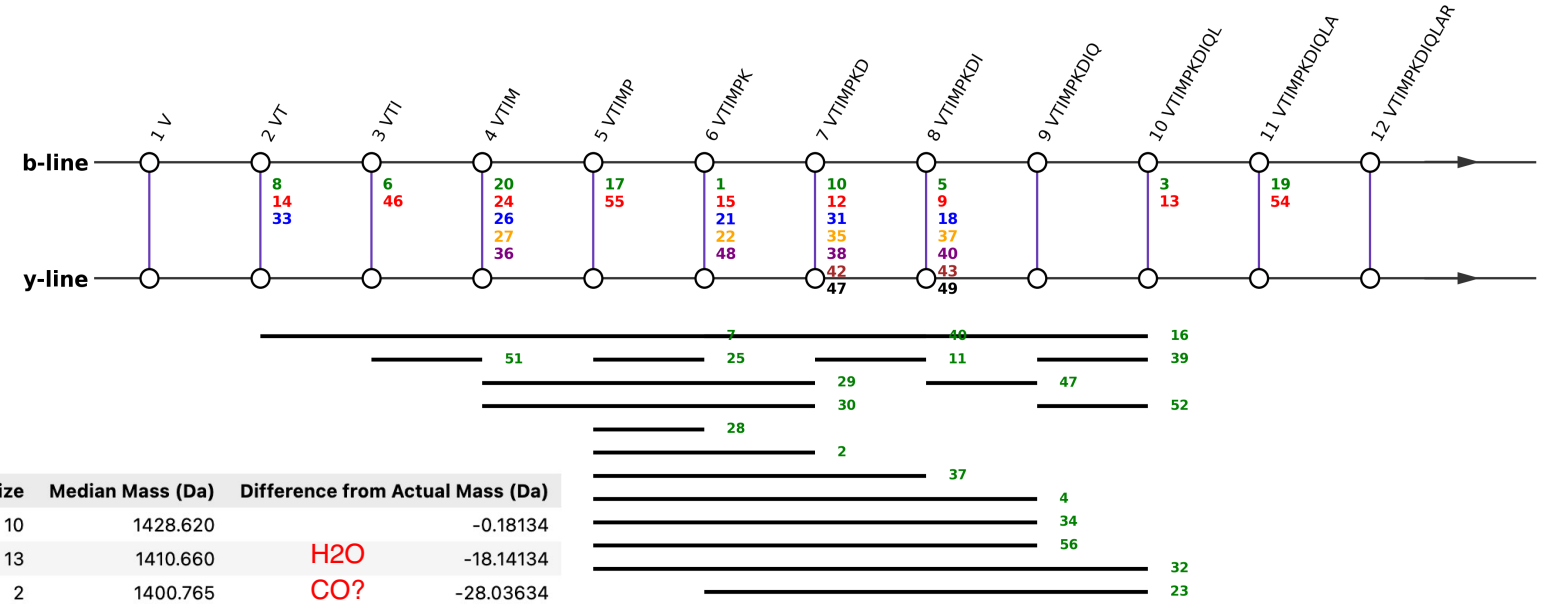
| n | classification | line | mass1 | correct_mass1 | mass2 | correct_mass2 | m1+m2 | 2m1+m2 | m1+2m2 | chosen_sum |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | usable | y5 (1+) @ 523.33 & [b9 - NH3] (2+) @ 394.0 | 523.33 | 523.26 | 394.0 | 394.18 | 917.33 | 1440.66 | 1311.33 | 1311.33 |
| 2 | usable | y5 (1+) @ 523.33 & b9 (2+) @ 402.67 | 523.33 | 523.26 | 402.67 | 402.69 | 926.0 | 1449.33 | 1328.67 | 1328.67 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | non_complementary | y7 (2+) @ 319.0 & [b11 - NH3] (2+) @ 496.0 | 319.0 | 319.16 | 496.0 | 496.22 | 815.0 | 1134.0 | 1311.0 | 1311.0 |
| 4 | usable | y9 (2+) @ 432.67 & b5 (1+) @ 463.0 | 432.67 | 432.73 | 463.0 | 463.19 | 895.67 | 1328.34 | 1358.67 | 1328.34 |
| 5 | usable | y5 (2+) @ 262.0 & b9 (1+) @ 804.33 | 262.0 | 262.13 | 804.33 | 804.37 | 1066.33 | 1328.33 | 1870.66 | 1328.33 |
| 6 | usable | y7 (1+) @ 637.33 & [b7 - NH3] (2+) @ 337.0 | 637.33 | 637.31 | 337.0 | 337.16 | 974.33 | 1611.66 | 1311.33 | 1311.33 |
| 7 | usable | y10 (2+) @ 476.33 & a4 (1+) @ 348.0 | 476.33 | 476.24 | 348.0 | 348.15 | 824.33 | 1300.66 | 1172.33 | 1300.66 |
| 8 | non_complementary | y7 (2+) @ 319.0 & b11 (2+) @ 504.67 | 319.0 | 319.16 | 504.67 | 504.74 | 823.67 | 1142.67 | 1328.34 | 1328.34 |
| 9 | usable | y4 (1+) @ 376.0 & [b10 - NH3] (2+) @ 467.67 | 376.0 | 376.19 | 467.67 | 467.71 | 843.67 | 1219.67 | 1311.34 | 1311.34 |
| 10 | usable | y7 (1+) @ 637.33 & b7 (2+) @ 345.67 | 637.33 | 637.31 | 345.67 | 345.67 | 983.0 | 1620.33 | 1328.67 | 1328.67 |
| 11 | usable | y6 (1+) @ 580.33 & [b8 - NH3] (2+) @ 365.33 | 580.33 | 580.28 | 365.33 | 365.67 | 945.66 | 1525.99 | 1310.99 | 1310.99 |
| 12 | usable | y11 (2+) @ 550.0 & [b3 - H2O] (1+) @ 210.67 | 550.0 | 549.78 | 210.67 | 211.08 | 760.67 | 1310.67 | 971.34 | 1310.67 |
| 13 | usable | y4 (1+) @ 375.67 & b10 (2+) @ 476.33 | 375.67 | 376.19 | 476.33 | 476.23 | 852.0 | 1227.67 | 1328.33 | 1328.33 |
| 14 | usable | y9 (2+) @ 432.67 & [b5 - NH3] (1+) @ 446.0 | 432.67 | 432.73 | 446.0 | 446.17 | 878.67 | 1311.34 | 1324.67 | 1324.67 |
| 15 | usable | y6 (1+) @ 580.33 & b8 (2+) @ 374.0 | 580.33 | 580.28 | 374.0 | 374.18 | 954.33 | 1534.66 | 1328.33 | 1328.33 |
| 16 | usable | y5 (1+) @ 523.33 & [b9 – H2O – NH3] (2+) @ 385.0 | 523.33 | 523.26 | 385.0 | 385.17 | 908.33 | 1431.66 | 1293.33 | 1293.33 |
| 17 | usable | y7 (1+) @ 637.33 & [b7 – H2O – NH3] (2+) @ 328.0 | 637.33 | 637.31 | 328.0 | 328.15 | 965.33 | 1602.66 | 1293.33 | 1293.33 |
| 18 | usable | y5 (2+) @ 262.0 & [b9 - NH3] (1+) @ 787.33 | 262.0 | 262.13 | 787.33 | 787.35 | 1049.33 | 1311.33 | 1836.66 | 1311.33 |
| 19 | usable | y11 (2+) @ 550.0 & b3 (1+) @ 228.67 | 550.0 | 549.78 | 228.67 | 229.09 | 778.67 | 1328.67 | 1007.34 | 1328.67 |
| 20 | usable | [b11 – H2O – NH3] (2+) @ 487.33 & y3 (1+) @ 319.0 | 487.33 | 487.22 | 319.0 | 319.17 | 806.33 | 1293.66 | 1125.33 | 1293.66 |
| 21 | usable | y6 (2+) @ 290.33 & b8 (1+) @ 747.33 | 290.33 | 290.65 | 747.33 | 747.35 | 1037.66 | 1327.99 | 1784.99 | 1327.99 |
| 22 | usable | y7 (2+) @ 319.0 & b7(1+) @ 690.33 | 319.0 | 319.16 | 690.33 | 690.33 | 1009.33 | 1328.33 | 1699.66 | 1328.33 |
| 23 | ambiguous | [y10 – NH3 – H2O] (2+) @ 458.67 & b4/y4 (1+) @ 376.0 | 458.67 | 458.72 | 376.0 | 376.16 | 834.67 | 1293.34 | 1210.67 | 1293.34 |
| 24 | usable | y6 (1+) @ 580.33 & [b8 – H2O - NH3] (2+) @ 356.67 | 580.33 | 580.28 | 356.67 | 356.66 | 937.0 | 1517.33 | 1293.67 | 1293.67 |
| 25 | usable | y6 (2+) @ 290.33 & [b8-NH3] (1+) @ 730.33 | 290.33 | 290.65 | 730.33 | 730.33 | 1020.66 | 1310.99 | 1750.99 | 1310.99 |
| 26 | internal_acid | [y11 + G] (2+) @ 578.33 & bi2-3 (1+) @ 171.67 | 578.33 | 578.29 | 171.67 | 172.07 | 750.0 | 1328.33 | 921.67 | 1328.33 |
| 27 | unclear | y9 (2+) @ 432.67 & ??? @ 383.0 | 432.67 | 432.73 | 383.0 | nan | 815.67 | 1248.34 | 1198.67 | 1248.34 |
| 28 | unclear | ??? @ 595.33 & [b8 - NH3] (2+) @ 366.0 | 595.33 | nan | 366.0 | 365.67 | 961.33 | 1556.66 | 1327.33 | 1327.33 |
| 29 | usable | [y4-NH3] (1+) @ 358.67 & b10 (2+) @ 476.33 | 358.67 | 359.17 | 476.33 | 476.23 | 835.0 | 1193.67 | 1311.33 | 1311.33 |
| 30 | usable | [y11 - G] (2+) @ 521.67 & [b3 + G] (1+) @ 285.67 | 521.67 | 521.26 | 285.67 | 286.11 | 807.34 | 1329.01 | 1093.01 | 1329.01 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | ambiguous | [b10/y10 – H2O – 2(NH3)] (2+) @ 450.0 & y4/b4 @ 376.0 | 450.0 | 450.19 | 376.0 | 376.19 | 826.0 | 1276.0 | 1202.0 | 1276.0 |
| 32 | usable | [b8 – NH3] (1+) @ 730.33 & ai9-10 (1+) @ 176.67 | 730.33 | 730.33 | 176.67 | 177.09 | 907.0 | 1637.33 | 1083.67 | 1083.67 |
| 33 | usable | b8 (1+) @ 747.33 & ai9-10 (1+) 176.67 | 747.33 | 747.35 | nan | nan | nan | nan | nan | nan |
| 34 | usable | y7 (2+) @ 319.0 & [b7-NH3] (1+) @ 673.33 | 319.0 | 319.16 | 673.33 | 673.31 | 992.33 | 1311.33 | 1665.66 | 1311.33 |
| 35 | non_complementary | y5 (2+) @ 262.0 & b12 (2+) @ 533.0 | 262.0 | 262.13 | 533.0 | 533.25 | 795.0 | 1057.0 | 1328.0 | 1328.0 |
| 36 | usable | b8 (1+) @ 748.0 & ai9-10 (1+) @ 204.67 | 748.0 | 747.35 | 204.67 | 177.09 | 952.67 | 1700.67 | 1157.34 | 1157.34 |
| 37 | usable | y11(2+) @ 549.67 & a3(1+) @ 201.67 | 549.67 | 549.78 | 201.67 | 201.08 | 751.34 | 1301.01 | 953.01 | 1301.01 |
| 38 | undefined | 549.67 & 165.33 | 549.67 | nan | 165.33 | nan | 715.0 | 1264.67 | 880.33 | 1264.67 |
| 39 | usable | y11 (2+) @ 550.0 & [a3 – 2(H2O)] (1+) @ 193.33 | 550.0 | 549.78 | 193.33 | 165.06 | 743.33 | 1293.33 | 936.66 | 1293.33 |
| 40 | undefined | 461.67 & 389.0 | 461.67 | nan | 389.0 | nan | 850.67 | 1312.34 | 1239.67 | 1312.34 |
| 41 | usable | y11 (2+) @ 550.0 & [a3-NH3] (1+) @ 183.33 | 550.0 | 549.78 | 183.33 | 184.06 | 733.33 | 1283.33 | 916.66 | 1283.33 |
| 42 | usable | y4 (2+) @ 188.0 & [b10-NH3] (1+) @ 934.33 | 188.0 | 188.6 | 934.33 | 934.42 | 1122.33 | 1310.33 | 2056.66 | 1310.33 |
| 43 | usable | b11 (1+) @ 504.67 & [y3 – CO2] (1+) @ 274.0 | 504.67 | 1008.46 | 274.0 | 275.18 | 778.67 | 1283.34 | 1052.67 | 1283.34 |
| 44 | usable | y4 (1+) @ 376.0 & ai9-10 (1+) @ 176.67 | 376.0 | 376.19 | 176.67 | 177.09 | 552.67 | 928.67 | 729.34 | 928.67 |
| 45 | usable | [b13-H2O-NH3] (2+) @ 559.33 & y1(1+) @ 175.0 | 559.33 | 559.24 | 175.0 | 175.12 | 734.33 | 1293.66 | 909.33 | 1293.66 |
| 46 | usable | y1 (1+) @ 174.67 & [b13-NH3] (2+) @ 567.67 | 174.67 | 175.12 | 567.67 | 568.25 | 742.34 | 917.01 | 1310.01 | 1310.01 |
| 47 | unclear | y5 (1+) @ 523.67 & ??? @ 370.33 | 523.67 | 523.26 | 370.33 | nan | 894.0 | 1417.67 | 1264.33 | 1264.33 |
| 48 | undefined | 637.0 & 314.33 | 637.0 | nan | 314.33 | nan | 951.33 | 1588.33 | 1265.66 | 1265.66 |
| 49 | undefined | 589.33 & 131.67 | 589.33 | nan | 131.67 | nan | 721.0 | 1310.33 | 852.67 | 1310.33 |
| 50 | internal_acid | [y10-H2O] (1+) @ 540.67 & [bi3-4 – 2(NH3)] (1+) @ 228.0 | 540.67 | 933.46 | 228.0 | 228.07 | 768.67 | 1309.34 | 996.67 | 1309.34 |

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

Fragmentation Diagram for: VTIMPKDIQLAR




| | Cluster ID | Cluster Size | Median Mass (Da) | Difference from Actual Mass (Da) | |
|---|---|---|---|---|---|
| 0 | 0 | 10 | 1428.620 | | -0.18134 |
| 1 | 1 | 13 | 1410.660 | H2O | -18.14134 |
| 2 | 2 | 2 | 1400.765 | CO? | -28.03634 |
| 3 | 3 | 2 | 1328.835 | H3PO4? | -99.96634 |

## Detailed Data

| n | classification | line | mass1 | correct_mass1 | mass2 | correct_mass2 | m1+m2 | 2m1+m2 | m1+2m2 | chosen_sum |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | usable | y6 (1+) @ 715.44 & b6 (2+) @ 356.66 | 715.44 | 715.41 | 356.66 | 356.71 | 1072.1 | 1787.54 | 1428.76 | 1428.76 |
| 2 | internal_acid | y5 (1+) @ 600.46 & bi5-7 (1+) @ 383.1 | 600.46 | 600.38 | 383.1 | 383.19 | 983.56 | 1584.02 | 1366.66 | 1366.66 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | usable | y2 (1+) @ 245.82 & b10 (2+) @ 591.38 | 245.82 | 246.16 | 591.38 | 591.33 | 837.2 | 1083.02 | 1428.58 | 1428.58 |
| 4 | internal_acid | bi5-9 (1+) @ 624.4 & y3 (1+) @ 359.18 | 624.4 | 624.34 | 359.18 | 359.24 | 983.58 | 1607.98 | 1342.76 | 1342.76 |
| 5 | usable | y4 (1+) @ 487.22 & a8(2+) @ 456.75 | 487.22 | 487.3 | 456.75 | 456.76 | 943.97 | 1431.19 | 1400.72 | 1431.19 |
| 6 | usable | y9 (2+) @ 557.42 & [b3-NH3] (1+) @ 296.01 | 557.42 | 557.31 | 296.01 | 297.18 | 853.43 | 1410.85 | 1149.44 | 1410.85 |
| 7 | non_complementary | y6 (2+) @ 359.14 & b9 (2+) @ 534.76 | 359.14 | 358.21 | 534.76 | 534.79 | 893.9 | 1253.04 | 1428.66 | 1428.66 |
| 8 | usable | y10 (2+) @ 614.08 & b2 (1+) @ 200.71 | 614.08 | 613.85 | 200.71 | 201.12 | 814.79 | 1428.87 | 1015.5 | 1428.87 |
| 9 | usable | [y4-NH3] (2+) @ 234.85 & b8 (1+) @ 940.45 | 234.85 | 235.64 | 940.45 | 940.52 | 1175.3 | 1410.15 | 2115.75 | 1410.15 |
| 10 | usable | y5 (1+) @ 600.38 & b7 (2+) @ 414.18 | 600.38 | 600.38 | 414.18 | 414.22 | 1014.56 | 1614.94 | 1428.74 | 1428.74 |
| 11 | non_complementary | y4 (1+) @ 487.33 & b7 (1+) @ 827.44 | 487.33 | 487.3 | 827.44 | 827.43 | 1314.77 | 1802.1 | 2142.21 | 1314.77 |
| 12 | usable | y5 (2+) @ 300.5 & b7 (1+) @ 827.42 | 300.5 | 300.69 | 827.42 | 827.43 | 1127.92 | 1428.42 | 1955.34 | 1428.42 |
| 13 | usable | y2 (1+) @ 245.82 & [b10-NH3] (2+) @ 582.35 | 245.82 | 246.16 | 582.35 | 582.82 | 828.17 | 1073.99 | 1410.52 | 1410.52 |
| 14 | usable | y10 (2+) @ 614.08 & a2 (1+) @ 172.63 | 614.08 | 613.85 | 172.63 | 173.11 | 786.71 | 1400.79 | 959.34 | 1400.79 |
| 15 | usable | y6 (1+) @ 715.45 & c5 (1+) @ 559.34 | 715.45 | 715.41 | 559.34 | nan | 1274.79 | 1990.24 | 1834.13 | 1274.79 |
| 16 | non_complementary | y2 (1+) @ 245.79 & b9 (1+) @ 1068.42 | 245.79 | 246.16 | 1068.42 | 1068.58 | 1314.21 | 1560.0 | 2382.63 | 1314.21 |
| 17 | usable | y7 (2+) @ 443.34 & b5 (1+) @ 542.33 | 443.34 | 443.26 | 542.33 | 542.3 | 985.67 | 1429.01 | 1528.0 | 1429.01 |
| 18 | usable | y4 (2+) @ 243.98 & b8 (1+) @ 940.41 | 243.98 | 244.15 | 940.41 | 940.52 | 1184.39 | 1428.37 | 2124.8 | 1428.37 |
| 19 | usable | y1 (1+) @ 174.58 & b11 (2+) @ 626.99 | 174.58 | 175.12 | 626.99 | 626.85 | 801.57 | 976.15 | 1428.56 | 1428.56 |
| 20 | usable | y8 (2+) @ 491.76 & b4 (1+) @ 444.98 | 491.76 | 491.79 | 444.98 | 445.25 | 936.74 | 1428.5 | 1381.72 | 1428.5 |
| 21 | usable | [y6-NH3] (1+) @ 698.39 & b6 (2+) @ 356.64 | 698.39 | 698.38 | 356.64 | 356.71 | 1055.03 | 1753.42 | 1411.67 | 1411.67 |
| 22 | usable | y6 (1+) @ 715.54 & [b6-NH3] (2+) @ 347.56 | 715.54 | 715.41 | 347.56 | 348.19 | 1063.1 | 1778.64 | 1410.66 | 1410.66 |
| 23 | non_complementary | b6 (1+) @ 712.43 & [y2 – H2O] (1+) @ 228.63 | 712.43 | 712.41 | 228.63 | 228.15 | 941.06 | 1653.49 | 1169.69 | 1653.49 |
| 24 | usable | y8 (2+) @ 491.82 & a4 (1+) @ 417.1 | 491.82 | 491.79 | 417.1 | 417.24 | 908.92 | 1400.74 | 1326.02 | 1400.74 |
| 25 | non_complementary | y6 (2+) @ 359.14 & [b5-NH3] (1+) @ 525.62 | 359.14 | 358.21 | 525.62 | 525.27 | 884.76 | 1243.9 | 1410.38 | 1410.38 |
| 26 | usable | y8 (2+) @ 491.96 & [b4 - CH3SH - CO] (1+) @ 369.04 | 491.96 | 491.79 | 369.04 | 369.25 | 861.0 | 1352.96 | 1230.04 | 1352.96 |
| 27 | usable | [y8-NH3] (2+) @ 482.8 & b4 (1+) @ 445.14 | 482.8 | 483.27 | 445.14 | 445.25 | 927.94 | 1410.74 | 1373.08 | 1410.74 |
| 28 | internal_acid | y6 (1+) @ 715.66 & bi5-6 @ 267.85 | 715.66 | 715.41 | 267.85 | 268.17 | 983.51 | 1699.17 | 1251.36 | 1251.36 |
| 29 | internal_acid | y4 (1+) @ 487.09 & [bi4-7 – HCOOH] (1+) @ 468.09 | 487.09 | 487.3 | 468.09 | 468.23 | 955.18 | 1442.27 | 1423.27 | 1423.27 |
| 30 | internal_acid | [bi4-7 – HCOOH] (1+) @ 468.13 & ??? @ 445.09 | 468.13 | 468.23 | 445.09 | nan | 913.22 | 1381.35 | 1358.31 | 1381.35 |

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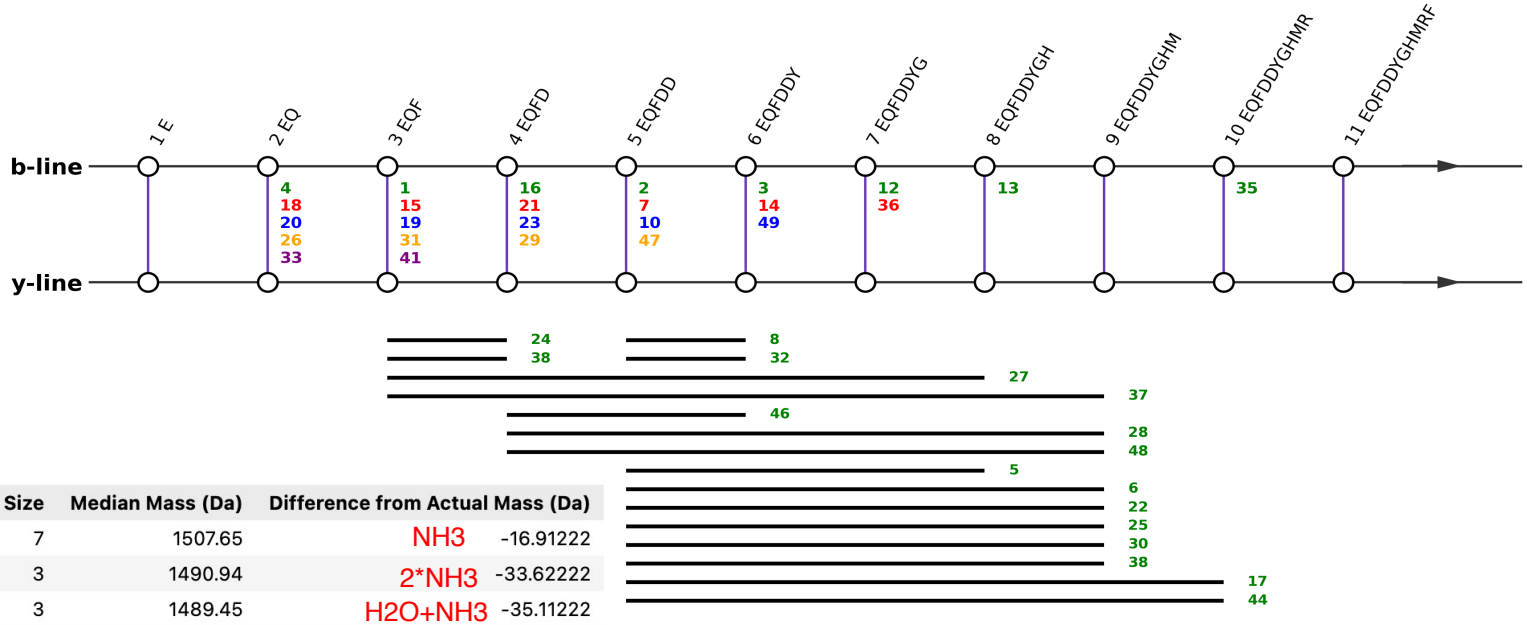
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | usable | y5(1+) @ 600.3 & [b7-NH3] (2+) @ 405.11 | 600.3 | 600.38 | 405.11 | 405.71 | 1005.41 | 1605.71 | 1410.52 | 1410.52 |
| 32 | internal_acid | bi5-10 (1+) @ 737.3 & y2 (1+) @ 245.92 | 737.3 | 737.42 | 245.92 | 246.16 | 983.22 | 1720.52 | 1229.14 | 1229.14 |
| 33 | usable | [y10-NH3] (2+) @ 604.93 & b2(1+) @ 200.68 | 604.93 | 605.34 | 200.68 | 201.12 | 805.61 | 1410.54 | 1006.29 | 1410.54 |
| 34 | internal_acid | bi5-9 (1+) @ 624.41 & b4 (1+) @ 444.93 | 624.41 | 624.34 | 444.93 | 445.25 | 1069.34 | 1693.75 | 1514.27 | 1514.27 |
| 35 | usable | y5(1+) @ 600.44 & a5 (1+) @ 514.24 | 600.44 | 600.38 | 514.24 | 514.29 | 1114.68 | 1715.12 | 1628.92 | 1628.92 |
| 36 | usable | y8(2+) @ 491.95 & [b4-NH3] (1+) @ 427.07 | 491.95 | 491.79 | 427.07 | 428.22 | 919.02 | 1410.97 | 1346.09 | 1410.97 |
| 37 | usable | bi (5-8) (1+) @ 496.41 & y4 (1+) @ 487.01 | 496.41 | 496.28 | 487.01 | 487.3 | 983.42 | 1479.83 | 1470.43 | 1470.43 |
| 38 | usable | [y5-NH3](2+) @ 291.64 & b7 (1+) @ 827.56 | 291.64 | 292.18 | 827.56 | 827.43 | 1119.2 | 1410.84 | 1946.76 | 1410.84 |
| 39 | non_complementary | y2(1+) @ 245.81 & [b9-NH3] (1+) @ 1051.61 | 245.81 | 246.16 | 1051.61 | 1051.55 | 1297.42 | 1543.23 | 2349.03 | 1543.23 |
| 40 | usable | bi (2-8) (1+) @ 841.49 & y4 (1+) @ 487.14 | 841.49 | 841.45 | 487.14 | 487.3 | 1328.63 | 2170.12 | 1815.77 | 1328.63 |
| 41 | unclear | b8(1+) @ 940.89 & ??? @ 195.81 | 940.89 | 940.52 | 195.81 | nan | 1136.7 | 2077.59 | 1332.51 | 1332.51 |
| 42 | usable | y5(2+) @ 300.61 & [b7-NH3] (1+) @ 809.82 | 300.61 | 300.69 | 809.82 | 810.41 | 1110.43 | 1411.04 | 1920.25 | 1411.04 |
| 43 | usable | y4(2+) @ 243.81 & [b8-NH3] (1+) @ 922.17 | 243.81 | 244.15 | 922.17 | 923.49 | 1165.98 | 1409.79 | 2088.15 | 1409.79 |
| 44 | unclear | b6(1+) @ 712.31 & ??? @ 200.73 | 712.31 | 712.41 | 200.73 | nan | 913.04 | 1625.35 | 1113.77 | 1625.35 |
| 45 | unclear | y9 (2+) @ 557.39 & ??? @ 250.74 | 557.39 | 557.31 | 250.74 | nan | 808.13 | 1365.52 | 1058.87 | 1365.52 |
| 46 | usable | [y9-NH3] (2+) @ 548.5 & [b3-NH3] (1+) @ 296.11 | 548.5 | 548.79 | 296.11 | 297.18 | 844.61 | 1393.11 | 1140.72 | 1393.11 |
| 47 | usable | b7 (1+) @ 827.88 & bi(8-9) (1+) @ 241.91 | 827.88 | 827.43 | 241.91 | 242.15 | 1069.79 | 1897.67 | 1311.7 | 1311.7 |
| 48 | usable | y6(1+) @ 715.27 & [a6-NH3] (2+) @ 335.69 | 715.27 | 715.41 | 335.69 | 334.19 | 1050.96 | 1766.23 | 1386.65 | 1386.65 |
| 49 | usable | [y4-NH3] (2+) @ 234.7 & [b8-NH3](1+) @ 922.41 | 234.7 | 235.64 | 922.41 | 923.49 | 1157.11 | 1391.81 | 2079.52 | 1391.81 |
| 50 | unclear | y8 (1+) @ 983.52 & ??? @ 216.78 | 983.52 | 982.57 | 216.78 | nan | 1200.3 | 2183.82 | 1417.08 | 1417.08 |
| 51 | non_complementary | y8(2+) @ 491.84 & b3(1+) @ 313.96 | 491.84 | 491.79 | 313.96 | 314.21 | 805.8 | 1297.64 | 1119.76 | 1297.64 |
| 52 | non_complementary | [b9-2(H2O)] (1+) @ 516.81 & y2 (1+) @ 245.85 | 516.81 | 1032.55 | 245.85 | 246.16 | 762.66 | 1279.47 | 1008.51 | 1279.47 |
| 53 | unclear | ??? @ 755.18 & y6(2+) @ 359.22 | 755.18 | nan | 359.22 | 358.21 | 1114.4 | 1869.58 | 1473.62 | 1473.62 |
| 54 | usable | y1 (1+) @ 174.8 & a10 (2+) @ 577.12 | 174.8 | 175.12 | 577.12 | 577.33 | 751.92 | 926.72 | 1329.04 | 1329.04 |
| 55 | usable | y7 (2+) @ 443.31 & [b5-NH3] (1+) @ 524.29 | 443.31 | 443.26 | 524.29 | 525.27 | 967.6 | 1410.91 | 1491.89 | 1410.91 |
| 56 | internal_acid | bi5-9 (1+) @ 624.36 & [b4- H2O] (1+) @ 427.13 | 624.36 | 624.34 | 427.13 | 427.24 | 1051.49 | 1675.85 | 1478.62 | 1478.62 |

# [EQFDDY(p)GHMRF(NH2) +3H]3+

Fragmentation Diagram for: EQFDDYGHMRF




| | Cluster ID | Cluster Size | Median Mass (Da) | Difference from Actual Mass (Da) | |
|---|---|---|---|---|---|
| 0 | 0 | 7 | 1507.65 | NH3 | -16.91222 |
| 1 | 1 | 3 | 1490.94 | 2*NH3 | -33.62222 |
| 2 | 2 | 3 | 1489.45 | H2O+NH3 | -35.11222 |
| 3 | 3 | 3 | 1479.51 | CO+H2O | -45.05222 |

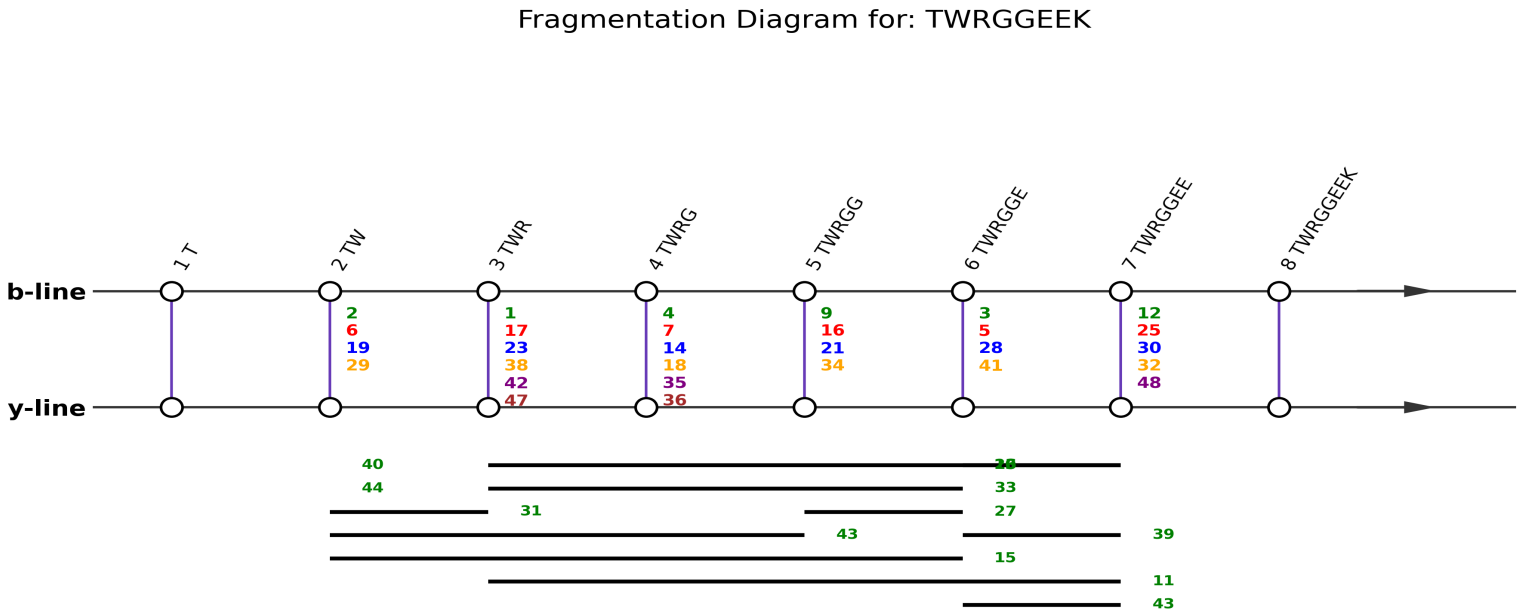
## Detailed Data

| n | classification | line | mass1 | correct_mass1 | mass2 | correct_mass2 | m1+m2 | 2m1+m2 | m1+2m2 | chosen_sum |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | usable | y8(2+) @ 560.4 & [b3-NH3] (1+) @ 387.05 | 560.4 | 559.7 | 387.05 | 388.15 | 947.45 | 1507.85 | 1334.5 | 1507.85 |
| 2 | usable | y6(2+) @ 445.29 & [b5-NH3] (1+) @ 617.14 | 445.29 | 444.68 | 617.14 | 618.2 | 1062.43 | 1507.72 | 1679.57 | 1507.72 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | usable | y5(2+) @ 323.67 & [b6-NH3] (1+) @ 860.17 | 323.67 | 323.16 | 860.17 | 861.23 | 1183.84 | 1507.51 | 2044.01 | 1507.51 |
| 4 | usable | y9(2+) @ 633.88 & [b2-NH3] (1+) @ 239.74 | 633.88 | 633.24 | 239.74 | 241.08 | 873.62 | 1507.5 | 1113.36 | 1507.5 |
| 5 | internal_acid | bi5-8 (1+) @ 1553.17 & y3 (1+) @ 452.35 | 1553.17 | 553.14 | 452.35 | 451.24 | 2005.52 | 3558.69 | 2457.87 | 2005.52 |
| 6 | internal_acid | bi5-9 (1+) @ 684.16 & y2 (1+) @ 321.1 | 684.16 | 684.18 | 321.1 | 320.2 | 1005.26 | 1689.42 | 1326.36 | 1689.42 |
| 7 | usable | y6(2+) @ 445.35 & a3(1+) @ 378.1 | 445.35 | 444.68 | 378.1 | 377.17 | 823.45 | 1268.8 | 1201.55 | 1268.8 |
| 8 | internal_acid | y5+ @ 646.41 & bi5-6 (1+) @ 359.02 | 646.41 | nan | 359.02 | 359.06 | 1005.43 | 1651.84 | 1364.45 | 1651.84 |
| 9 | undefined | 503.73 & 498.42 | 503.73 | nan | 498.42 | nan | 1002.15 | 1505.88 | 1500.57 | 1505.88 |
| 10 | usable | [b5-H2O-NH3] (1+) @ 599.96 & y6 (2+) @ 445.31 | 599.96 | 600.19 | 445.31 | 444.68 | 1045.27 | 1645.23 | 1490.58 | 1490.58 |
| 11 | usable | y5 (1+) 646.38 & ai5-6 (1+) @ 330.84 | nan | nan | 330.84 | 331.05 | nan | nan | nan | nan |
| 12 | usable | y4(1+) @ 589.39 & [a6-NH3](2+) @ 416.05 | 589.39 | 588.29 | 416.05 | 417.12 | 1005.44 | 1594.83 | 1421.49 | 1594.83 |
| 13 | usable | y3(1+) @ 452.19 & [b8-NH3](2+) @ 527.73 | 452.19 | 451.24 | 527.73 | 528.16 | 979.92 | 1432.11 | 1507.65 | 1507.65 |
| 14 | usable | [b6-2(H2O)] (1+) @ 842.68 & y5 (2+) @ 323.57 | 842.68 | 842.24 | 323.57 | 323.16 | 1166.25 | 2008.93 | 1489.82 | 1489.82 |
| 15 | usable | y8(2+) @ 560.27 & [a3-NH3](1+) @ 358.97 | 560.27 | 559.7 | 358.97 | 360.14 | 919.24 | 1479.51 | 1278.21 | 1479.51 |
| 16 | usable | [b4-H2O-NH3] (1+) @ 485.79 & [y7- CHONH2] (2+) @ 480.35 | 485.79 | 485.17 | 480.35 | 479.68 | 966.14 | 1451.93 | 1446.49 | 1451.93 |
| 17 | internal_acid | bi5-10 (1+) @ 840.5 & y1 (1+) 164.73 | 840.5 | 840.29 | nan | nan | nan | nan | nan | nan |
| 18 | usable | y9(2+) @ 633.84 & [a2-NH3](1+) @ 211.71 | 633.84 | 633.24 | 211.71 | 213.07 | 845.55 | 1479.39 | 1057.26 | 1479.39 |
| 19 | usable | [y8-NH3](2+) @ 551.2 & [b3-NH3](1+) @ 387.05 | 551.2 | 551.19 | 387.05 | 388.15 | 938.25 | 1489.45 | 1325.3 | 1489.45 |
| 20 | usable | y9(2+) @ 634.16 & b2(1+) @ 257.79 | 634.16 | 633.24 | 257.79 | 258.11 | 891.95 | 1526.11 | 1149.74 | 1526.11 |
| 21 | usable | [y7-NH3] (2+) @ 494.13 & [b4-HCOH – H2O] (1+) @ 456.16 | 494.13 | 493.68 | 456.16 | 472.18 | 950.29 | 1444.42 | 1406.45 | 1444.42 |
| 22 | internal_acid | bi5-9 (1+) @ 656.39 & y2 (1+) @ 321.11 | 656.39 | 684.18 | 321.11 | 320.2 | 977.5 | 1633.89 | 1298.61 | 1633.89 |
| 23 | usable | y7 (2+) @ 502.88 & [b4-HCOH – H2O] (1+) @ 455.94 | 502.88 | 502.19 | 455.94 | 472.18 | 958.82 | 1461.7 | 1414.76 | 1461.7 |
| 24 | internal_acid | [y7 – NH3] 2+ @ 494.11 & bi3-4 @ 262.78 | 494.11 | nan | 262.78 | 263.1 | 756.89 | 1251.0 | 1019.67 | 1251.0 |
| 25 | internal_acid | [bi5-9 – CH3CH2SCH3] (1+) @ 608.2 & y2 (1+) @ 320.89 | 608.2 | 608.15 | 320.89 | 320.2 | 929.09 | 1537.29 | 1249.98 | 1537.29 |
| 26 | usable | [y9-NH3] (2+) @ 624.77 & [b2-NH3] (1+) @ 239.79 | 624.77 | 624.72 | 239.79 | 241.08 | 864.56 | 1489.33 | 1104.35 | 1489.33 |
| 27 | internal_acid | bi3-8 (1+) @ 815.6 & y3 (1+) @ 452.34 | 815.6 | 815.24 | 452.34 | 451.24 | 1267.94 | 2083.54 | 1720.28 | 1720.28 |
| 28 | non_complementary | [b4-HCOH – H2O] (1+) @ 456.12 & y2 (1+) @ 321.07 | 456.12 | 472.18 | 321.07 | 320.2 | 777.19 | 1233.31 | 1098.26 | 1233.31 |
| 29 | usable | [y7 – NH3] (2+) @ 494.28 & [b4 - H2O – NH3] (1+) @ 484.76 | 494.28 | 493.68 | 484.76 | 485.17 | 979.04 | 1473.32 | 1463.8 | 1473.32 |
| 30 | internal_acid | [bi5-9] (1+) @ 683.79 & [b4 - HCOH – H2O] (1+) @ 456.23 | 683.79 | 684.18 | 456.23 | 472.18 | 1140.02 | 1823.81 | 1596.25 | 1596.25 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 31 | usable | y8 (2+) @ 560.59 & [b3 – 2(H2O)] (1+) @ 369.82 | 560.59 | 559.7 | 369.82 | 369.16 | 930.41 | 1491.0 | 1300.23 | 1491.0 |
| 32 | internal_acid | y5 (1+) @ 646.41 & bi5-6 (1+) @ 312.22 | 646.41 | 645.32 | 312.22 | 359.06 | 958.63 | 1605.04 | 1270.85 | 1605.04 |
| 33 | usable | y9 (2+) @ 634.11 & [b2 – H2O – NH3] (1+) @ 222.72 | 634.11 | 633.24 | 222.72 | 223.07 | 856.83 | 1490.94 | 1079.55 | 1490.94 |
| 34 | unclear | b8 (2+) @ 536.55 & ??? @ 454.17 | 536.55 | 536.67 | 454.17 | nan | 990.72 | 1527.27 | 1444.89 | 1527.27 |
| 35 | usable | y1(1+) @ 164.91 & [b10-NH3](2+) @ 671.48 | 164.91 | 164.09 | 671.48 | 671.73 | 836.39 | 1001.3 | 1507.87 | 1507.87 |
| 36 | usable | y4(2+) @ 294.78 & [b7-NH3](1+) @ 917.61 | 294.78 | 294.65 | 917.61 | 918.26 | 1212.39 | 1507.17 | 2130.0 | 1507.17 |
| 37 | internal_acid | bi3-9 (1+) @ 946.47 & y2 (1+) 321.09 | 946.47 | 946.28 | nan | nan | nan | nan | nan | nan |
| 38 | internal_acid | bi5-9 (1+) @ 683.85 & bi3-4 (1+) @ 263.1 | 683.85 | 684.18 | 263.1 | 263.1 | 946.95 | 1630.8 | 1210.05 | 1630.8 |
| 39 | undefined | 591.11 & 398.48 | 591.11 | nan | 398.48 | nan | 989.59 | 1580.7 | 1388.07 | 1580.7 |
| 40 | unclear | y9 (2+) @ 634.11 & ??? @ 194.76 | 634.11 | 633.24 | 194.76 | nan | 828.87 | 1462.98 | 1023.63 | 1462.98 |
| 41 | usable | [y8-NH3] (2+) @ 551.28 & [a3-H2O] (1+) @ 358.64 | 551.28 | 551.19 | 358.64 | 359.16 | 909.92 | 1461.2 | 1268.56 | 1461.2 |
| 42 | unclear | y8(2+) @ 560.81 & ??? @ 342.47 | 560.81 | 559.7 | 342.47 | nan | 903.28 | 1464.09 | 1245.75 | 1464.09 |
| 43 | unclear | y4(1+) @ 589.96 & ??? @ 329.12 | 589.96 | 588.29 | 329.12 | nan | 919.08 | 1509.04 | 1248.2 | 1509.04 |
| 44 | internal_acid | bi5-10 (1+) @ 840.36 & [b4 – H2O – NH3] (1+) @ 485.91 | 840.36 | 840.29 | 485.91 | 485.17 | 1326.27 | 2166.63 | 1812.18 | 1326.27 |
| 45 | undefined | 518.97 & 454.06 | 518.97 | nan | 454.06 | nan | 973.03 | 1492.0 | 1427.09 | 1492.0 |
| 46 | non_complementary | y5 (1+) @ 646.3 & [b4-HCOH – H2O] (1+) @ 456.09 | 646.3 | 645.32 | 456.09 | 472.18 | 1102.39 | 1748.69 | 1558.48 | 1558.48 |
| 47 | usable | y6 (1+) @ 889.27 & a3 (1+) @ 378.19 | 889.27 | 888.35 | 378.19 | 377.17 | 1267.46 | 2156.73 | 1645.65 | 1645.65 |
| 48 | non_complementary | [b4 – H2O – NH3] (1+) @ 484.86 & y2 (1+) @ 320.83 | 484.86 | 485.17 | 320.83 | 320.2 | 805.69 | 1290.55 | 1126.52 | 1290.55 |
| 49 | usable | y5 (2+) @ 323.7 & [a6-NH3] (1+) @ 832.58 | 323.7 | 323.16 | 832.58 | 833.22 | 1156.28 | 1479.98 | 1988.86 | 1479.98 |
| 50 | undefined | 567.88 & 374.49 | 567.88 | nan | 374.49 | nan | 942.37 | 1510.25 | 1316.86 | 1510.25 |

# [TWR(Me2)GGEEK+3H]3+




| | Cluster ID | Cluster Size | Median Mass (Da) | Difference from Actual Mass (Da) | |
|---|---|---|---|---|---|
| 0 | 0 | 7 | 992.300 | | -0.19302 |
| 1 | 1 | 9 | 974.240 | NH3/H2O | -18.25302 |
| 2 | 2 | 4 | 956.255 | NH3+H2O/2H2O/2NH3 | -36.23802 |

## Detailed Data

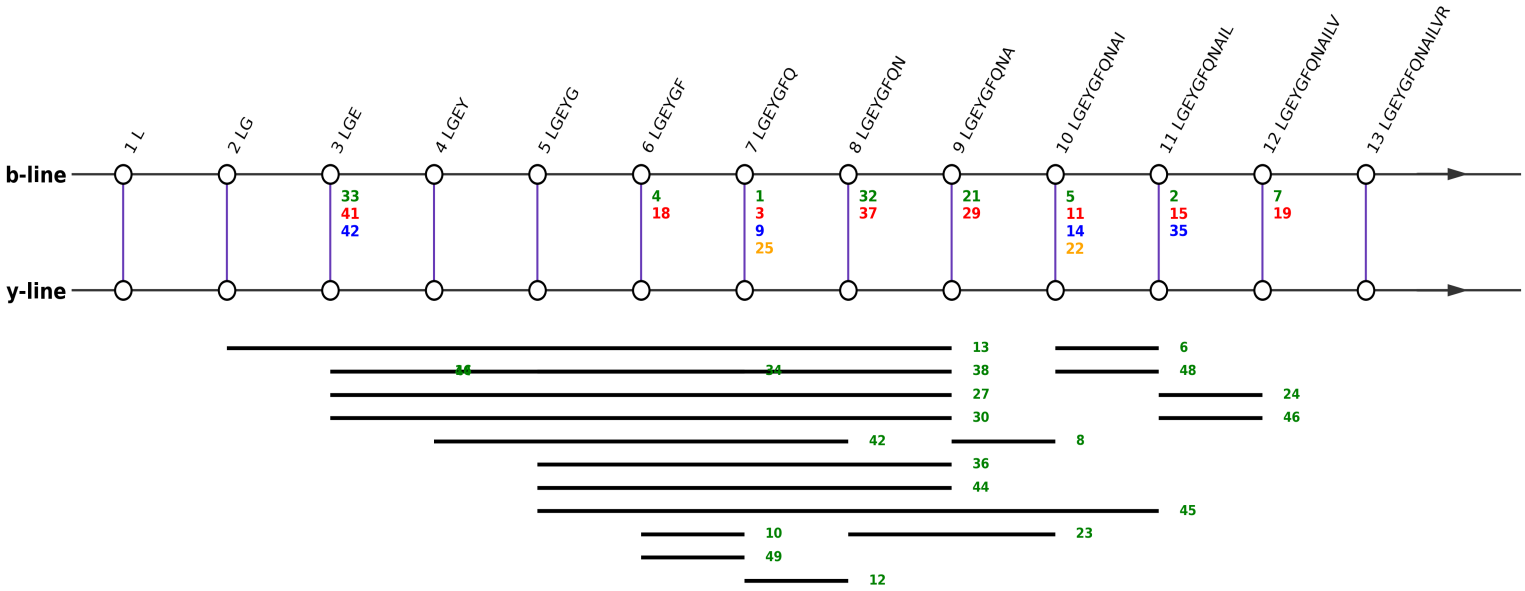
| n | classification | line | mass1 | correct_mass1 | mass2 | correct_mass2 | m1+m2 | 2m1+m2 | m1+2m2 | chosen_sum |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | usable | y5 (1+) @ 519.33 & b3 (2+) @ 236.46 | 519.33 | 519.24 | 236.46 | 236.64 | 755.79 | 1275.12 | 992.25 | 992.25 |
| 2 | usable | y6 (2+) @ 352.17 & b2 (1+) @ 287.97 | 352.17 | 352.19 | 287.97 | 288.13 | 640.14 | 992.31 | 928.11 | 992.31 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | usable | y2 (1+) @ 276.0 & b6 (2+) @ 358.22 | 276.0 | 276.16 | 358.22 | 358.18 | 634.22 | 910.22 | 992.44 | 992.44 |
| 4 | usable | y4 (1+) @ 462.2 & b4 (2+) @ 265.05 | 462.2 | 462.22 | 265.05 | 265.15 | 727.25 | 1189.45 | 992.3 | 992.3 |
| 5 | usable | y2 (1+) @ 275.95 & [b6-NH3] (2+) @ 349.0 | 275.95 | 276.16 | 349.0 | 349.67 | 624.95 | 900.9 | 973.95 | 973.95 |
| 6 | usable | y6 (2+) @ 352.25 & a2 (1+) @ 260.09 | 352.25 | 352.19 | 260.09 | 260.12 | 612.34 | 964.59 | 872.43 | 964.59 |
| 7 | usable | b4 (1+) @ 529.34 & Im(W) @ 158.68 | 529.34 | 529.29 | 158.68 | nan | 688.02 | 1217.36 | 846.7 | 846.7 |
| 8 | undefined | 379.75 & 197.76 | 379.75 | nan | 197.76 | nan | 577.51 | 957.26 | 775.27 | 957.26 |
| 9 | usable | [y3-NH3] (1+) @ 387.08 & [b5-NH3] (2+) @ 284.5 | 387.08 | 388.17 | 284.5 | 285.15 | 671.58 | 1058.66 | 956.08 | 956.08 |
| 10 | non_complementary | [y2-NH3] (2+) @ 129.42 & b7 (2+) @ 422.56 | 129.42 | 130.07 | 422.56 | 422.7 | 551.98 | 681.4 | 974.54 | 974.54 |
| 11 | internal_acid | [bi3-7 - HCOOH] (1+) @ 511.25 & Im (W) @ 158.67 | 511.25 | 511.26 | 158.67 | nan | 669.92 | 1181.17 | 828.59 | 828.59 |
| 12 | usable | y1(1+) @ 146.68 & [b7-NH3](2+) @ 413.81 | 146.68 | 147.11 | 413.81 | 414.19 | 560.49 | 707.17 | 974.3 | 974.3 |
| 13 | internal_acid | bi3-6 (1+) @ 428.14 & y2 (1+) @ 276.01 | 428.14 | 428.23 | 276.01 | 276.16 | 704.15 | 1132.29 | 980.16 | 980.16 |
| 14 | usable | y4 (1+) @ 462.16 & [b4-NH3] (2+) @ 255.92 | 462.16 | 462.22 | 255.92 | 256.63 | 718.08 | 1180.24 | 974.0 | 974.0 |
| 15 | internal_acid | bi2-6 (1+) @ 614.19 & y2 (1+) @ 276.05 | 614.19 | 614.3 | 276.05 | 276.16 | 890.24 | 1504.43 | 1166.29 | 890.24 |
| 16 | usable | y3 (1+) @ 405.15 & [b5-NH3] (2+) @ 284.45 | 405.15 | 405.2 | 284.45 | 285.15 | 689.6 | 1094.75 | 974.05 | 974.05 |
| 17 | usable | y5 (1+) @ 519.29 & [b3-NH3] (2+) @ 227.3 | 519.29 | 519.24 | 227.3 | 228.12 | 746.59 | 1265.88 | 973.89 | 973.89 |
| 18 | usable | y4 (2+) @ 231.48 & [b4-NH3] (1+) @ 511.28 | 231.48 | 231.61 | 511.28 | 512.26 | 742.76 | 974.24 | 1254.04 | 974.24 |
| 19 | usable | [y6 - CH3NHCH3] (1+) @ 658.39 & Im(W) 158.65 | 658.39 | 658.32 | nan | nan | nan | nan | nan | nan |
| 20 | undefined | 519.31 & 343.18 | 519.31 | nan | 343.18 | nan | 862.49 | 1381.8 | 1205.67 | 862.49 |
| 21 | usable | [y3-NH3] (1+) @ 387.17 & b5 (2+) @ 293.58 | 387.17 | 388.17 | 293.58 | 293.66 | 680.75 | 1067.92 | 974.33 | 974.33 |
| 22 | undefined | 583.42 & 243.89 | 583.42 | nan | 243.89 | nan | 827.31 | 1410.73 | 1071.2 | 1071.2 |
| 23 | usable | y5 (1+) @ 519.34 & [b3-H2O-NH3] (2+) @ 218.59 | 519.34 | 519.24 | 218.59 | 219.12 | 737.93 | 1257.27 | 956.52 | 956.52 |
| 24 | undefined | 360.8 & 257.89 | 360.8 | nan | 257.89 | nan | 618.69 | 979.49 | 876.58 | 979.49 |
| 25 | usable | y1 (1+) @ 146.68 & b7 (2+) @ 422.86 | 146.68 | 147.11 | 422.86 | 422.7 | 569.54 | 716.22 | 992.4 | 992.4 |
| 26 | non_complementary | [y2-NH3] (2+) @ 129.33 & [b7-NH3] (2+) @ 413.55 | 129.33 | 130.07 | 413.55 | 414.19 | 542.88 | 672.21 | 956.43 | 956.43 |
| 27 | internal_acid | [b4-NH3] (1+) @ 511.38 & bi5-6 (1+) @ 186.59 | 511.38 | 512.26 | 186.59 | 187.07 | 697.97 | 1209.35 | 884.56 | 884.56 |
| 28 | usable | [y2-NH3] (2+) @ 129.46 & a6(2+) @ 342.91 | 129.46 | 130.07 | 342.91 | 344.17 | 472.37 | 601.83 | 815.28 | 815.28 |
| 29 | usable | y6(2+) @ 353.02 & [b2-H2O] (1+) @ 268.68 | 353.02 | 352.19 | 268.68 | 270.12 | 621.7 | 974.72 | 890.38 | 974.72 |
| 30 | usable | y6 (2+) @ 352.16 & [y1-H2O] (1+) @ 117.43 | 352.16 | 352.19 | 117.43 | 129.1 | 469.59 | 821.75 | 587.02 | 821.75 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | internal_acid | bi2-3 (1+) @ 370.7 & ??? @ 197.72 | 370.7 | 371.22 | 197.72 | nan | 568.42 | 939.12 | 766.14 | 939.12 |
| 32 | usable | [b7+H2O] (2+) @ 431.82 & y1-H2O (1+)128.45 | 431.82 | 431.71 | nan | nan | nan | nan | nan | nan |
| 33 | internal_acid | bi3-6 (1+) @ 428.11 & b2 (1+) @ 287.75 | 428.11 | 428.23 | 287.75 | 288.13 | 715.86 | 1143.97 | 1003.61 | 1003.61 |
| 34 | usable | y3 (1+) @ 405.0 & b5 (2+) @ 293.55 | 405.0 | 405.2 | 293.55 | 293.66 | 698.55 | 1103.55 | 992.1 | 992.1 |
| 35 | usable | y4 (1+) @ 462.22 & [a4-NH3] (2+) @ 242.05 | 462.22 | 462.22 | 242.05 | 242.63 | 704.27 | 1166.49 | 946.32 | 946.32 |
| 36 | usable | y4 (2+) @ 230.81 & [a4-NH3] (1+) @ 485.42 | 230.81 | 231.61 | 485.42 | 484.25 | 716.23 | 947.04 | 1201.65 | 947.04 |
| 37 | unclear | y7-H2O (2+) 436.23 & ??? @ 118.35 | nan | nan | 118.35 | nan | nan | nan | nan | nan |
| 38 | usable | y5 (1+) @ 519.35 & [b3 - CH3NHCH3 – H2O] (2+) @ 205.31 | 519.35 | 519.24 | 205.31 | 205.1 | 724.66 | 1244.01 | 929.97 | 929.97 |
| 39 | non_complementary | y1 (1+) @ 147.54 & b6 (1+) @ 715.4 | 147.54 | 147.11 | 715.4 | 715.35 | 862.94 | 1010.48 | 1578.34 | 1010.48 |
| 40 | internal_acid | [y6 - CH3-NH-CH3] (1+) @ 658.42 & bi2-2 (1+) @ 186.66 | 658.42 | 658.32 | 186.66 | 187.09 | 845.08 | 1503.5 | 1031.74 | 1031.74 |
| 41 | usable | [b6 – H3C-N=CH2 - NH3] (1+) @ 654.37 & y2 (1+) @ y2 (1+) 275.92 | 654.37 | 655.28 | nan | nan | nan | nan | nan | nan |
| 42 | usable | y5 (1+) @ 519.11 & a2 (2+) @ 129.47 | 519.11 | 519.24 | 129.47 | 130.57 | 648.58 | 1167.69 | 778.05 | 1167.69 |
| 43 | usable | bi 2-5 (1+) @ 485.29 & [bi 6-7 – HCOOH] (1+) @ 212.85 | 485.29 | 485.26 | 212.85 | 213.09 | 698.14 | 1183.43 | 910.99 | 910.99 |
| 44 | internal_acid | y6 (2+) @ 352.4 & bi2-2 (1+) @ 186.67 | 352.4 | 352.19 | 186.67 | 187.09 | 539.07 | 891.47 | 725.74 | 891.47 |
| 45 | unclear | y5 (1+) @ 519.0 & ??? @ 177.74 | 519.0 | 519.24 | 177.74 | nan | 696.74 | 1215.74 | 874.48 | 874.48 |
| 46 | undefined | 697.71 & 101.31 | 697.71 | nan | 101.31 | nan | 799.02 | 1496.73 | 900.33 | 900.33 |
| 47 | usable | y5 (2+) @ 259.95 & b3 (1+) @ 472.14 | 259.95 | 260.12 | 472.14 | 472.27 | 732.09 | 992.04 | 1204.23 | 992.04 |
| 48 | usable | y1 (1+) @ 146.75 & a5 (1+) @ 557.2 | 146.75 | 147.11 | 557.2 | 558.3 | 703.95 | 850.7 | 1261.15 | 850.7 |
| 49 | undefined | 404.6 & 146.46 | 404.6 | nan | 146.46 | nan | 551.06 | 955.66 | 697.52 | 955.66 |
| 50 | undefined | 352.05 & 131.78 | 352.05 | nan | 131.78 | nan | 483.83 | 835.88 | 615.61 | 835.88 |

# [LGEY(nitro)GFQNAILVR+3H]3+

Fragmentation Diagram for: LGEYGFQNAILVR




| | Cluster ID | Cluster Size | Median Mass (Da) | Difference from Actual Mass (Da) |
|---|---|---|---|---|
| 0 | 0 | 8 | 1526.665 | -0.10821 |
| 1 | 1 | 2 | 1412.500 | -114.27321 |
| 2 | 2 | 2 | 1397.975 | -128.79821 |
| 3 | 3 | 11 | 1509.040 | NH3/H2O -17.73321 |

## Detailed Data

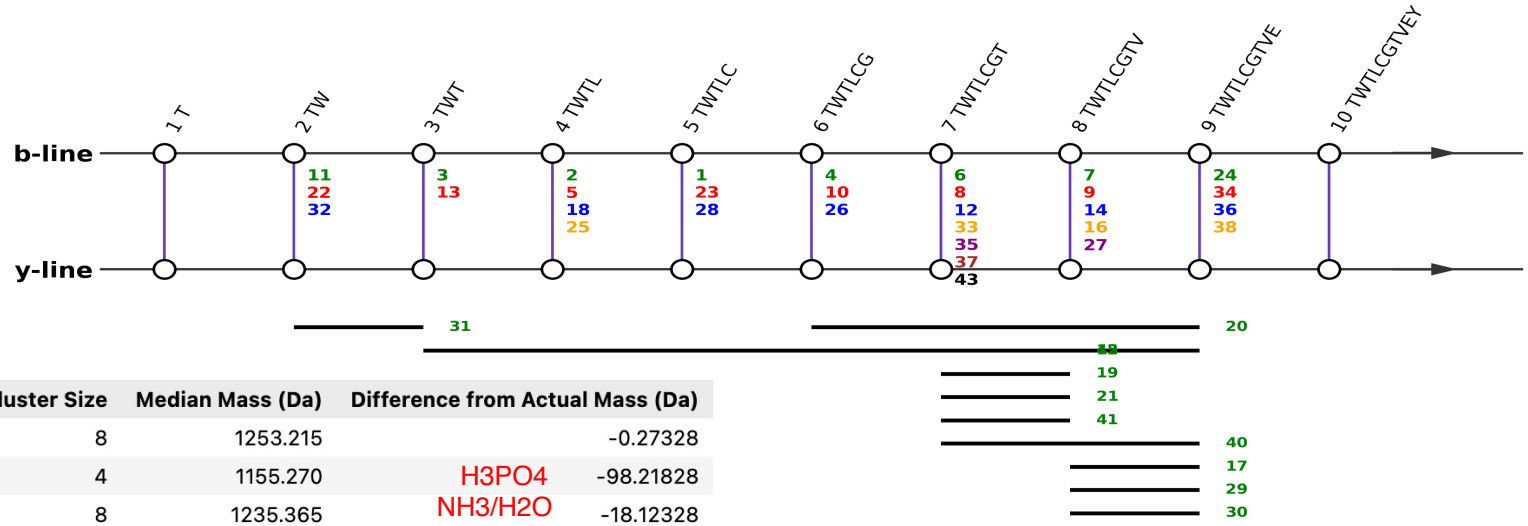
| n | classification | line | mass1 | correct_mass1 | mass2 | correct_mass2 | m1+m2 | 2m1+m2 | m1+2m2 | chosen_sum |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | usable | y6 (1+) @ 685.47 & b7 (2+) @ 420.68 | 685.47 | 685.44 | 420.68 | 420.68 | 1106.15 | 1791.62 | 1526.83 | 1526.83 |
| 2 | usable | y2 (1+) @ 274.0 & b11 (2+) @ 626.38 | 274.0 | 274.19 | 626.38 | 626.3 | 900.38 | 1174.38 | 1526.76 | 1526.76 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | usable | y6 (2+) @ 343.18 & b7 (1+) @ 840.4 | 343.18 | 343.22 | 840.4 | 840.35 | 1183.58 | 1526.76 | 2023.98 | 1526.76 |
| 4 | usable | y7 (2+) @ 407.31 & b6 (1+) @ 712.37 | 407.31 | 407.25 | 712.37 | 712.29 | 1119.68 | 1526.99 | 1832.05 | 1526.99 |
| 5 | usable | y3 (1+) @ 387.15 & b10 (2+) @ 569.71 | 387.15 | 387.27 | 569.71 | 569.76 | 956.86 | 1344.01 | 1526.57 | 1526.57 |
| 6 | non_complementary | y2 (1+) @ 273.94 & b10 (1+) @ 1138.46 | 273.94 | 274.19 | 1138.46 | 1138.52 | 1412.4 | 1686.34 | 2550.86 | 1412.4 |
| 7 | usable | y1 (1+) @ 174.65 & b12 (2+) @ 675.8 | 174.65 | 175.12 | 675.8 | 675.84 | 850.45 | 1025.1 | 1526.25 | 1526.25 |
| 8 | non_complementary | y3 (1+) @ 387.19 & b9 (1+) @ 1025.41 | 387.19 | 387.27 | 1025.41 | 1025.43 | 1412.6 | 1799.79 | 2438.01 | 1412.6 |
| 9 | usable | c6 (1+) @ 729.52 & y6 (1+) @ 685.6 | 729.52 | nan | 685.6 | 685.44 | 1415.12 | 2144.64 | 2100.72 | 1415.12 |
| 10 | non_complementary | y6 (1+) @ 685.52 & b6(1+) @ 712.65 | 685.52 | 685.44 | 712.65 | 712.29 | 1398.17 | 2083.69 | 2110.82 | 1398.17 |
| 11 | usable | y3 (2+) @ 193.8 & [b10-NH3] (1+) @ 1121.15 | 193.8 | 194.14 | 1121.15 | 1121.49 | 1314.95 | 1508.75 | 2436.1 | 1508.75 |
| 12 | internal_acid | b6 (1+) @ 712.35 & bi7-8 (1+) @ 242.83 | 712.35 | 712.29 | 242.83 | 243.11 | 955.18 | 1667.53 | 1198.01 | 1667.53 |
| 13 | internal_acid | bi2-9 (1+) @ 912.43 & y4 (1+) 500.2 | 912.43 | 912.35 | nan | nan | nan | nan | nan | nan |
| 14 | usable | y3 (1+) @ 387.1 & [b10-NH3] (2+) @ 560.95 | 387.1 | 387.27 | 560.95 | 561.25 | 948.05 | 1335.15 | 1509.0 | 1509.0 |
| 15 | usable | y2 (1+) @ 274.1 & [b11-NH3] (2+) @ 617.47 | 274.1 | 274.19 | 617.47 | 617.79 | 891.57 | 1165.67 | 1509.04 | 1509.04 |
| 16 | non_complementary | [y9-NH3] (2+) @ 500.36 & b8 (1+) @ 954.34 | 500.36 | 500.78 | 954.34 | 954.4 | 1454.7 | 1955.06 | 2409.04 | 1454.7 |
| 17 | internal_acid | B6 (1+) 712.44 & [bi7-10 – HCONH2] (1+) 382.53 | nan | nan | nan | nan | nan | nan | nan | nan |
| 18 | usable | [y7-NH3] (2+) @ 398.45 & b6 (1+) @ 712.41 | 398.45 | 398.74 | 712.41 | 712.29 | 1110.86 | 1509.31 | 1823.27 | 1509.31 |
| 19 | usable | y1(1+) @ 174.59 & [b12-NH3] (2+) @ 666.97 | 174.59 | 175.12 | 666.97 | 667.32 | 841.56 | 1016.15 | 1508.53 | 1508.53 |
| 20 | undefined | 518.11 & 319.86 | 518.11 | nan | 319.86 | nan | 837.97 | 1356.08 | 1157.83 | 1356.08 |
| 21 | usable | y4 (2+) @ 250.34 & b9 (1+) @ 1025.4 | 250.34 | 250.68 | 1025.4 | 1025.43 | 1275.74 | 1526.08 | 2301.14 | 1526.08 |
| 22 | usable | y3 (1+) @ 387.14 & [a10-NH3] (2+) @ 547.28 | 387.14 | 387.27 | 547.28 | 547.24 | 934.42 | 1321.56 | 1481.7 | 1481.7 |
| 23 | internal_acid | b7 (1+) @ 840.43 & [bi8-10 – HCONH2] (1+) @ 253.8 | 840.43 | 840.35 | 253.8 | 254.15 | 1094.23 | 1934.66 | 1348.03 | 1348.03 |
| 24 | non_complementary | y1 (1+) @ 174.67 & b11 (1+) @ 1251.44 | 174.67 | 175.12 | 1251.44 | 1251.6 | 1426.11 | 1600.78 | 2677.55 | 1600.78 |
| 25 | usable | y6 (2+) @ 343.17 & [b7-NH3] (1+) @ 822.63 | 343.17 | 343.22 | 822.63 | 823.33 | 1165.8 | 1508.97 | 1988.43 | 1508.97 |
| 26 | internal_acid | b6 (1+) @ 712.2 & [bi7-8 – NH3] (1+) 225.78 | 712.2 | 712.29 | nan | nan | nan | nan | nan | nan |
| 27 | internal_acid | bi3-9 (1+) @ 855.2 & y4 (1+) 500.38 | 855.2 | 855.33 | nan | nan | nan | nan | nan | nan |
| 28 | undefined | 840.47 & 298.93 | 840.47 | nan | 298.93 | nan | 1139.4 | 1979.87 | 1438.33 | 1438.33 |
| 29 | usable | y4 (2+) @ 250.5 & [b9-NH3] (1+) @ 1008.11 | 250.5 | 250.68 | 1008.11 | 1008.41 | 1258.61 | 1509.11 | 2266.72 | 1509.11 |
| 30 | internal_acid | [bi3-9 -H2O] (1+) @ 837.58 & y4 (1+) @ 500.18 | 837.58 | 837.32 | 500.18 | 500.36 | 1337.76 | 2175.34 | 1837.94 | 1337.76 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | usable | c7 (1+) @ 857.81 & [z6 – H2O] (1+) @ 325.64 | 857.81 | nan | 325.64 | nan | 1183.45 | 2041.26 | 1509.09 | 1509.09 |
| 32 | usable | y5 (2+) @ 286.06 & b8 (1+) @ 954.34 | 286.06 | 286.2 | 954.34 | 954.4 | 1240.4 | 1526.46 | 2194.74 | 1526.46 |
| 33 | usable | y10 (2+) @ 613.96 & b3 (1+) @ 299.83 | 613.96 | 613.32 | 299.83 | 300.16 | 913.79 | 1527.75 | 1213.62 | 1527.75 |
| 34 | non_complementary | y6 (1+) @ 685.7 & b5 (1+) @ 565.38 | 685.7 | 685.44 | 565.38 | 565.23 | 1251.08 | 1936.78 | 1816.46 | 1251.08 |
| 35 | usable | y2 (1+) @ 273.99 & ai10-11 (1+) @ 198.67 | 273.99 | 274.19 | 198.67 | 199.16 | 472.66 | 746.65 | 671.33 | 746.65 |
| 36 | internal_acid | bi5-9 (1+) @ 518.33 & y4 (1+) @ 500.42 | 518.33 | 518.24 | 500.42 | 500.36 | 1018.75 | 1537.08 | 1519.17 | 1519.17 |
| 37 | usable | y5 (2+) @ 286.06 & [b8-NH3] (1+) @ 937.39 | 286.06 | 286.2 | 937.39 | 937.37 | 1223.45 | 1509.51 | 2160.84 | 1509.51 |
| 38 | internal_acid | b7 (1+) @ 840.79 & bi8-9 (1+) @ 185.67 | 840.79 | 840.35 | 185.67 | 186.09 | 1026.46 | 1867.25 | 1212.13 | 1212.13 |
| 39 | usable | c11 (2+) @ 634.43 & [z2-H2O] (1+) @ 239.69 | 634.43 | nan | 239.69 | nan | 874.12 | 1508.55 | 1113.81 | 1508.55 |
| 40 | undefined | 447.1 & 337.82 | 447.1 | nan | 337.82 | nan | 784.92 | 1232.02 | 1122.74 | 1232.02 |
| 41 | usable | [y10-NH3] (2+) @ 604.9 & b3 (1+) @ 299.81 | 604.9 | 604.81 | 299.81 | 300.16 | 904.71 | 1509.61 | 1204.52 | 1509.61 |
| 42 | usable | bi(4-8) (1+) @ 655.43 & b3 (1+) @ 299.94 | 655.43 | 655.25 | 299.94 | 300.16 | 955.37 | 1610.8 | 1255.31 | 1610.8 |
| 43 | undefined | 537.05 & 461.15 | 537.05 | nan | 461.15 | nan | 998.2 | 1535.25 | 1459.35 | 1535.25 |
| 44 | internal_acid | bi5-9 (1+) @ 518.15 & [bi3-4 – HCOOH] (1+) @ 291.85 | 518.15 | 518.24 | 291.85 | 292.09 | 810.0 | 1328.15 | 1101.85 | 1328.15 |
| 45 | internal_acid | bi5-11 (1+) @ 744.47 & y2 (1+) @ 274.17 | 744.47 | 744.4 | 274.17 | 274.19 | 1018.64 | 1763.11 | 1292.81 | 1292.81 |
| 46 | non_complementary | y1 (1+) @ 174.58 & b11 (2+) @ 626.04 | 174.58 | 175.12 | 626.04 | 626.3 | 800.62 | 975.2 | 1426.66 | 1426.66 |
| 47 | undefined | 524.22 & 313.54 | 524.22 | nan | 313.54 | nan | 837.76 | 1361.98 | 1151.3 | 1361.98 |
| 48 | non_complementary | y2 (1+) @ 273.88 & [b10-NH3] (1+) @ 1122.11 | 273.88 | 274.19 | 1122.11 | 1121.49 | 1395.99 | 1669.87 | 2518.1 | 1395.99 |
| 49 | non_complementary | y6 (1+) @ 685.28 & b6 (2+) @ 356.25 | 685.28 | 685.44 | 356.25 | 356.65 | 1041.53 | 1726.81 | 1397.78 | 1397.78 |
| 50 | undefined | 395.09 & 332.94 | 395.09 | nan | 332.94 | nan | 728.03 | 1123.12 | 1060.97 | 1123.12 |

# [TWT(p)LCGTVEY+2H]2+

Fragmentation Diagram for: TWTLCGTVEY




| | Cluster ID | Cluster Size | Median Mass (Da) | Difference from Actual Mass (Da) | |
|---|---|---|---|---|---|
| 0 | 0 | 8 | 1253.215 | | -0.27328 |
| 1 | 1 | 4 | 1155.270 | H3PO4 | -98.21828 |
| 2 | 2 | 8 | 1235.365 | NH3/H2O | -18.12328 |
| 3 | 3 | 2 | 1217.560 | NH3 + H2O | -35.92828 |
| 4 | 4 | 4 | 1137.625 | H3PO4 + NH3/H2O | -115.86328 |
| 5 | 5 | 2 | 1216.720 | 2H2O | -36.76828 |

## Detailed Data

| n | classification | line | mass1 | correct_mass1 | mass2 | correct_mass2 | m1+m2 | 2m1+m2 | m1+2m2 | chosen_sum |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | usable | y5 (1+) @ 568.12 & b5 (1+) @ 685.12 | 568.12 | 568.26 | 685.12 | 685.24 | 1253.24 | 1821.36 | 1938.36 | 1253.24 |
| 2 | usable | y6 (1+) @ 671.16 & b4 (1+) @ 582.03 | 671.16 | 671.27 | 582.03 | 582.23 | 1253.19 | 1924.35 | 1835.22 | 1253.19 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | usable | y7 (1+) @ 784.38 & b3 (1+) @ 469.1 | 784.38 | 784.35 | 469.1 | 469.15 | 1253.48 | 2037.86 | 1722.58 | 1253.48 |
| 4 | usable | y4 (1+) @ 511.14 & b6 (1+) @ 742.16 | 511.14 | 511.24 | 742.16 | 742.26 | 1253.3 | 1764.44 | 1995.46 | 1253.3 |
| 5 | usable | y6 (1+) @ 671.17 & [b4-H3PO4] (1+) @ 484.11 | 671.17 | 671.27 | 484.11 | 484.26 | 1155.28 | 1826.45 | 1639.39 | 1155.28 |
| 6 | usable | y3 (1+) @ 410.06 & b7 (1+) @ 843.07 | 410.06 | 410.19 | 843.07 | 843.31 | 1253.13 | 1663.19 | 2096.2 | 1253.13 |
| 7 | usable | [y2-NH3 ] (1+) @ 292.81 & b8 (1+) @ 942.06 | 292.81 | 294.1 | 942.06 | 942.38 | 1234.87 | 1527.68 | 2176.93 | 1234.87 |
| 8 | usable | y3 (1+) @ 410.14 & [b7-H3PO4] (1+) @ 745.45 | 410.14 | 410.19 | 745.45 | 745.33 | 1155.59 | 1565.73 | 1901.04 | 1155.59 |
| 9 | usable | [y2-H2O] (1+) @ 292.99 & [b8-NH3] (1+) @ 924.66 | 292.99 | 293.11 | 924.66 | 925.35 | 1217.65 | 1510.64 | 2142.31 | 1217.65 |
| 10 | usable | y4 (1+) @ 511.35 & [b6-H3PO4] (1+) @ 644.83 | 511.35 | 511.24 | 644.83 | 644.29 | 1156.18 | 1667.53 | 1801.01 | 1156.18 |
| 11 | usable | [y8-NH3] (1+) @ 949.32 & b2 (1+) @ 287.66 | 949.32 | 948.34 | 287.66 | 288.13 | 1236.98 | 2186.3 | 1524.64 | 1236.98 |
| 12 | usable | y3 (1+) @ 410.08 & [b7-NH3] (1+) @ 825.18 | 410.08 | 410.19 | 825.18 | 826.28 | 1235.26 | 1645.34 | 2060.44 | 1235.26 |
| 13 | usable | [y7-NH3] (1+) @ 766.69 & b3 (1+) @ 469.17 | 766.69 | 767.33 | 469.17 | 469.15 | 1235.86 | 2002.55 | 1705.03 | 1235.86 |
| 14 | usable | y2 (1+) @ 310.82 & b8 (1+) @ 941.96 | 310.82 | 311.12 | 941.96 | 942.38 | 1252.78 | 1563.6 | 2194.74 | 1252.78 |
| 15 | non_complementary | b9 (1+) @ 942.37 & [y2 – HCOOH – H2O] (1+) @ 246.94 | 942.37 | 1071.42 | 246.94 | 247.11 | 1189.31 | 2131.68 | 1436.25 | 1189.31 |
| 16 | usable | y2 (1+) @ 310.96 & [b8-NH3] (1+) @ 924.24 | 310.96 | 311.12 | 924.24 | 925.35 | 1235.2 | 1546.16 | 2159.44 | 1235.2 |
| 17 | internal_acid | b7 (1+) @ 843.12 & bi8-9 (1+) @ 228.81 | 843.12 | 843.31 | 228.81 | 229.12 | 1071.93 | 1915.05 | 1300.74 | 1300.74 |
| 18 | usable | [y6-NH3] (1+) @ 653.25 & [b4-H3PO4] (1+) @ 484.86 | 653.25 | 654.24 | 484.86 | 484.26 | 1138.11 | 1791.36 | 1622.97 | 1138.11 |
| 19 | non_complementary | [y2-NH3] (1+) @ 292.74 & b7 (1+) @ 844.74 | 292.74 | 294.1 | 844.74 | 843.31 | 1137.48 | 1430.22 | 1982.22 | 1137.48 |
| 20 | internal_acid | b5 (1+) @ 685.65 & bi6-9 (1+) @ 387.07 | 685.65 | 685.24 | 387.07 | 387.19 | 1072.72 | 1758.37 | 1459.79 | 1072.72 |
| 21 | non_complementary | y2 (1+) @ 310.67 & b7 (1+) @ 844.47 | 310.67 | 311.12 | 844.47 | 843.31 | 1155.14 | 1465.81 | 1999.61 | 1155.14 |
| 22 | usable | [y8-NH3] (1+) @ 947.45 & a2 (1+) @ 259.8 | 947.45 | 948.34 | 259.8 | 260.12 | 1207.25 | 2154.7 | 1467.05 | 1207.25 |
| 23 | usable | y5 (1+) @ 568.07 & [b5-H3PO4] (1+) @ 587.19 | 568.07 | 568.26 | 587.19 | 587.26 | 1155.26 | 1723.33 | 1742.45 | 1155.26 |
| 24 | usable | y1 (1+) @ 181.5 & [b9-NH3] (1+) @ 1053.38 | 181.5 | 182.08 | 1053.38 | 1054.4 | 1234.88 | 1416.38 | 2288.26 | 1234.88 |
| 25 | usable | [y6-NH3] (1+) @ 653.29 & b4 (1+) @ 582.18 | 653.29 | 654.24 | 582.18 | 582.23 | 1235.47 | 1888.76 | 1817.65 | 1235.47 |
| 26 | usable | y4 (1+) @ 511.3 & [b6-NH3] (1+) @ 724.3 | 511.3 | 511.24 | 724.3 | 725.24 | 1235.6 | 1746.9 | 1959.9 | 1235.6 |
| 27 | usable | [b8-H2O] (1+) @ 924.37 & [y2 – HCOOH – H2O] (1+) @ 246.98 | 924.37 | 924.37 | 246.98 | 247.11 | 1171.35 | 2095.72 | 1418.33 | 1171.35 |
| 28 | usable | [y5-NH3] (1+) @ 550.54 & b5 (1+) @ 685.25 | 550.54 | 551.23 | 685.25 | 685.24 | 1235.79 | 1786.33 | 1921.04 | 1235.79 |
| 29 | internal_acid | [b7-H2O] (1+) @ 825.19 & bi8-9 (1+) @ 228.81 | 825.19 | 825.3 | 228.81 | 229.12 | 1054.0 | 1879.19 | 1282.81 | 1282.81 |
| 30 | internal_acid | [b7-H3PO4] (1+) 745.72 & bi8-9 (1+) @ 228.74 | nan | nan | 228.74 | 229.12 | nan | nan | nan | nan |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | non_complementary | y7 (1+) @ 784.12 & b2 (1+) @ 287.76 | 784.12 | 784.35 | 287.76 | 288.13 | 1071.88 | 1856.0 | 1359.64 | 1359.64 |
| 32 | usable | y8 (1+) @ 965.41 & b2 (1+) @ 287.94 | 965.41 | 965.37 | 287.94 | 288.13 | 1253.35 | 2218.76 | 1541.29 | 1253.35 |
| 33 | usable | [b7-2(H2O)]/[b7-NH3-H2O] (1+) @ 807.36 & y3 (1+) @ 410.11 | 807.36 | nan | 410.11 | 410.19 | 1217.47 | 2024.83 | 1627.58 | 1217.47 |
| 34 | usable | y1(1+) @ 181.74 & [b9-H3PO4] (1+) @ 973.65 | 181.74 | 182.08 | 973.65 | 973.44 | 1155.39 | 1337.13 | 2129.04 | 1337.13 |
| 35 | usable | [b7-H3PO4-H2O] (1+) @ 727.27 & y3 (1+) @ 410.25 | 727.27 | 727.32 | 410.25 | 410.19 | 1137.52 | 1864.79 | 1547.77 | 1137.52 |
| 36 | usable | y1 (1+) @ 181.38 & b9 (1+) @ 1071.1 | 181.38 | 182.08 | 1071.1 | 1071.42 | 1252.48 | 1433.86 | 2323.58 | 1252.48 |
| 37 | usable | b7 (1+) @ 843.61 & ai8-9 (1+) @ 200.62 | 843.61 | 843.31 | 200.62 | 201.11 | 1044.23 | 1887.84 | 1244.85 | 1244.85 |
| 38 | usable | [b9-H3PO4-H2O] (1+) @ 955.76 & y1 (1+) 181.5 | 955.76 | 955.43 | nan | nan | nan | nan | nan | nan |
| 39 | unclear | ??? @ 867.7 & [y2 – H2O] (1+) @ 291.9 | 867.7 | nan | 291.9 | 293.11 | 1159.6 | 2027.3 | 1451.5 | 1159.6 |
| 40 | internal_acid | b6 (1+) @ 743.52 & bi7-9 (1+) @ 329.71 | 743.52 | 742.26 | 329.71 | 330.17 | 1073.23 | 1816.75 | 1402.94 | 1402.94 |
| 41 | non_complementary | y2 (1+) @ 311.27 & [b7-NH3] (1+) @ 826.46 | 311.27 | 311.12 | 826.46 | 826.28 | 1137.73 | 1449.0 | 1964.19 | 1137.73 |
| 42 | internal_acid | bi3-8 (1+) @ 627.78 & y2 (1+) @ 310.79 | 627.78 | 655.25 | 310.79 | 311.12 | 938.57 | 1566.35 | 1249.36 | 1249.36 |
| 43 | usable | [y3-NH3] (1+) @ 392.06 & [b7-NH3] (1+) @ 824.85 | 392.06 | 393.17 | 824.85 | 826.28 | 1216.91 | 1608.97 | 2041.76 | 1216.91 |
| 44 | undefined | 728.32 & 569.4 | 728.32 | nan | 569.4 | nan | 1297.72 | 2026.04 | 1867.12 | 1297.72 |
| 45 | undefined | 844.84 & 274.35 | 844.84 | nan | 274.35 | nan | 1119.19 | 1964.03 | 1393.54 | 1119.19 |
| 46 | undefined | 844.25 & 806.82 | 844.25 | nan | 806.82 | nan | 1651.07 | 2495.32 | 2457.89 | 1651.07 |
| 47 | undefined | 587.33 & 538.42 | 587.33 | nan | 538.42 | nan | 1125.75 | 1713.08 | 1664.17 | 1125.75 |
| 48 | undefined | 535.98 & 435.95 | 535.98 | nan | 435.95 | nan | 971.93 | 1507.91 | 1407.88 | 1407.88 |
| 49 | undefined | 939.22 & 609.33 | 939.22 | nan | 609.33 | nan | 1548.55 | 2487.77 | 2157.88 | 1548.55 |
| 50 | undefined | 941.73 & 274.8 | 941.73 | nan | 274.8 | nan | 1216.53 | 2158.26 | 1491.33 | 1216.53 |