

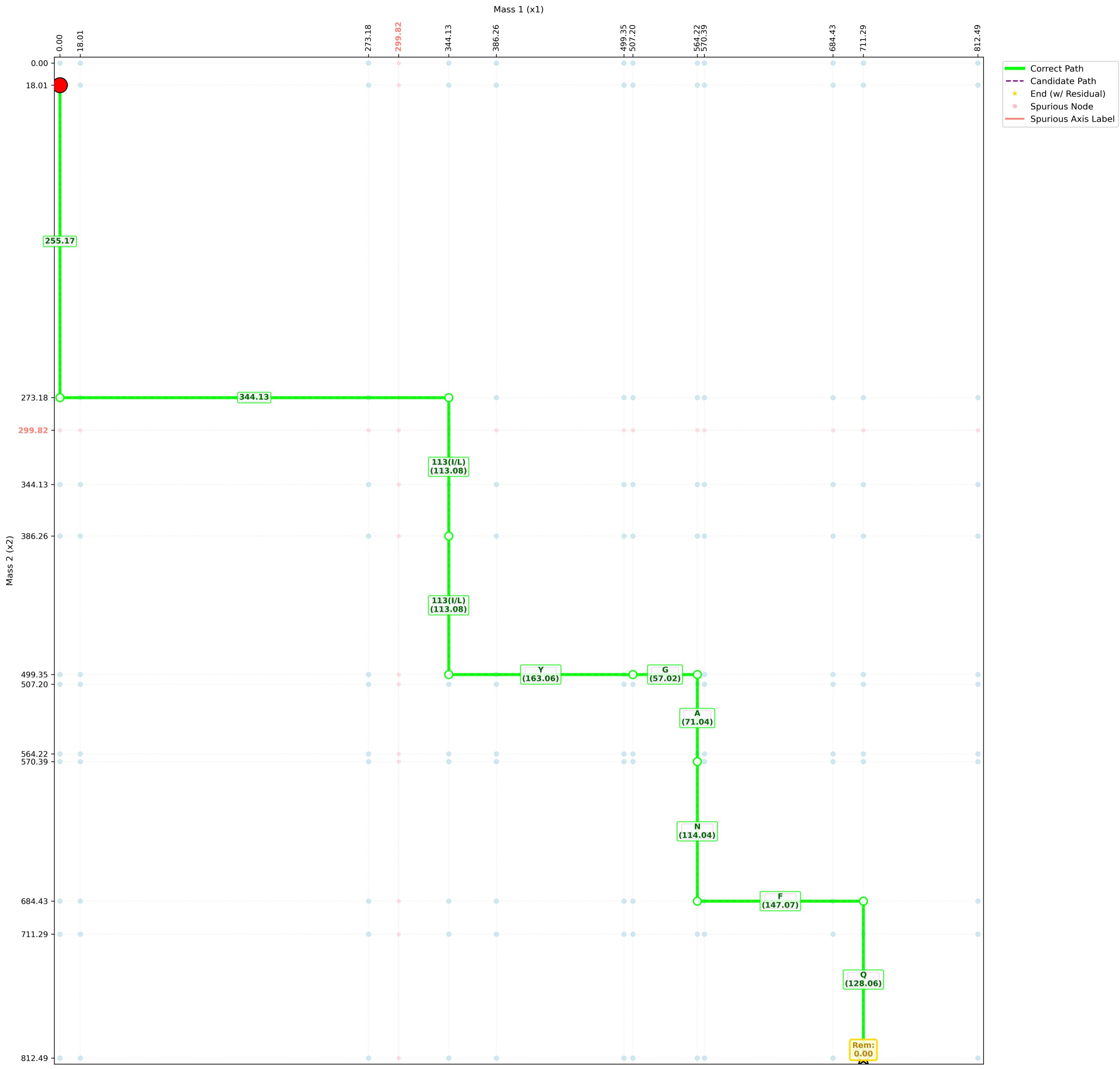
b-ion

y-ion

Spurious

| | LGE(nitro) | A | Y | G | F | Q | N | A | I | L | VR | | | | |
|---------------------|------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|----------|----------|----------|----------|----------|
| Ground Truth | 273.180 | 344.133 | 386.264 | 499.348 | 507.196 | 564.218 | 570.385 | 684.428 | 812.487 | 953.388 | 1024.425 | 1137.509 | 1179.640 | 1250.593 | 1487.752 |
| Peptide 1 | | 344.133 | | | 507.196 | 564.218 | | 711.286 | | 839.345 | 1024.425 | 1137.509 | | 1250.593 | |

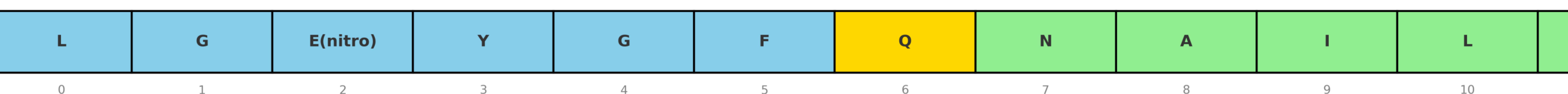
ME4_2+: [LGE(nitro)YGFQNAILVR+2H]2+



| | b1y12(L) | b2y11(G) | b3y10(E(nitro)) | b4y9(Y) | b5y8(G) | b6y7(F) | b7y6(Q) | b8y5(N) | b9y4(A) | b10y3(I) | b11y2(L) | b12y1(V) | Row_Count | Unexplained Count | Abs Average Mass Difference | Unexplained Pairs | |
|-----------|---------------------|----------------------|----------------------|---|---|--|--|---|---|--|--|----------------------|-----------|-------------------|-----------------------------|-------------------|---|
| Parent | -- | -- | -- | (b4,y9) (1+, 1+) (-0.05, 0.16) 1 | (b5,y8) (1+, 1+) (0.05, 0.15) 11 | (b6,y7) (1+, 1+) (0.11, 0.03) 4 | (b7,y6) (1+, 1+) (0.04, 0.07) 2 | (b8,y5) (1+, 1+) (0.03, 0.0) 5 | (b9,y4) (1+, 1+) (0.03, -0.01) 7 | (b10,y3) (1+, 1+) (-0.19, -0.19) 12 | (b11,y2) (1+, 1+) (-0.31, -0.19) 18 | -- | 8 | 1 | 0.2 | -0.3(26) | |
| Col_Count | 0 | 0 | 0 | 3 | 4 | 4 | 3 | 3 | 2 | 3 | 2 | 0 | 24 | 2 | 0.34 | nan | |
| Ion Mass | (114.09, 1411.7) | (171.11, 1354.67) | (345.14, 1180.65) | (508.2, 1017.58) | (565.23, 960.56) | (712.29, 813.49) | (840.35, 685.44) | (954.4, 571.39) | (1025.43, 500.36) | (1138.52, 387.27) | (1251.6, 274.19) | (1350.67, 175.12) | 0 | 0 | 0 | 0.0 | 0 |

Array Visualization (Target Index: 6)

- Before Index
- At Index
- After Index



b-ion

y-ion

Middle Point

273.18 **344.133** **386.264** **499.348** **507.196** **564.218** **570.385** **684.428** **711.286** **812.487** **812.487**