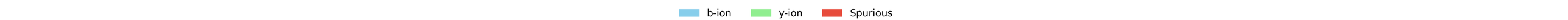
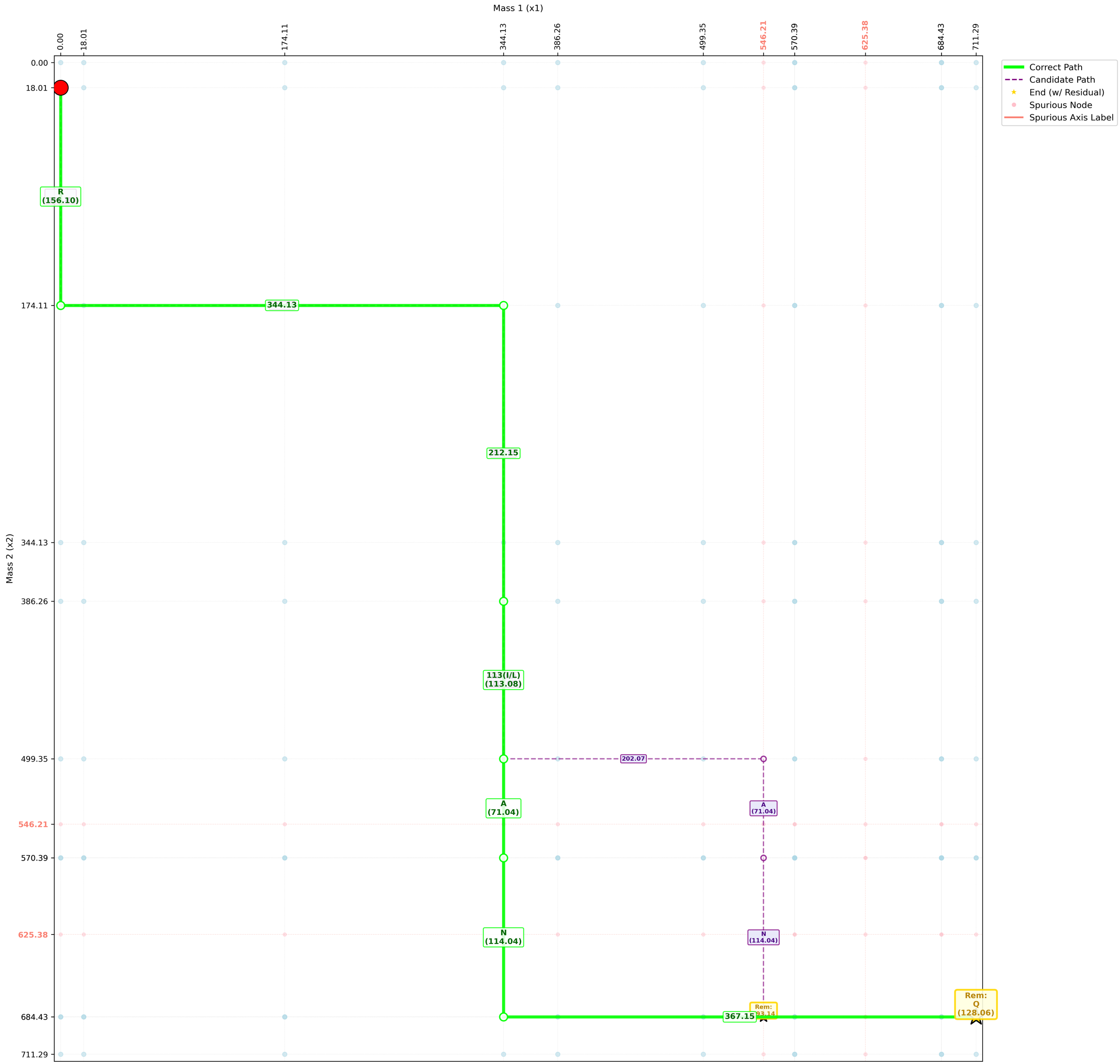
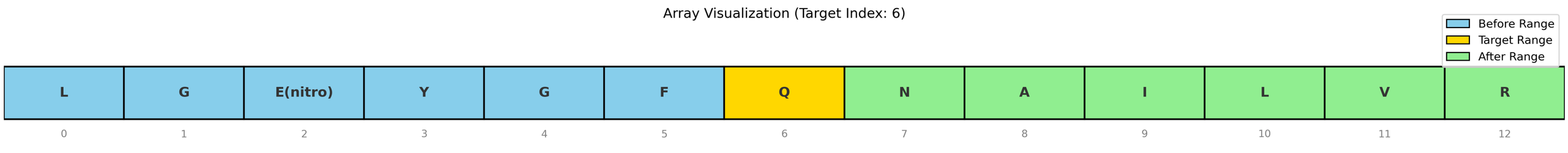
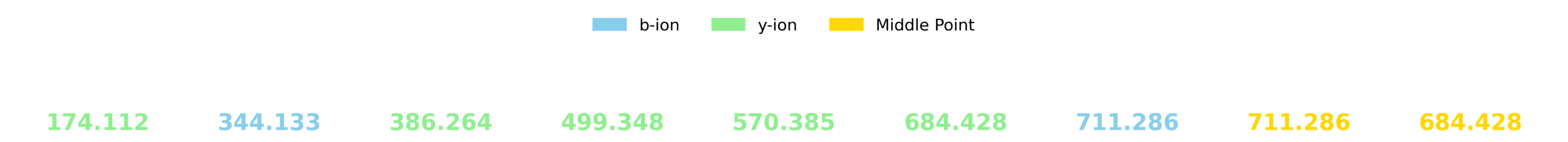

b-ion
y-ion
Spurious
LGE(nitro)
YGF
Q
N
A
I
LV
R
Ground Truth
174.112
344.133
386.264
499.348
546.207
570.385
625.380
684.428
711.286
812.487
839.345
953.388
1024.425
1137.509
1179.640
1349.661
1505.763
Peptide 1
344.133
546.207
839.345
953.388
1024.425
1137.509
1349.661

ME4_3+: [LGE(nitro)YGFQNAILVR+3H]3+



	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	--	--	--	--	--	(b6,y7) (1+ , 2+) (0.06, 0.08) 4	(b7,y6) (1+ , 2+) (-0.04, 0.05) 3	(b8,y5) (1+ , 2+) (-0.14, -0.06) 33	(b9,y4) (1+ , 2+) (-0.34, -0.03) 22	(b10,y3) (2+ , 1+) (-0.12, -0.05) 5	--	(b12,y1) (2+ , 1+) (-0.47, -0.04) 7	6	0	0.24	
Col_Count	0	0	0	0	0	2	2	2	2	2	1	2	13	2	0.12	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


Array Visualization (Target Index: 6)
Before Range
Target Range
After Range
L
G
E(nitro)
Y
G
F
Q
N
A
I
L
V
R
0
1
2
3
4
5
6
7
8
9
10
11
12


b-ion
y-ion
Middle Point
174.112
344.133
386.264
499.348
570.385
684.428
711.286
711.286
684.428