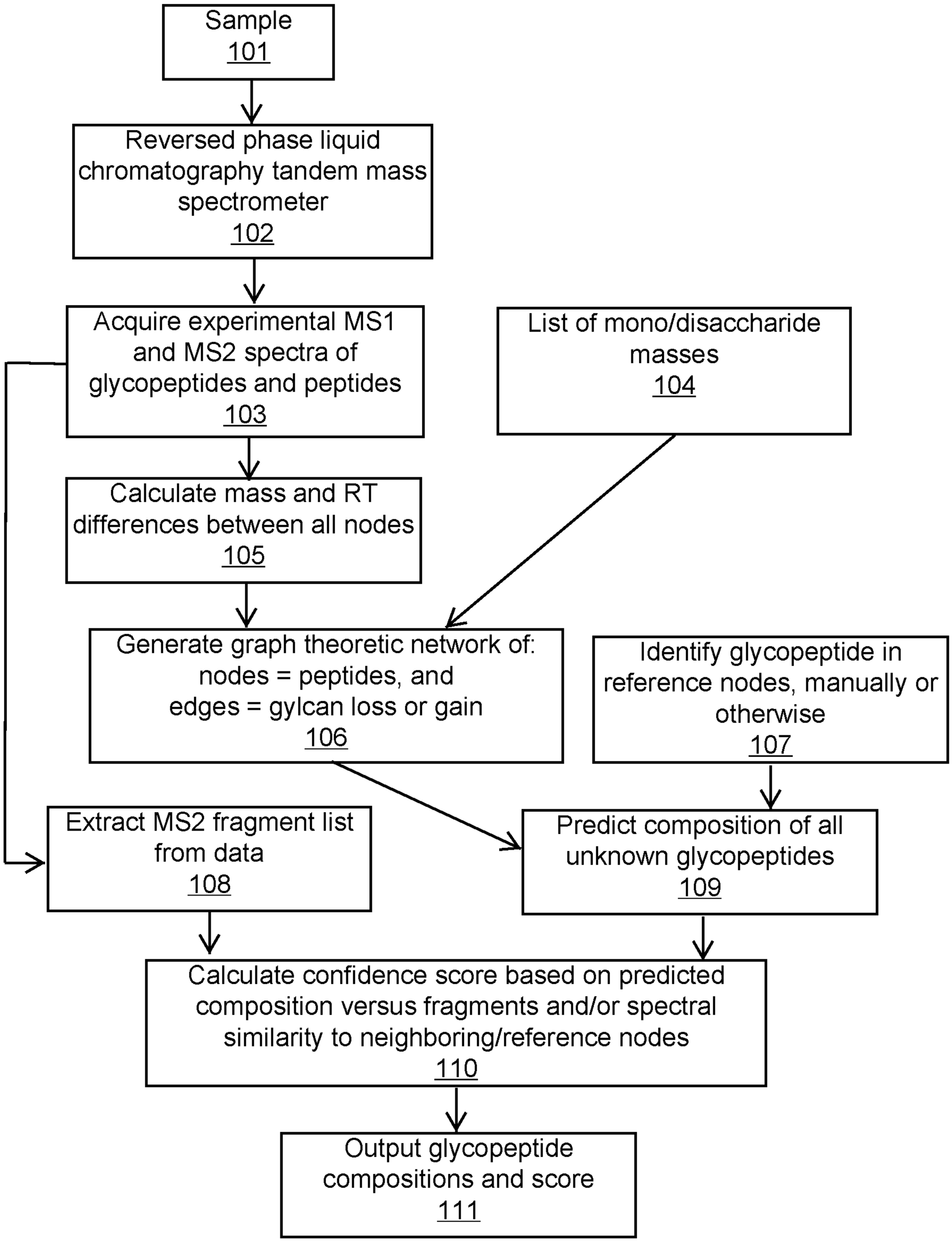

Sample
101
Reversed phase liquid chromatography tandem mass spectrometer
102
Acquire experimental MS1 and MS2 spectra of glycopeptides and peptides
103
List of mono/disaccharide masses
104
Calculate mass and RT differences between all nodes
105
Generate graph theoretic network of:
nodes = peptides, and
edges = gylcan loss or gain
106
Identify glycopeptide in reference nodes, manually or otherwise
107
Extract MS2 fragment list from data
108
Predict composition of all unknown glycopeptides
109
Calculate confidence score based on predicted composition versus fragments and/or spectral similarity to neighboring/reference nodes
110
Output glycopeptide compositions and score
111

Figure 1

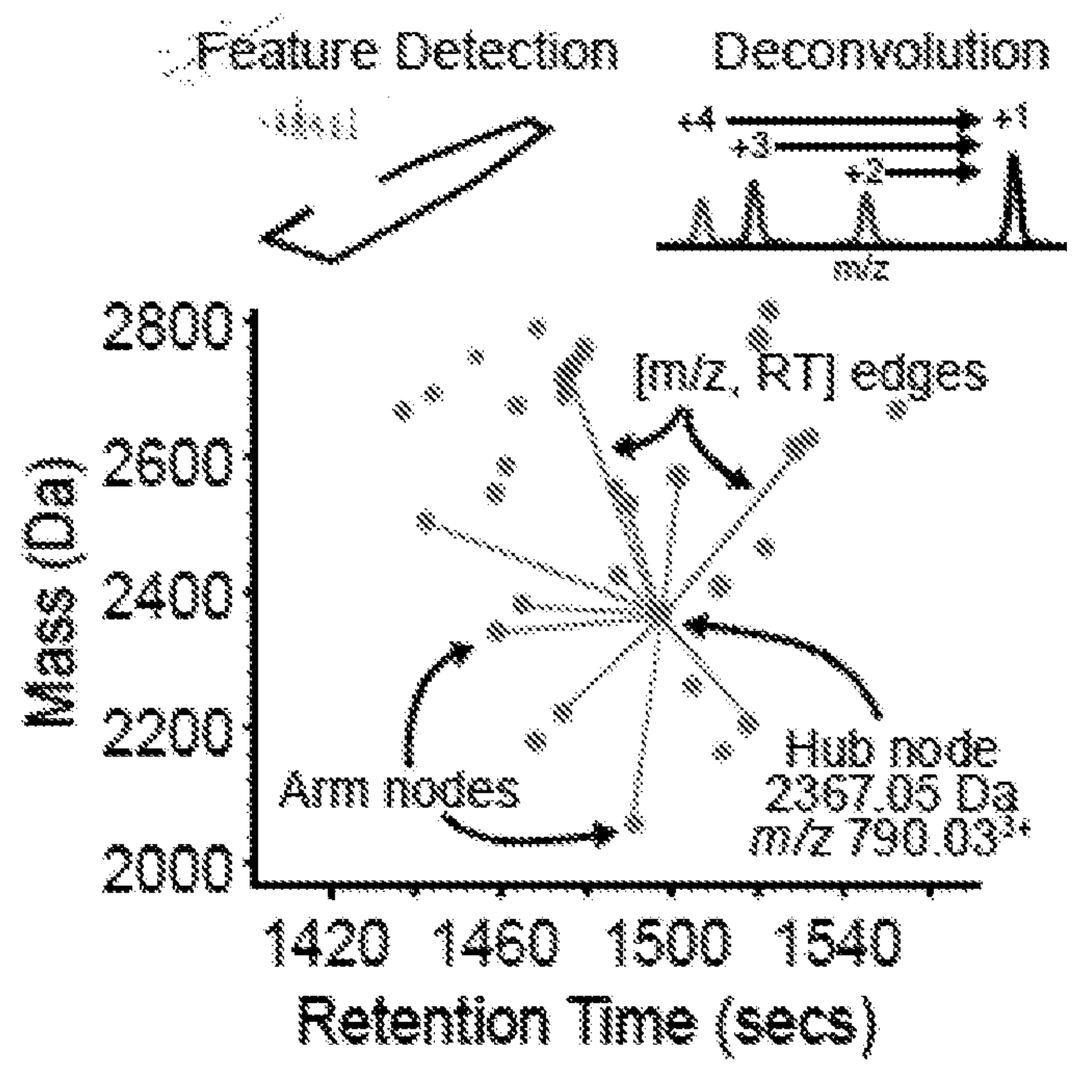


Figure 2a

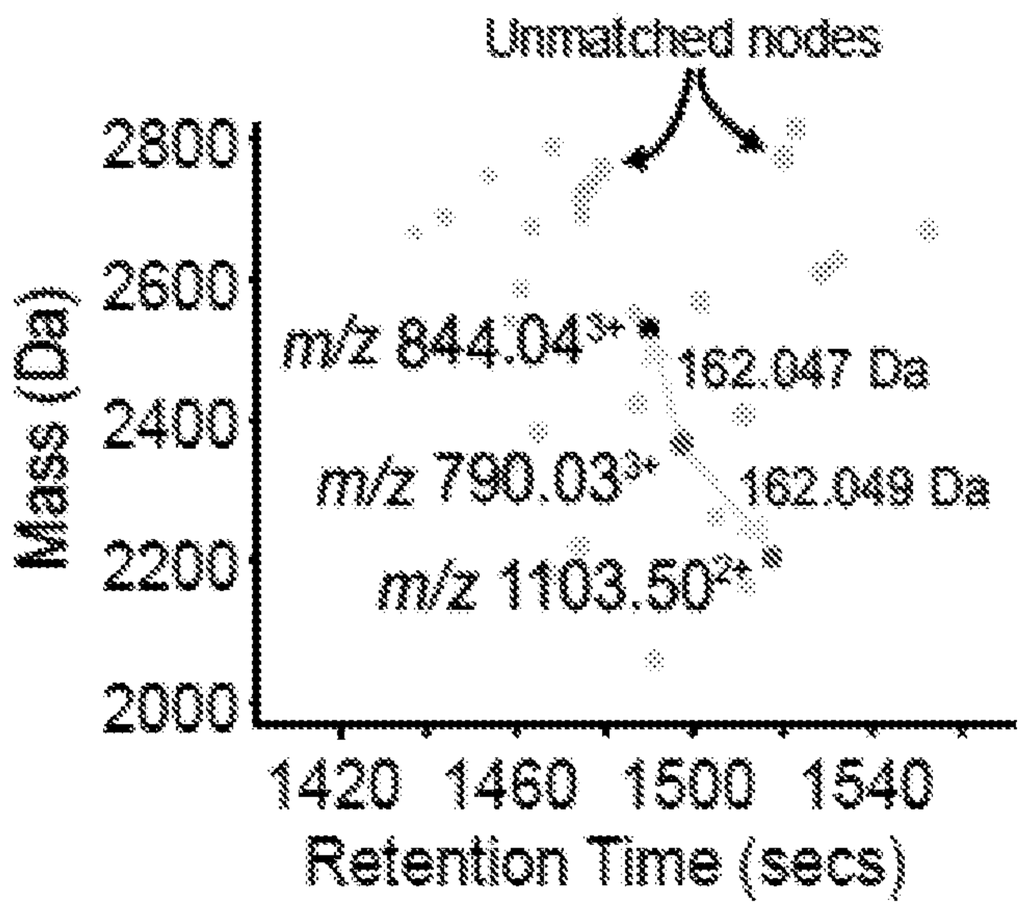


Figure 2b

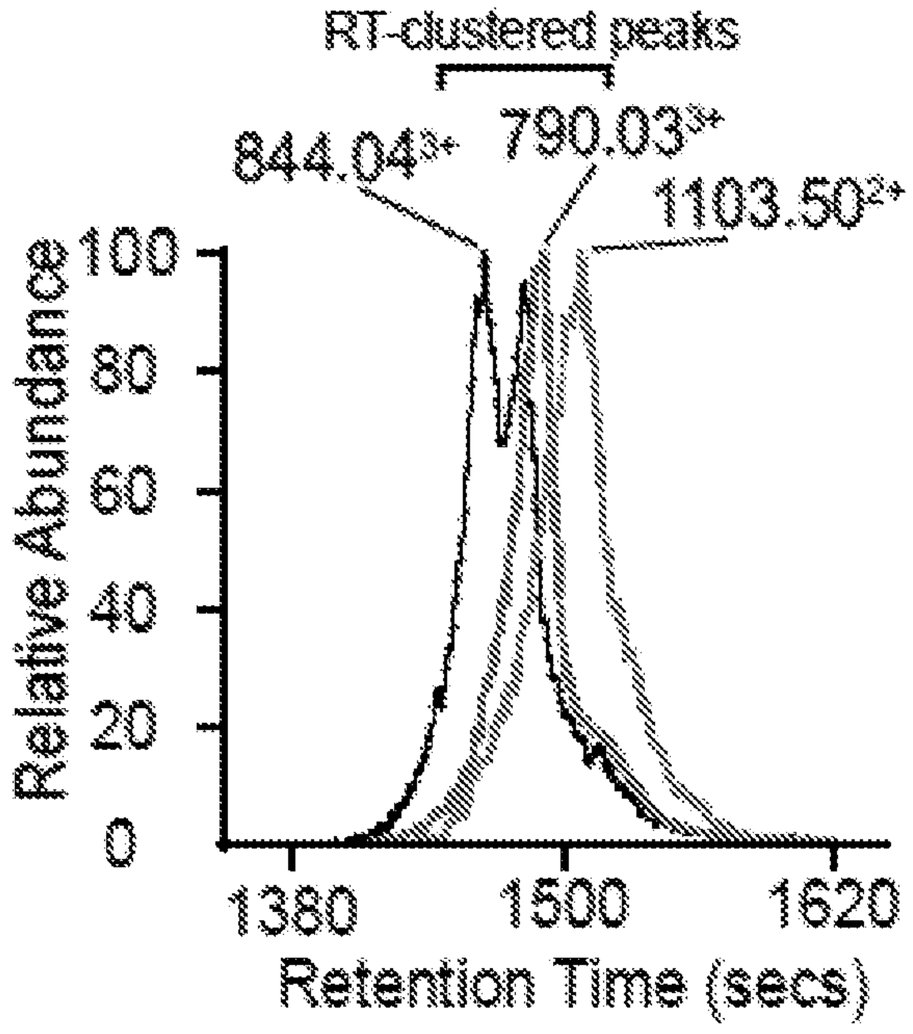


Figure 2c

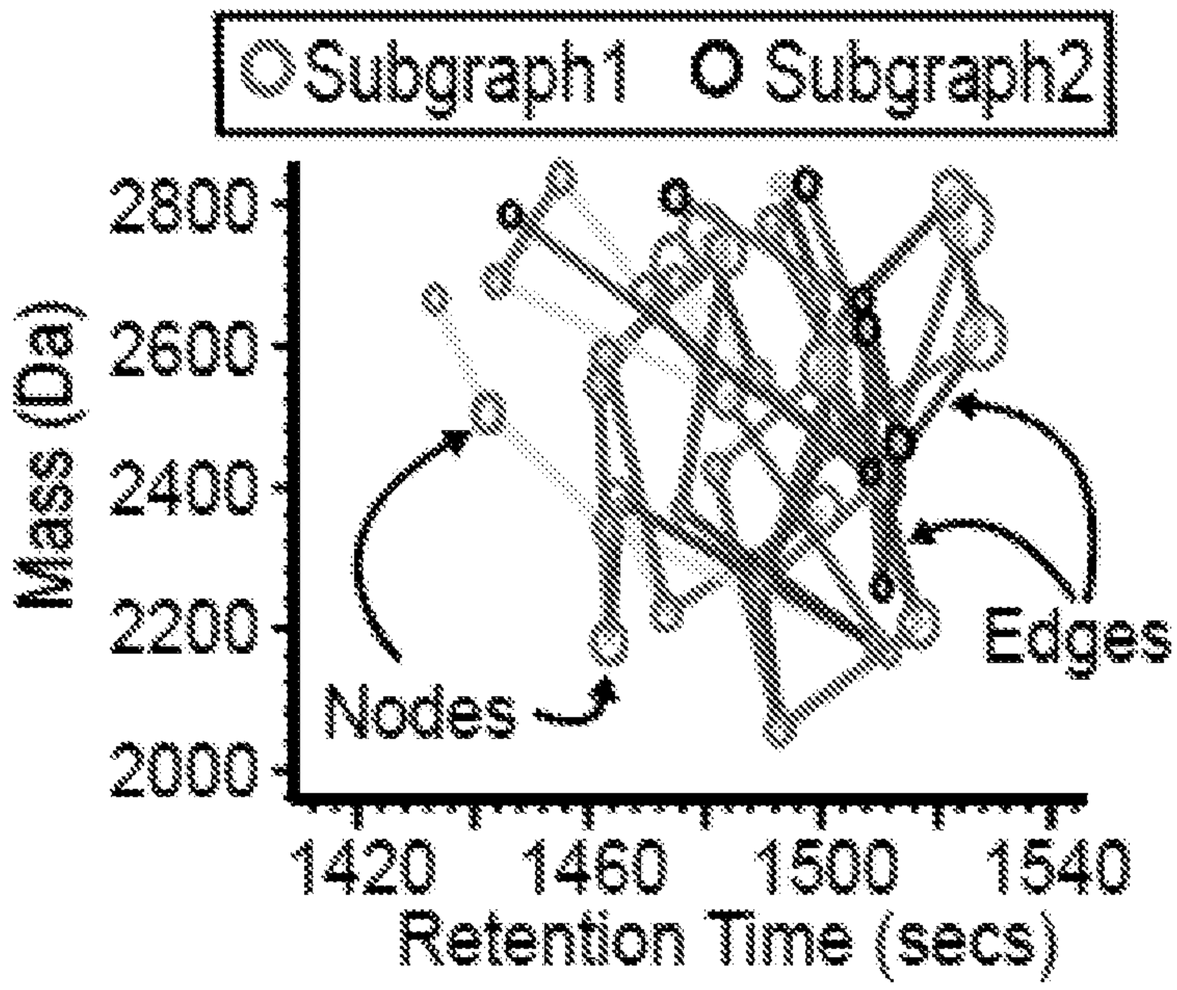


Figure 2d

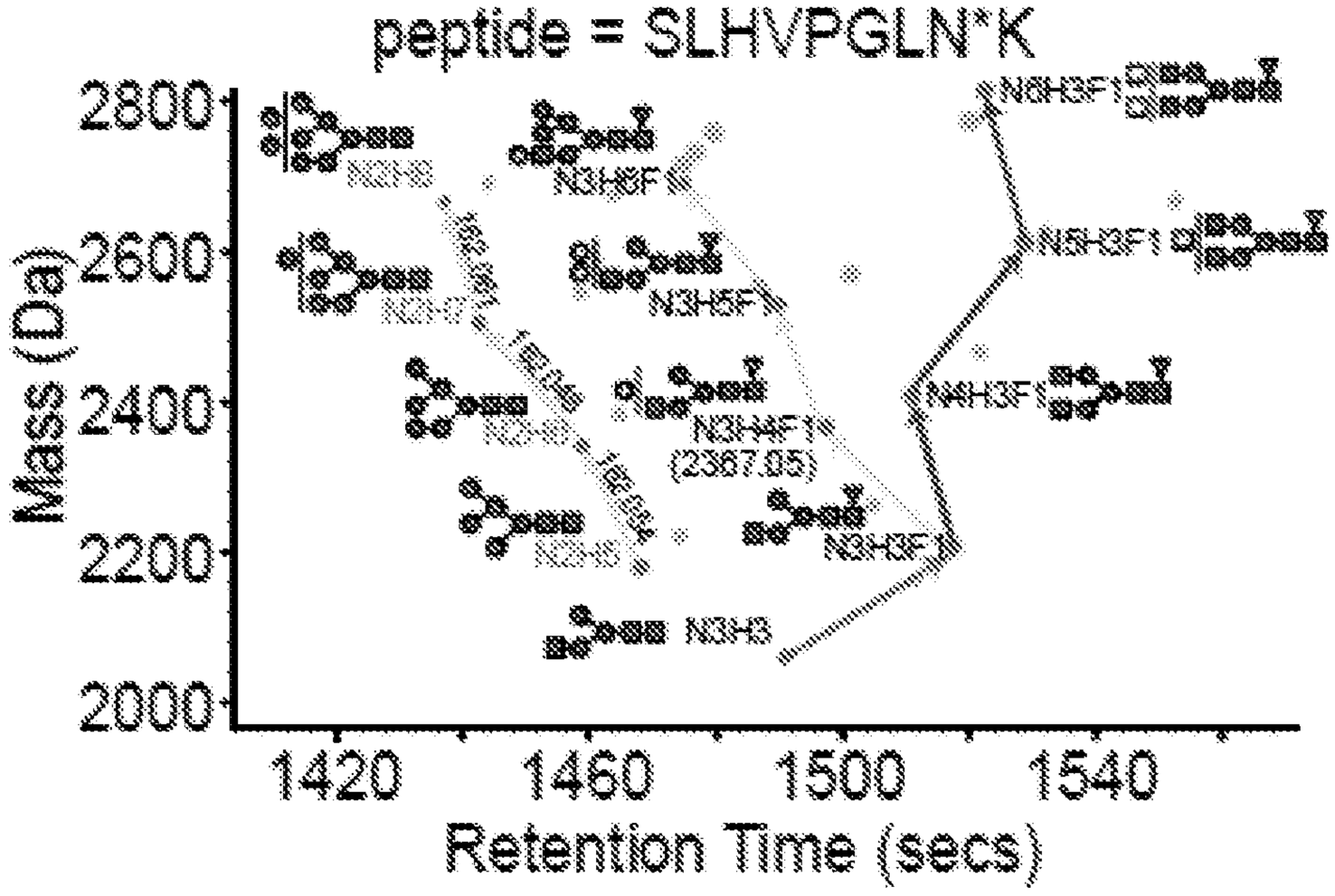

peptide = SLHVPGLN*K
Mass (Da)
2800
2600
2400
2200
2000
1420
1460
1500
1540
Retention Time (secs)
N3H3F1
N3H5F1
N3H4F1*
(2367.05)
N3H3
N5H3F1
N4H3F1
Legend
HexNAc
NeuAc
GlcNAc
Fuc
Man
Gal
Hex
Hex
HexNAc
Fuc
HexHexNAc

Figure 2e

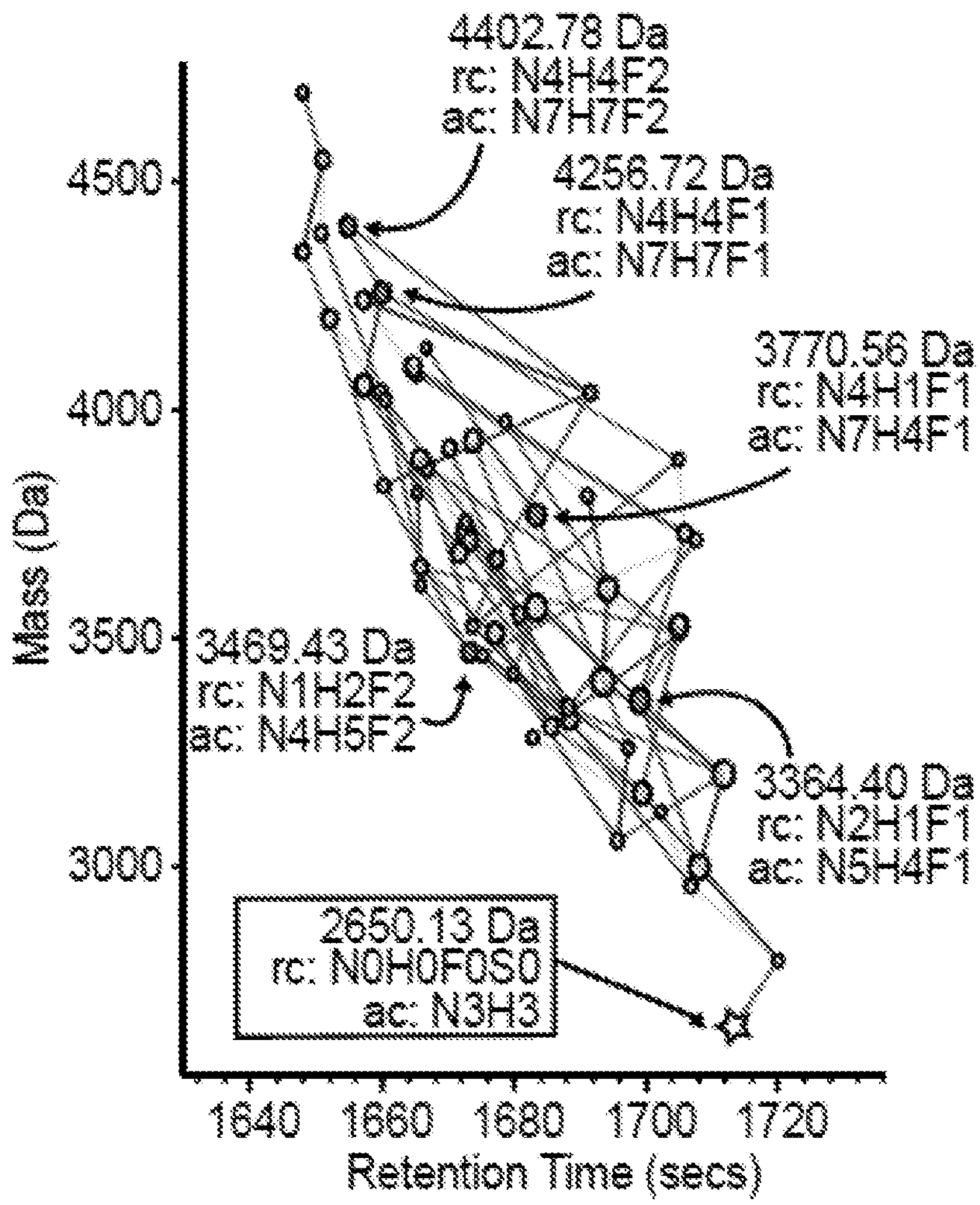
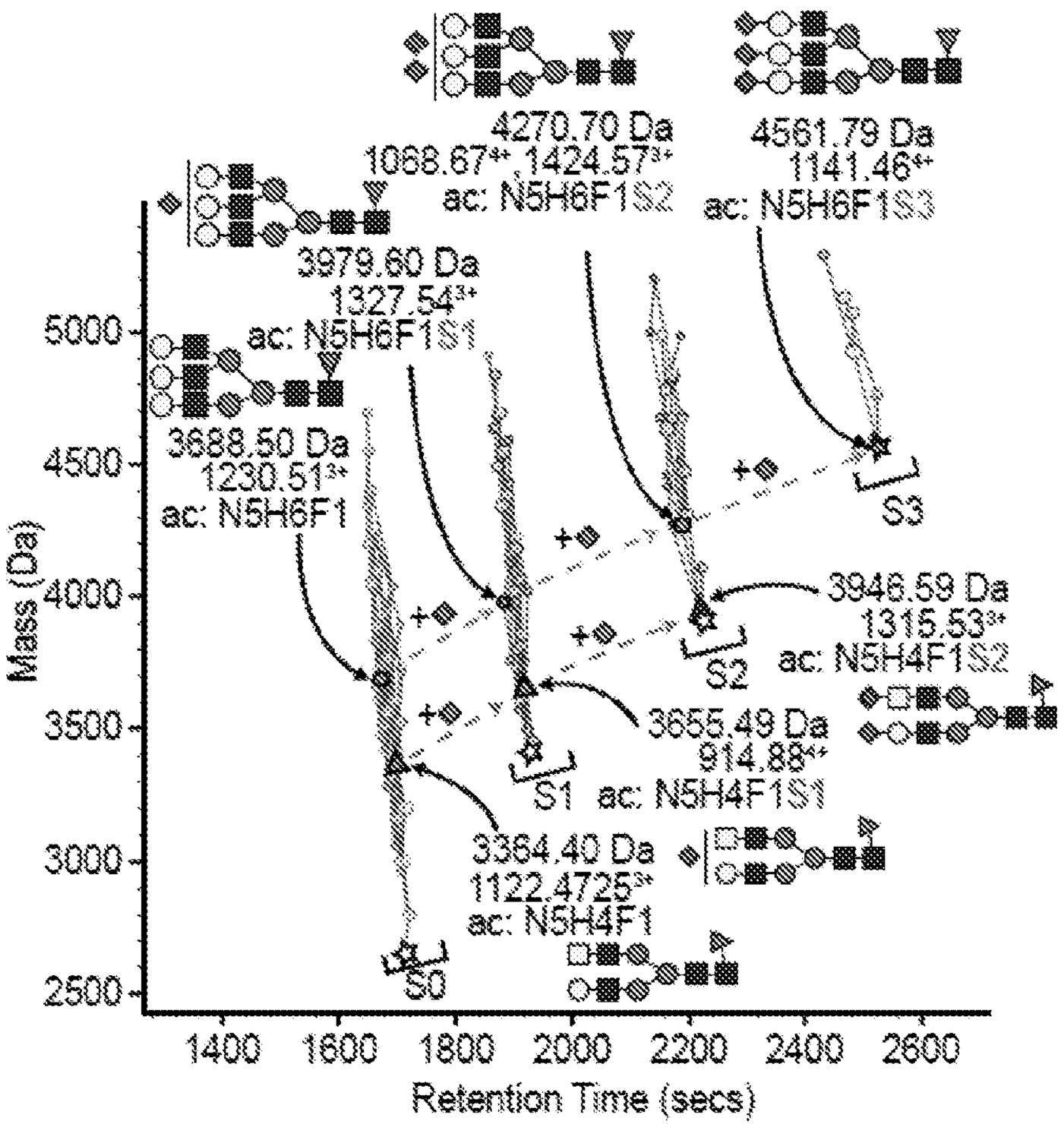

4402.78 Da
rc: N4H4F2
ac: N7H7F2
4258.72 Da
rc: N4H4F1
ac: N7H7F1
3770.56 Da
rc: N4H1F1
ac: N7H4F1
3469.43 Da
rc: N1H2F2
ac: N4H5F2
3364.40 Da
rc: N2H1F1
ac: N5H4F1
2650.13 Da
rc: N0H0F0S0
ac: N3H3
Mass (Da)
4500
4000
3500
3000
1640
1660
1680
1700
1720
Retention Time (secs)

Figure 3a


4270.70 Da
1068.67⁴⁺, 1424.57³⁺
ac: N5H6F1S2
4561.79 Da
1141.46⁴⁺
ac: N5H6F1S3
3979.60 Da
1327.54³⁺
ac: N5H6F1S1
3688.50 Da
1230.51³⁺
ac: N5H6F1
3946.59 Da
1315.53³⁺
ac: N5H4F1S2
3655.49 Da
914.88⁴⁺
ac: N5H4F1S1
3364.40 Da
1122.4725³⁺
ac: N5H4F1
S3
S2
S1
S0
Mass (Da)
5000
4500
4000
3500
3000
2500
1400
1600
1800
2000
2200
2400
2600
Retention Time (secs)

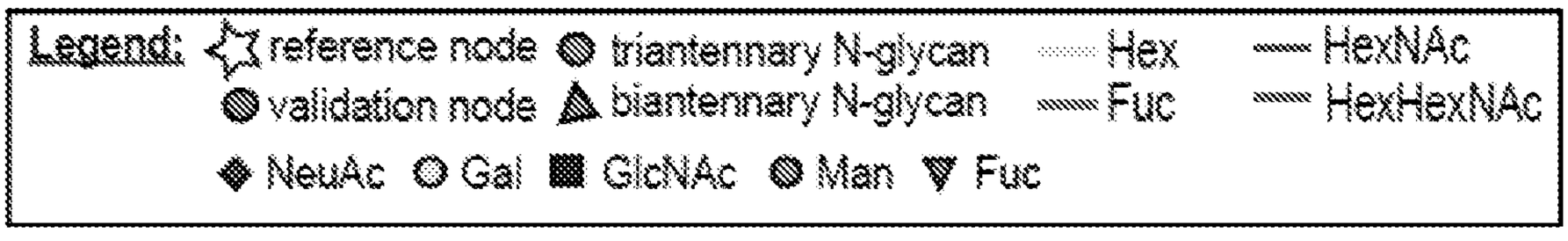

Legend:
reference node
validation node
triantennary N-glycan
biantennary N-glycan
Hex
Fuc
HexNAc
HexHexNAc
NeuAc
Gal
GlcNAc
Man
Fuc

Figure 3b

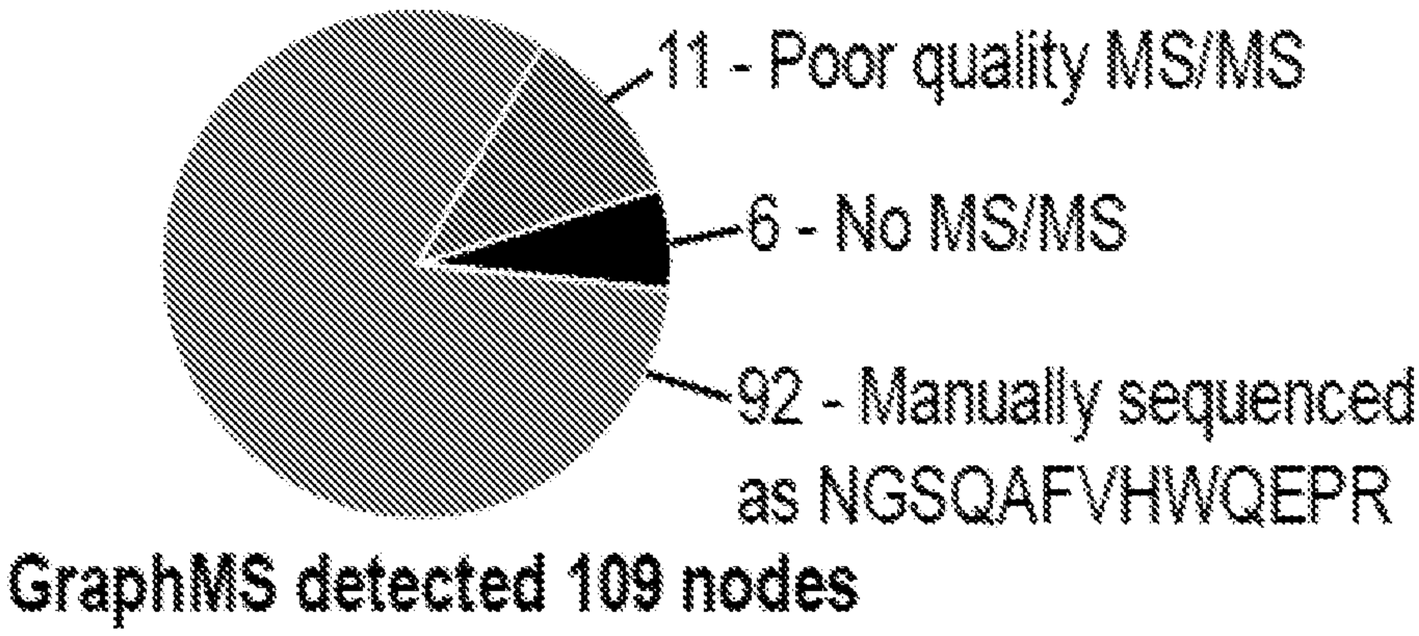


Figure 3c

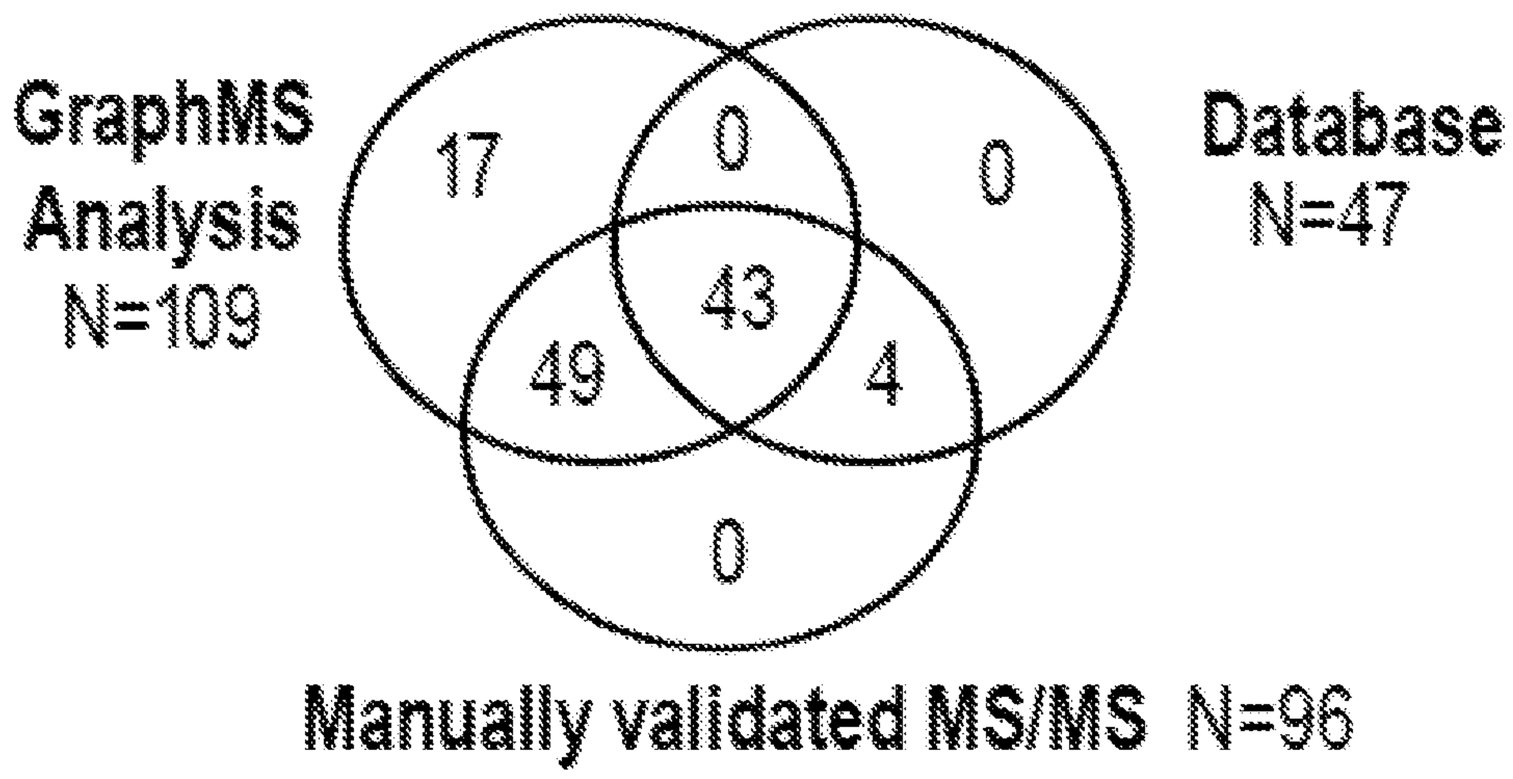


Figure 3d

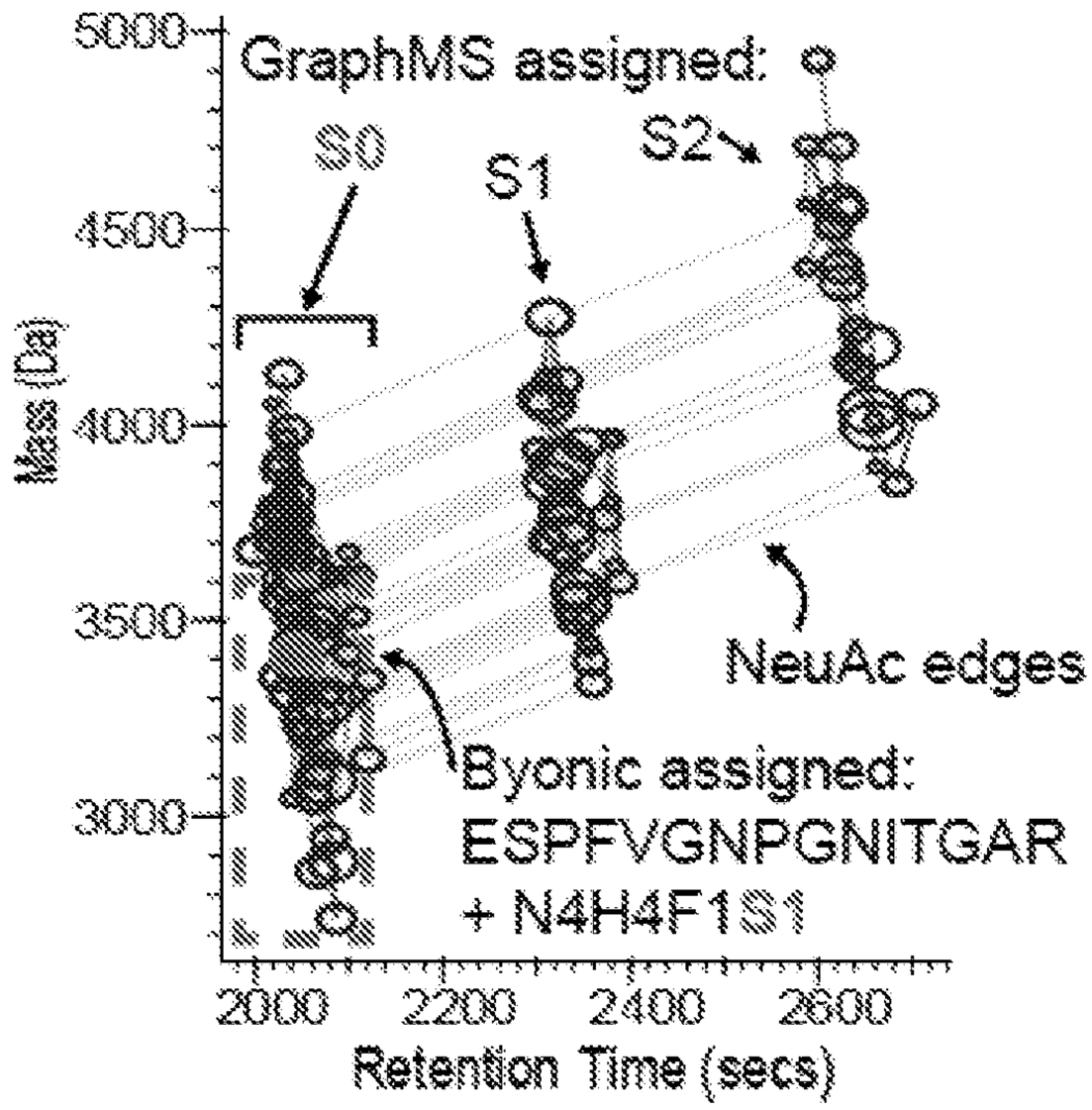


Figure 4a

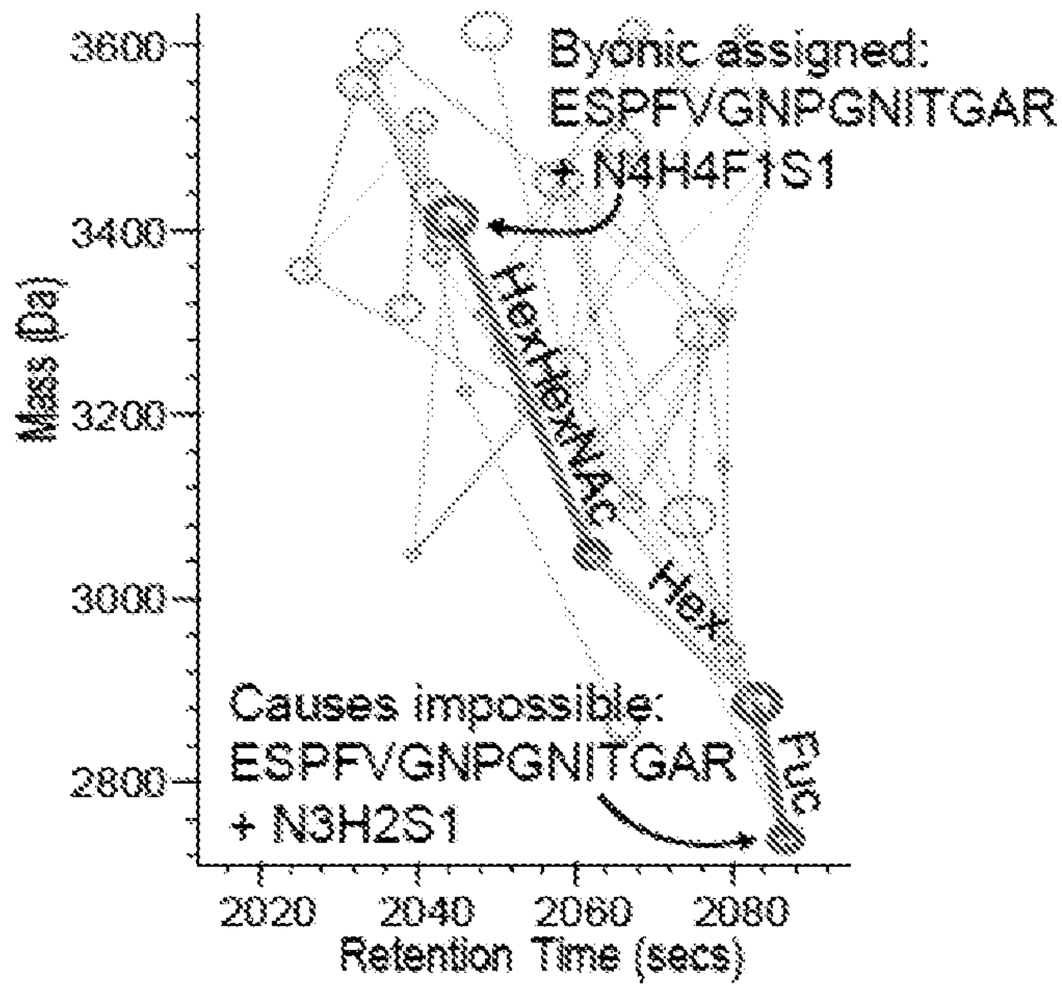


Figure 4b

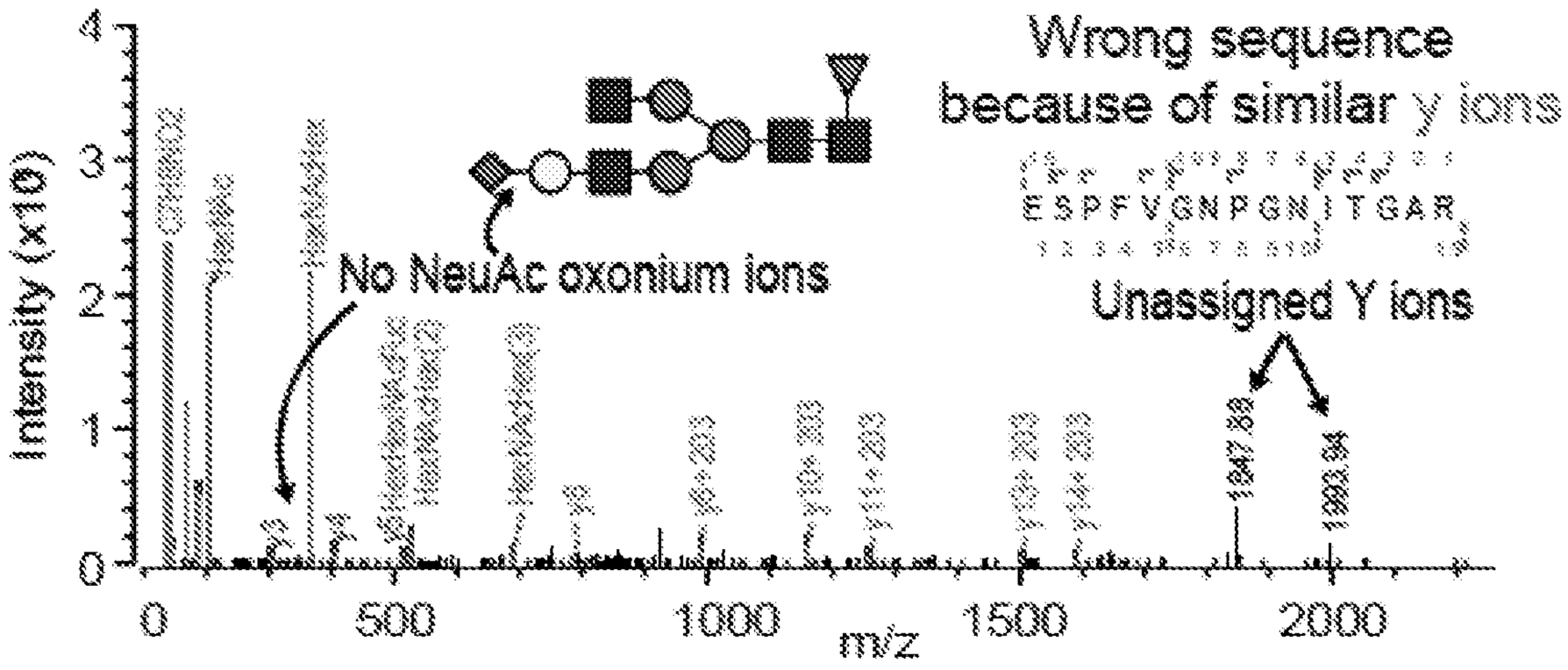


Figure 4c

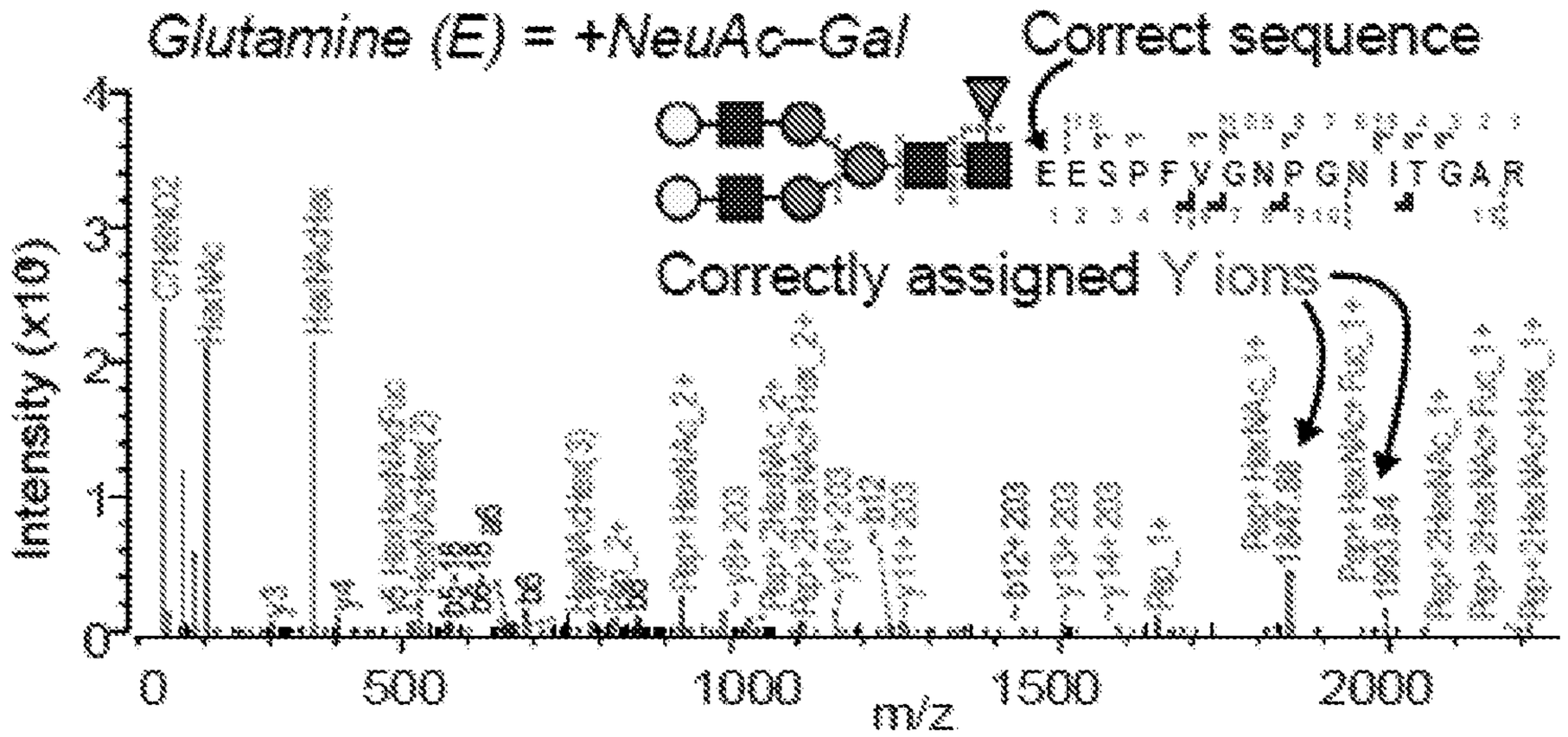


Figure 4d

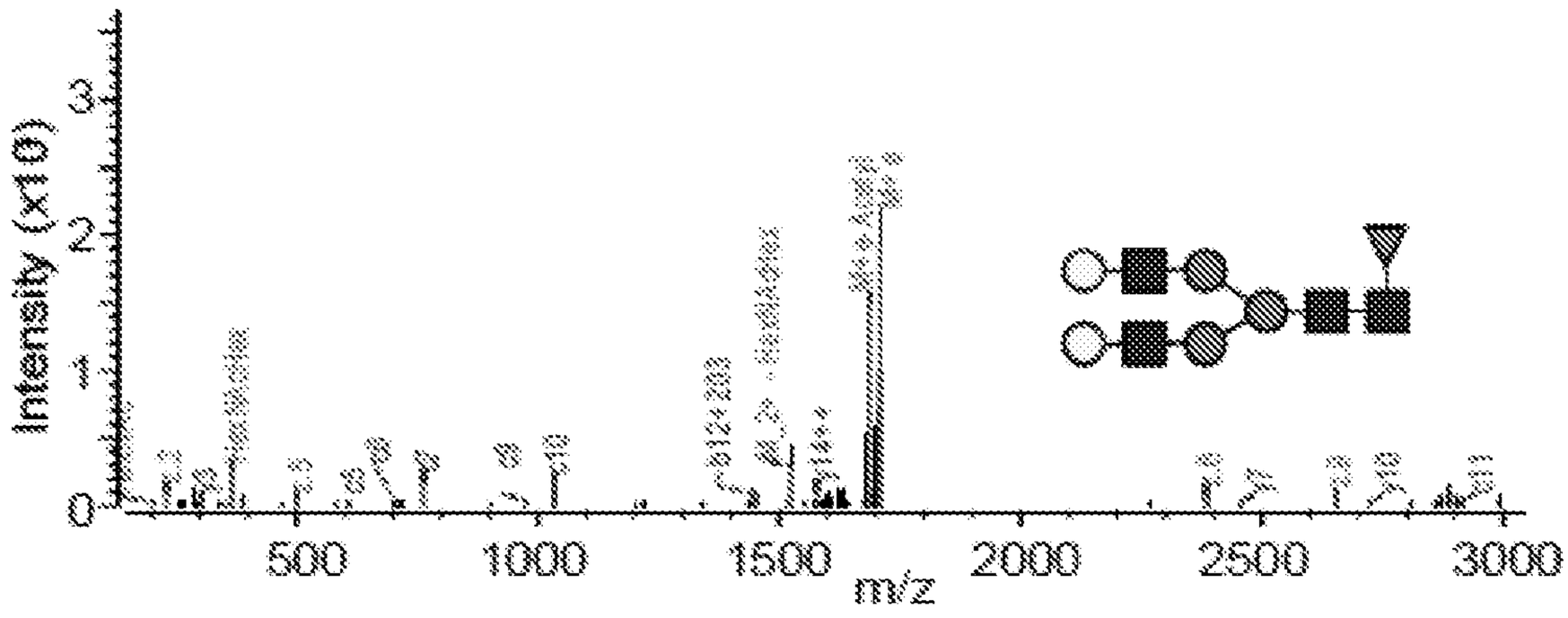


Figure 4e

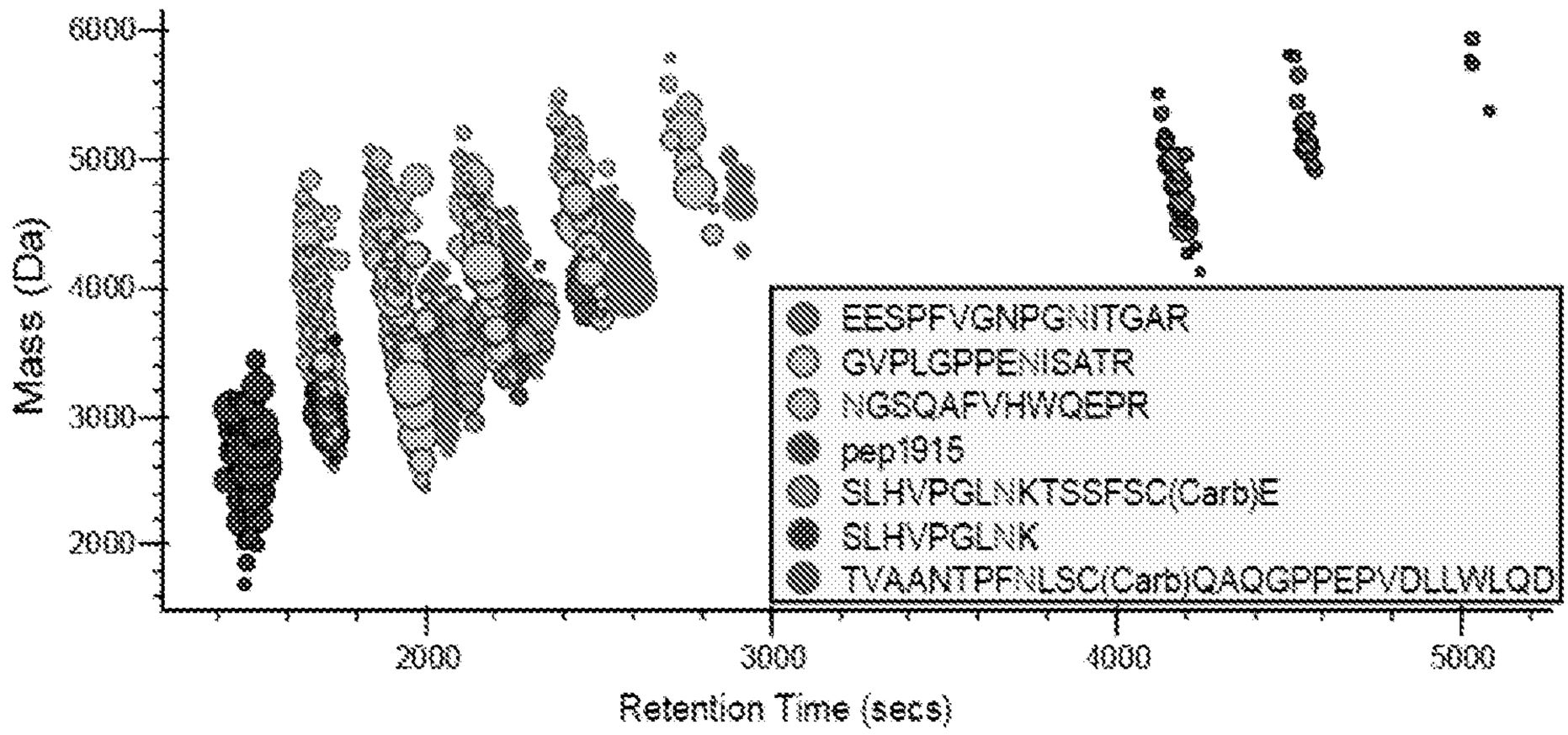


Figure 4f

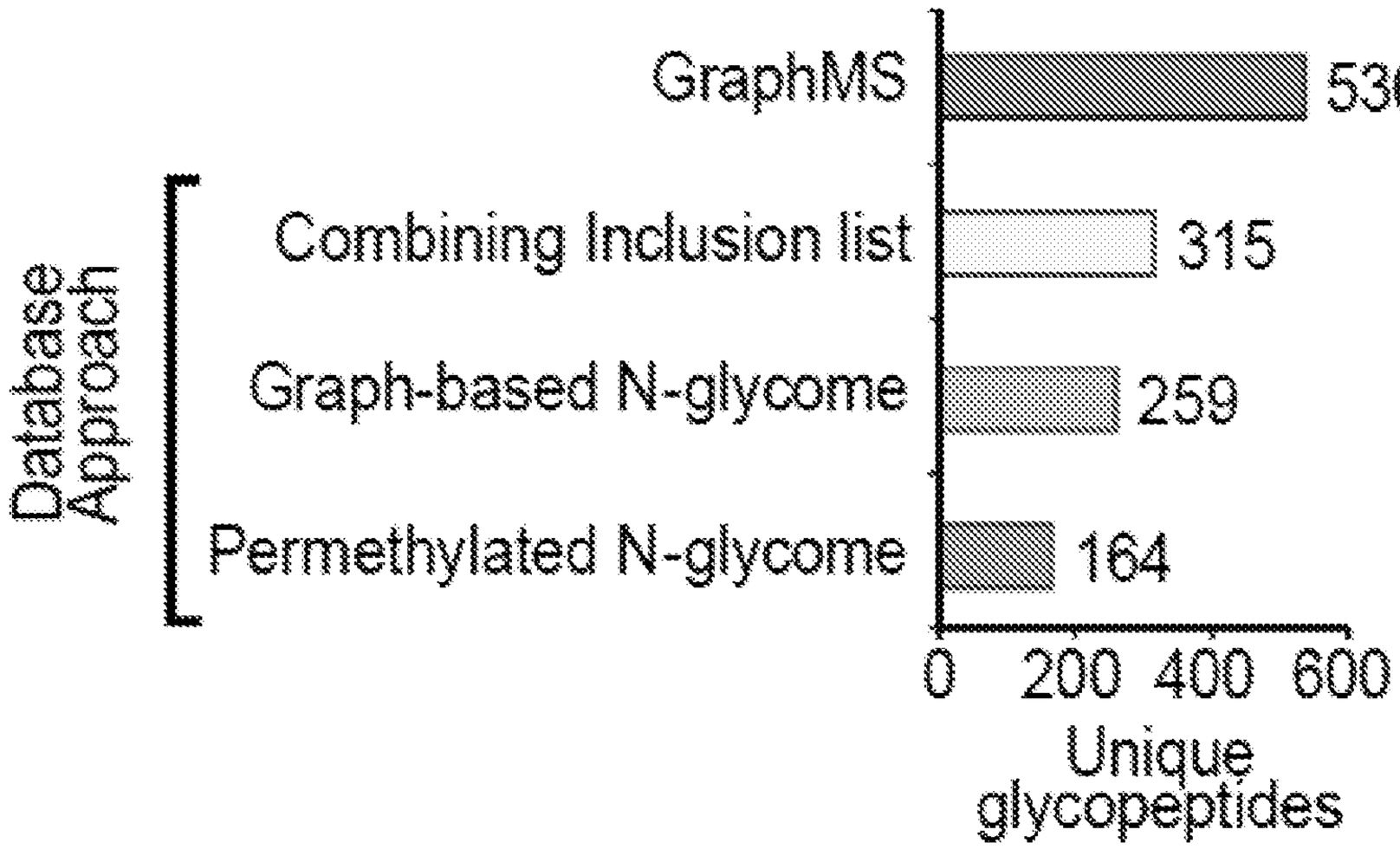


Figure 5a

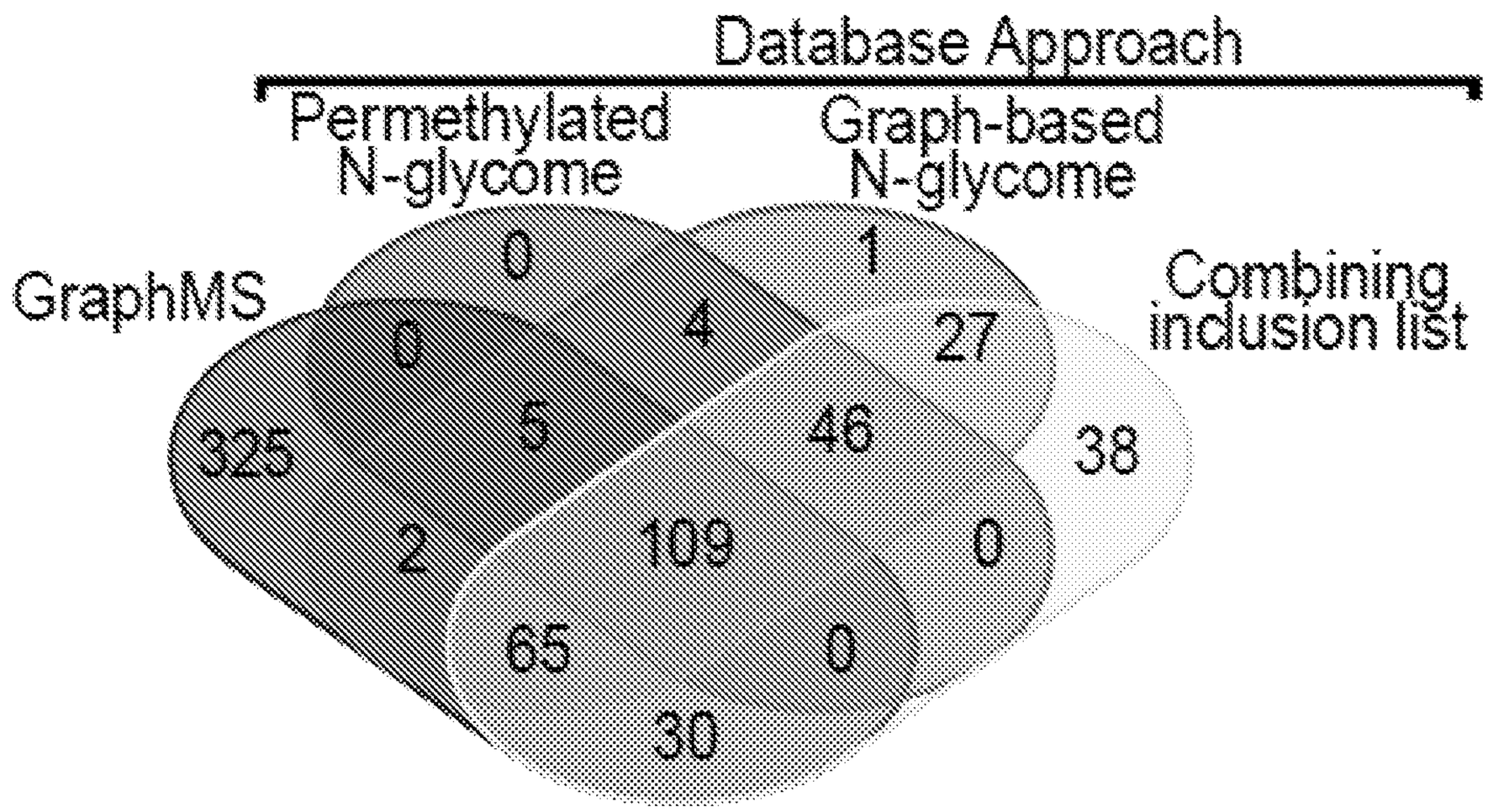


Figure 5b

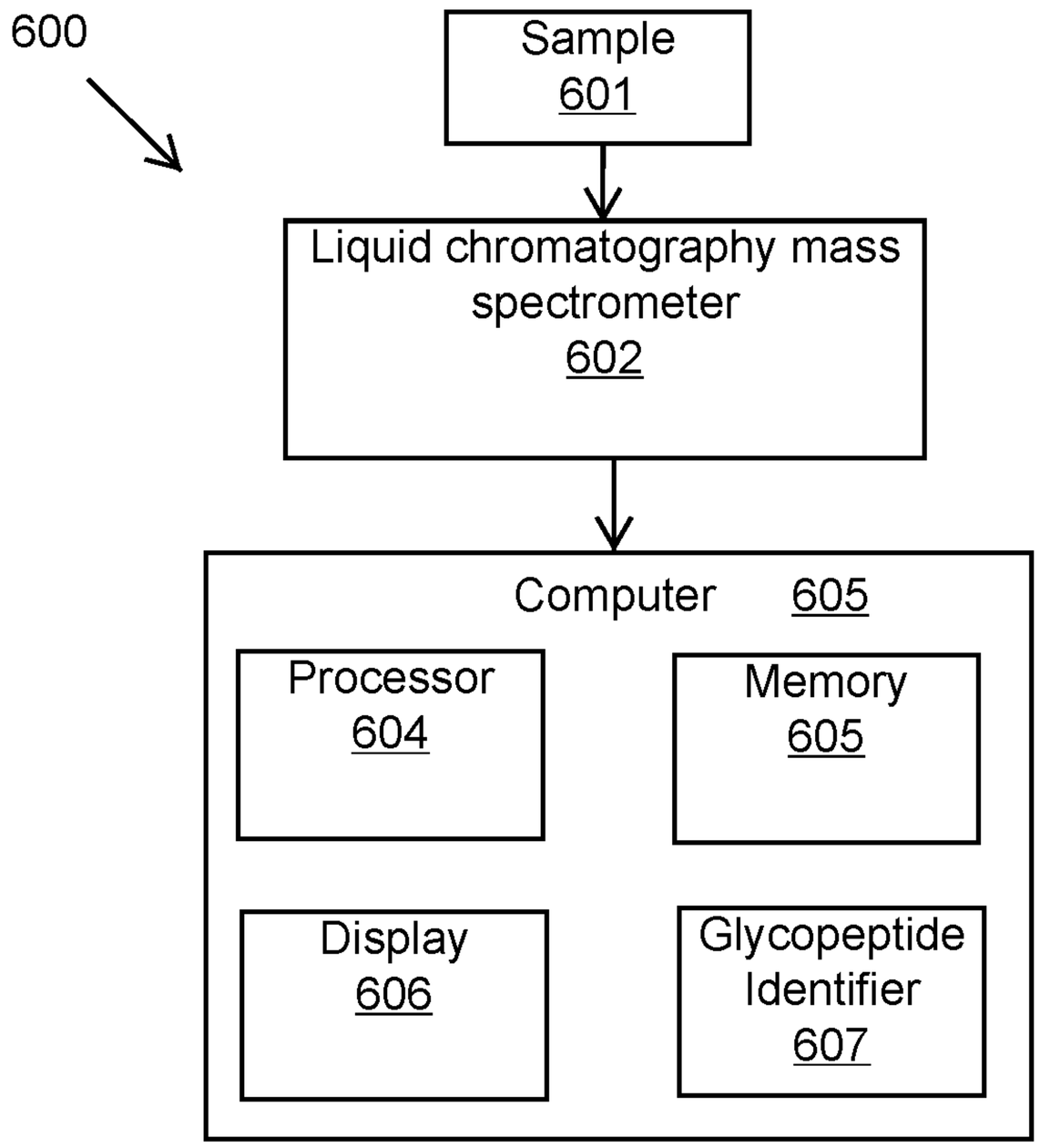

600
Sample
601
Liquid chromatography mass spectrometer
602
Computer 605
Processor
604
Memory
605
Display
606
Glycopeptide Identifier
607

Figure 6