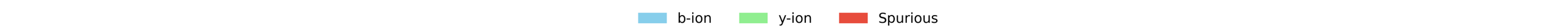
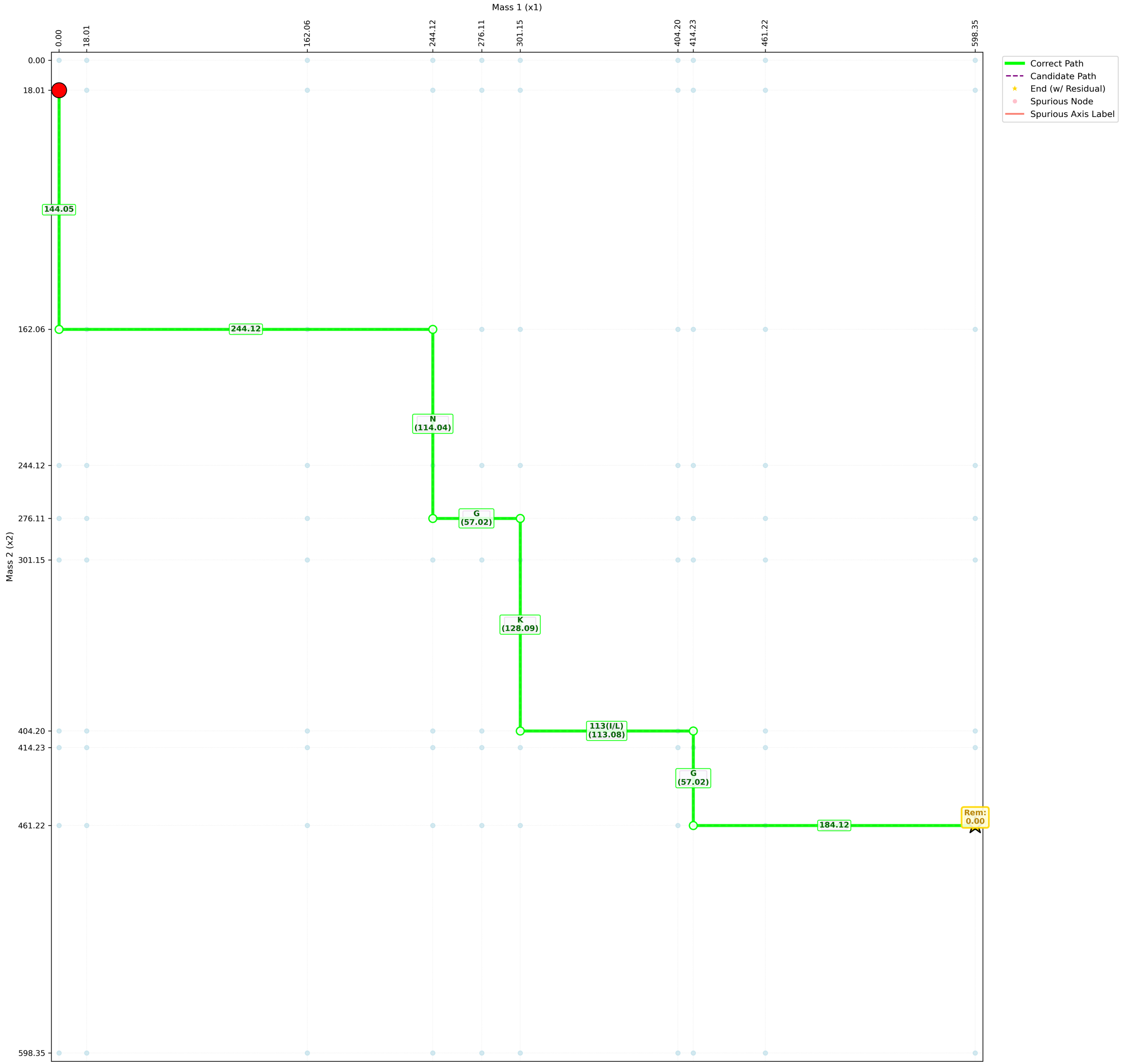
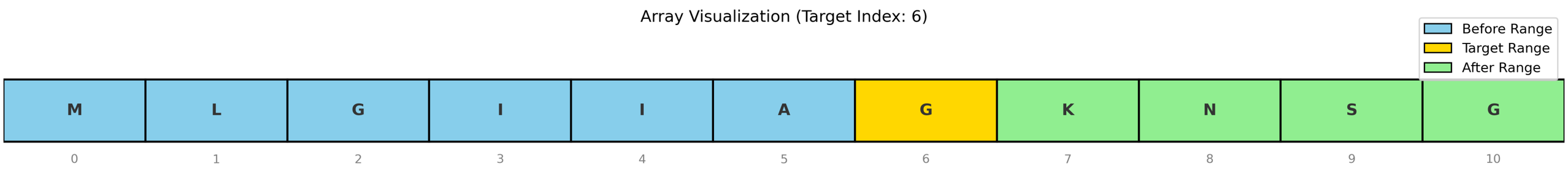

b-ion
y-ion
Spurious
ML
G
I
IA
G
K
N
SG
Ground Truth
162.064
244.125
276.107
301.146
404.202
414.230
461.223
598.351
645.345
655.373
758.429
783.468
815.450
897.511
1041.564
Peptide 1
244.125
301.146
414.230
598.351
655.373
783.468
897.511

UN15_2+: [MLGIIAGKNSG+2H]2+



	b1y10(M)	b2y9(L)	b3y8(G)	b4y7(I)	b5y6(I)	b6y5(A)	b7y4(G)	b8y3(K)	b9y2(N)	b10y1(S)	Row_Count	Unexplained Count	Abs Average Mass Difference	Unexplained Pairs
Parent	--	(b2,y9) (1+ , 1+) (-0.39, 0.17) 6	(b3,y8) (1+ , 1+) (-0.15, 0.0) 7	(b4,y7) (1+ , 1+) (-0.21, -0.05) 4	--	(b6,y5) (1+ , 1+) (-0.08, -0.04) 1	(b7,y4) (1+ , 1+) (-0.11, 0.03) 2	(b8,y3) (1+ , 1+) (-0.29, -0.04) 9	(b9,y2) (1+ , 1+) (-0.42, 0.16) 11	--	7	0	0.31	
Col_Count	0	3	1	3	0	4	2	2	2	0	17	1	0.14	nan
Ion Mass	(132.05, 929.54)	(245.13, 816.46)	(302.15, 759.44)	(415.24, 646.35)	(528.32, 533.27)	(599.36, 462.23)	(656.38, 405.21)	(784.47, 277.11)	(898.52, 163.07)	(985.55, 76.04)	0	0	0.0	0


Array Visualization (Target Index: 6)
Before Range
Target Range
After Range
M
L
G
I
I
A
G
K
N
S
G
0
1
2
3
4
5
6
7
8
9
10

b-ion
y-ion
Middle Point
162.064
244.125
276.107
301.146
404.202
414.23
461.223
598.351
598.351
461.223