

Dataset S3





for

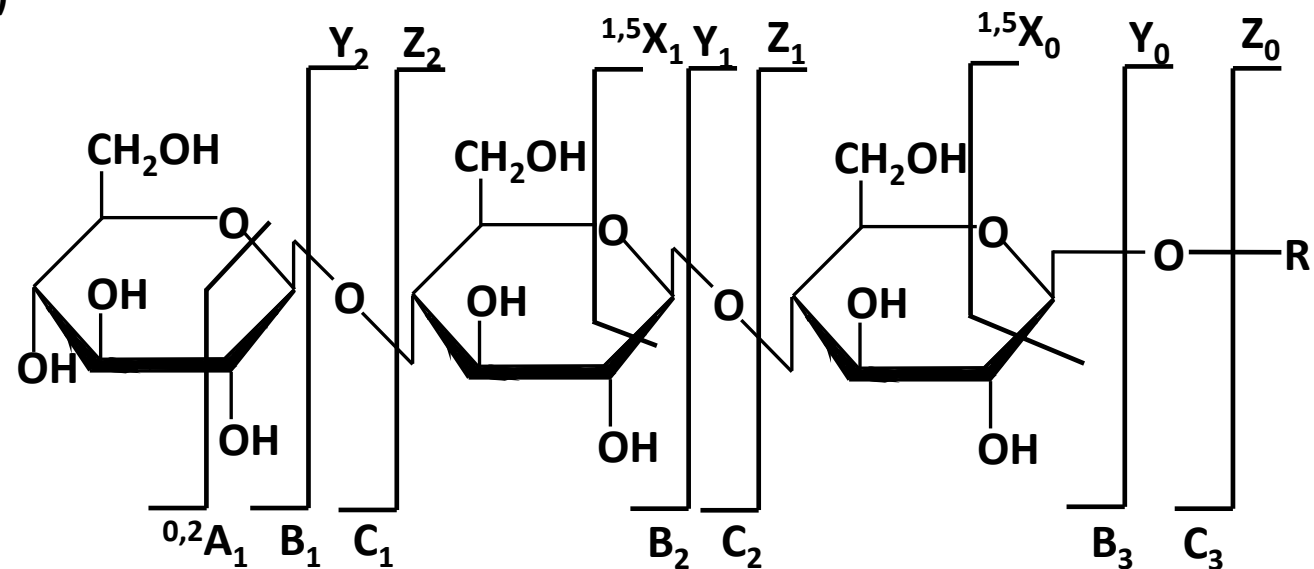
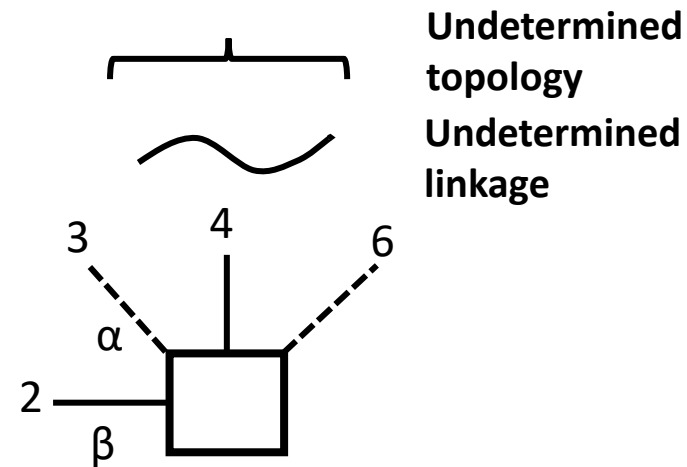
Glycoproteome remodelling and organelle-specific *N*-glycosylation accompany neutrophil granulopoiesis

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Dataset S3: Structural evidence for reported *N*-glycans based on PGC-LC-MS/MS *N*-Glycomics data

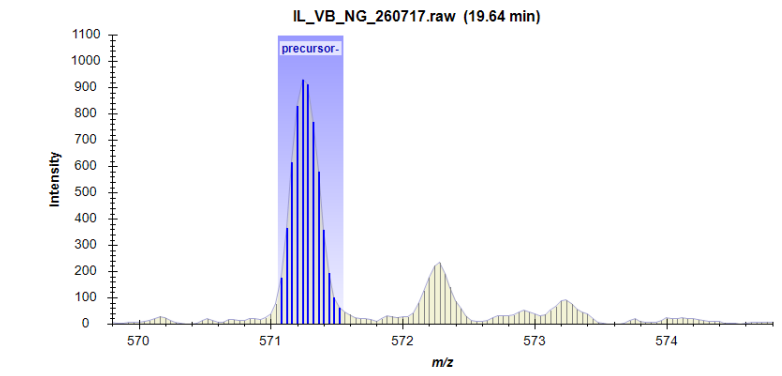
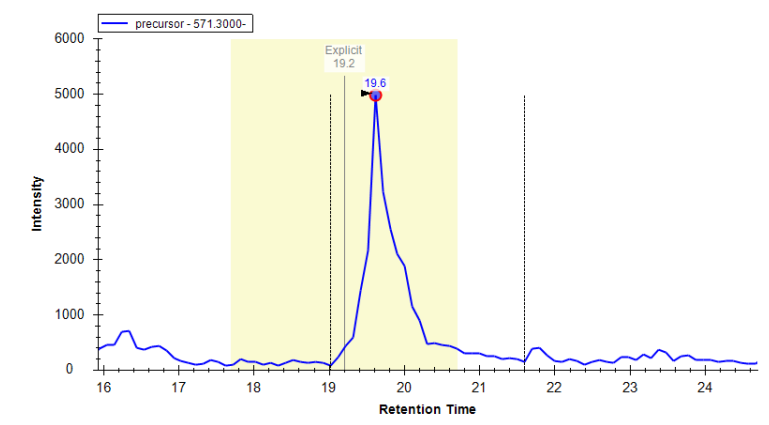
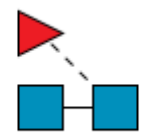
Annotation and fragmentation key

- Mannose (162.0528 Da)
- Galactose (162.0528 Da)
- N-Acetylglucosamine (203.0794 Da)
- N-Acetylgalactosamine (203.0794 Da)
- ◆ N-Acetylneuraminic acid (291.0954 Da)
- ▲ Fucose (146.0579 Da)
-  Cross-ring fragment (unspecified)
-  Indicates mostly Y ions (includes oxygen of glycosidic linkage)
-  Indicates mostly Z ions (excludes oxygen of glycosidic linkage)
-  Reduced reducing end
- P Phosphate

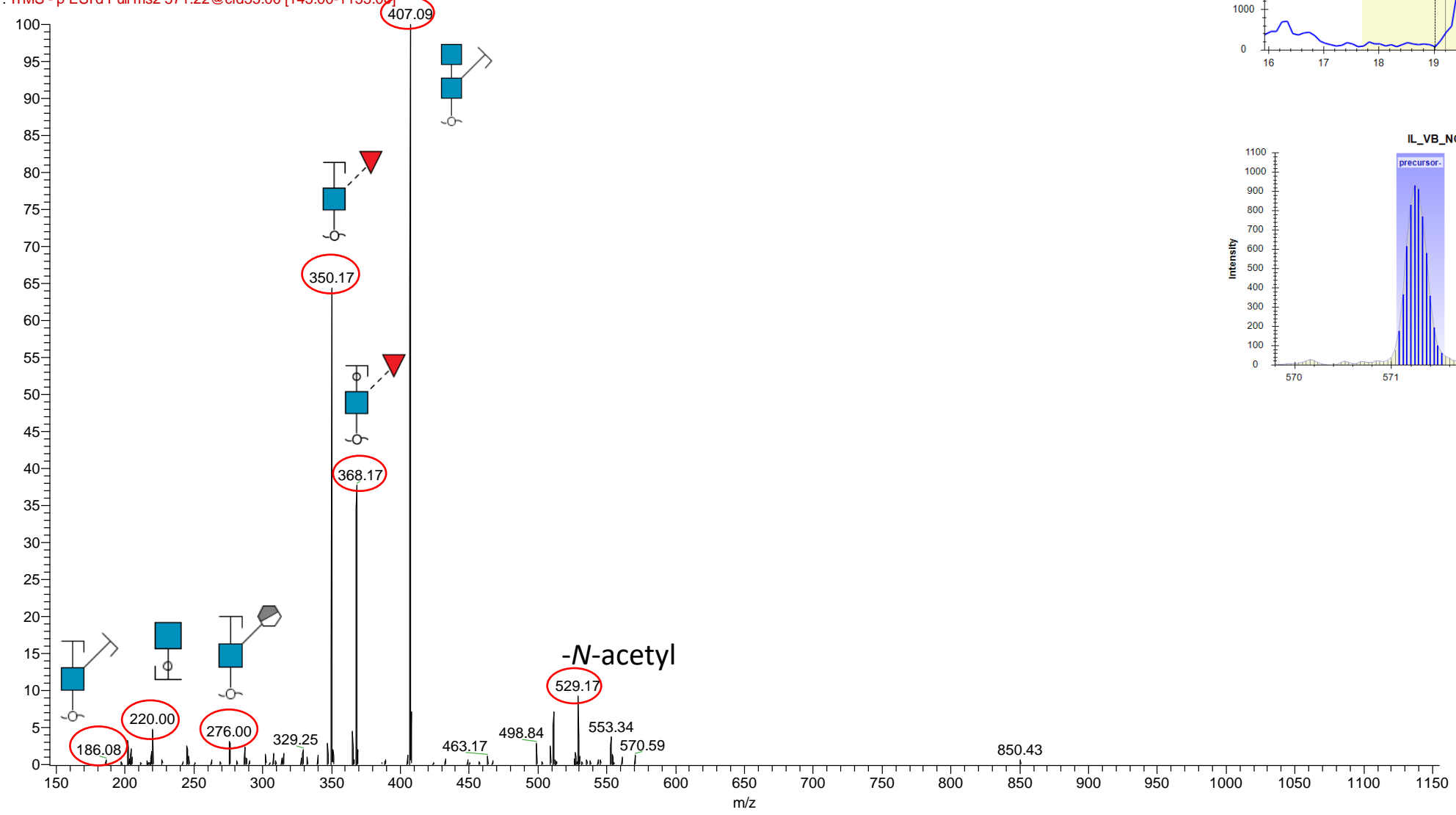


Note 1: All glycans contain reducing end which is not depicted in the reported N-glycan structure cartoon but are shown in the fragments.
 Note 2: Glycan #1-#3 were not observed with N-glycomics (only with glycopeptide analysis), hence have been left out here.

Glycan #4
 Chitobiose core
 HexNAc₂Fuc₁ (MOF)
m/z: 571.3 (1-)



IL_VB_NG_260717 #1972 RT: 19.65 AV: 1 NL: 1.57E2
 F: ITMS - p ESI d Full ms2 571.22@cid35.00 [145.00-1155.00]



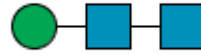
-N-acetyl

Glycan #5

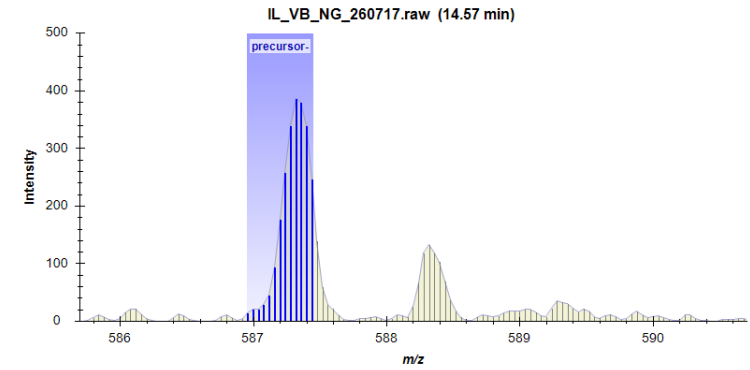
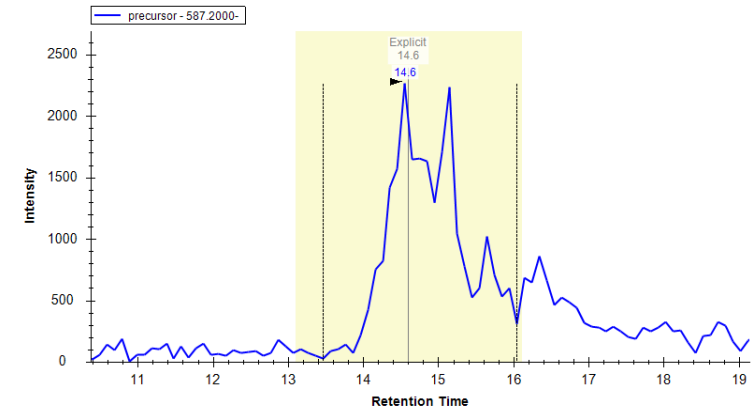
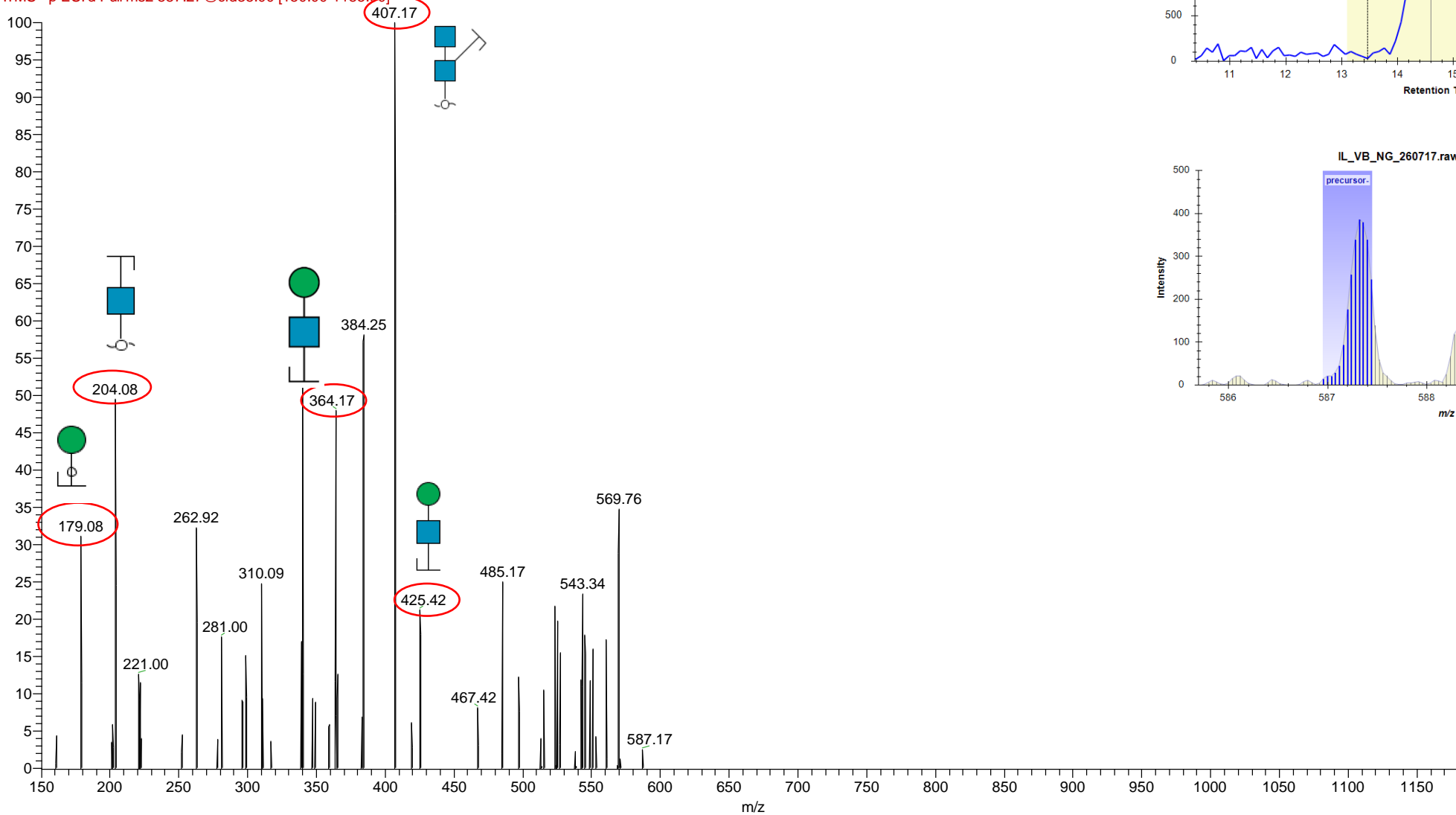
Paucimannose

Hex₁HexNAc₂ (M1)

m/z: 587.2 (1-)



IL_YA_NG_260717 #1500 RT: 14.96 AV: 1 NL: 1.21E1
F: ITMS - p ESI d Full ms2 587.27 @cid35.00 [150.00-1185.00]

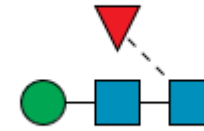


Glycan #6

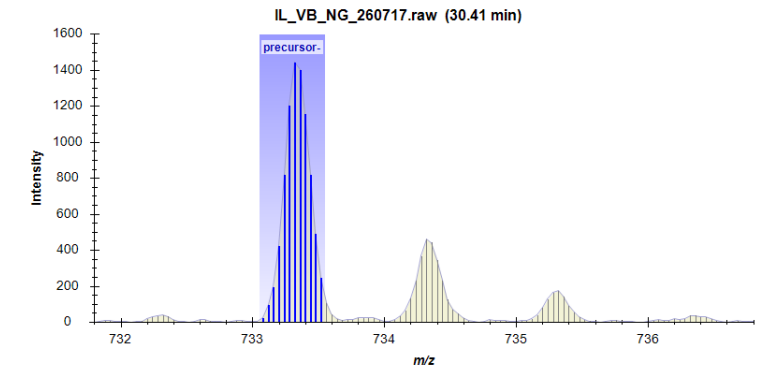
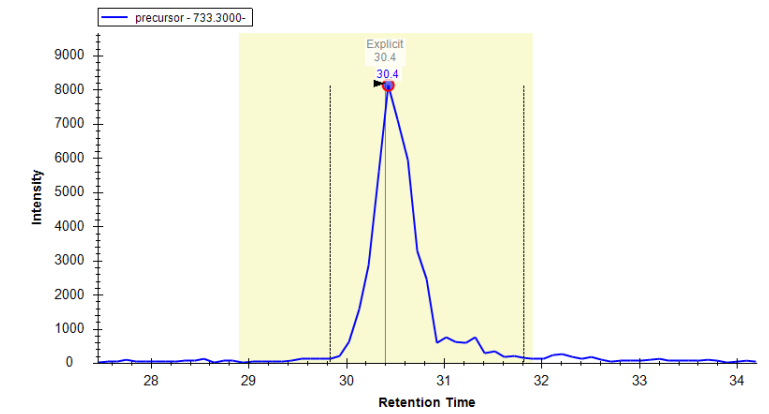
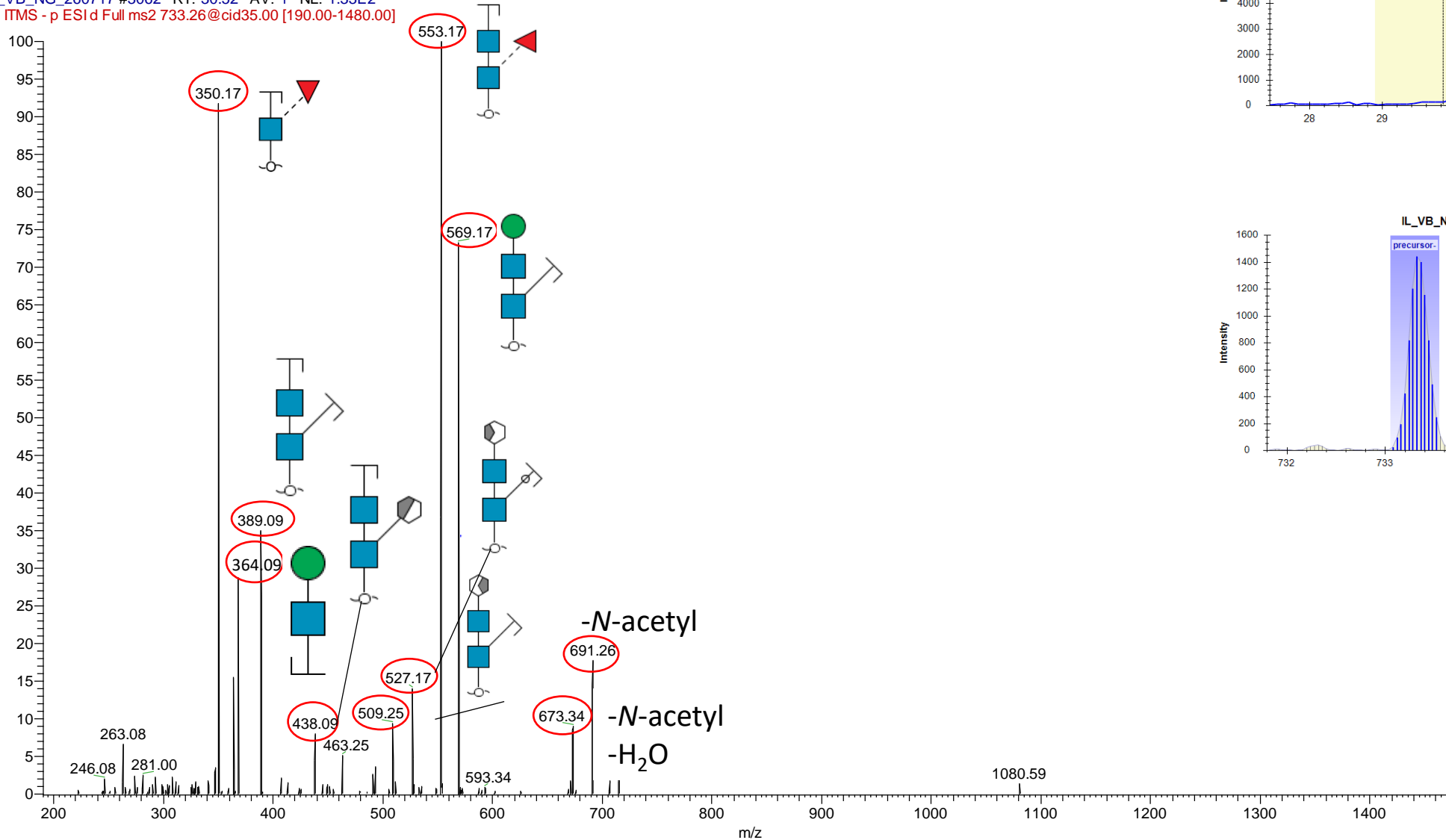
Paucimannose

Hex₁HexNAc₂Fuc₁ (M1F)

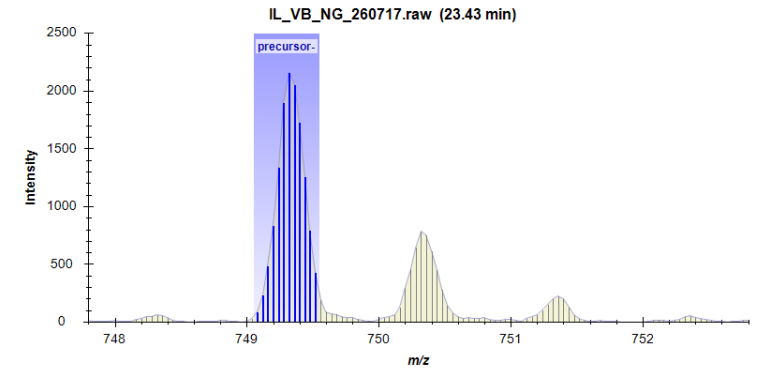
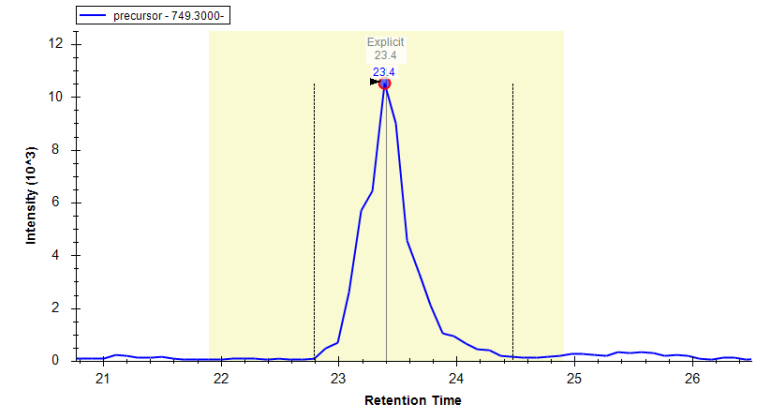
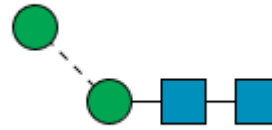
m/z: 733.3 (1-)



IL_VB_NG_260717 #3062 RT: 30.52 AV: 1 NL: 1.33E2
F: ITMS - p ESI d Full ms2 733.26@cid35.00 [190.00-1480.00]

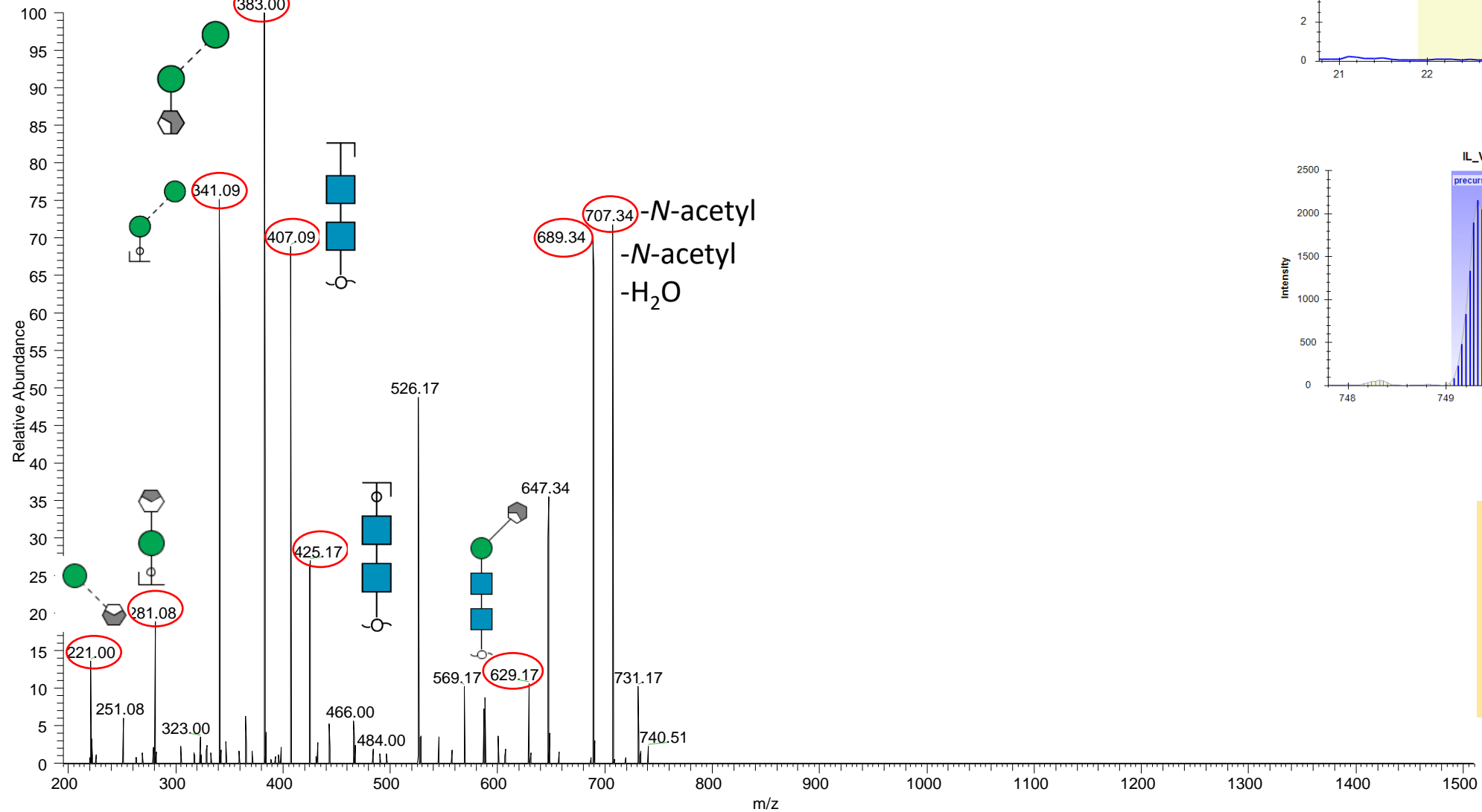


Glycan #7
 Paucimannose
 Hex₂HexNAc₂ (M2)
 m/z: 749.3 (1-)

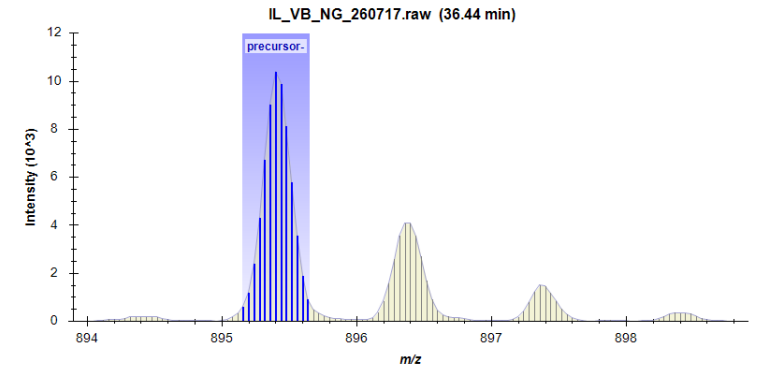
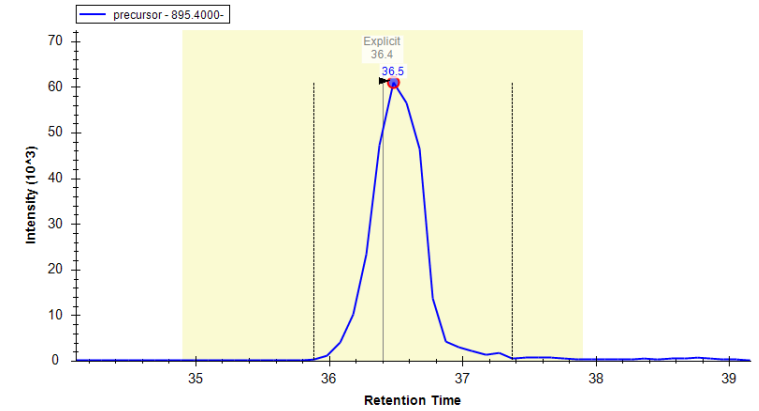
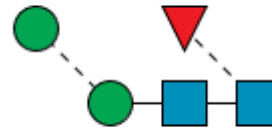


Note: Determined as alpha1,6-arm structure based on past observations reported in other neutrophil N-glycome studies

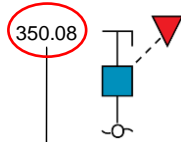
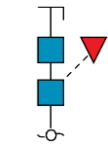
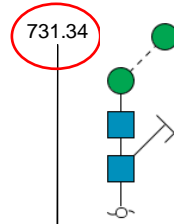
IL_VB_NG_260717#2352 RT: 23.43 AV: 1 NL: 5.16E1
 F: ITMS - p ESI d Full ms2 749.32 @cid35.00 [195.00-1510.00]



Glycan #8
Paucimannose
Hex₂HexNAc₂Fuc₁ (M2F)
***m/z*: 895.4 (1⁻)**



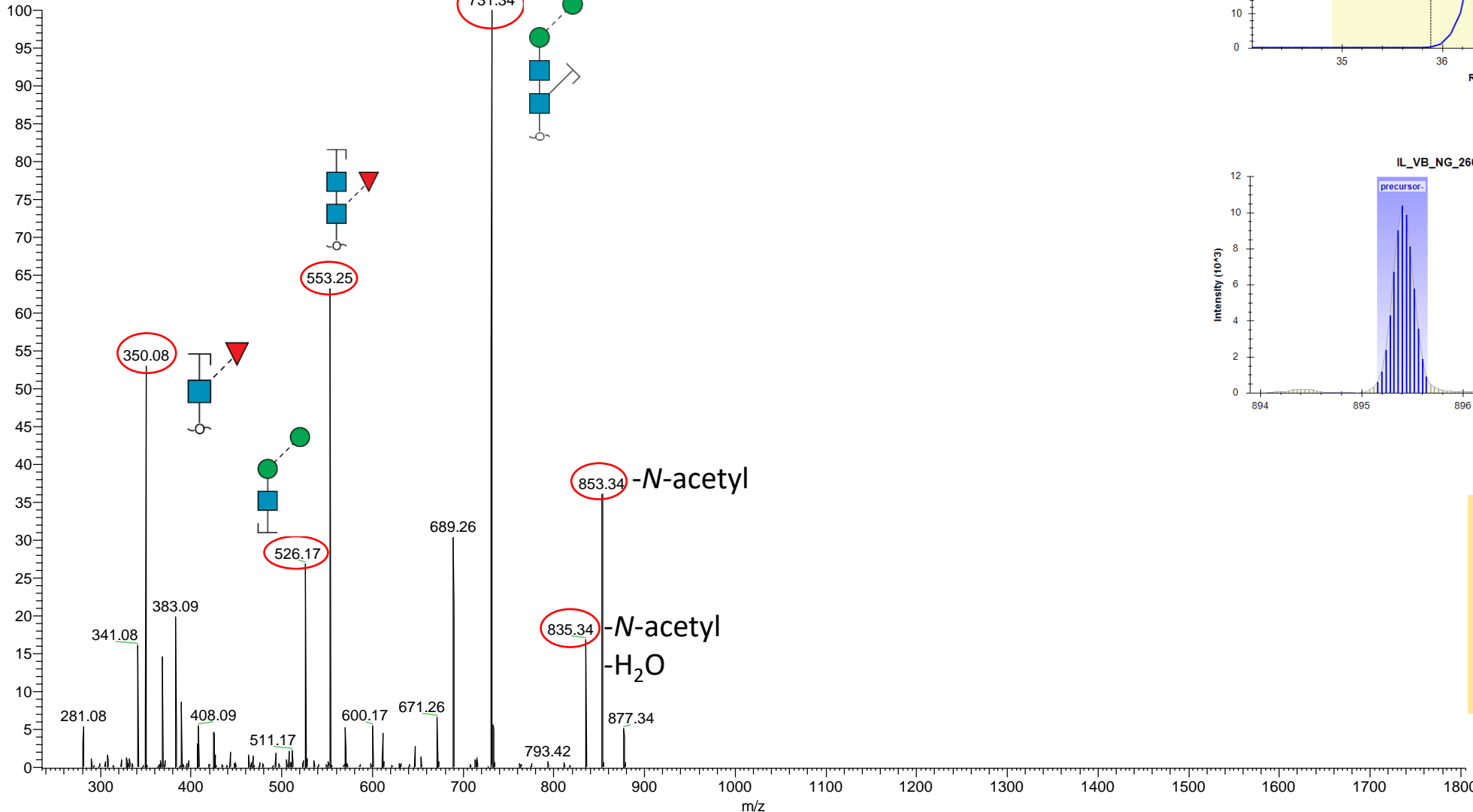
Note: Determined as alpha1,6-arm structure based on past observations reported in other neutrophil N-glycome studies



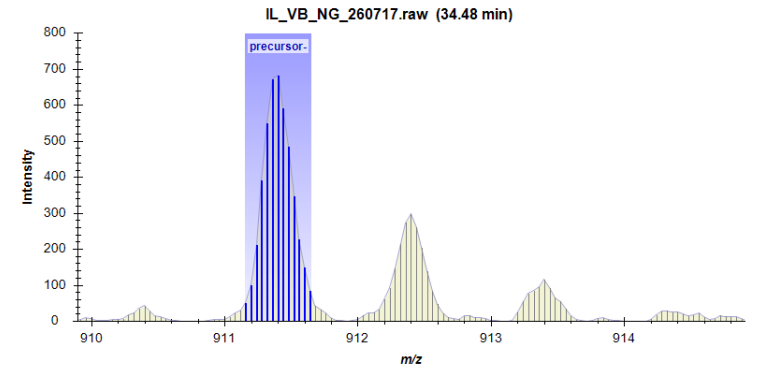
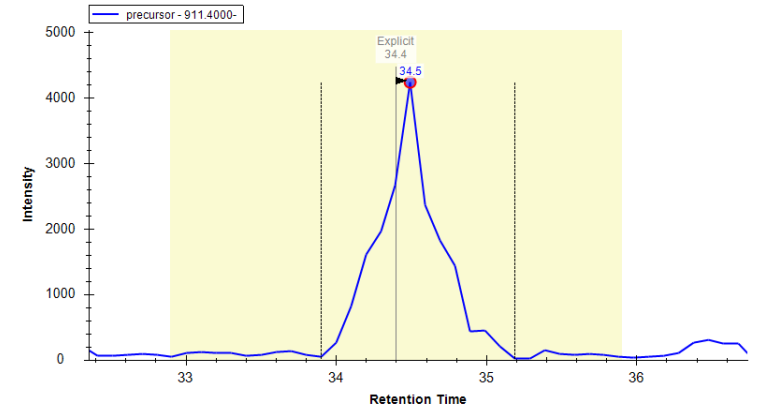
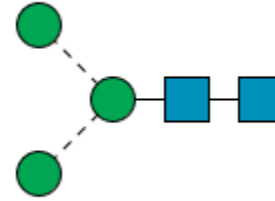
853.34 -N-acetyl

835.34 -N-acetyl
 -H₂O

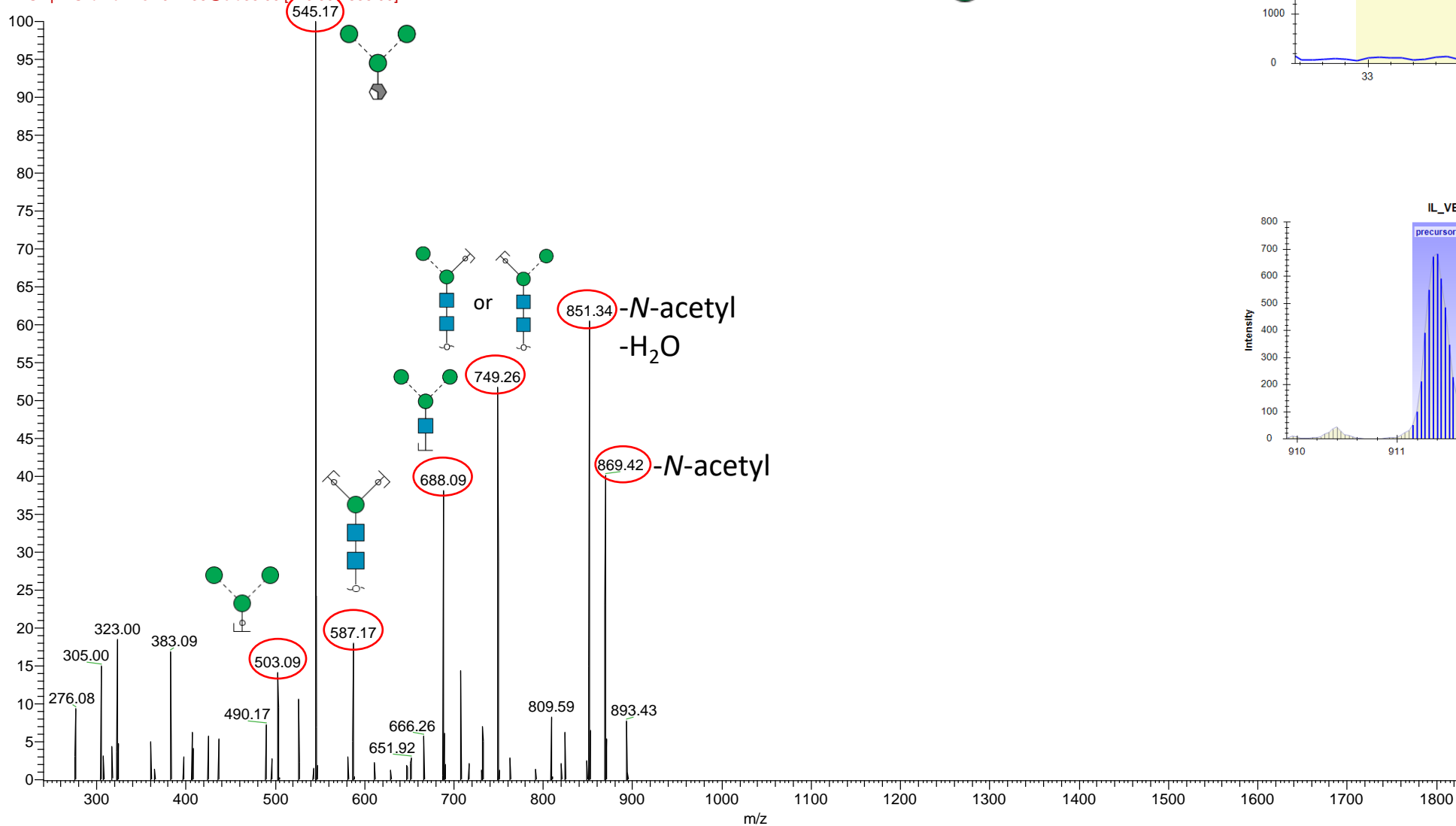
IL_VB_NG_260717 #3642 RT: 36.45 AV: 1 NL: 4.34E2
 F: ITMS - p ESI d Full ms2 895.39@cid35.00 [235.00-1805.00]



Glycan #9
 Paucimannose
 Hex₃HexNAc₂ (M3)
 m/z: 911.4 (1⁻)



IL_VB_NG_260717 #3452 RT: 34.49 AV: 1 NL: 3.76E1
 F: ITMS - p ESI d Full ms2 911.38@cid35.00 [240.00-1835.00]

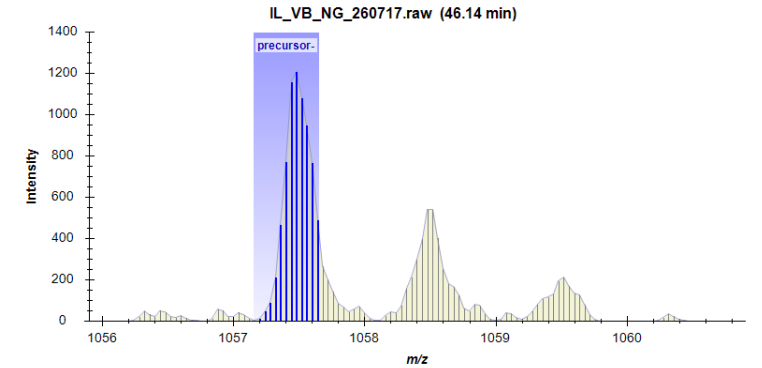
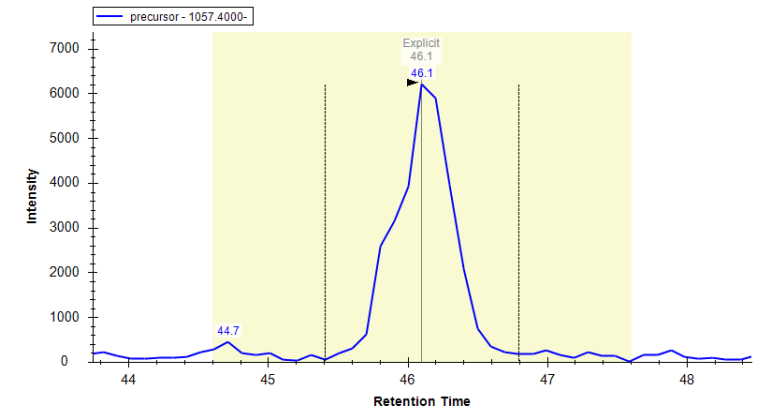
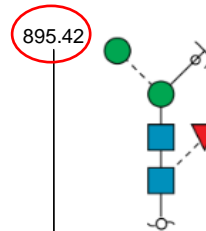
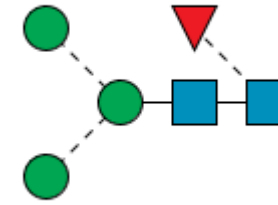


Glycan #10

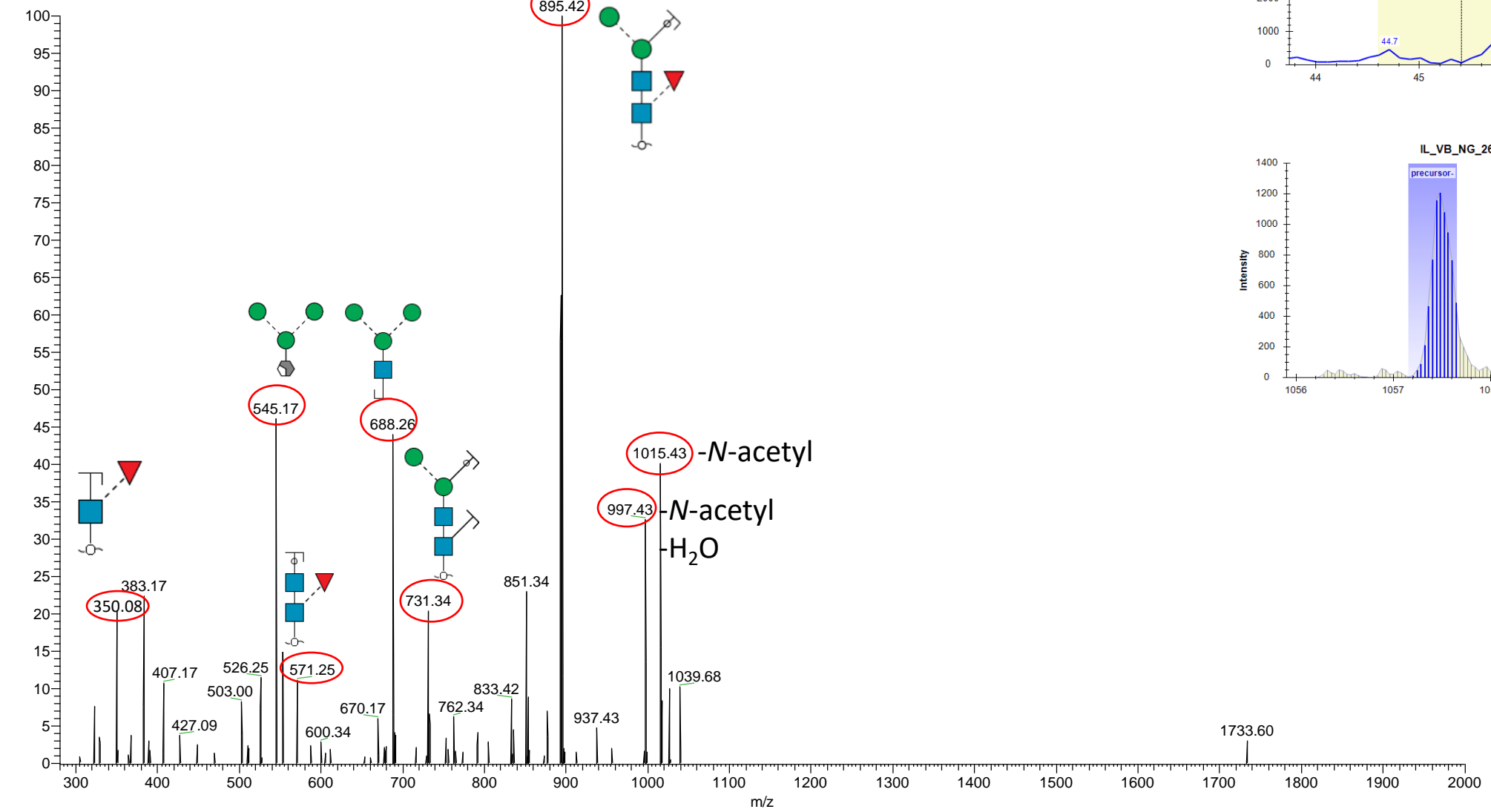
Paucimannose

Hex₃HexNAc₂Fuc₁ (M3F)

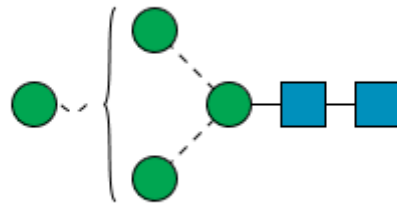
m/z: 1057.4⁽¹⁻⁾



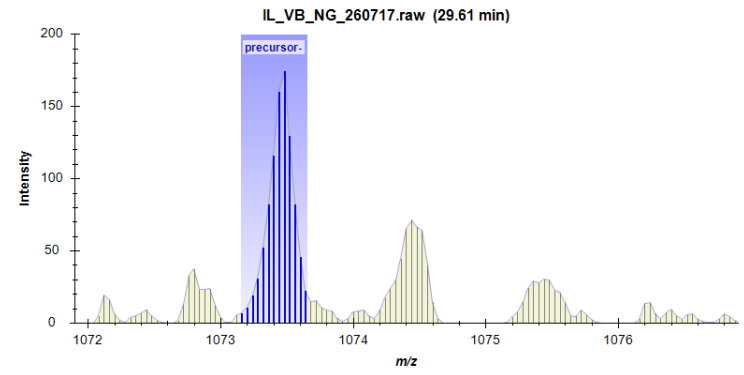
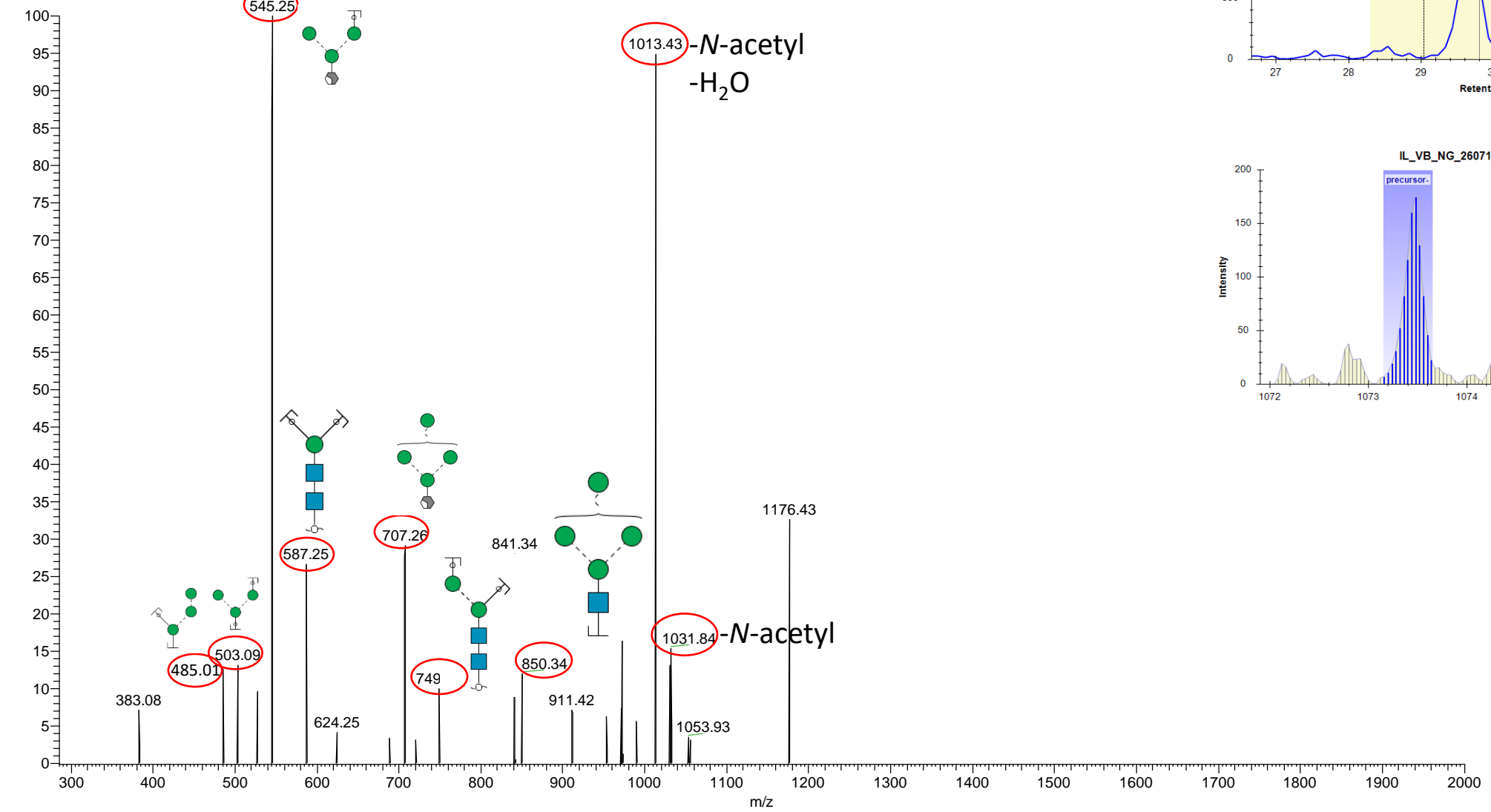
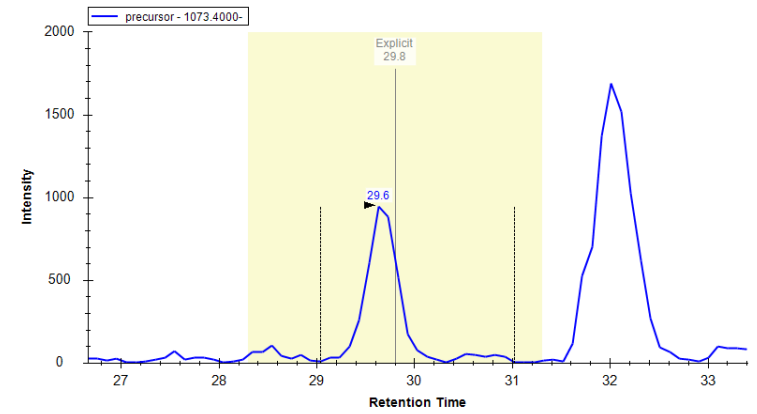
L_VB_NG_260717 #4583 RT: 46.05 AV: 1 NL: 3.97E1
 F: ITMS - p ESI d Full ms2 1057.44@cid35.00 [280.00-2000.00]



Glycan #11a
 Oligomannose
 Hex₄HexNAc₂ (Man4)
 m/z: 1073.4 (1-)



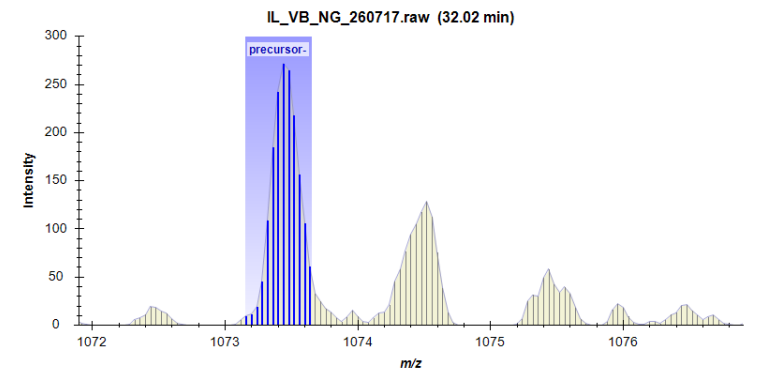
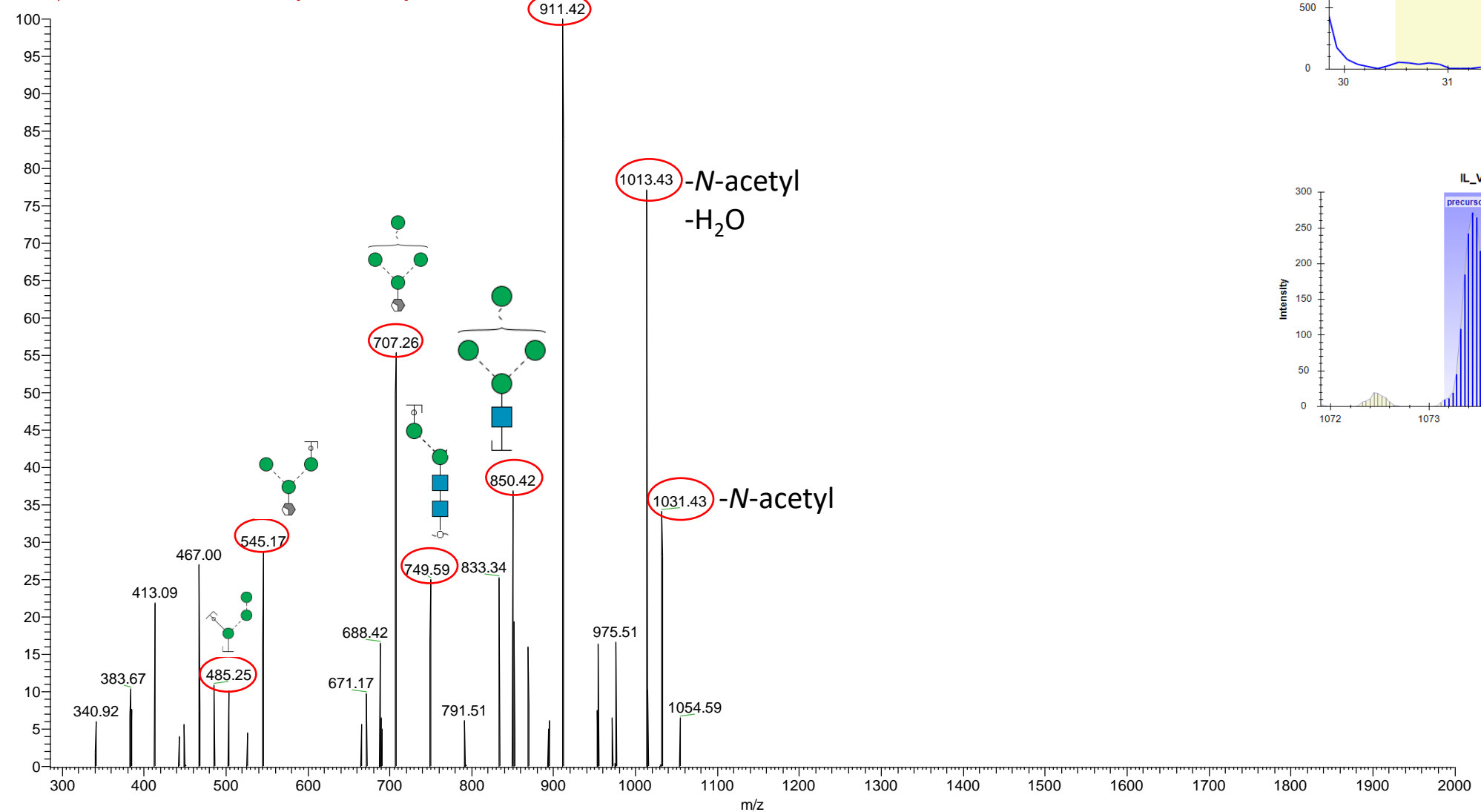
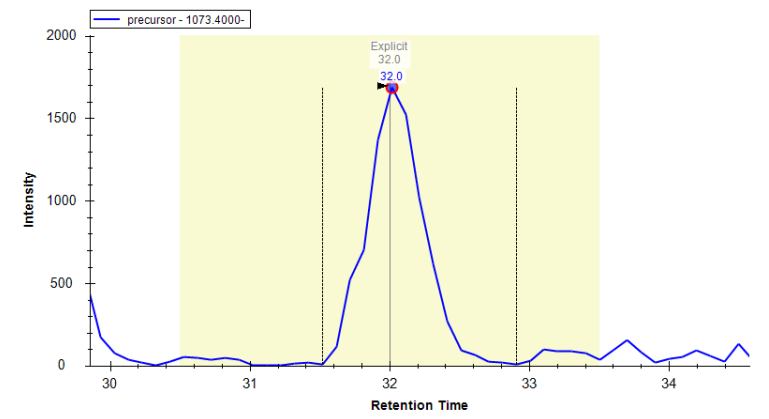
IL_VB_NG_260717 #2990 RT: 29.80 AV: 1 NL: 1.26E1
 F: ITMS - p ESI d Full ms2 1073.47 @ cid 35.00 [285.00-2000.00]



Glycan #11b
 Oligomannose
 Hex₄HexNAc₂ (Man4)
m/z: 1073.4 (1-)

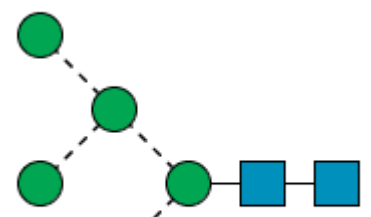
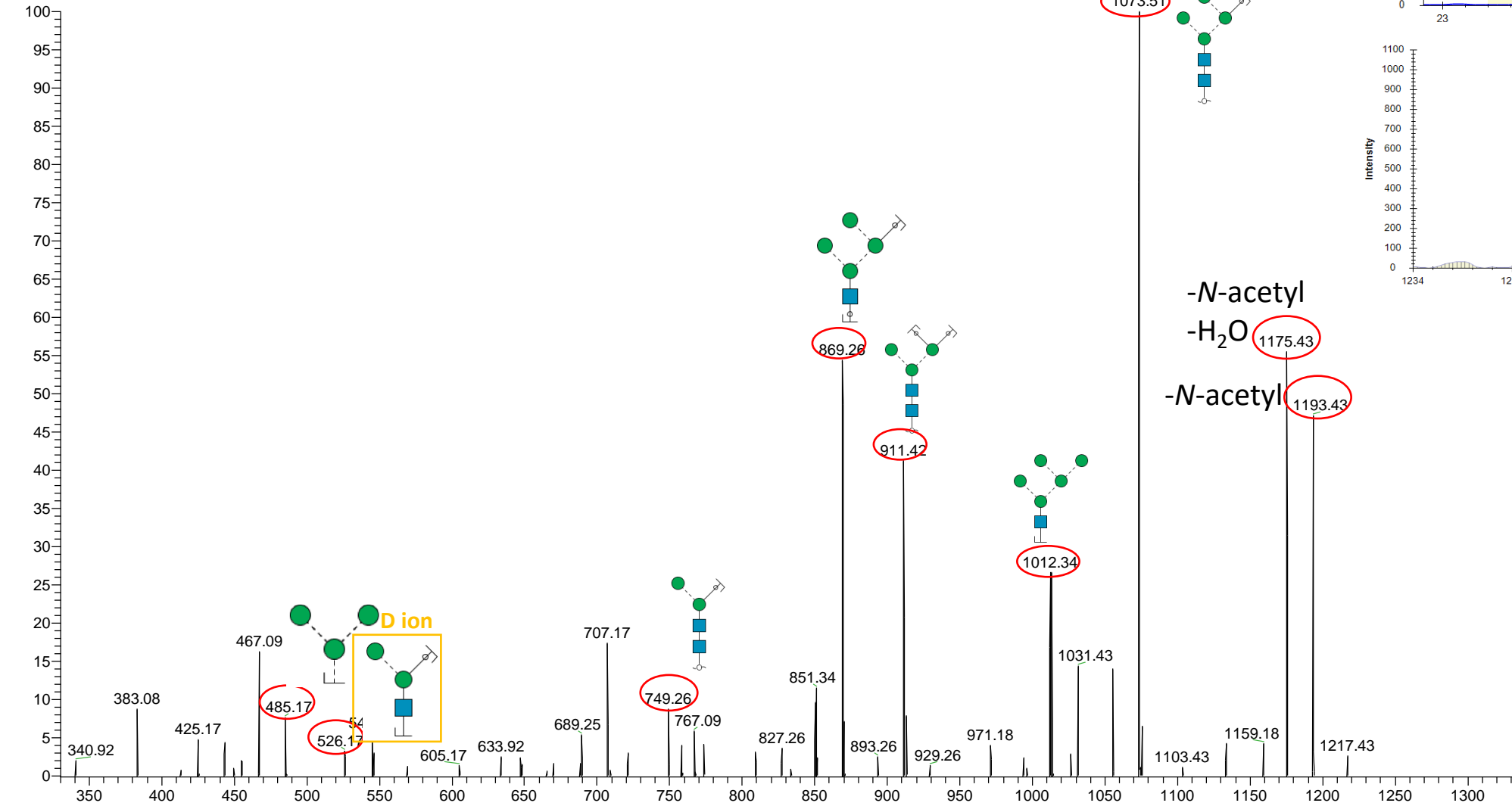


IL_VB_NG_260717 #3209 RT: 32.00 AV: 1 NL: 1.64E1
 F: ITMS - p ESI d Full ms2 1073.47@cid35.00 [285.00-2000.00]



Glycan #12a
 Oligomannose
 Hex₅HexNAc₂ (Man5)
m/z: 1235.5⁽¹⁻⁾

il_vb_ng_260717 #2502 RT: 24.94 AV: 1 NL: 4.52E1
 F: ITMS - p ESI d Full ms2 1235.49@cid35.00 [330.00-2000.00]



1073.51

869.26

911.42

1012.34

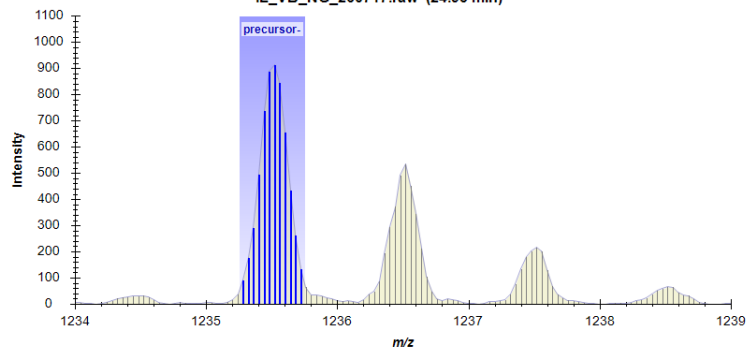
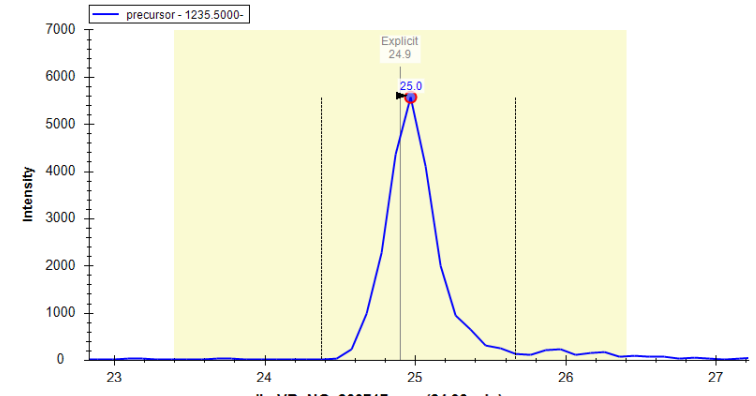
-N-acetyl

-H₂O

1175.43

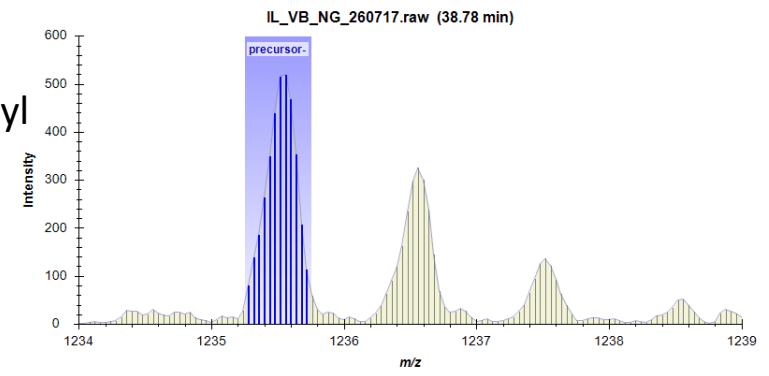
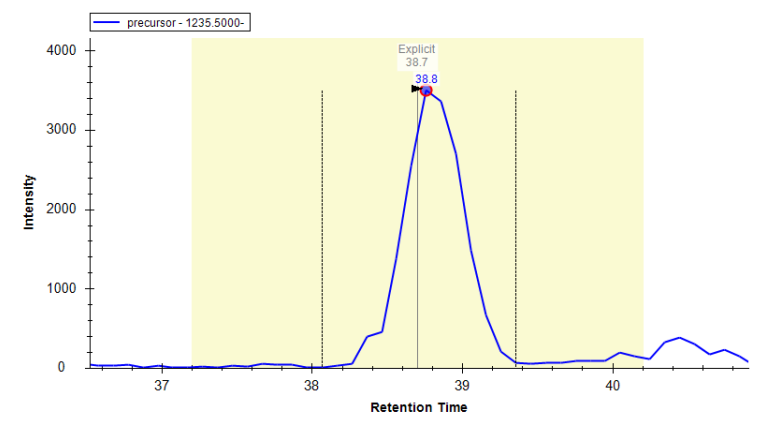
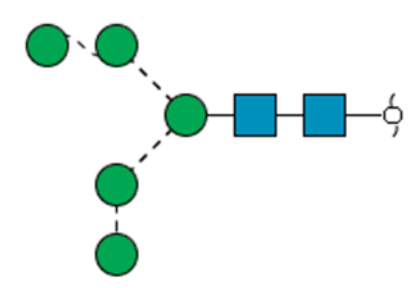
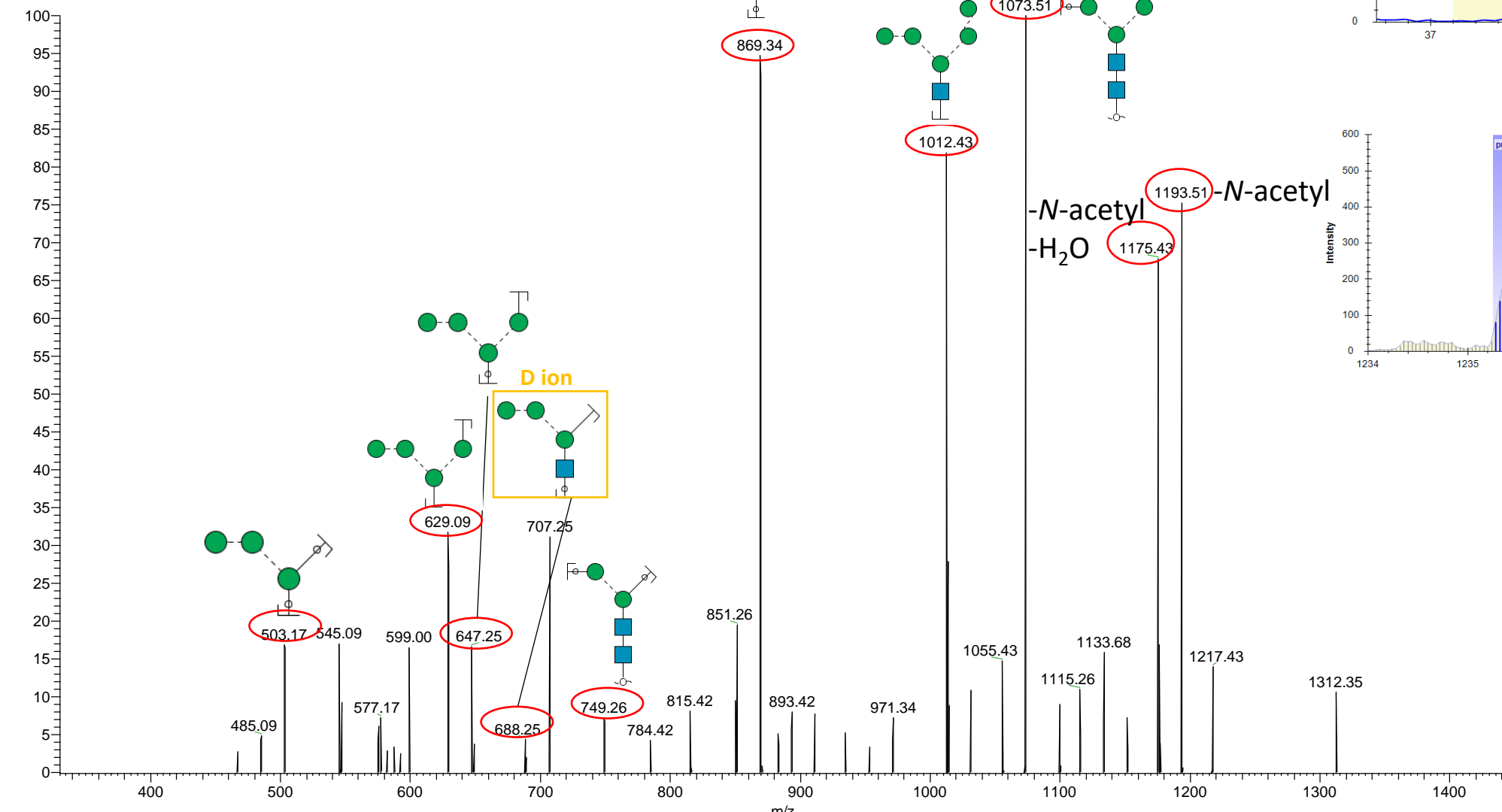
-N-acetyl

1193.43



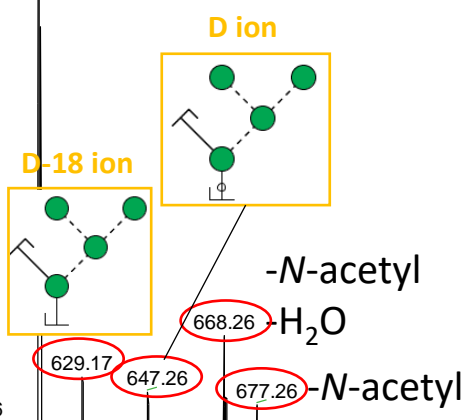
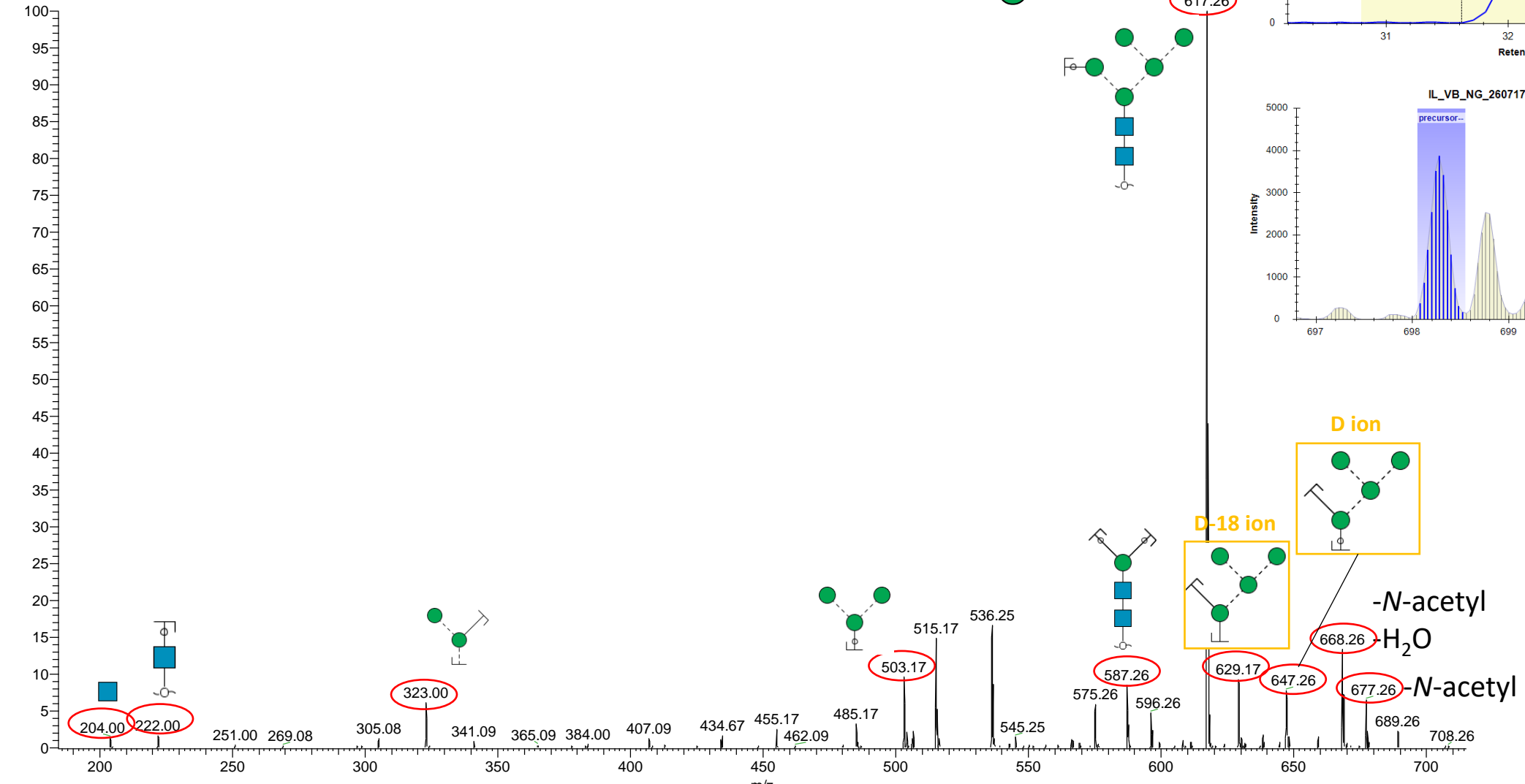
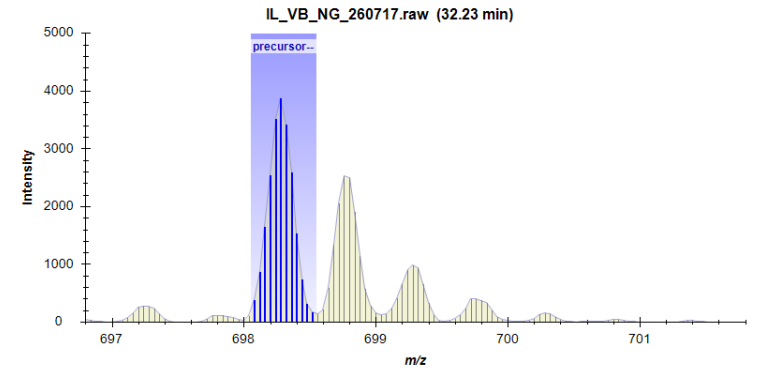
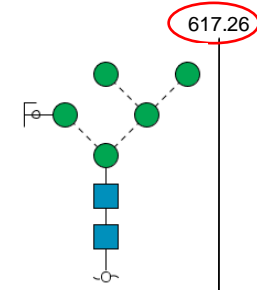
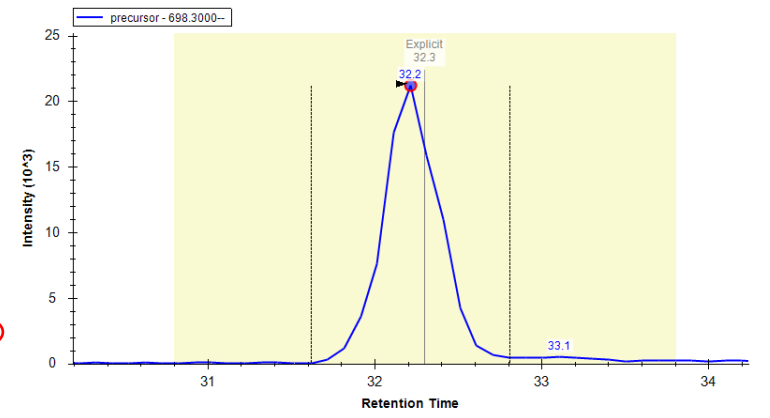
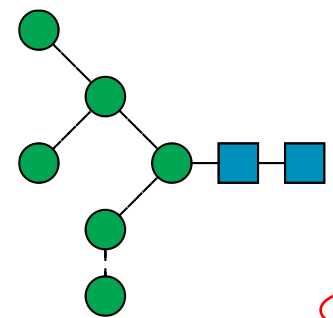
Glycan #12b
 Oligomannose
 Hex₅HexNAc₂ (Man5)
 m/z: 1235.5⁽¹⁻⁾

il_vb_ng_260717 #3869 RT: 38.76 AV: 1 NL: 1.77E1
 F: ITMS - p ESI d Full ms2 1235.49@cid35.00 [330.00-2000.00]



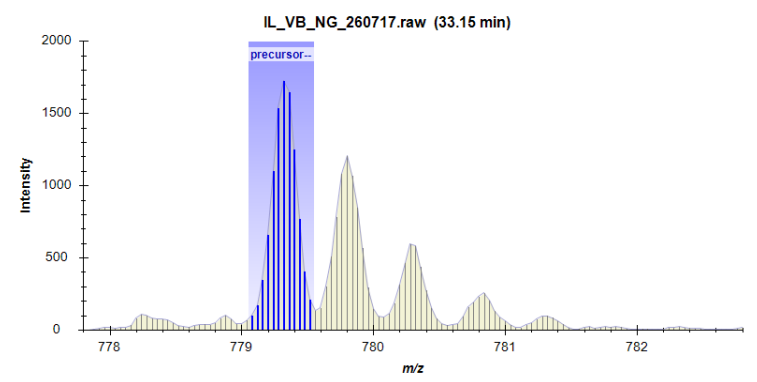
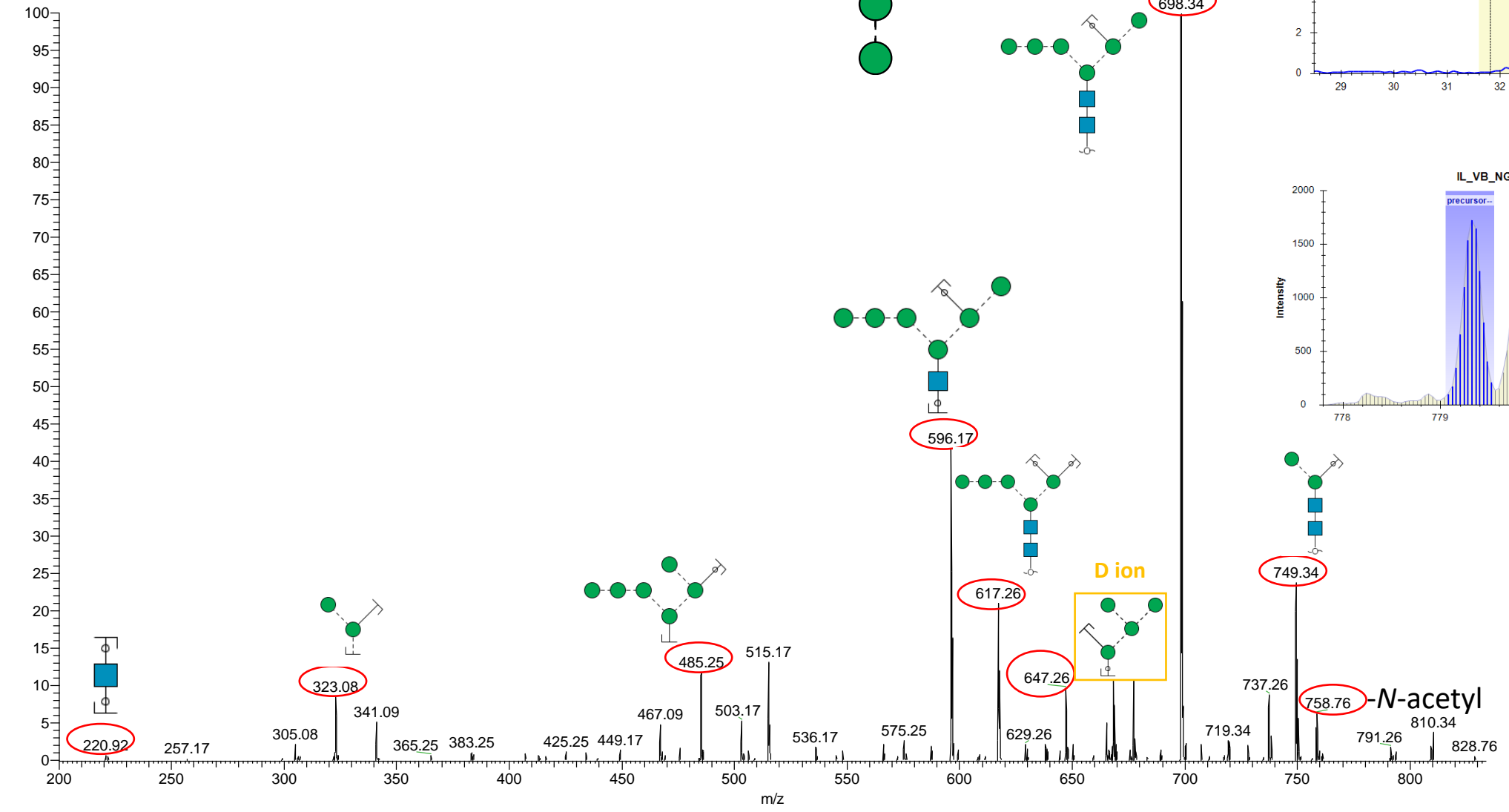
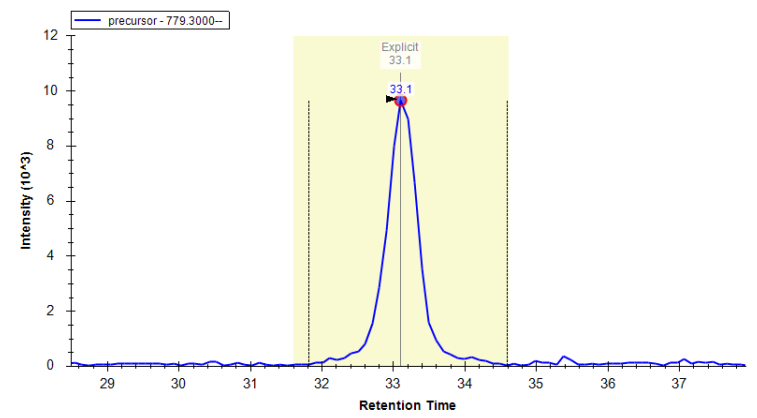
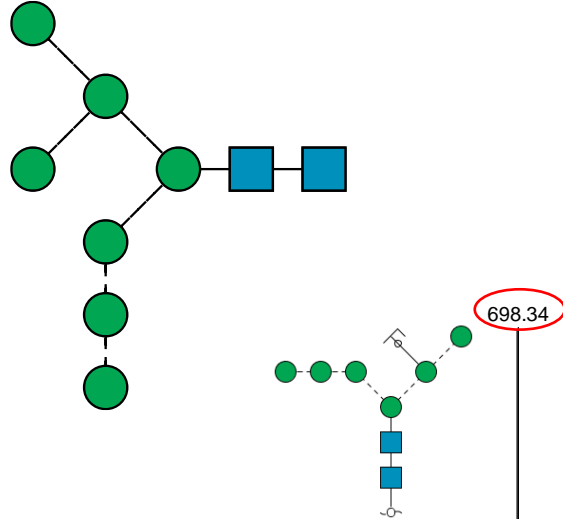
Glycan #13
 Oligomannose
 Hex₆HexNAc₂ (Man6)
m/z: 698.3⁽²⁻⁾

il_vb_ng_260717 #3232 RT: 32.23 AV: 1 NL: 4.62E2
 F: ITMS - p ESI d Full ms2 698.27@cid35.00 [180.00-1410.00]



Glycan #14
 Oligomannose
 Hex₇HexNAc₂ (Man7)
m/z: 779.3⁽²⁻⁾

il_vb_ng_260717 #3312 RT: 33.05 AV: 1 NL: 2.01E2
 F: ITMS - p ESI d Full ms2 779.30@cid35.00 [200.00-1570.00]

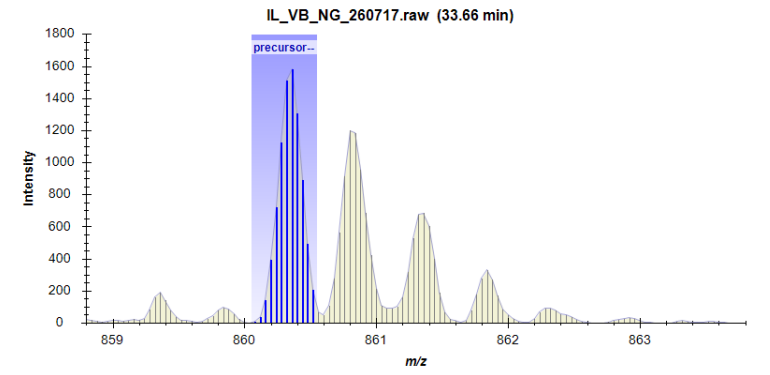
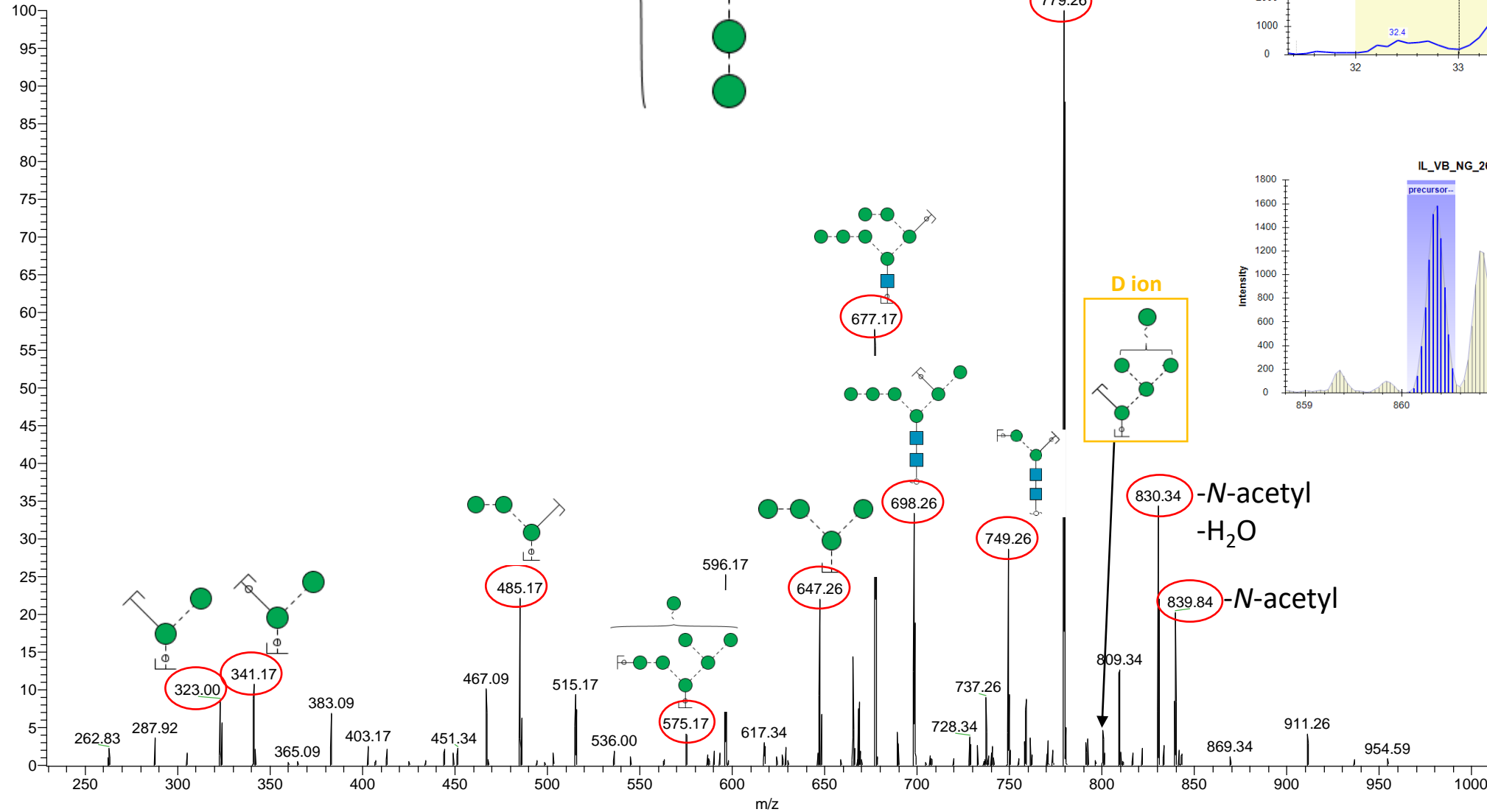
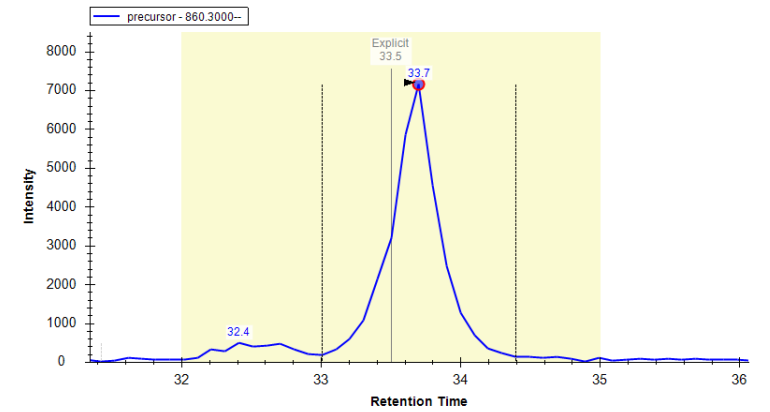
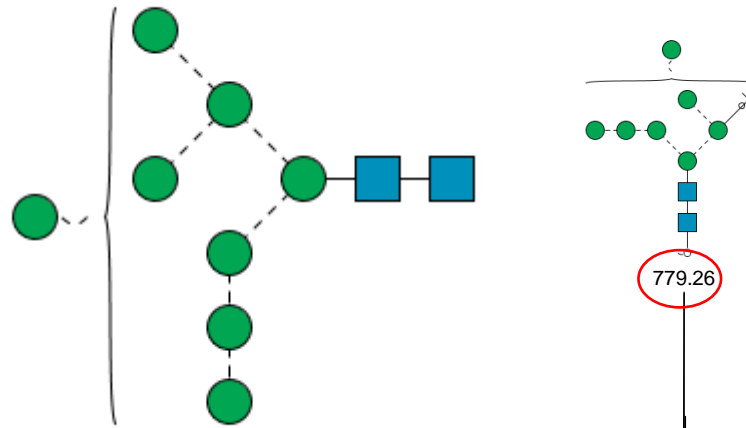


D ion

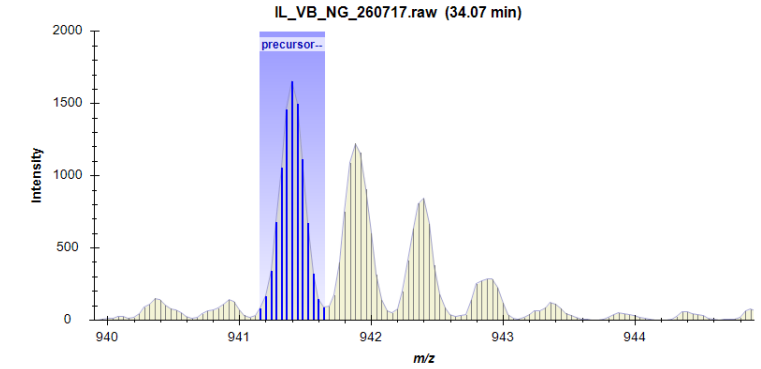
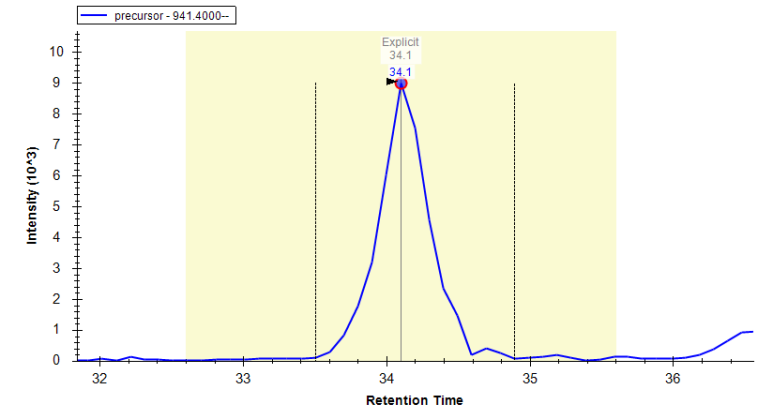
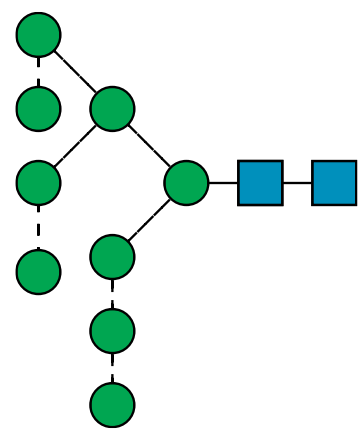
-N-acetyl

Glycan #15
 Oligomannose
 Hex₈HexNAc₂ (Man8)
 m/z: 860.3⁽²⁻⁾

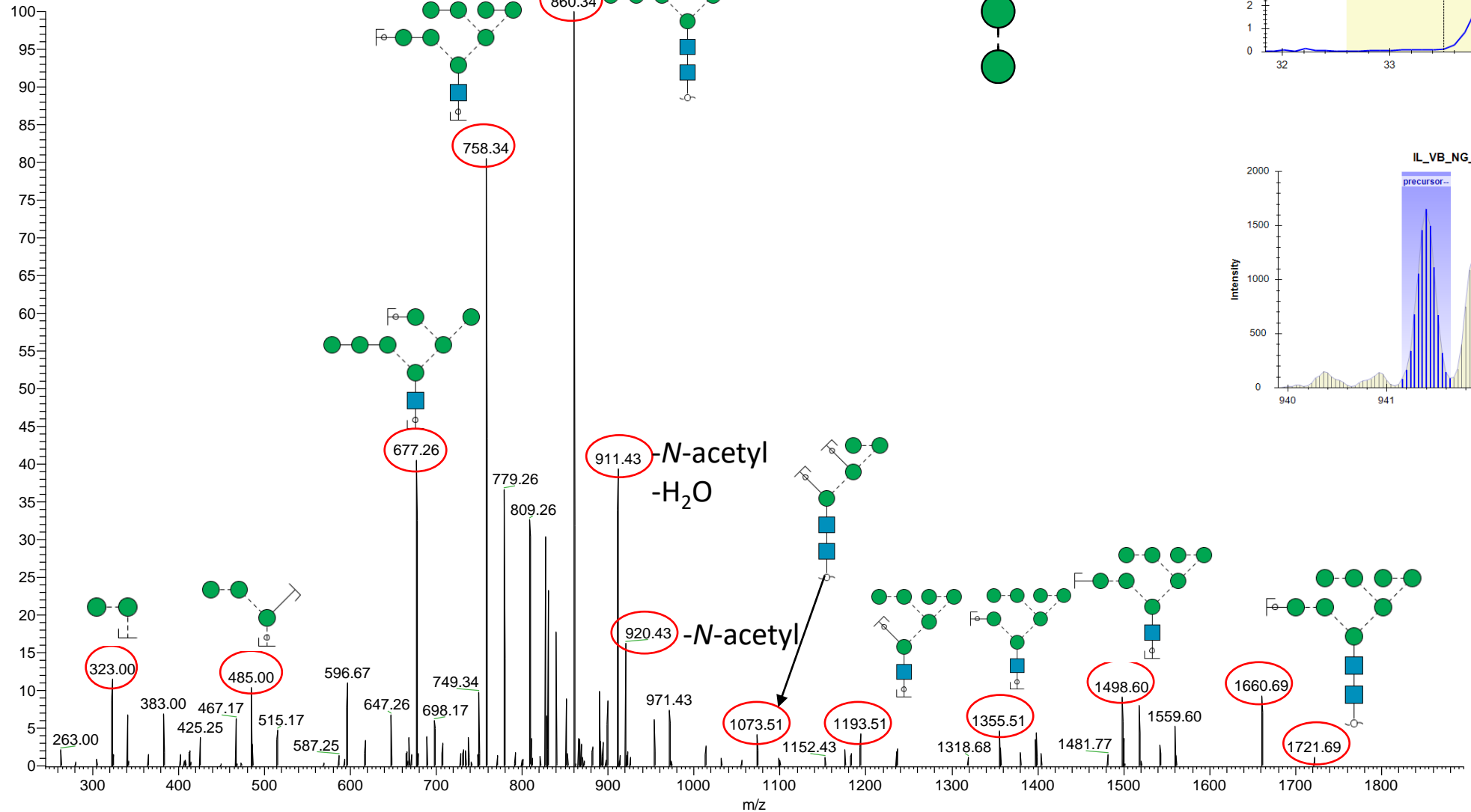
il_vb_ng_260717 #3372 RT: 33.66 AV: 1 NL: 8.68E1
 F: ITMS -p ESI d Full ms2 860.32@cid35.00 [225.00-1735.00]



Glycan #16
 Oligomannose
 Hex₉HexNAc₂ (Man9)
 m/z: 941.4 (2-)



IL_VB_NG_260717 #3422 RT: 34.18 AV: 1 NL: 8.49E1
 F: ITMS - p ESI d Full ms2 941.34@cid35.00 [245.00-1895.00]



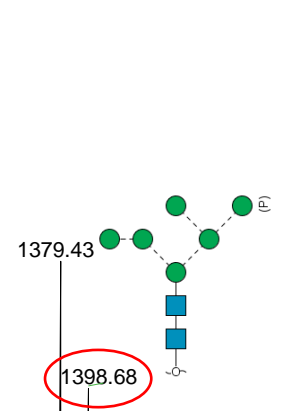
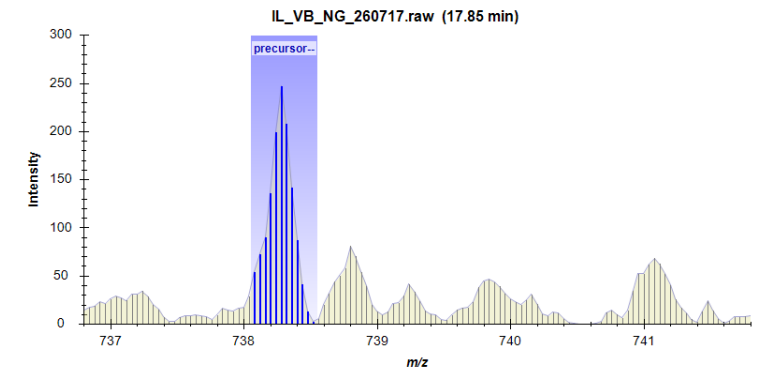
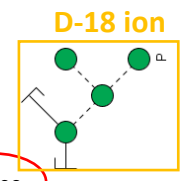
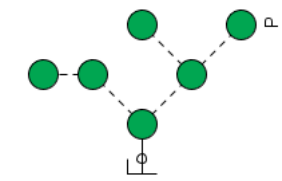
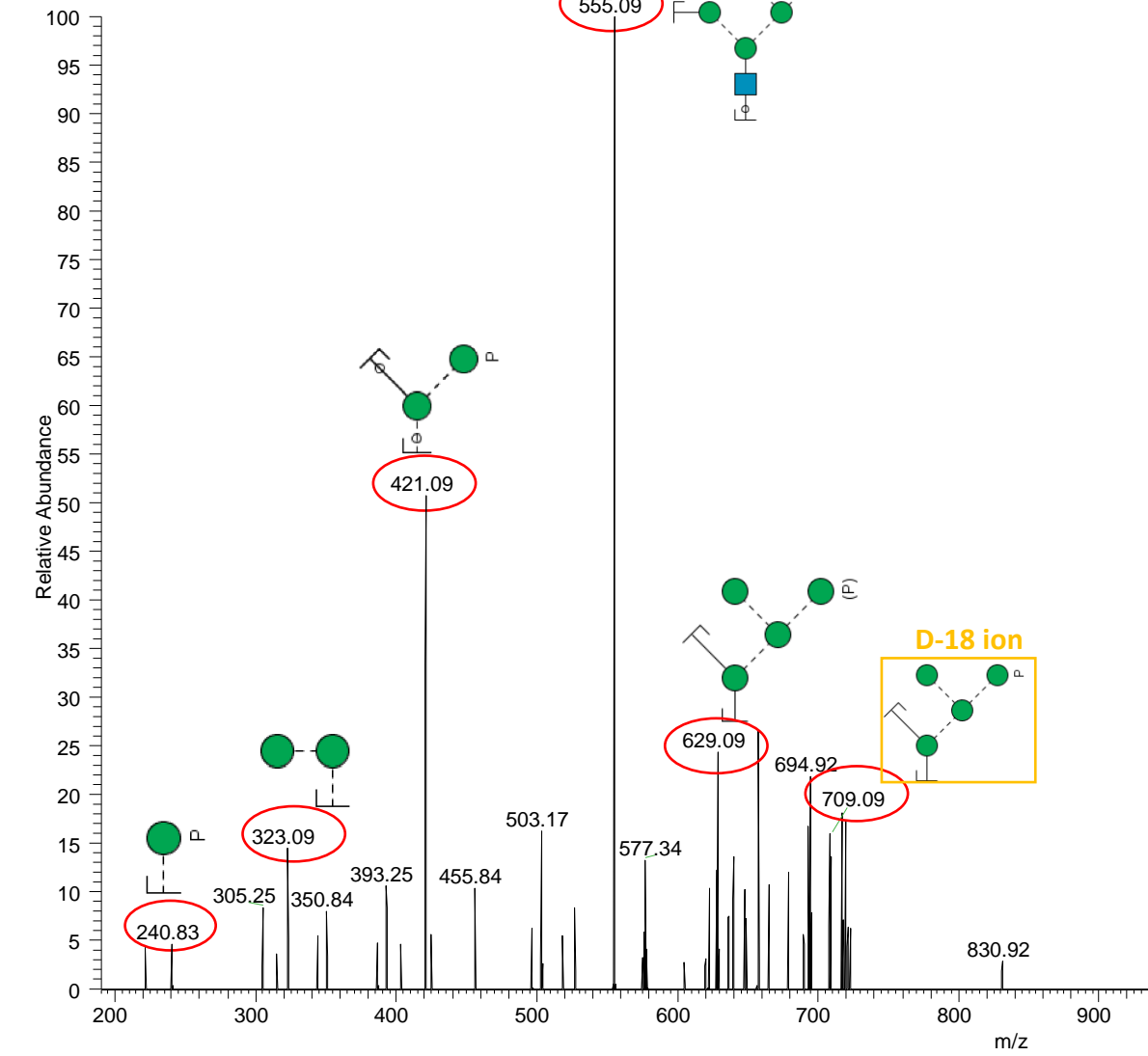
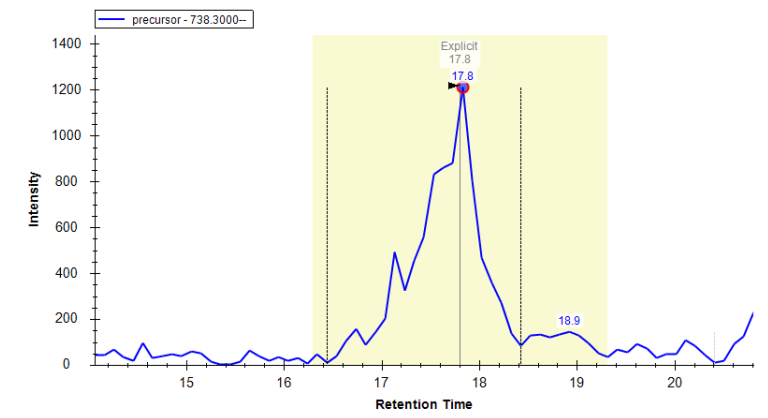
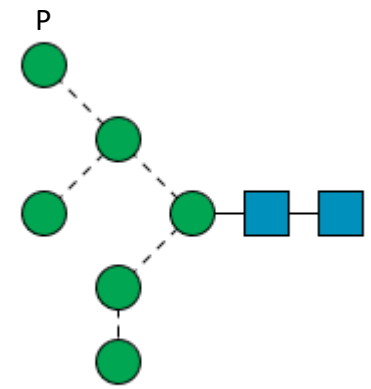
Glycan #17

Oligomannose

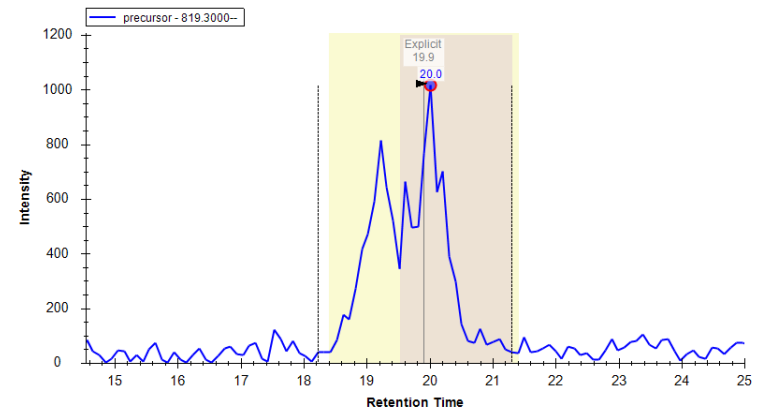
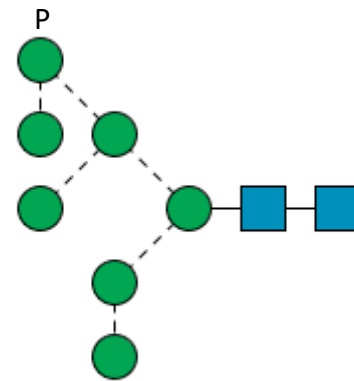
Hex₆HexNAc₂Phos₁ (M6P1)

m/z: 738.3⁽²⁻⁾

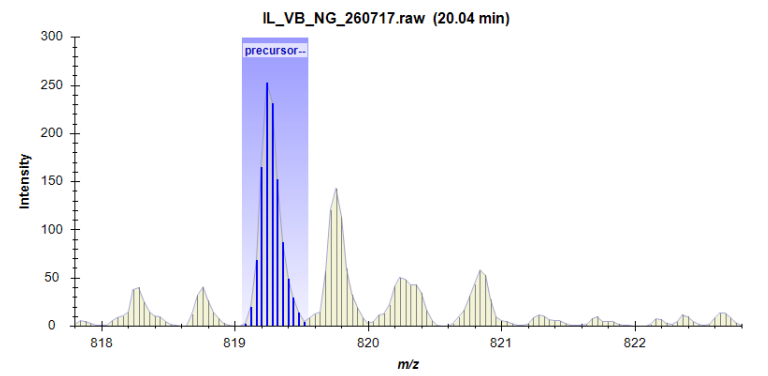
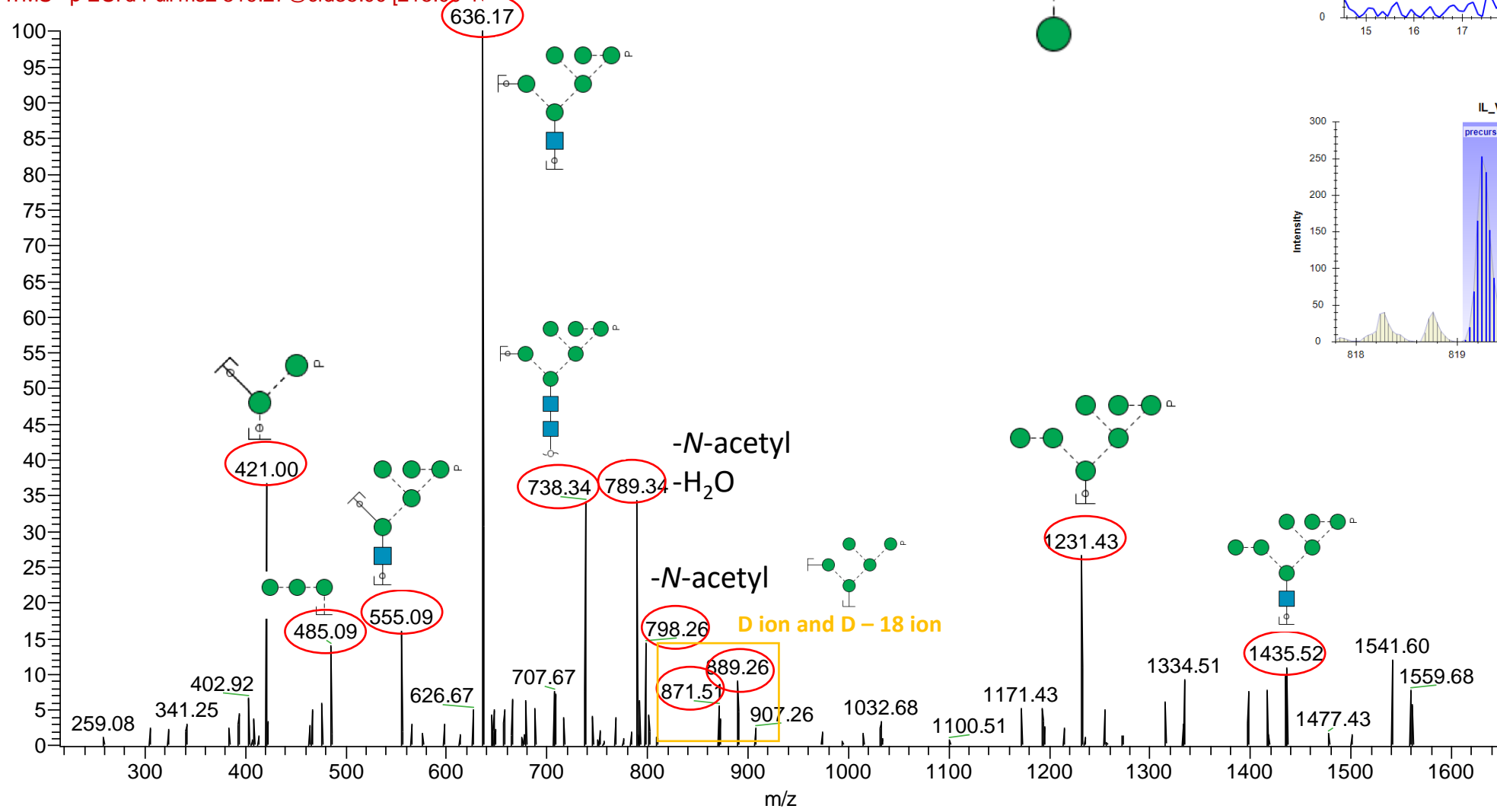
IL_VB_NG_260717#1797 RT: 17.91 AV: 1 NL: 1.59E1
 F: ITMS - p ESI d Full ms2 738.22@cid35.00 [190.00-1490.00]



Glycan #18
 Oligomannose
 Hex₇HexNAc₂Phos₁ (M7P1)
 m/z: 819.3⁽²⁻⁾



IL_XB_NG_260717 #1995 RT: 19.90 AV: 1 NL: 5.55E1
 F: ITMS - p ESI d Full ms2 819.27@cid35.00 [215.00-11



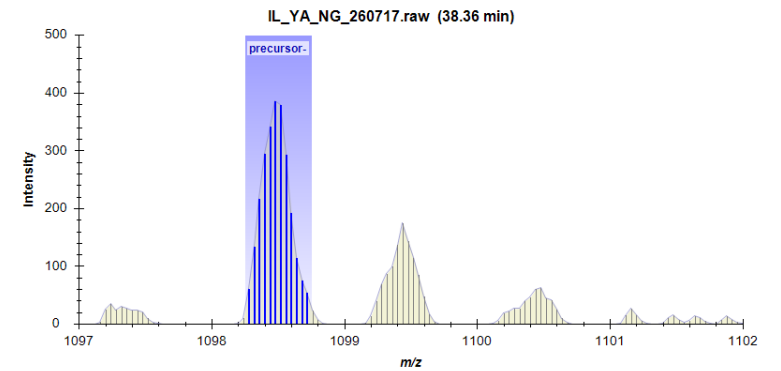
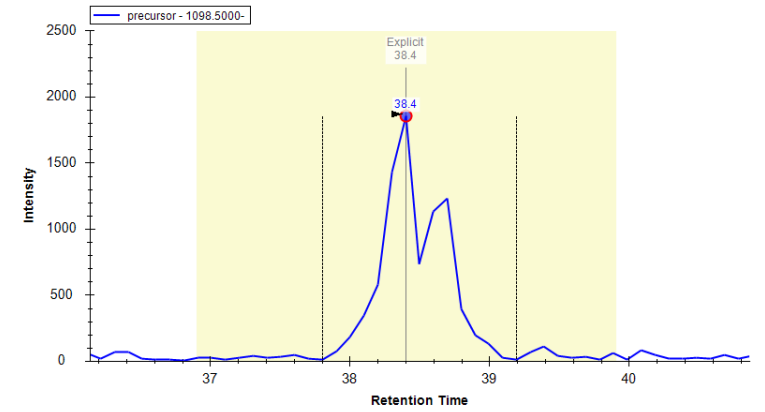
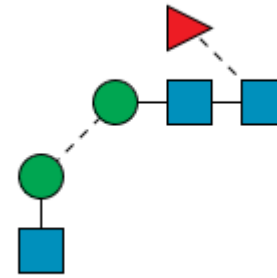
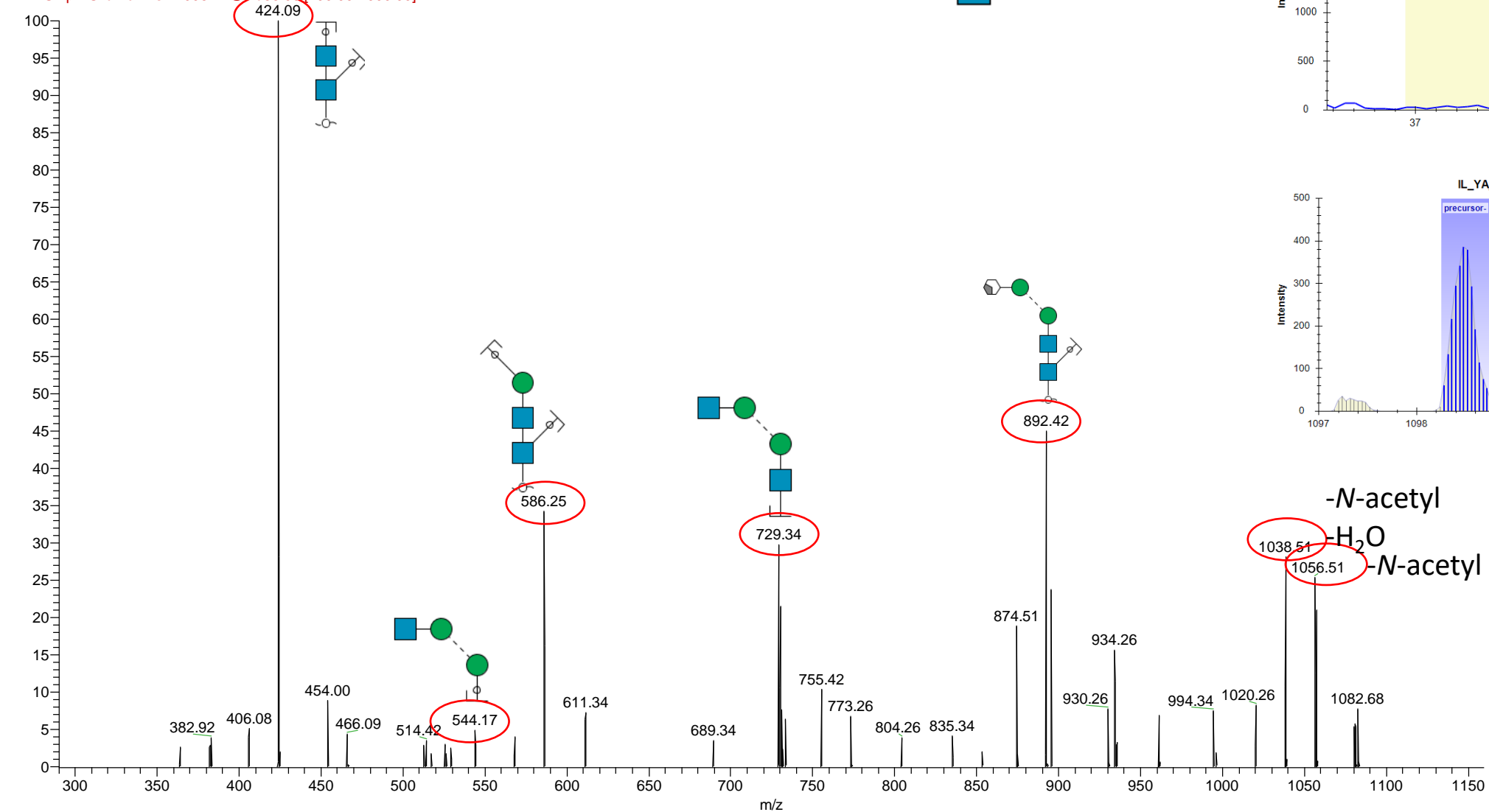
Glycan #19

Complex

HexNAc₁+ Hex₂HexNAc₂Fuc₁

m/z: 1098.5 (1-)

IL_YA_NG_260717 #3848 RT: 38.43 AV: 1 NL: 2.21E1
F: ITMS - p ESI d Full ms2 1098.47 @ 38.43 [290.00-2000.00]



-N-acetyl
-H₂O
-N-acetyl

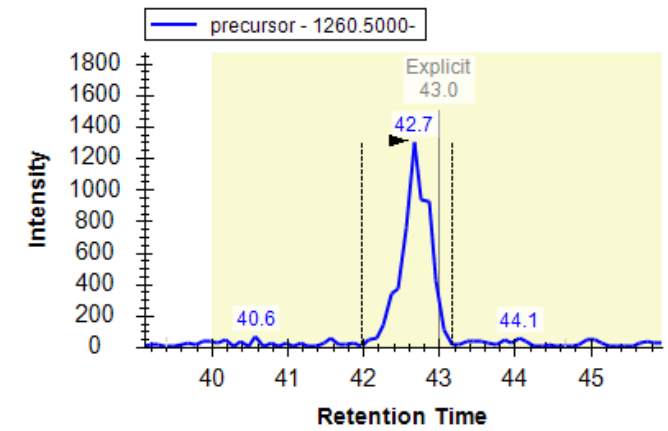
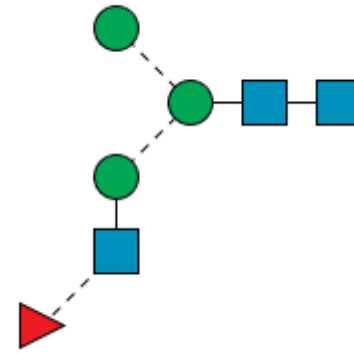
Note: From biosynthetic pathway and lack of D and D-18 ions, extension is predicted at α -1,3 arm.

Glycan #20a

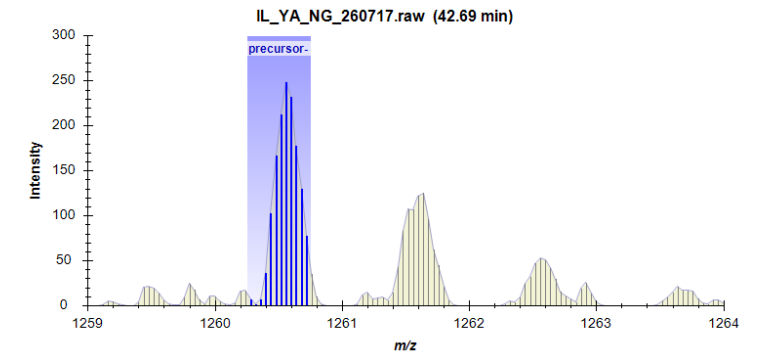
Complex

HexNAc₁Fuc₁+ Hex₃HexNAc₂

m/z: 1260.5⁽¹⁻⁾



No MS/MS available in N-glycomics data



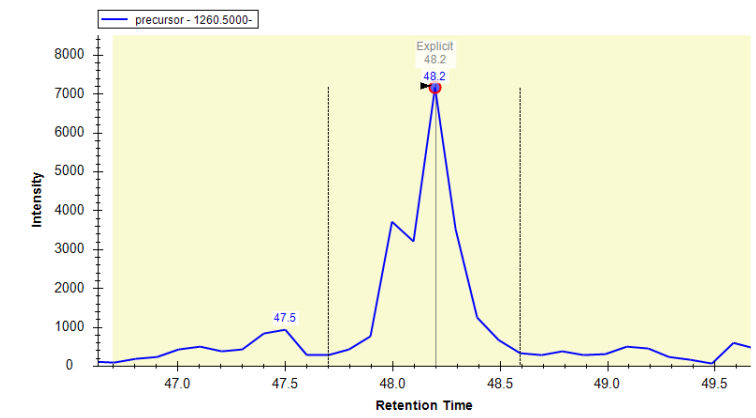
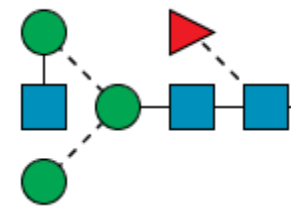
Note: There is a lack of tandem mass spectral data to evidence the glycan structure. However, based on early PGC-LC elution and the expected biosynthetic relationships between observed structures, this glycan is annotated as the antenna fucosylated isomer of glycan #20a. The exact antennary fucosyl linkage(s) (here drawn as alpha1,3) remains undetermined.

Glycan #20b

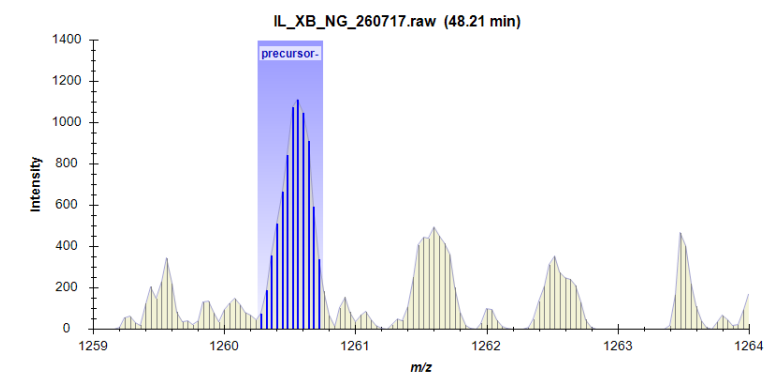
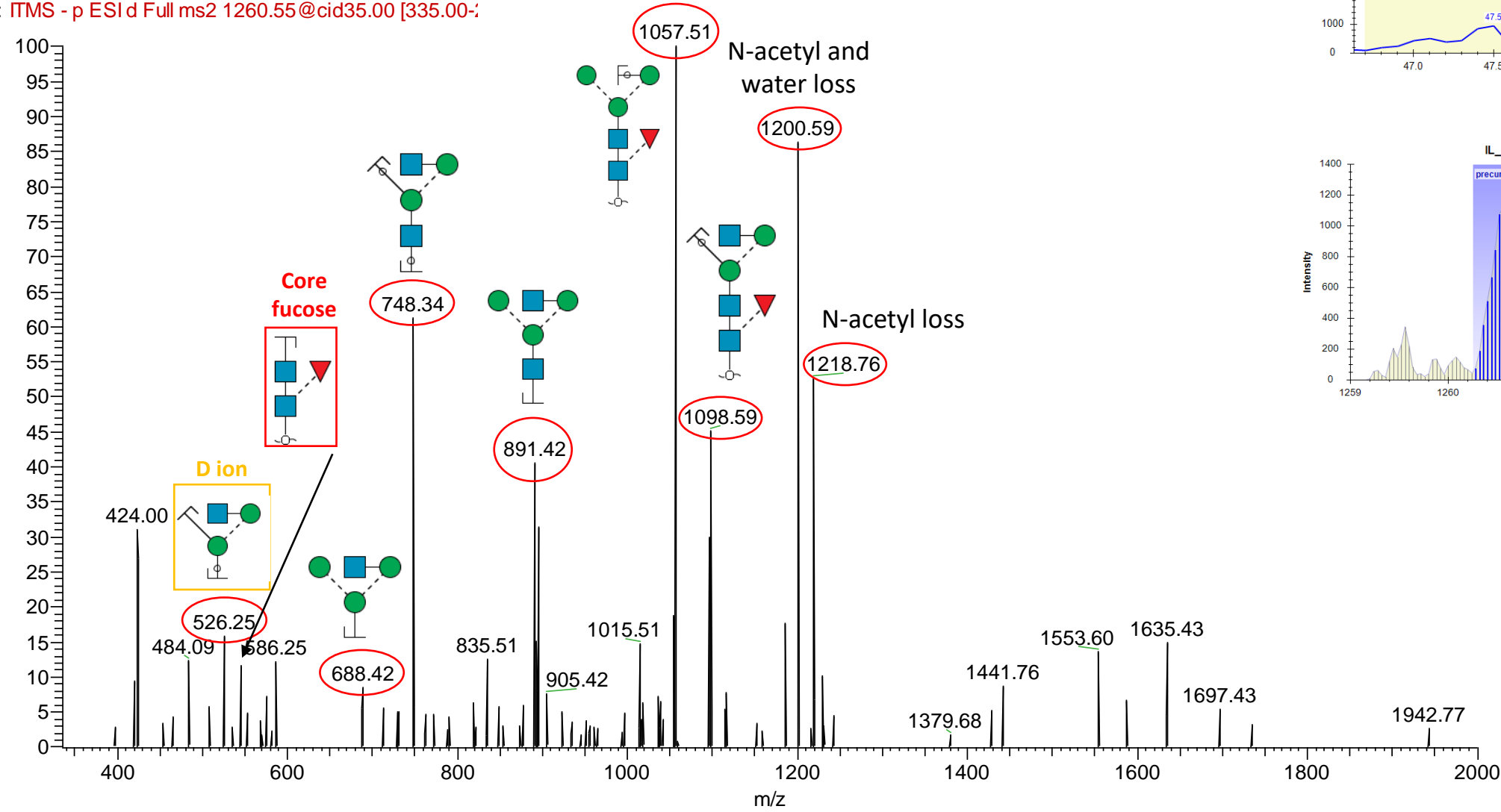
Complex

HexNAc₁ + Hex₃HexNAc₂Fuc₁

m/z: 1260.5 (1-)



IL_XB_NG_260717 #4787 RT: 48.27 AV: 1 NL: 2.03E1
F: ITMS - p ESI d Full ms2 1260.55@cid35.00 [335.00-;



Note: Evidence of core fucose and GlcNAc extension of α 1,6 arm as evidenced by D ion.

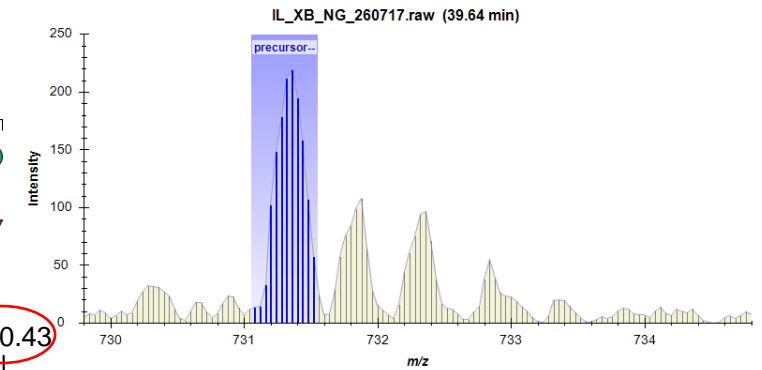
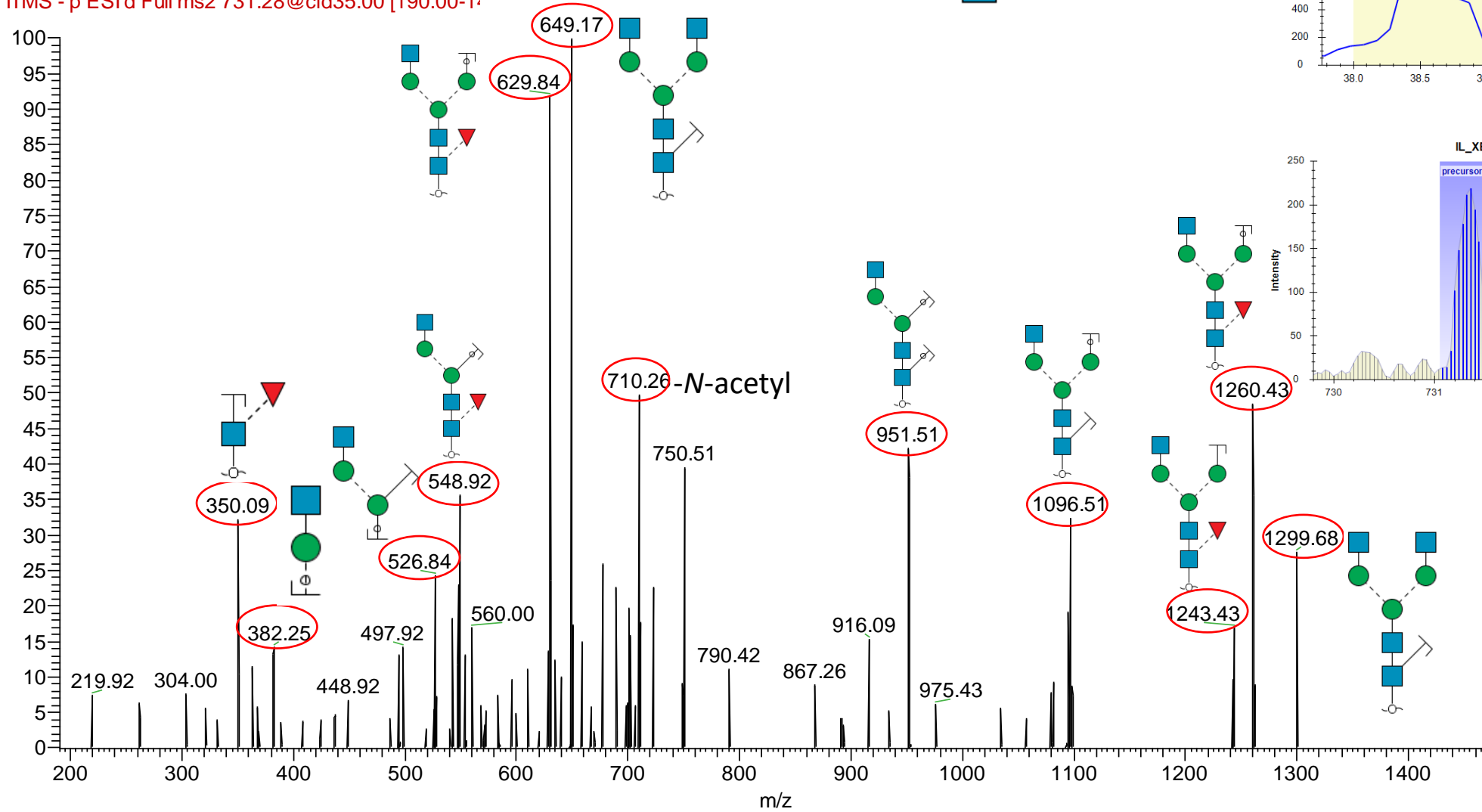
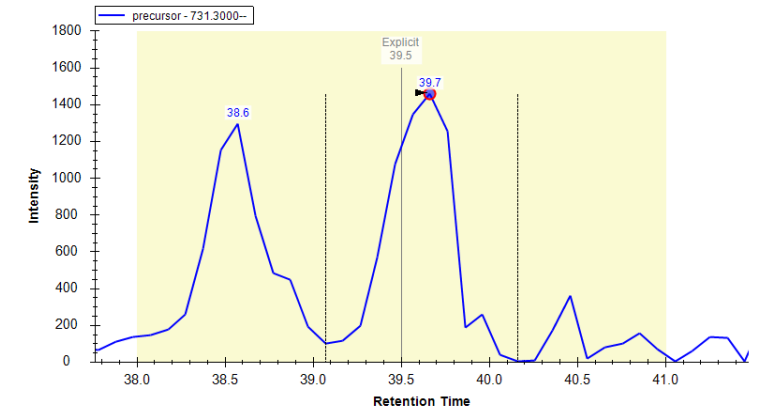
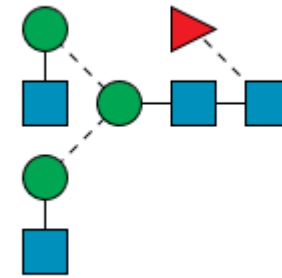
Glycan #21

Complex

HexNAc₂ + Hex₃HexNAc₂Fuc₁

m/z: 731.3⁽²⁻⁾

IL_XB_NG_260717 #3936 RT: 39.59 AV: 1 NL: 1.53E1
F: ITMS - p ESI d Full ms2 731.28@cid35.00 [190.00-1]



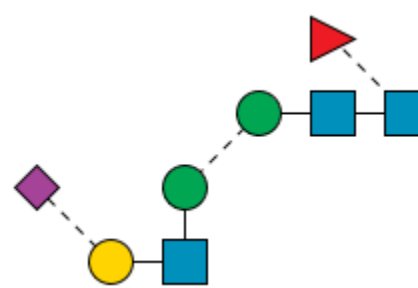
Note: Evidence of core fucose.

Glycan #22a

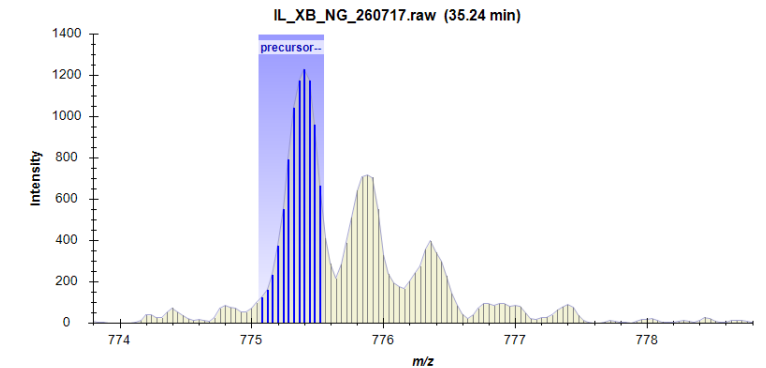
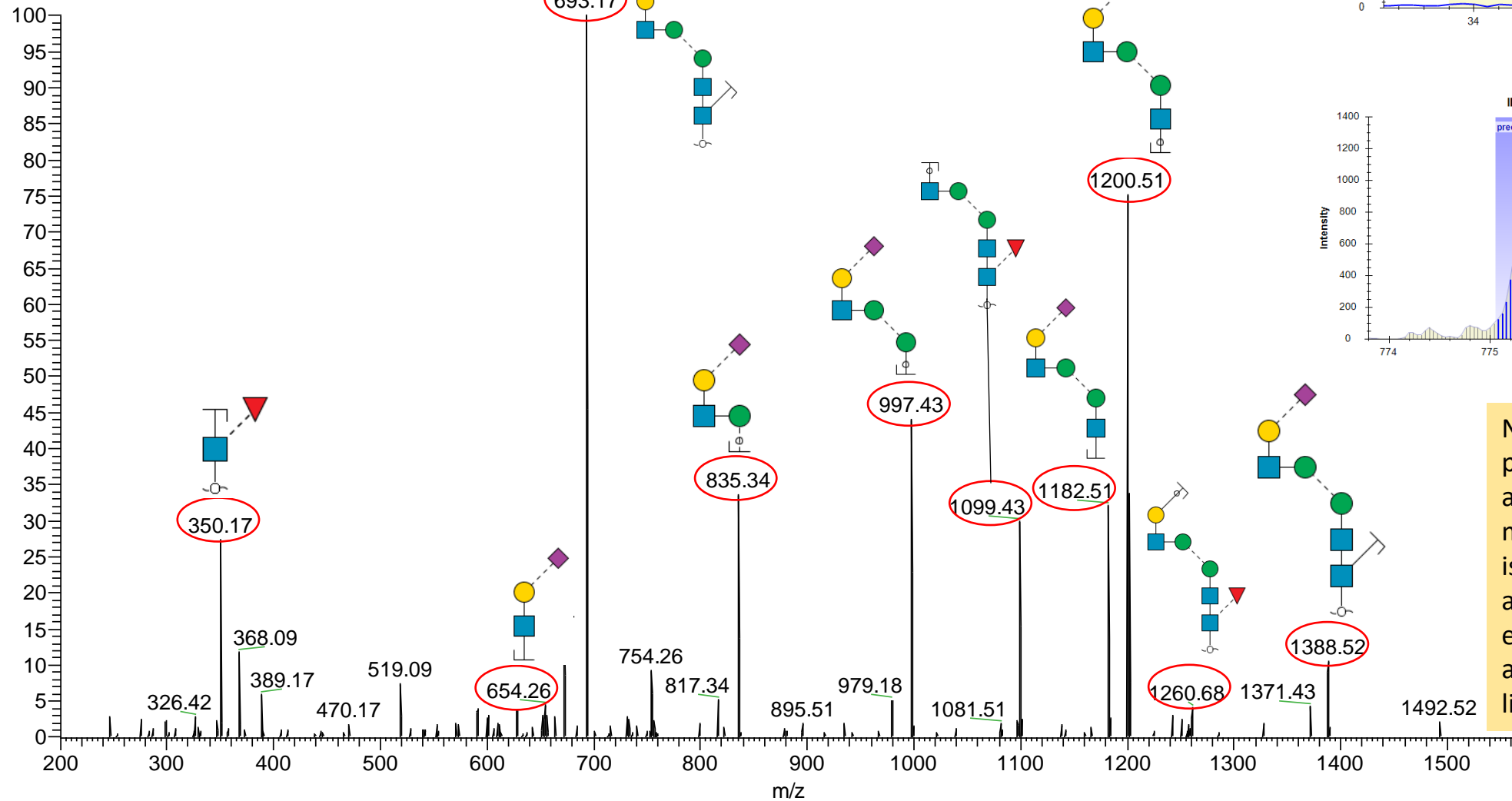
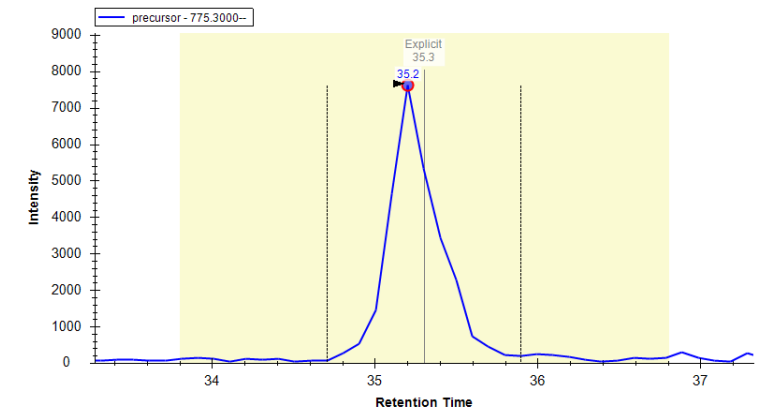
Complex

Hex₁HexNAc₁NeuAc₁ + Hex₂HexNAc₂Fuc₁

m/z: 775.3⁽²⁻⁾



IL_VB_NG_260717 #3534 RT: 35.34 AV: 1 NL: 8.53E1
F: ITMS - p ESI d Full ms2 775.33@cid35.00 [200.00-1!



Note: From biosynthetic pathway and the lack of D and/or D-18 ions, monoantennary sialyl LacNAc is predicted to occupy the α 1,3 arm. Based on early PGC-LC elution, this glycan is annotated as the α 2,6-sialyl linkage isomer.

Glycan #22b

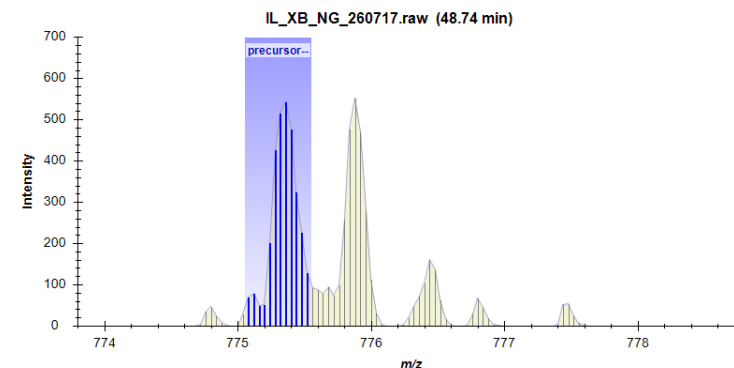
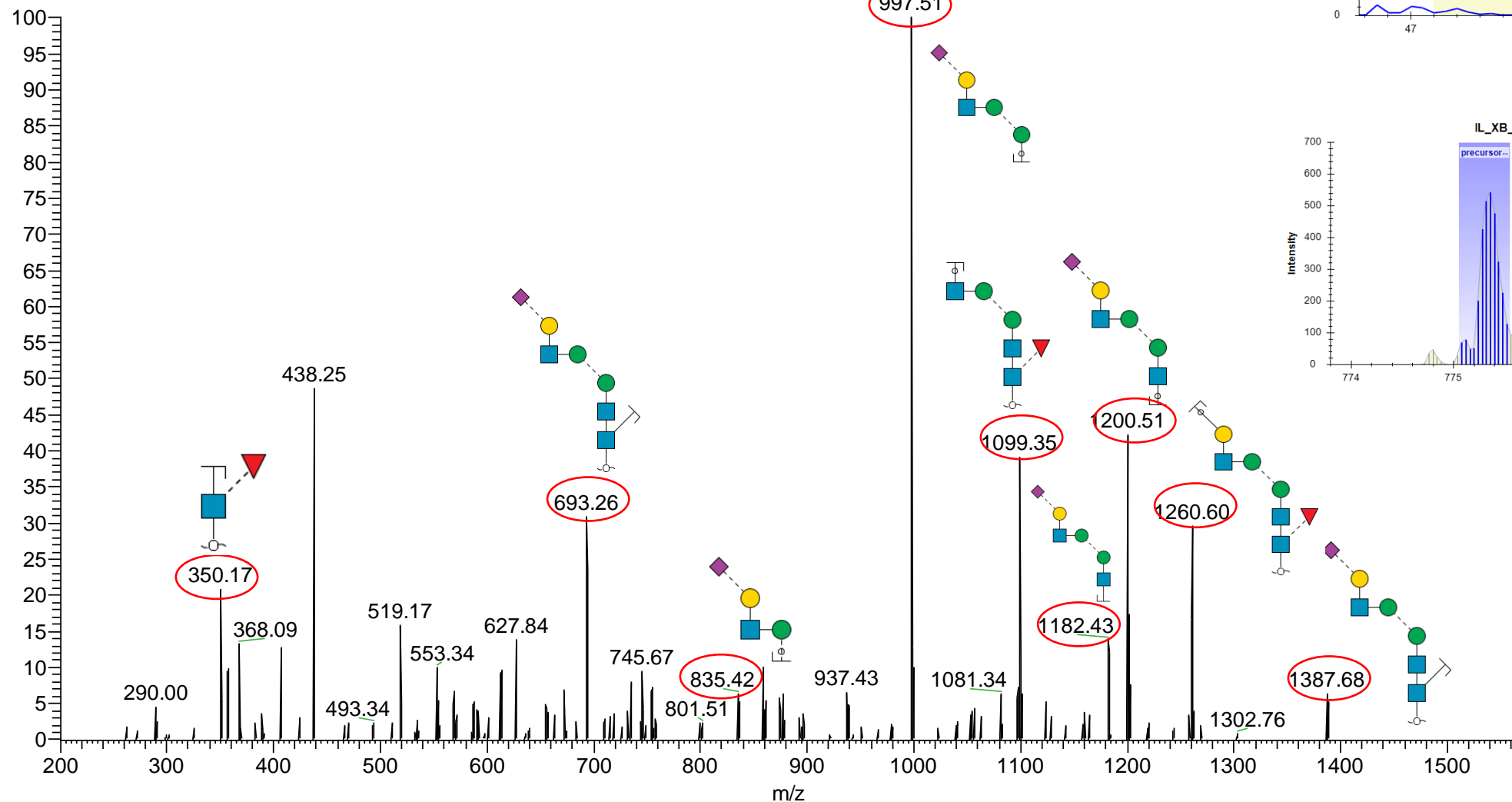
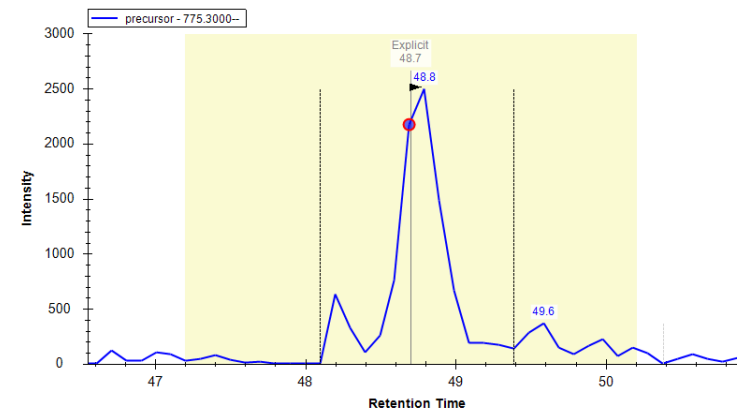
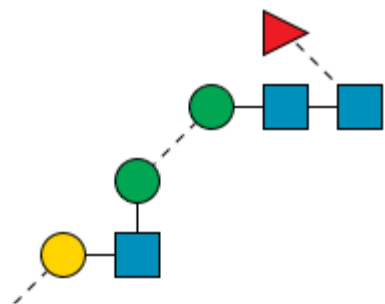
Complex

Hex₁HexNAc₁NeuAc₁ + Hex₂HexNAc₂Fuc₁

m/z: 775.3⁽²⁻⁾

IL_VB_NG_260717 #4838 RT: 48.72 AV: 1 NL: 4.31E1

F: ITMS - p ESI d Full ms2 775.33@cid35.00 [200.00-1!



Note: From biosynthetic pathway and the lack of D and/or D-18 ions, monoantennary sialyl LacNAc is predicted to occupy the α 1,3 arm. Based on late PGC-LC elution, this glycan is annotated as the α 2,3-sialyl linkage isomer.

Glycan #23

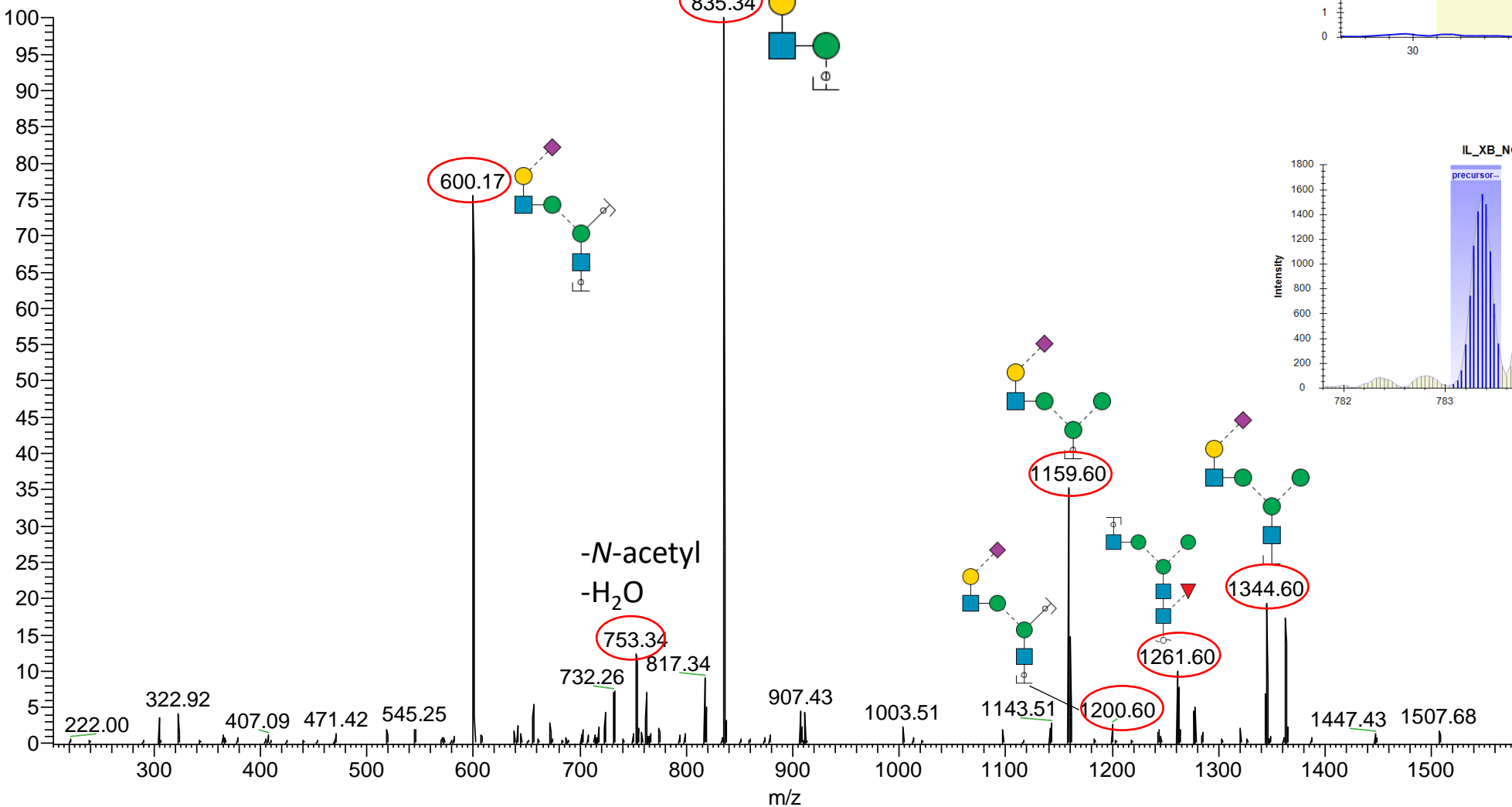
Complex

Hex₁HexNAc₁NeuAc₁ + Hex₃HexNAc₂

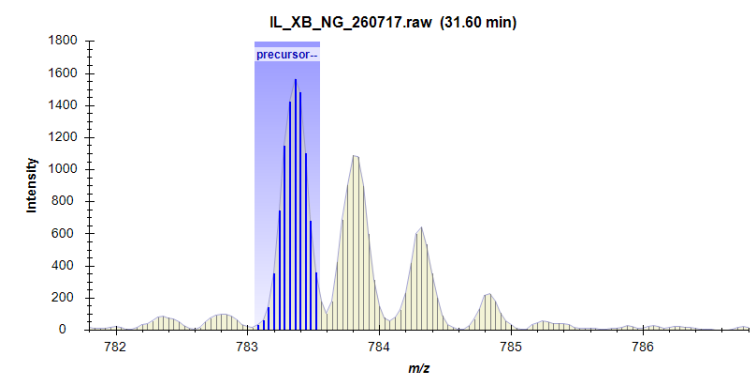
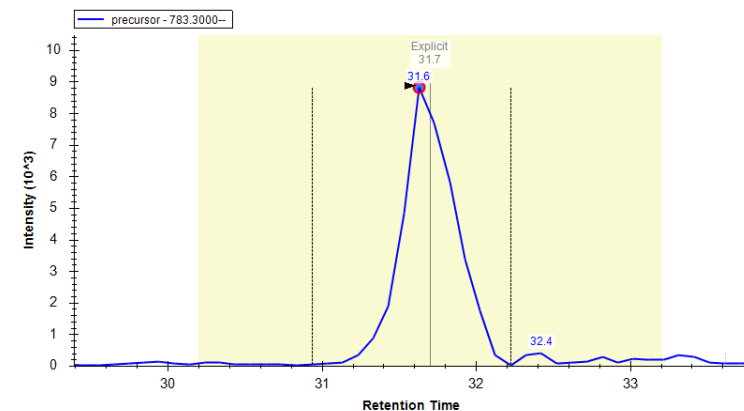
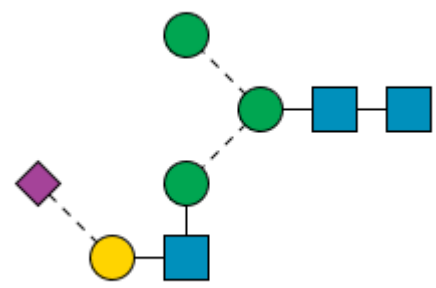
m/z: 783.3⁽²⁻⁾

IL_VB_NG_260717 #3182 RT: 31.72 AV: 1 NL: 1.20E2

F: ITMS - p ESI d Full ms2 783.20@cid35.00 [205.00-1!]



-N-acetyl
-H₂O



Note: From biosynthetic pathway and the lack of D and/or D-18 ions, monoantennary sialyl LacNAc is predicted to occupy the α1,3 arm. Based on early PGC-LC elution, this glycan is annotated as the α2,6-sialyl linkage isomer.

Glycan #24

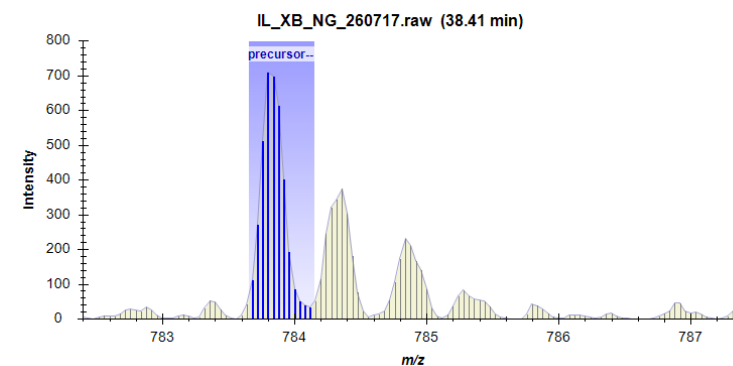
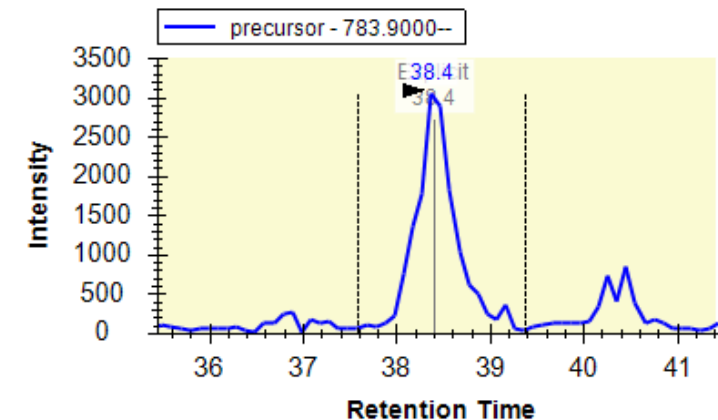
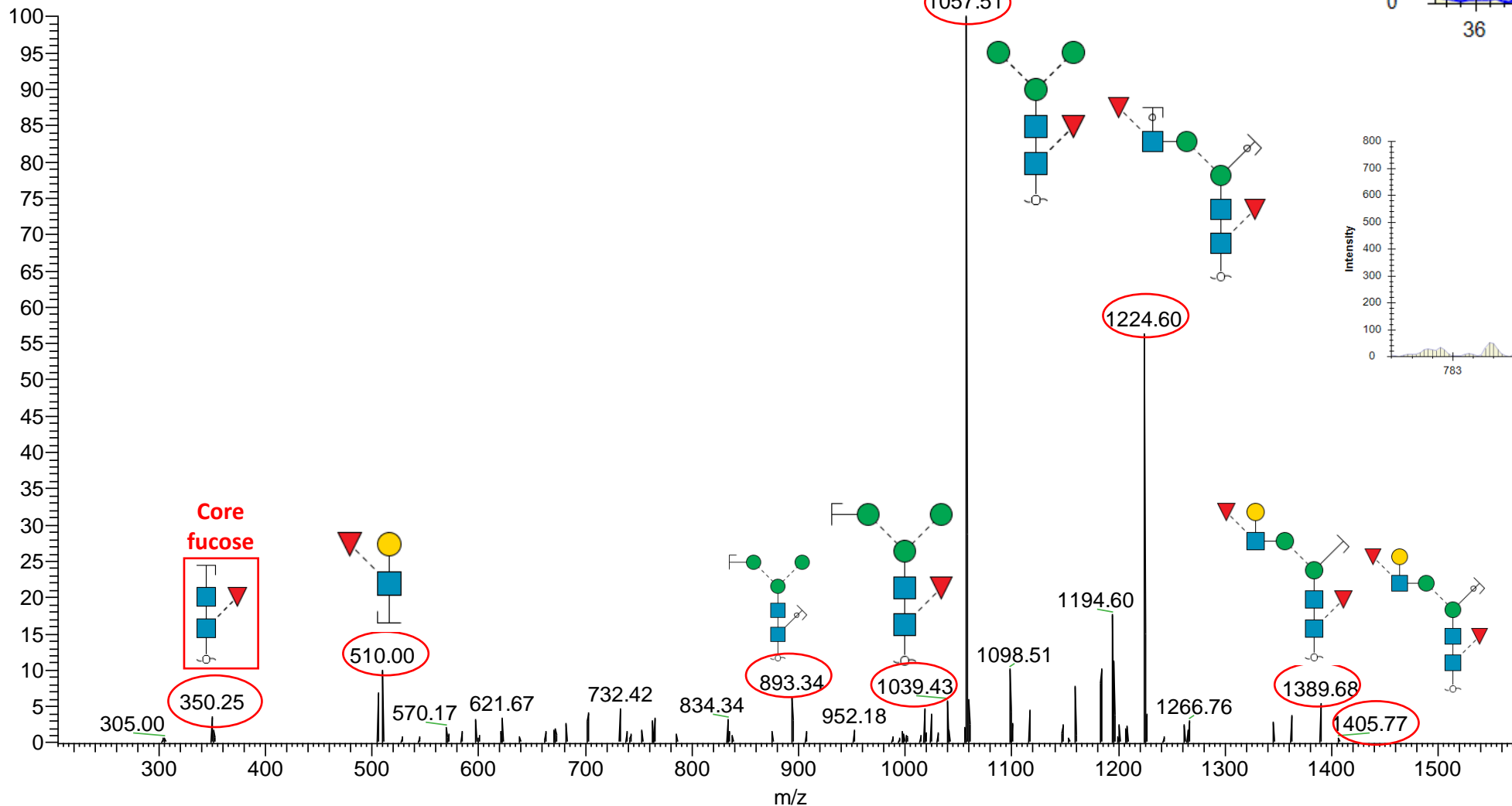
Complex

Hex₁HexNAc₁Fuc₁ + Hex₃HexNAc₂Fuc₁

m/z: 783.6⁽²⁻⁾

IL_XB_NG_260717 #3823 RT: 38.43 AV: 1 NL: 6.28E1

F: ITMS - p ESI d Full ms2 783.83@cid35.00 [205.00-1!



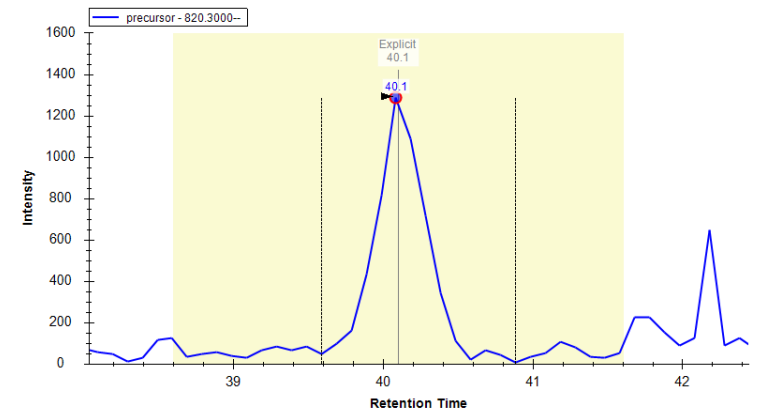
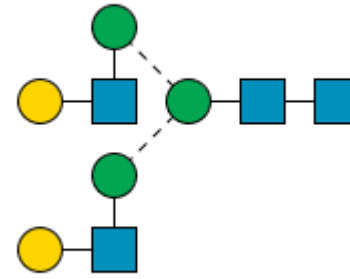
Note: Both evidence of core and antenna fucosylation. From biosynthetic pathway and the lack of D and/or D-18 ions, monoantennary Le x/a is predicted to occupy the α 1,3 arm. The exact antennary fucosyl linkage(s) (here drawn as alpha1,3) remains undetermined.

Glycan #25

Complex

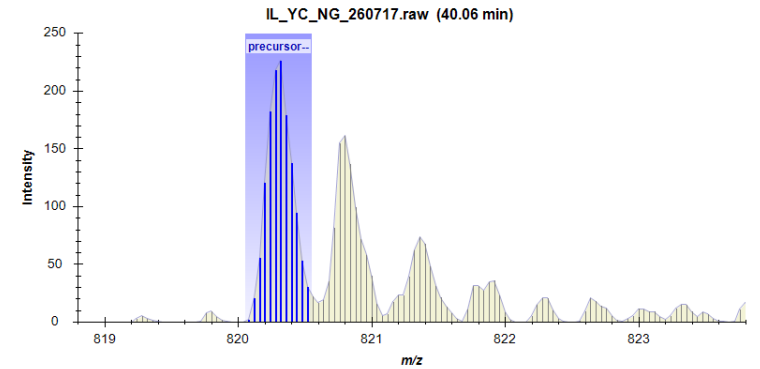
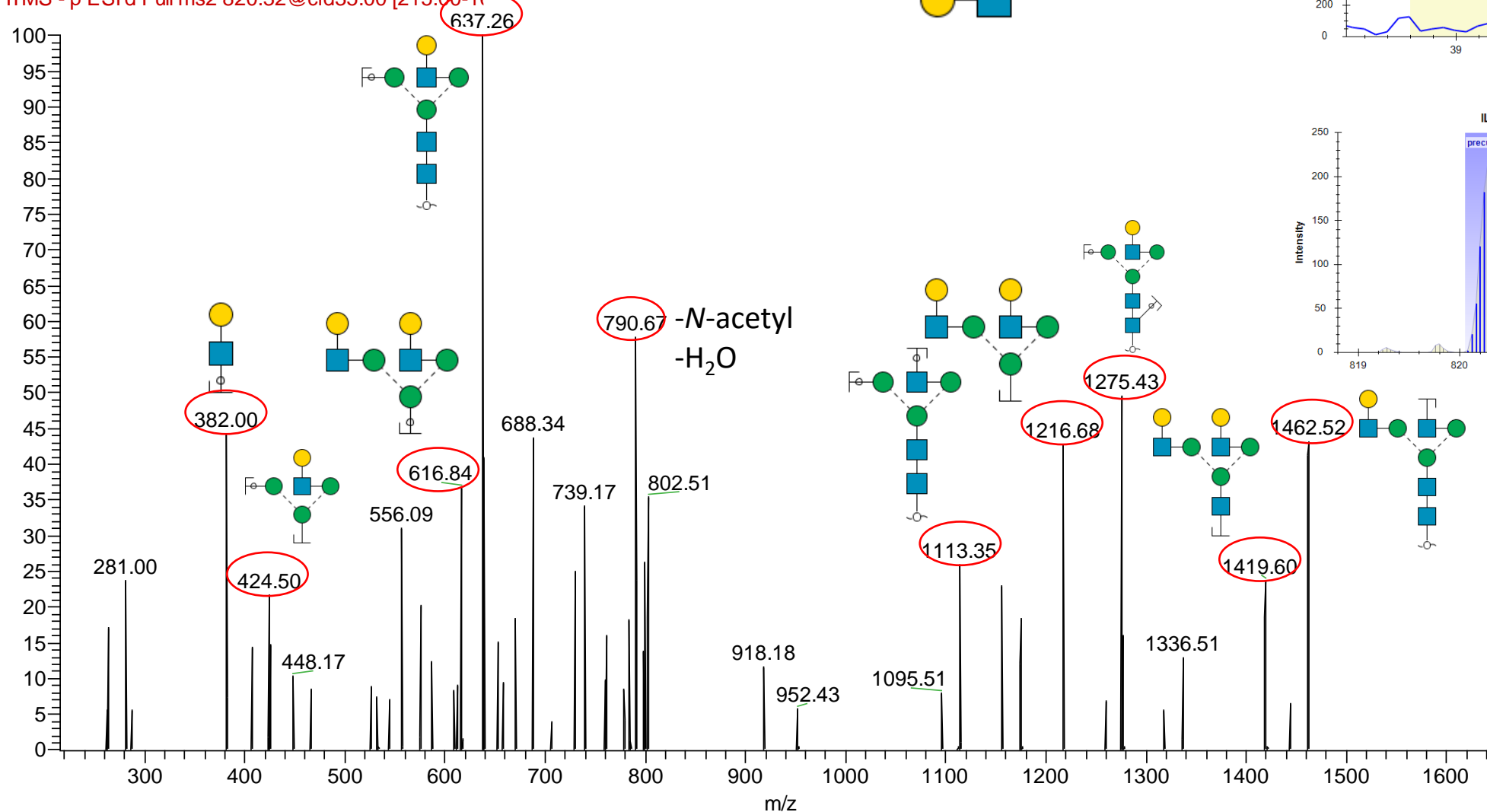
Hex₂HexNAc₂ + Hex₃HexNAc₂

m/z: 820.3⁽²⁻⁾



IL_YC_NG_260717 #4007 RT: 40.12 AV: 1 NL: 7.88

F: ITMS - p ESI d Full ms2 820.32@cid35.00 [215.00-11



Note: Assigned from good tandem mass spectral evidence and from known biosynthetic pathway

Glycan #26a

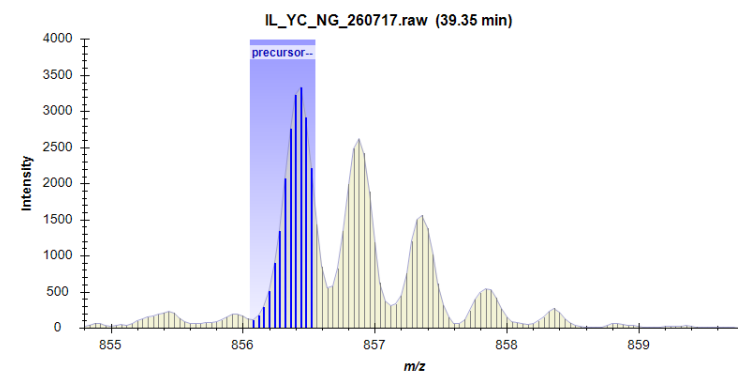
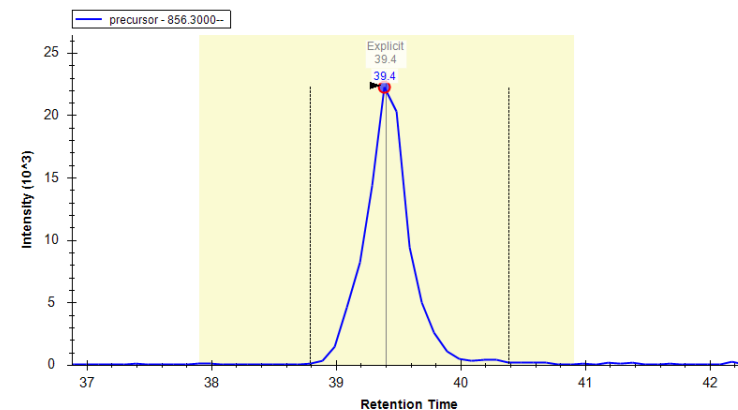
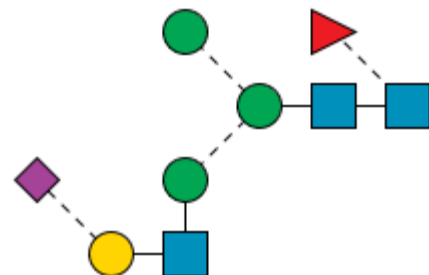
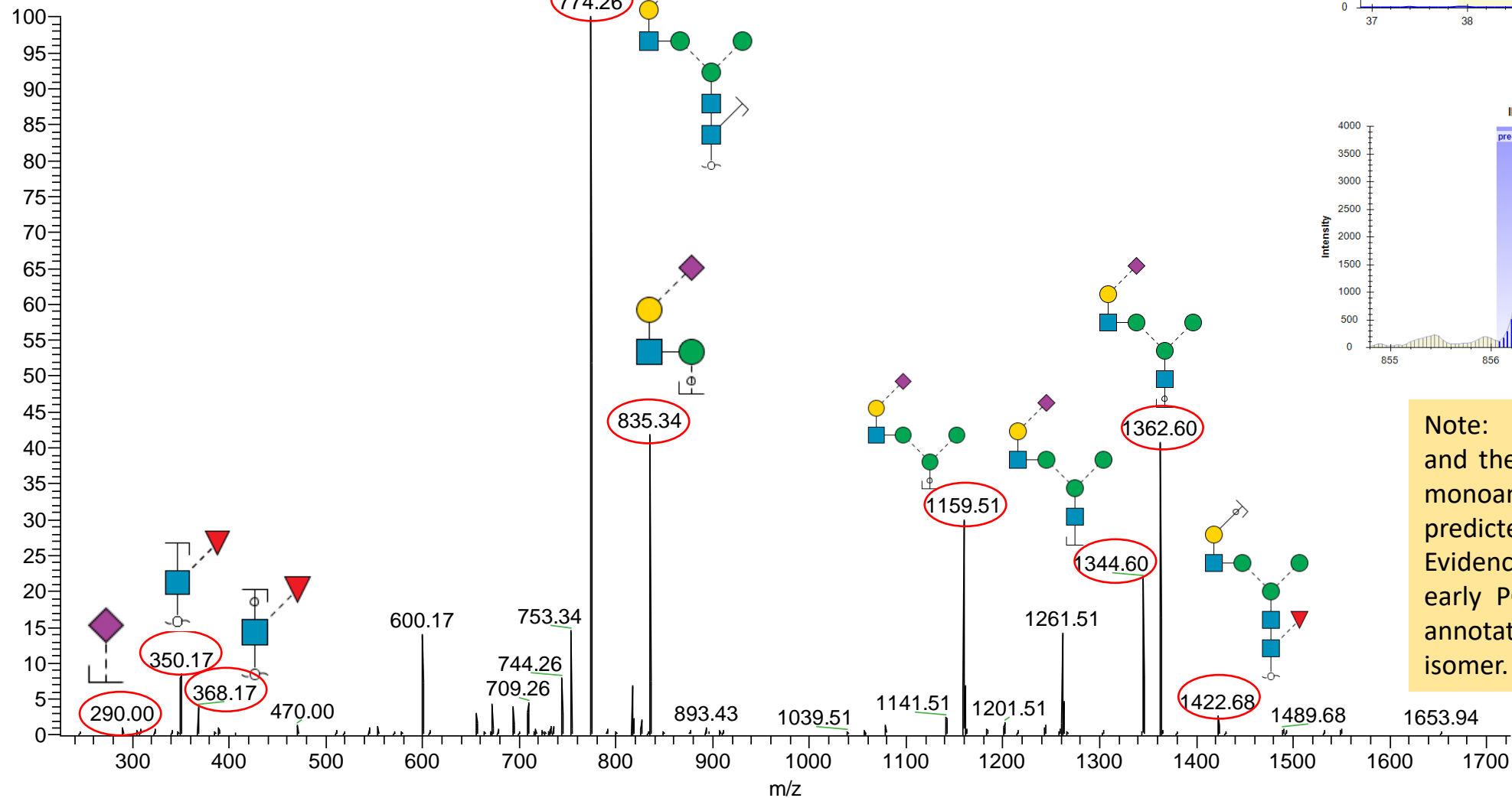
Complex

Hex₁HexNAc₁NeuAc₁ + Hex₃HexNAc₂Fuc₁

m/z: 856.3⁽²⁻⁾

IL_YC_NG_260717 #3942 RT: 39.46 AV: 1 NL: 4.46E2

F: ITMS - p ESI d Full ms2 856.31 @cid35.00 [225.00-1]



Note: From biosynthetic pathway and the lack of D and/or D-18 ions, monoantennary sialyl LacNAc is predicted to occupy the α 1,3 arm. Evidence of core fucose. Based on early PGC-LC elution, this glycan is annotated as the α 2,6-sialyl linkage isomer.

Glycan #26b

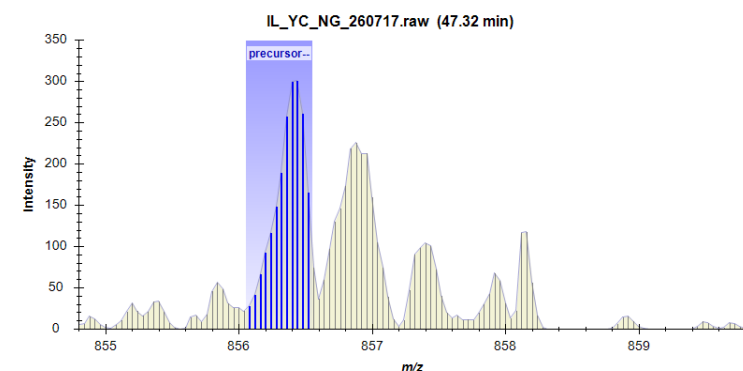
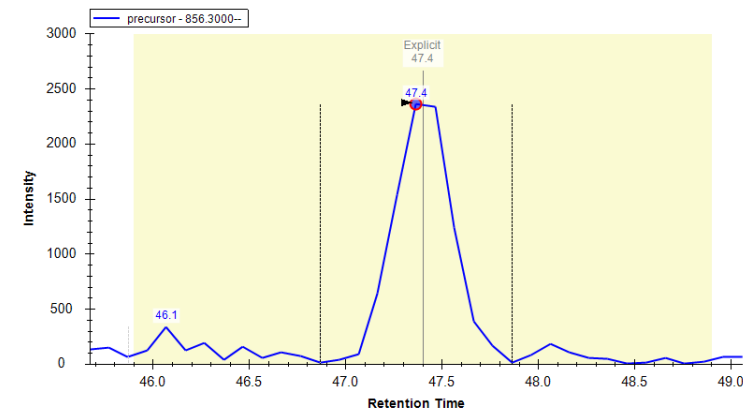
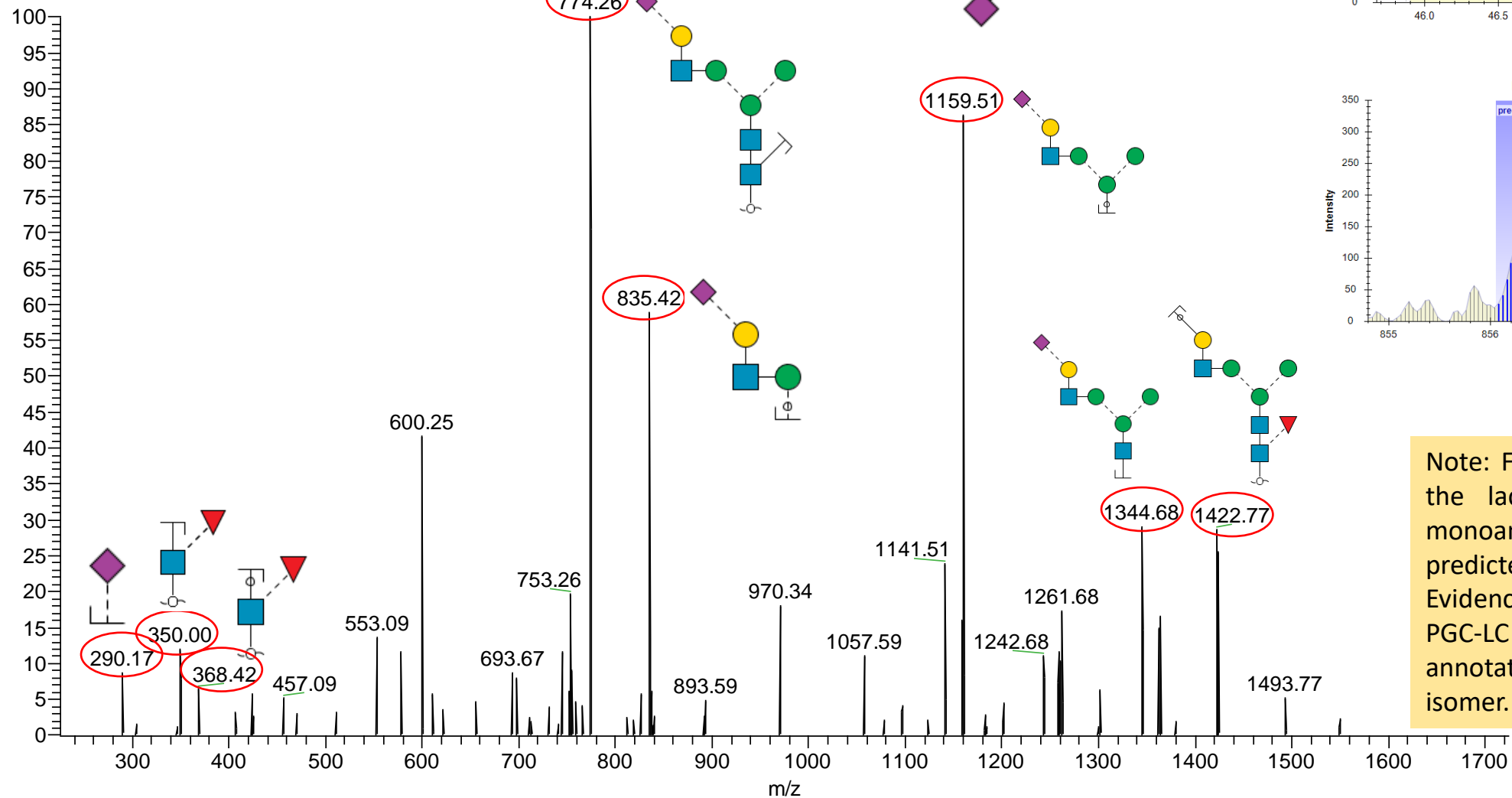
Complex

Hex₁HexNAc₁NeuAc₁ + Hex₃HexNAc₂Fuc₁

m/z: 856.3⁽²⁻⁾

IL_YC_NG_260717 #4726 RT: 47.47 AV: 1 NL: 3.04E1

F: ITMS - p ESI d Full ms2 856.31 @cid35.00 [225.00-1]



Note: From biosynthetic pathway and the lack of D and/or D-18 ions, monoantennary sialyl LacNAc is predicted to occupy the α 1,3-arm. Evidence of core fucose. Based on late PGC-LC elution, this glycan is annotated as the α 2,6-sialyl linkage isomer.

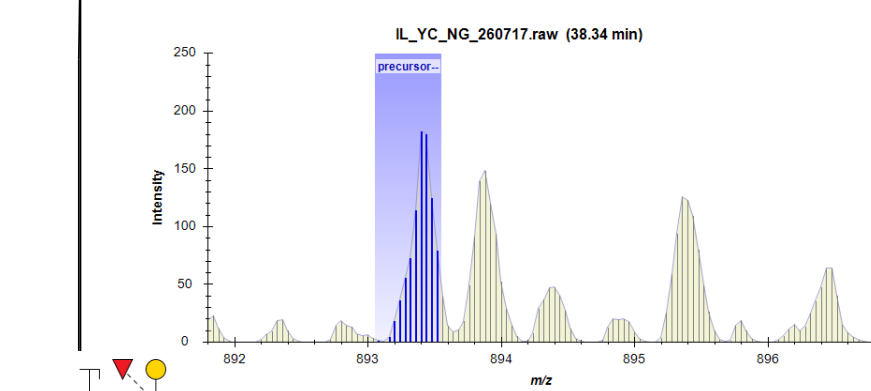
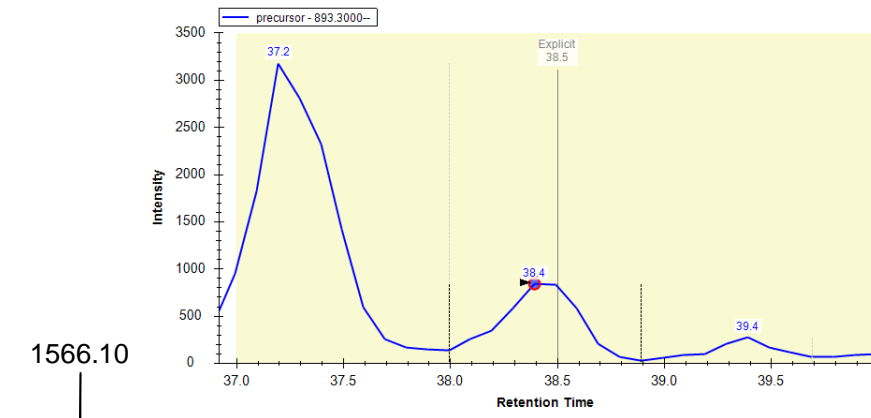
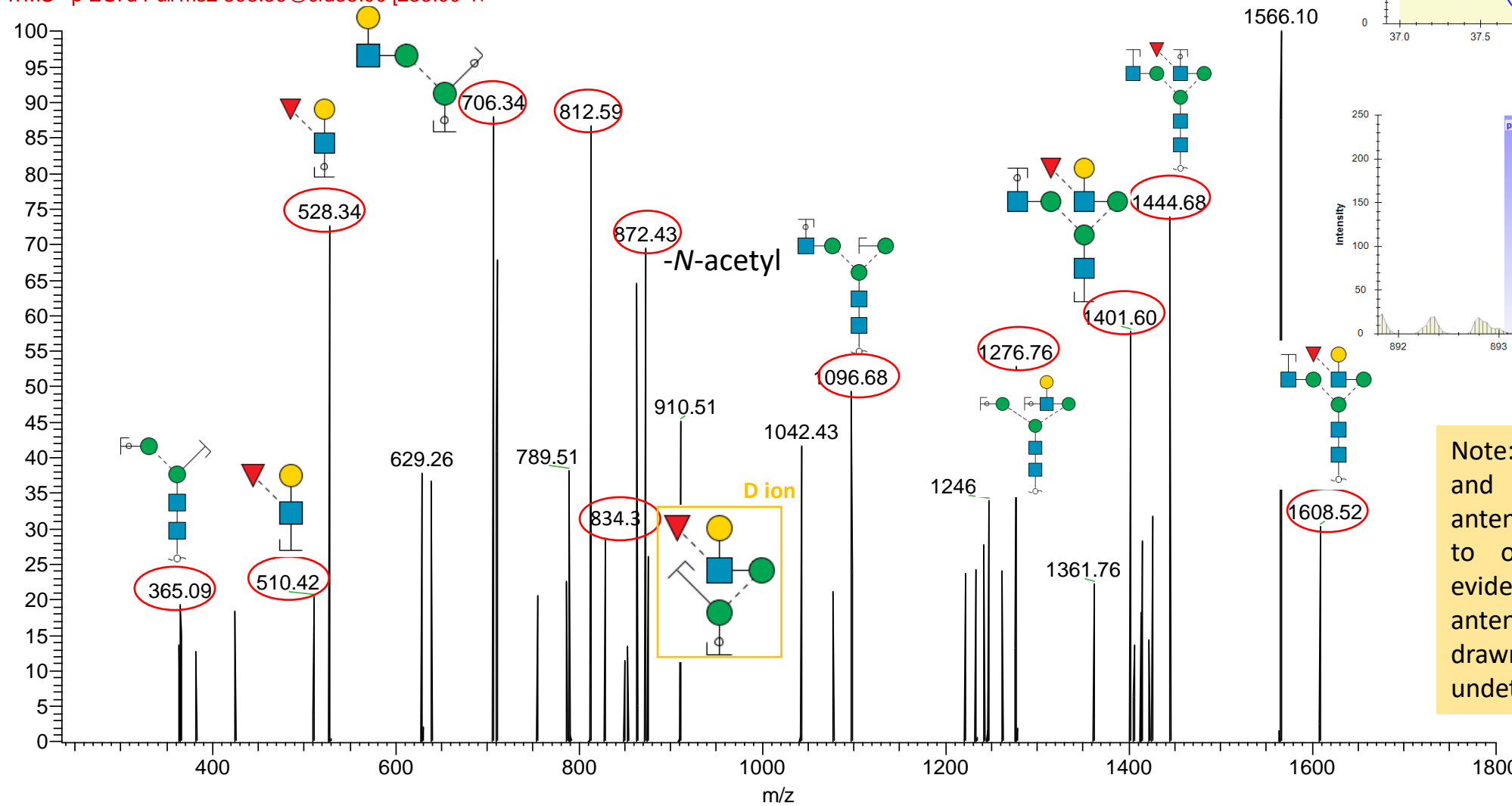
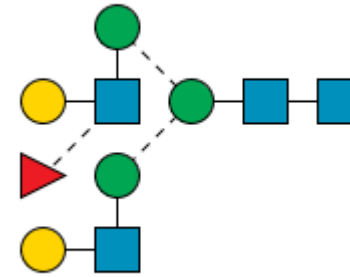
Glycan #27a

Complex

Hex₂HexNAc₂Fuc₁ + Hex₃HexNAc₂

m/z: 893.3⁽²⁻⁾

IL_YC_NG_260717 #3848 RT: 38.51 AV: 1 NL: 4.61
F: ITMS - p ESI d Full ms2 893.36@cid35.00 [235.00-1]



Note: From biosynthetic pathway and presence of D and ions, antenna fucosylation is predicted to occupy the α 1,6 arm. No evidence of core fucose. The exact antennary fucosyl linkage(s) (here drawn as alpha1,3) remains undetermined.

Glycan #27b

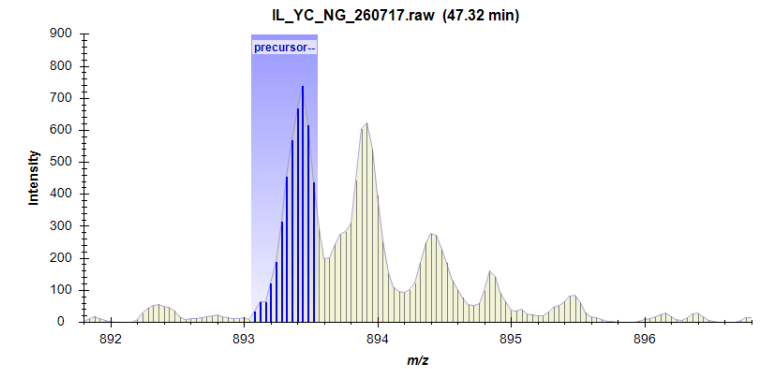
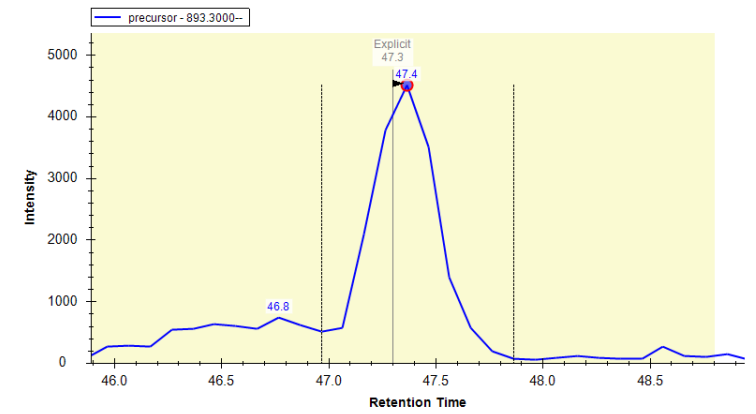
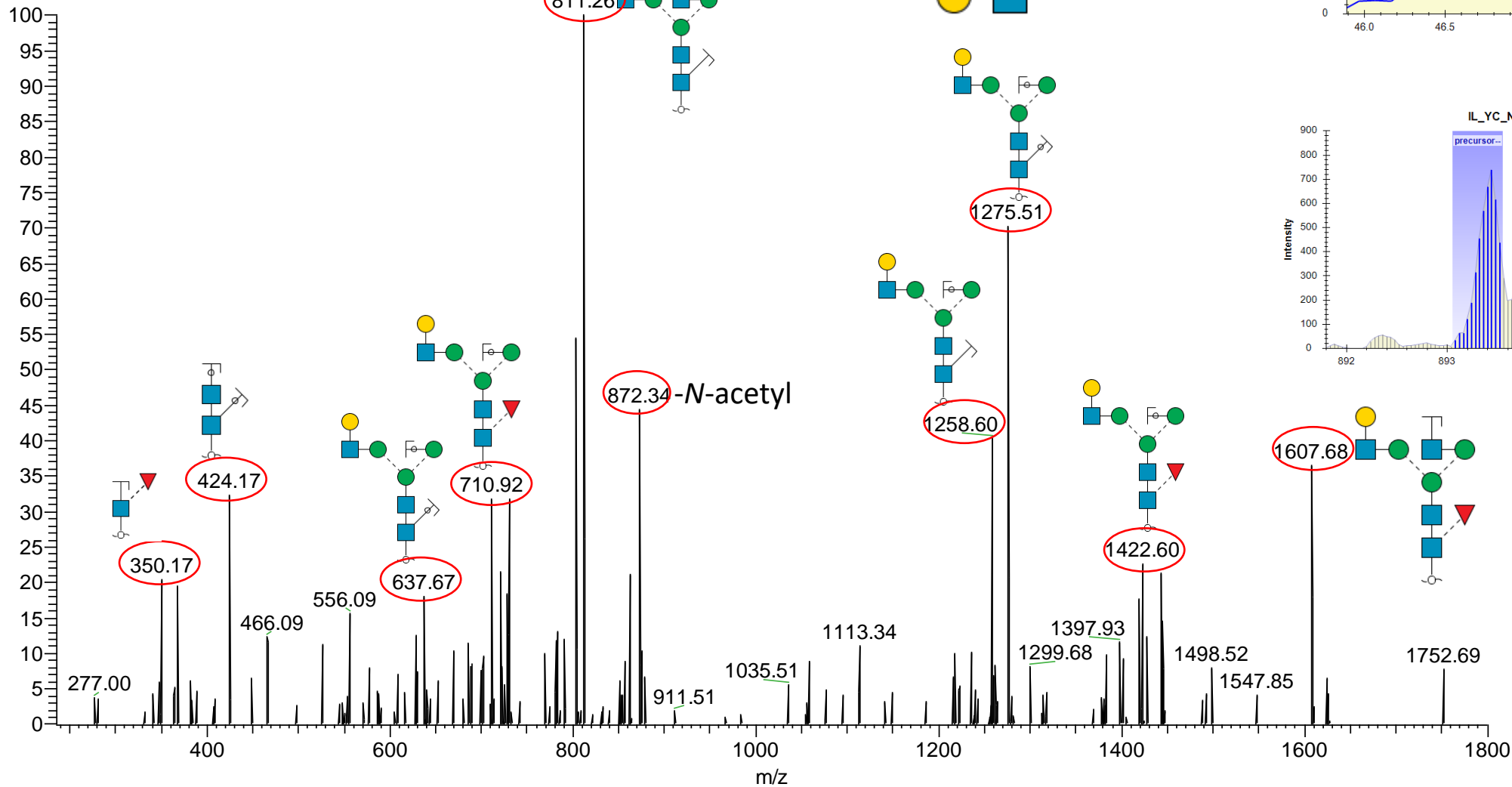
Complex

Hex₂HexNAc₂ + Hex₃HexNAc₂Fuc₁

m/z: 893.3 (2-)

IL_YC_NG_260717 #4722 RT: 47.43 AV: 1 NL: 3.52E1

F: ITMS - p ESI d Full ms2 893.36@cid35.00 [235.00-1}



Note: Evidence of core fucose and no indication of antenna fucose

Glycan #28

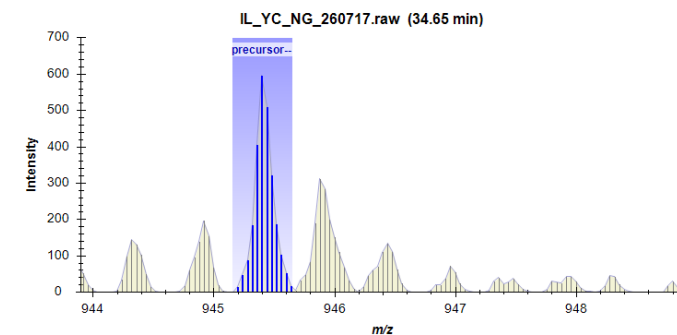
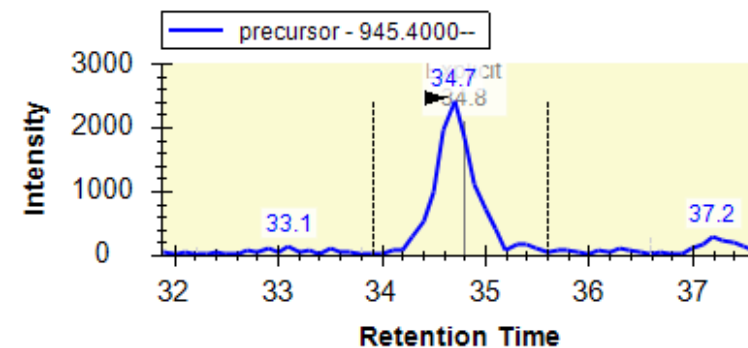
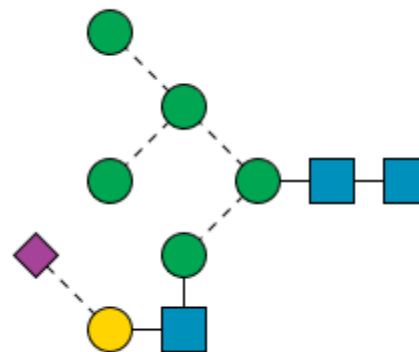
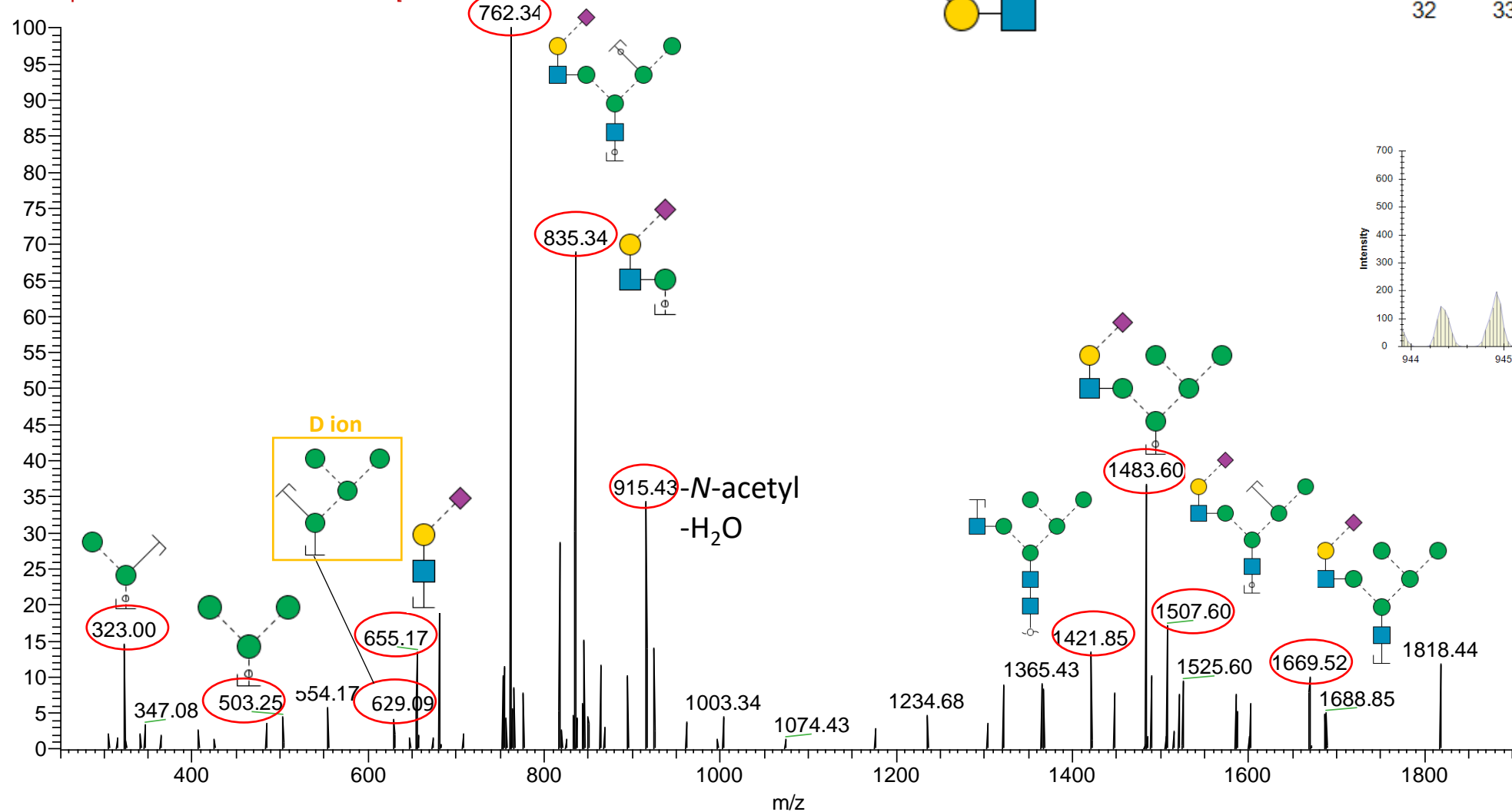
Complex (hybrid, but classified under complex)

Hex₃HexNAc₁NeuAc₁+ Hex₃HexNAc₂

m/z: 945.4⁽²⁻⁾

IL_YC_NG_260717 #3487 RT: 34.81 AV: 1 NL: 3.53E1

F: ITMS - p ESI d Full ms2 945.41 @cid35.00 [250.00-1500.00]



Note: From biosynthetic pathway and the D and/or D-18 ions, sialyl LacNAc is expected to occupy the α 1,3 arm. Based on early PGC-LC elution, this glycan is annotated as the α 2,6-sialyl linkage isomer.

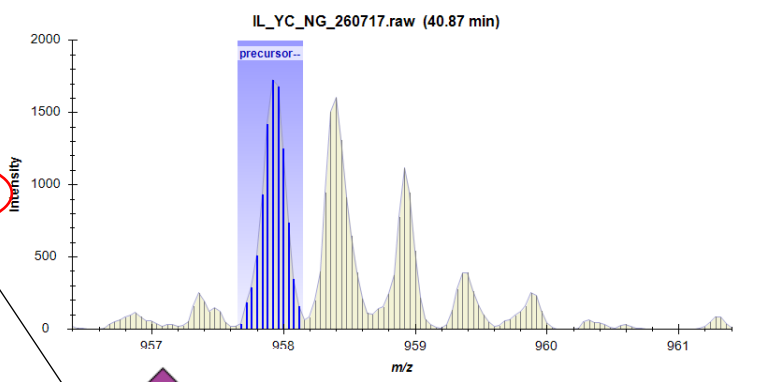
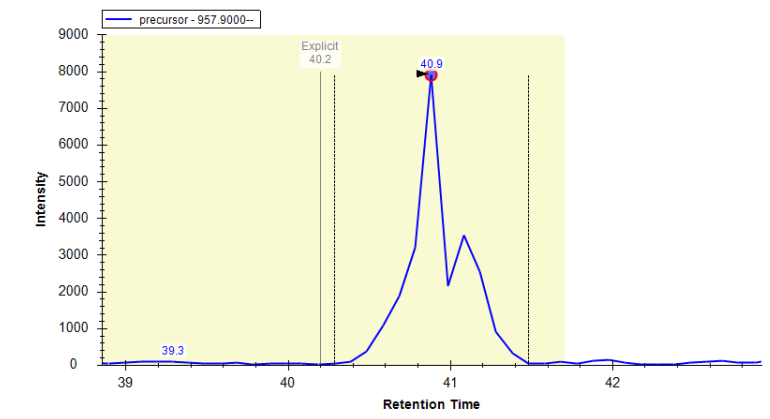
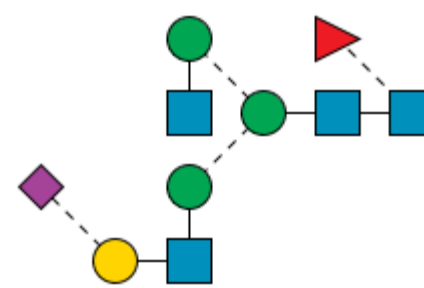
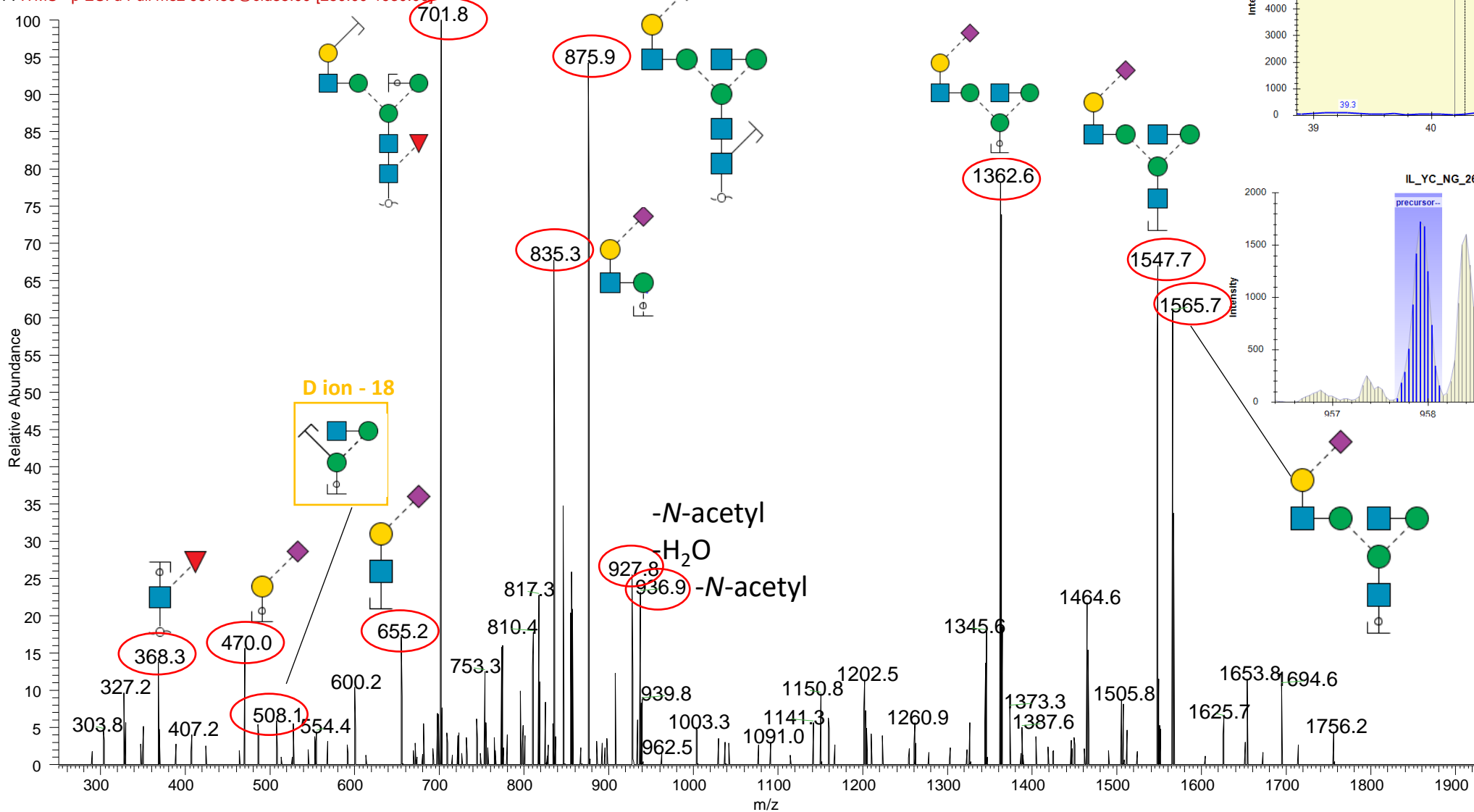
Glycan #29a

Complex

Hex₁HexNAc₂NeuAc₁ + Hex₃HexNAc₂Fuc₁

m/z: 957.9 (2-)

IL_YC_NG_260717#4079 RT: 40.84 AV: 1 NL: 3.24E1
F: ITMS - p ESI d Full ms2 957.89@cid35.00 [250.00-1930.00]



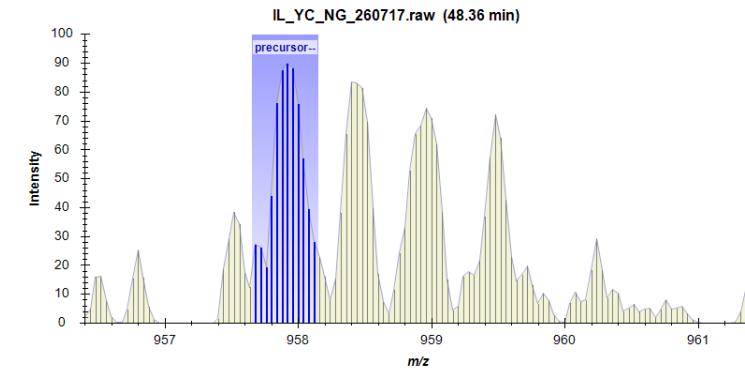
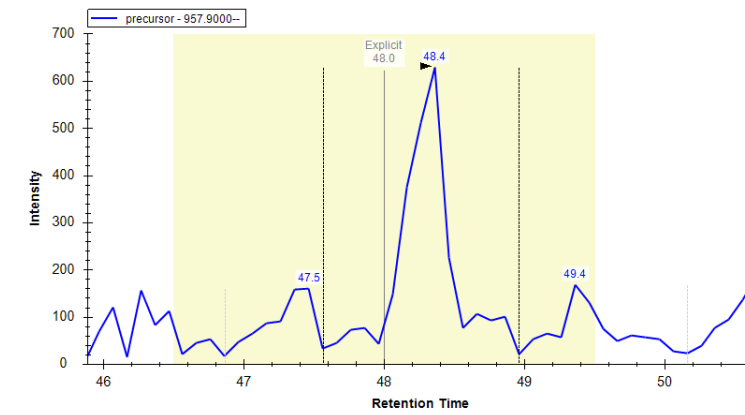
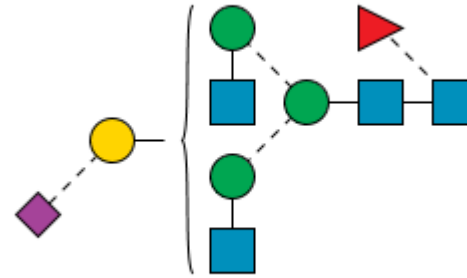
Note: From biosynthetic pathway and the D and/or D-18 ions, the sialyl LacNAc is expected to occupy the α 1,3 arm. Evidence of core fucose. Based on early PGC-LC elution, this glycan is annotated as the α 2,6-sialyl linkage isomer.

Glycan #29b

Complex

Hex₁HexNAc₂NeuAc₁ + Hex₃HexNAc₂Fuc₁

m/z: 957.9⁽²⁻⁾



No MS/MS available in glycomics data

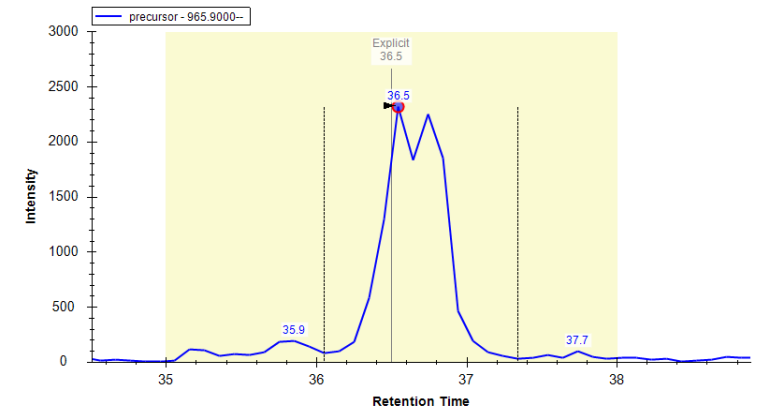
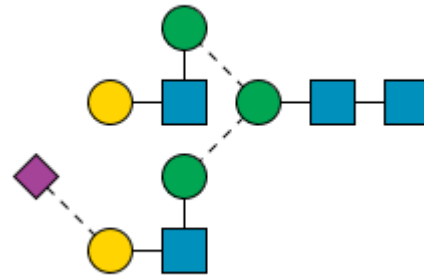
Note: There is a lack of tandem mass spectral data to evidence the glycan structure. However, based on late PGC-LC elution and the expected biosynthetic relationships between observed structures, this glycan is annotated as the α 2,3-sialyl linkage isomer of glycan #29a.

Glycan #30

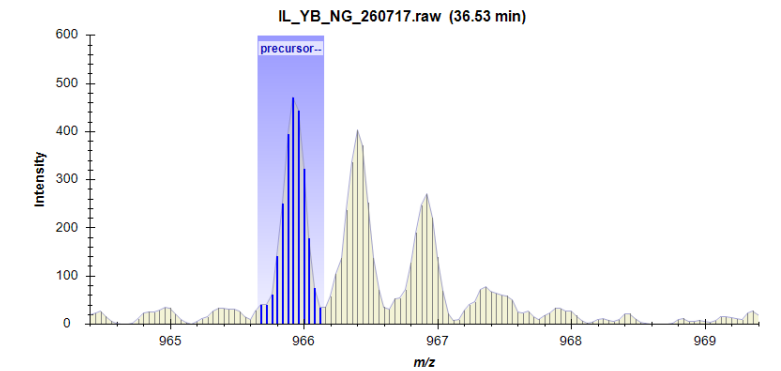
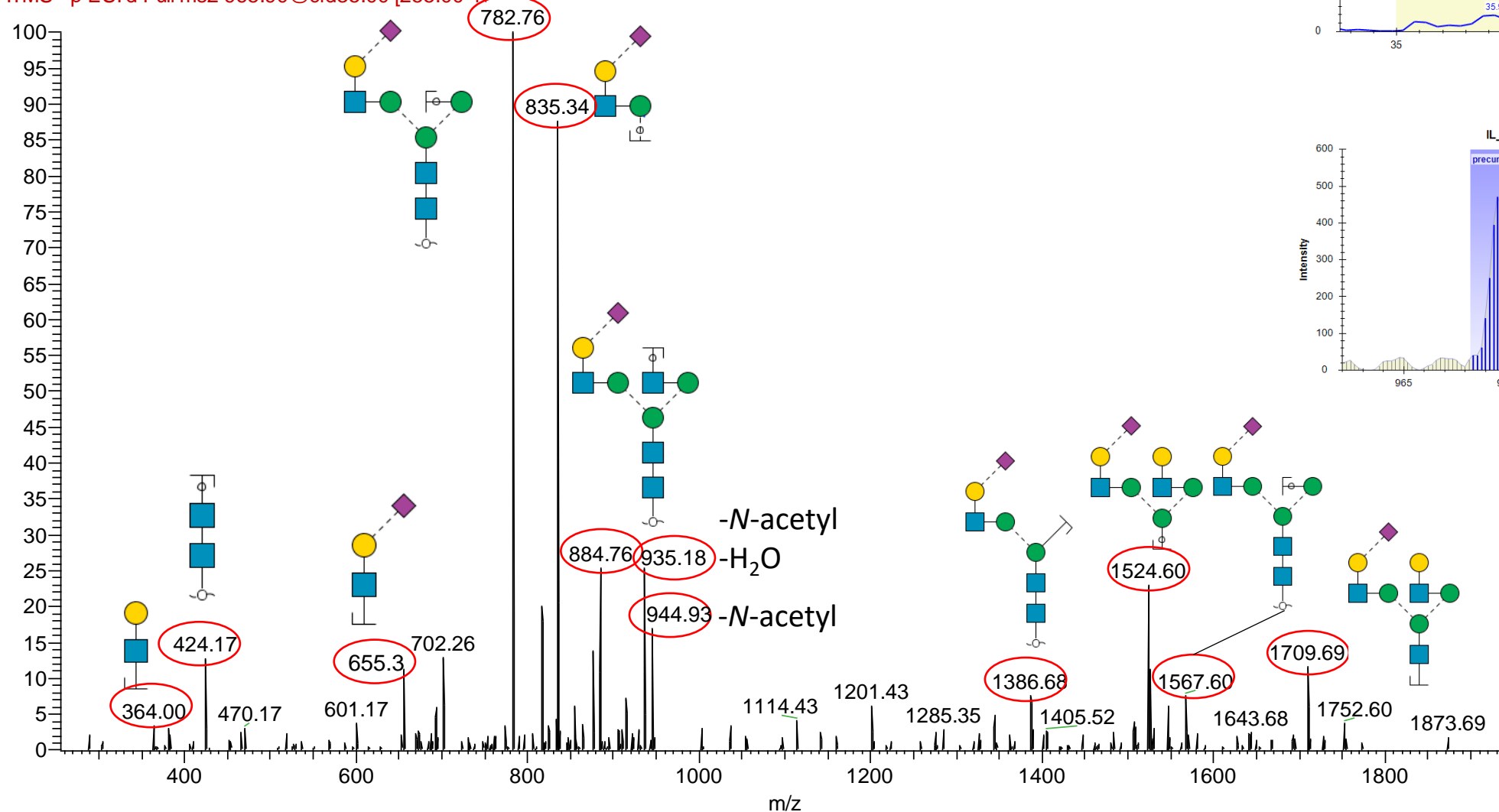
Complex

Hex₂HexNAc₂NeuAc₁ + Hex₃HexNAc₂

m/z: 965.9 (2-)



IL_VB_NG_260717 #3648 RT: 36.51 AV: 1 NL: 1.29E2
F: ITMS - p ESI d Full ms2 965.90@cid35.00 [255.00-14



Note: From biosynthetic pathway and the lack of D and/or D-18 ions, the sialyl LacNAc is predicted to occupy the α 1,3 arm. Based on early PGC-LC elution, this glycan is annotated as the α 2,6-sialyl linkage isomer.

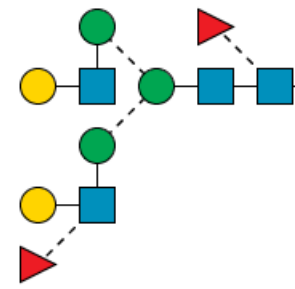
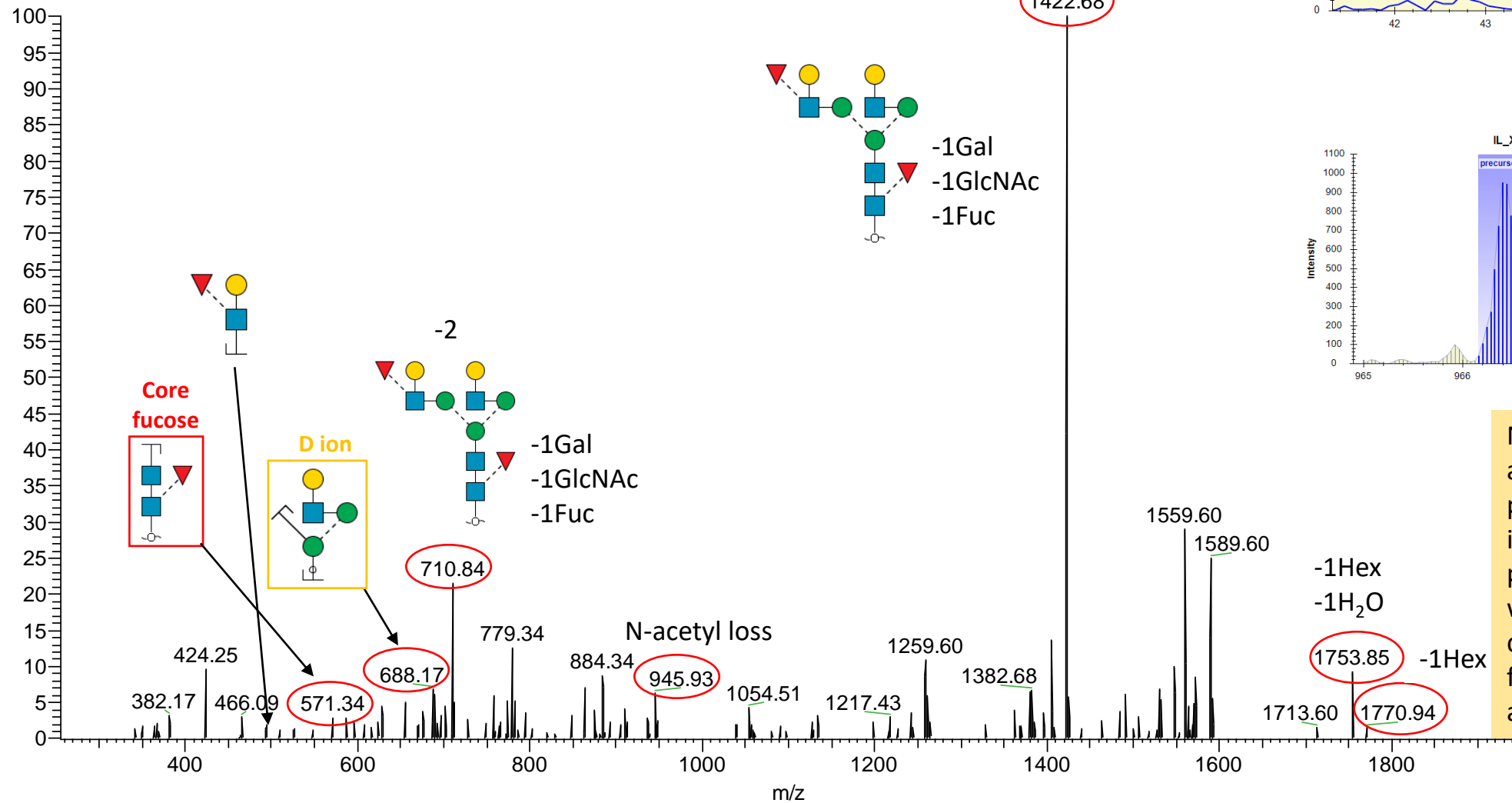
Glycan #31a

Complex

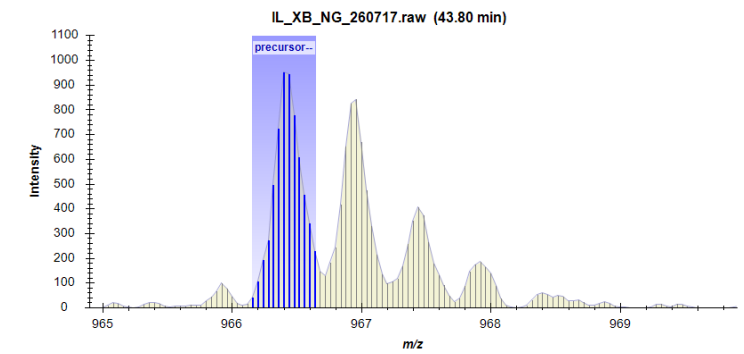
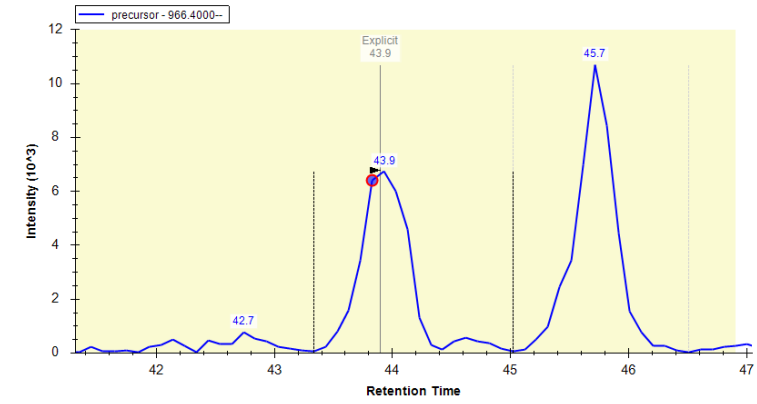
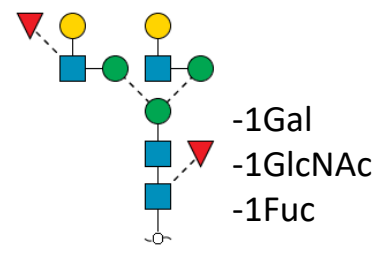
Hex₂HexNAc₂Fuc₁ + Hex₃HexNAc₂Fuc₁

m/z: 966.4⁽²⁻⁾

IL_XB_NG_260717 #4362 RT: 43.81 AV: 1 NL: 6.91E1
F: ITMS - p ESI d Full ms2 966.40@cid35.00 [255.00-1!



1422.68



Note: Indication of both core and antenna fucose. From biosynthetic pathway and the D and/or D-18 ions, the unmodified LacNAc is predicted to occupy the α 1,6 arm with the Lewis x/a to occupy the α 1,3 arm. The exact antennary fucosyl linkage(s) (here drawn as α 1,3) remains undetermined.

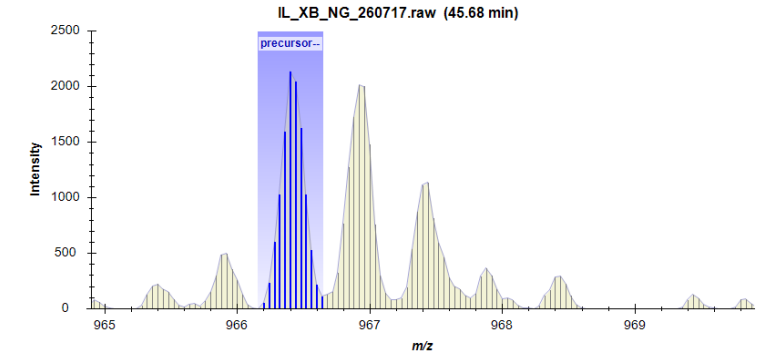
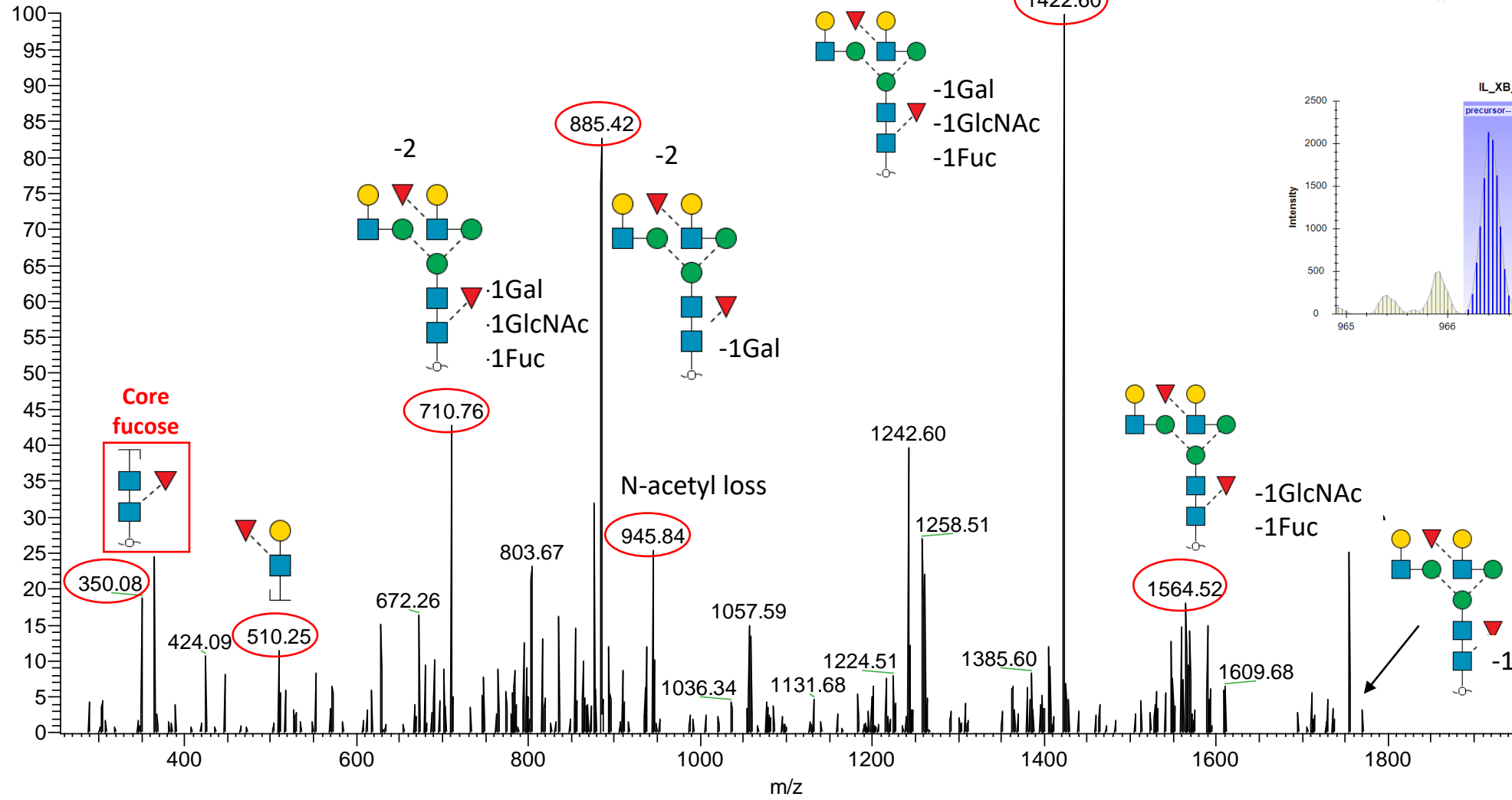
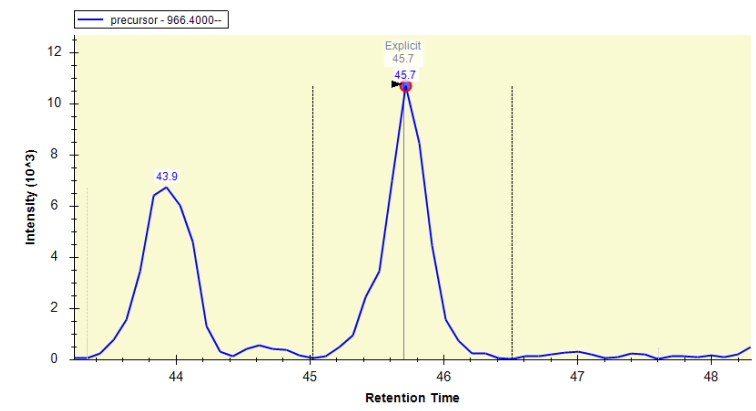
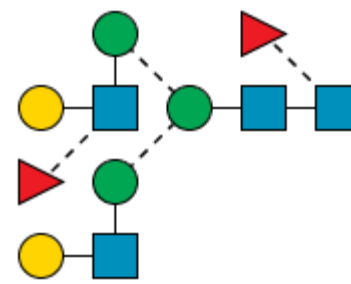
Glycan #31b

Complex

Hex₂HexNAc₂Fuc₁ + Hex₃HexNAc₂Fuc₁

m/z: 966.4⁽²⁻⁾

IL_XB_NG_260717 #4543 RT: 45.69 AV: 1 NL: 5.53E1
F: ITMS - p ESI d Full ms2 966.40@cid35.00 [255.00-1!



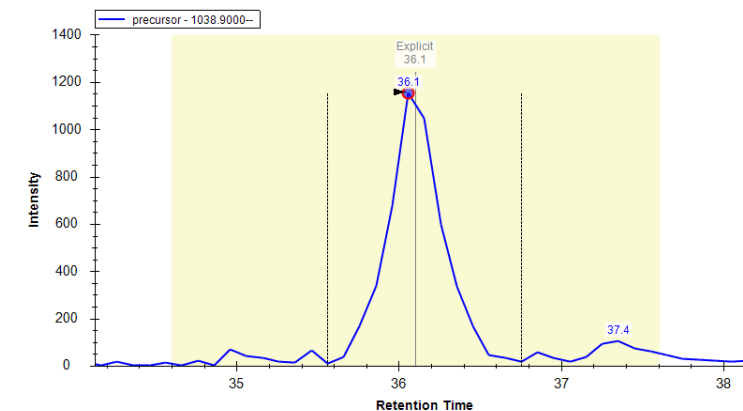
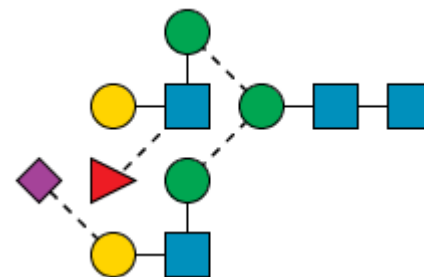
Note: Indication of both core and antenna fucose. The exact antennary fucosyl linkage(s) (here drawn as alpha1,3) remains undetermined.

Glycan #32a

Complex

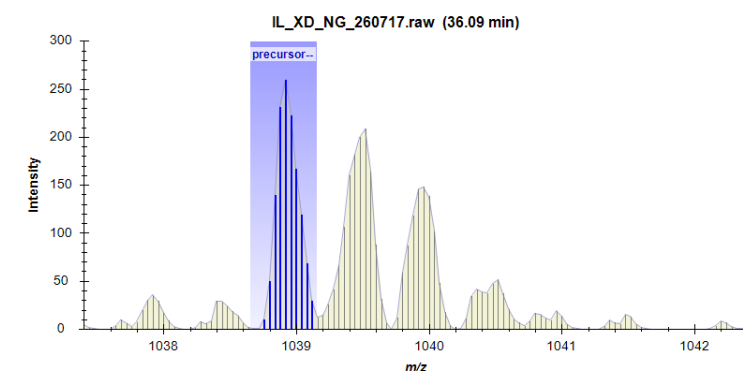
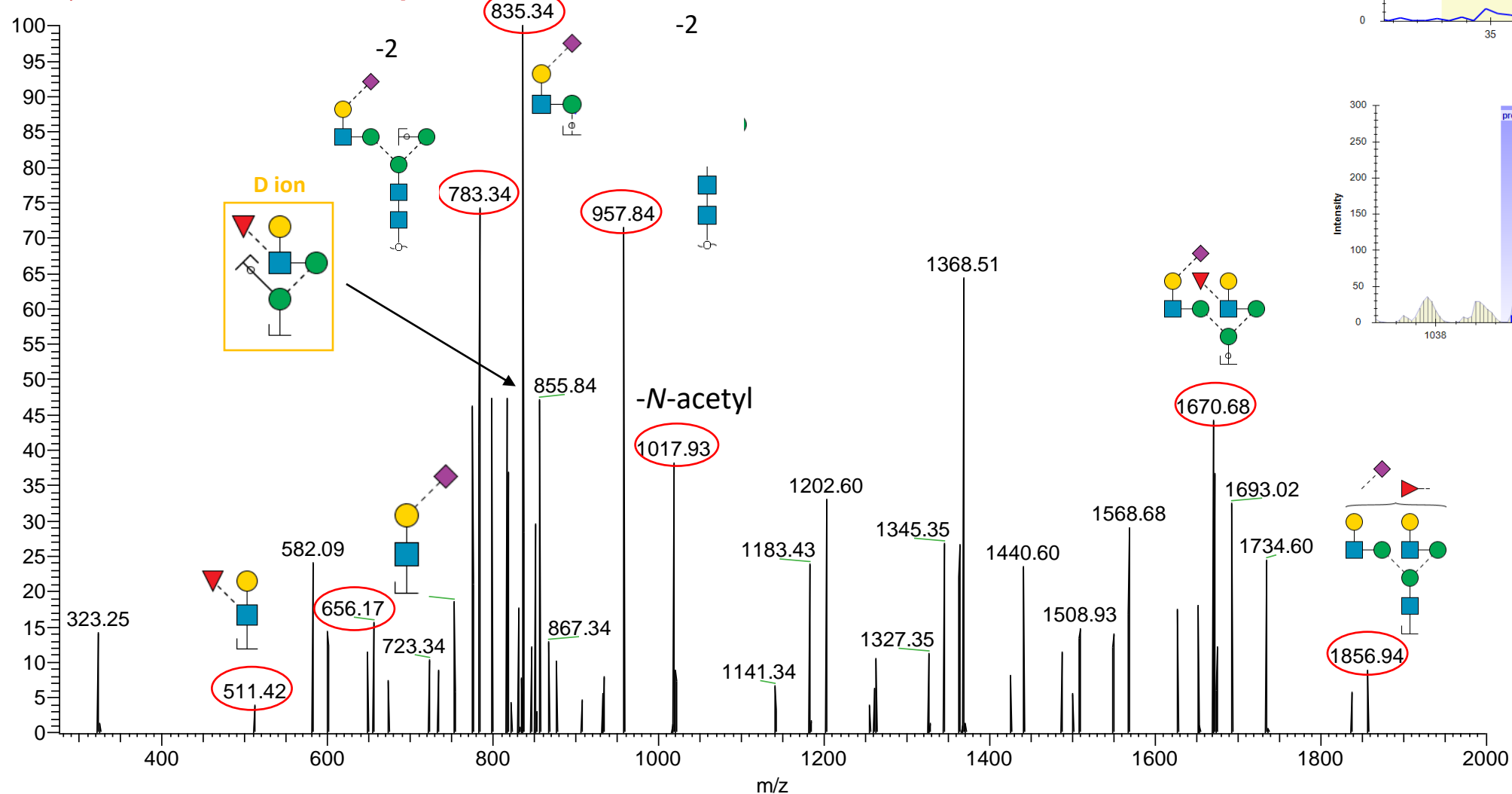
Hex₂HexNAc₂Fuc₁NeuAc₁ + Hex₃HexNAc₂

m/z: 1038.9⁽²⁻⁾



IL_XD_NG_260717 #3630 RT: 36.18 AV: 1 NL: 1.40E1

F: ITMS - p ESI d Full ms2 1038.92@cid35.00 [275.00-;



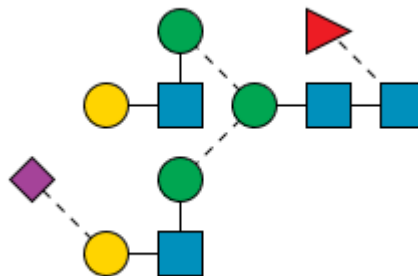
Note: Based on early PGC-LC elution, this glycan is annotated as the α 2,6-sialyl linkage isomer. No indication of core fucose. The exact antennary fucosyl linkage(s) (here drawn as α 1,3) remains undetermined.

Glycan #32b

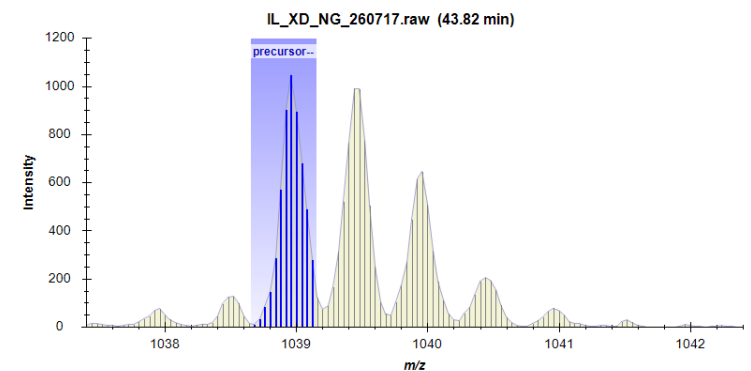
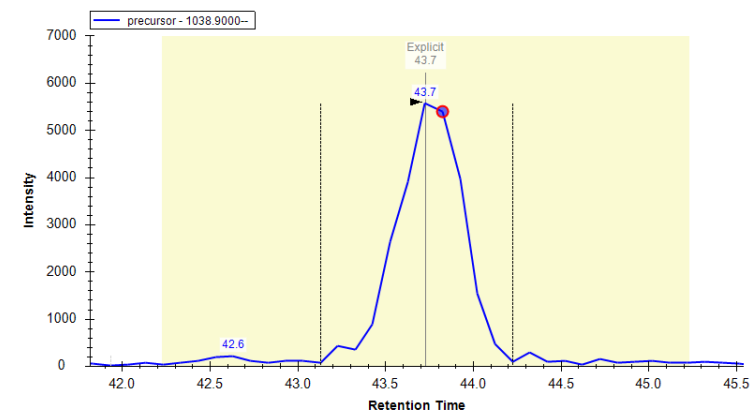
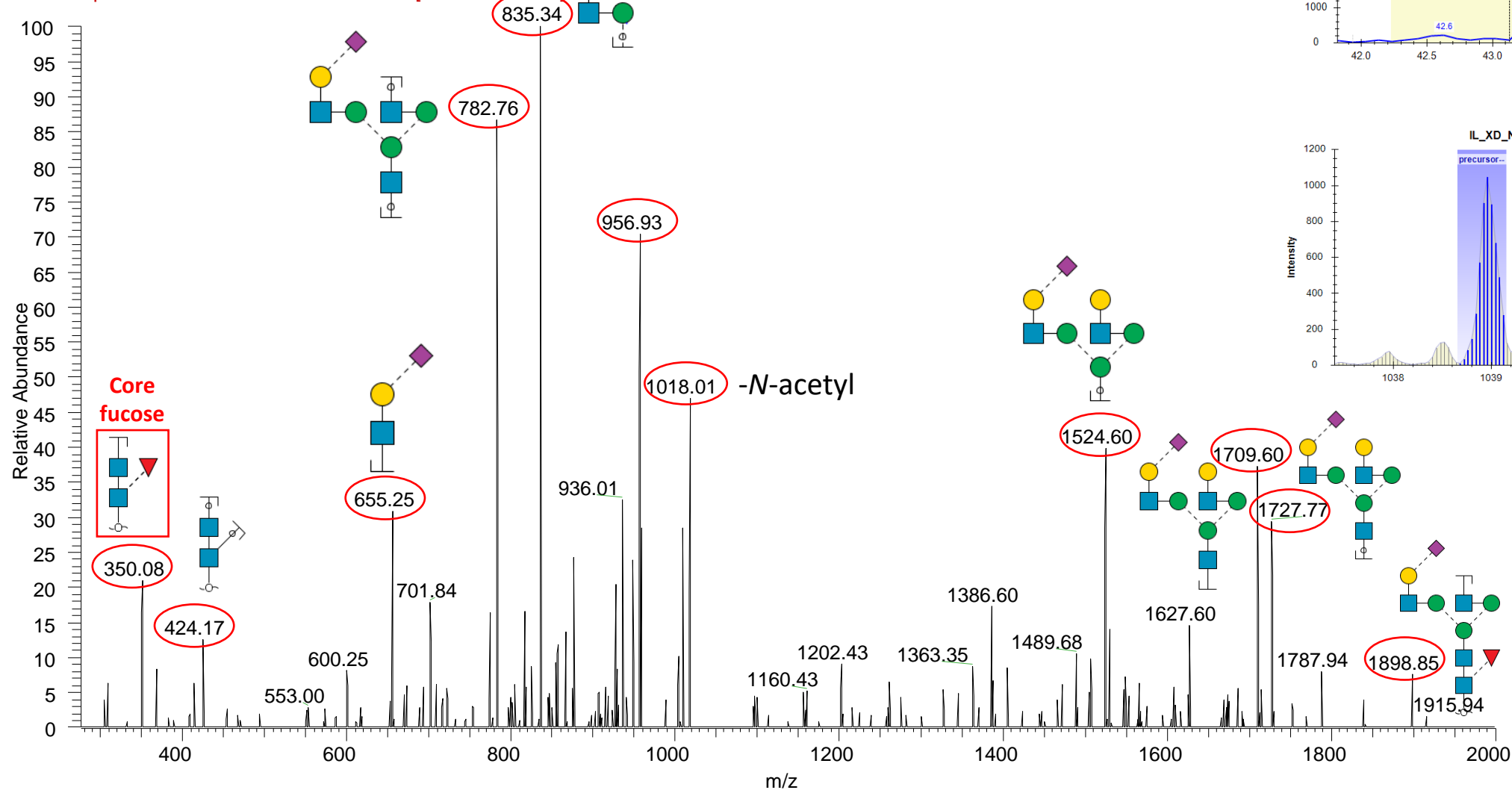
Complex

Hex₂HexNAc₂NeuAc₁ + Hex₃HexNAc₂Fuc₁

m/z: 1038.9 (2-)



IL_XD_NG_260717 #4382 RT: 43.73 AV: 1 NL: 4.21E1
F: ITMS - p ESI d Full ms2 1038.92@cid35.00 [275.00-2000.00]



Note: From biosynthetic pathway and the lack of D and/or D-18 ions, the sialyl LacNAc is predicted to occupy the α 1,3 arm. Evidence of core fucose. Based on early PGC-LC elution, this glycan is annotated as the α 2,6-sialyl linkage isomer.

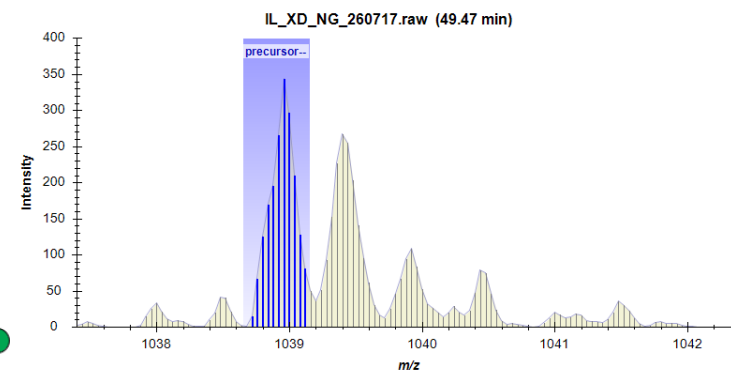
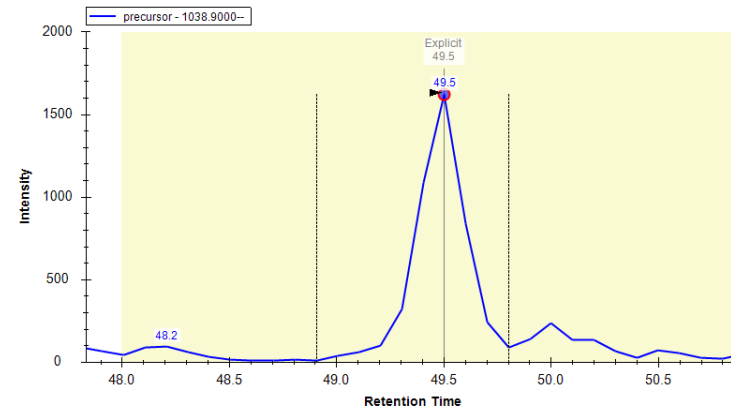
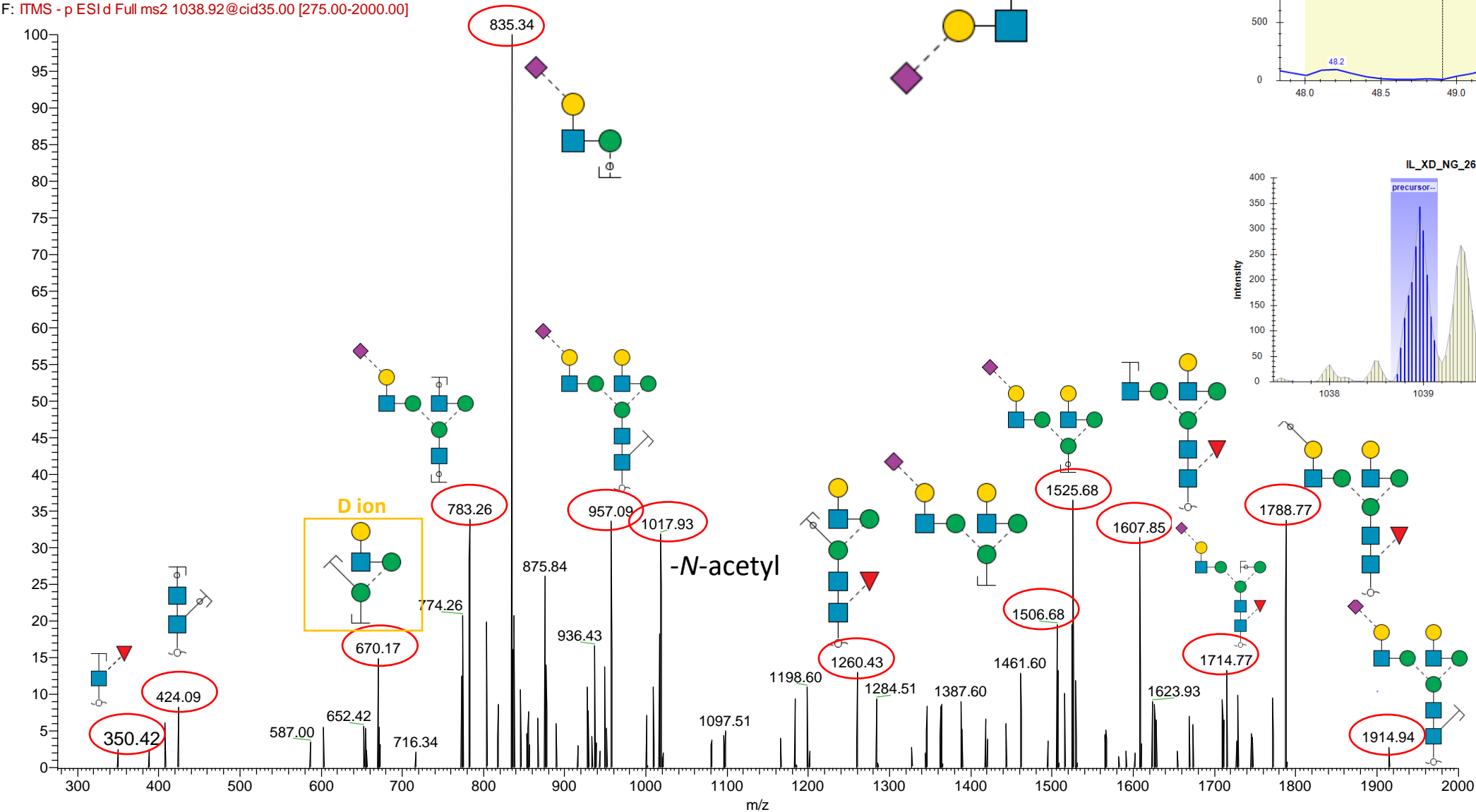
Glycan #32c

Complex

Hex₂HexNAc₂NeuAc₁ + Hex₃HexNAc₂Fuc₁

m/z: 1038.9 (2-)

IL_XD_NG_260717 #4955 RT: 49.51 AV: 1 NL: 1.82E1
F: ITMS - p ESI d Full ms2 1038.92@cid35.00 [275.00-2000.00]



Note: From biosynthetic pathway and presence of D-18 ions, the sialyl LacNAc is predicted to occupy the α 1,3 arm. Evidence of core fucose. Based on late PGC-LC elution, this glycan is annotated as the α 2,3-sialyl linkage isomer.

Glycan #33a

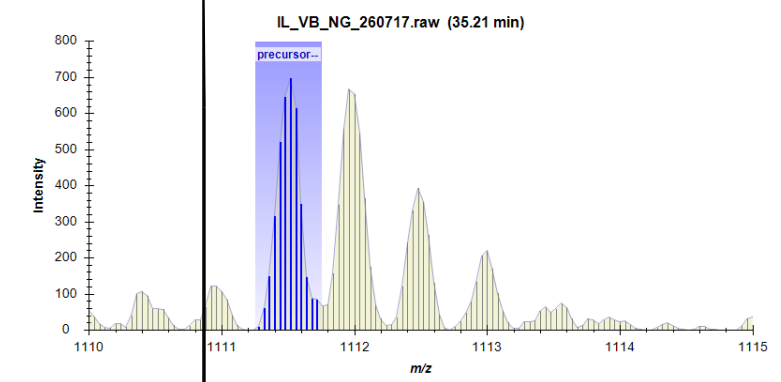
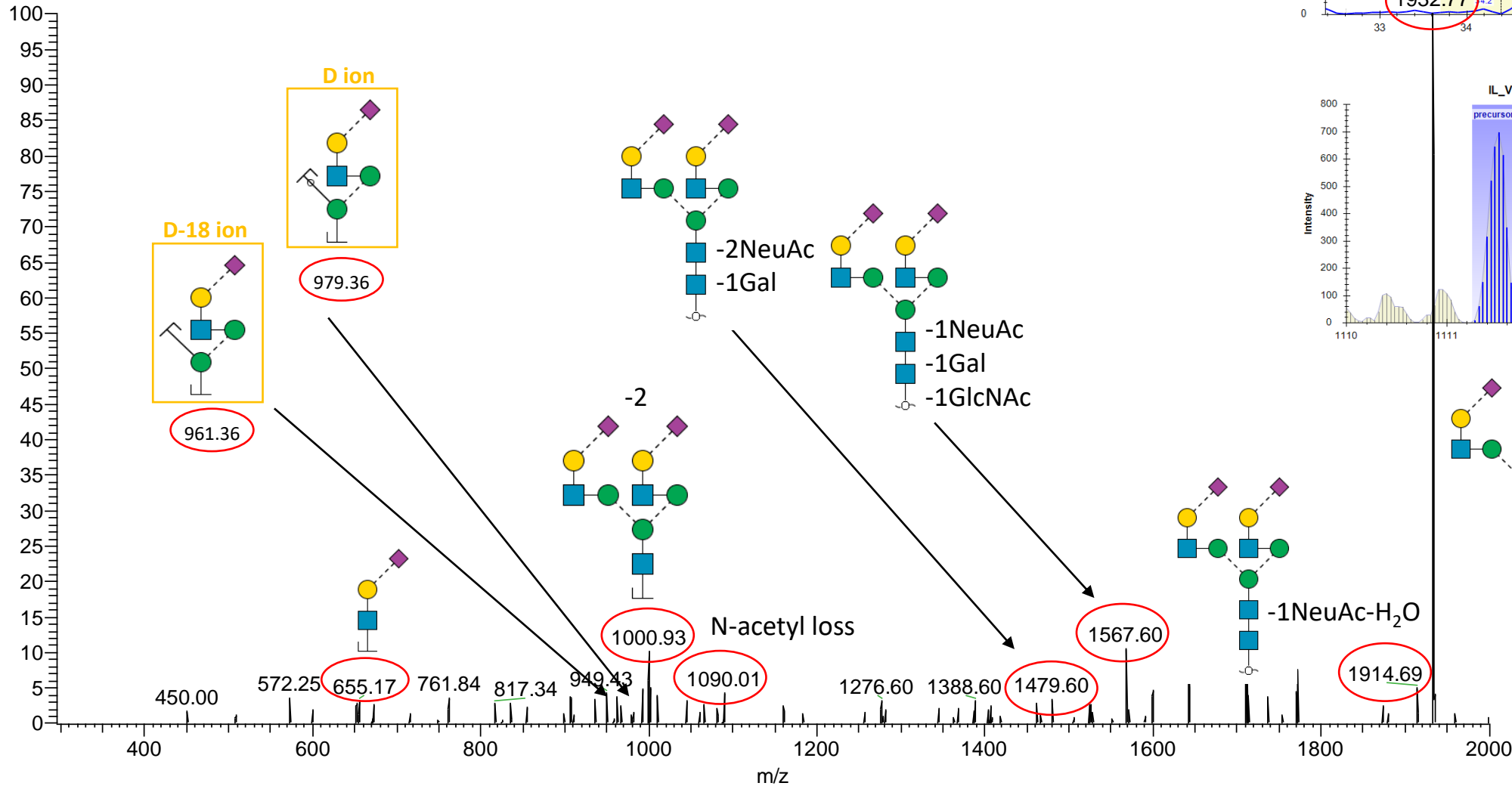
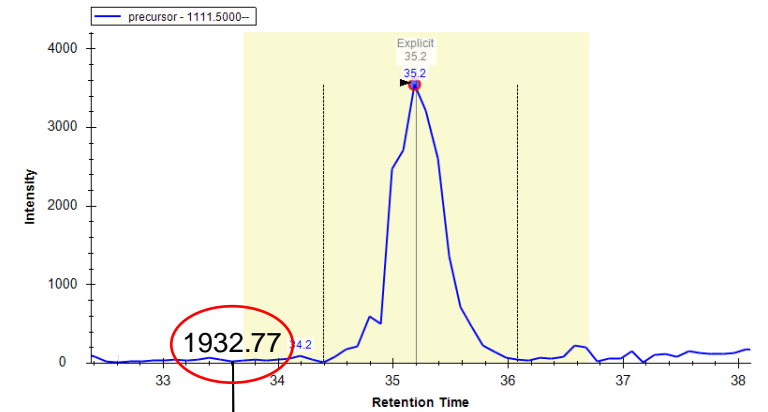
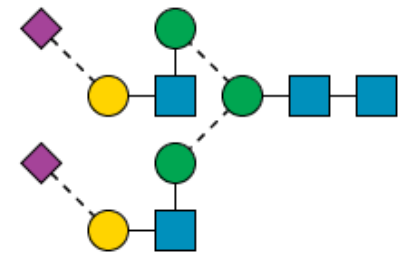
Complex

Hex₂HexNAc₂NeuAc₂ + Hex₃HexNAc₂

m/z: 1111.5⁽²⁻⁾

IL_VB_NG_260717 #3529 RT: 35.29 AV: 1 NL: 7.18E1

F: TMS - p ESI d Full ms2 1111.45@cid35.00 [295.00-:



Note: Based on PGC-LC elution pattern, this glycan is annotated as the α 2,6- α 2,6-sialyl linkage isomer.

Glycan #33b

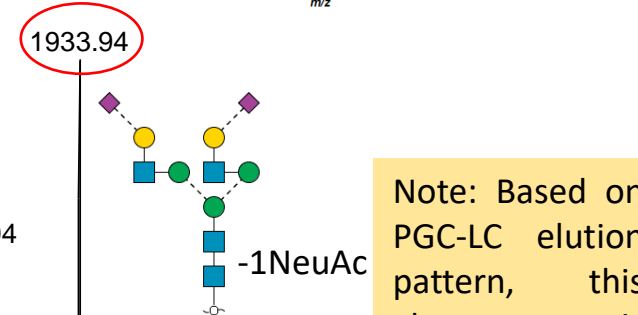
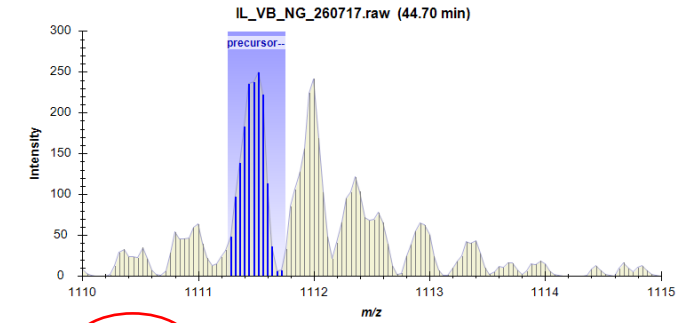
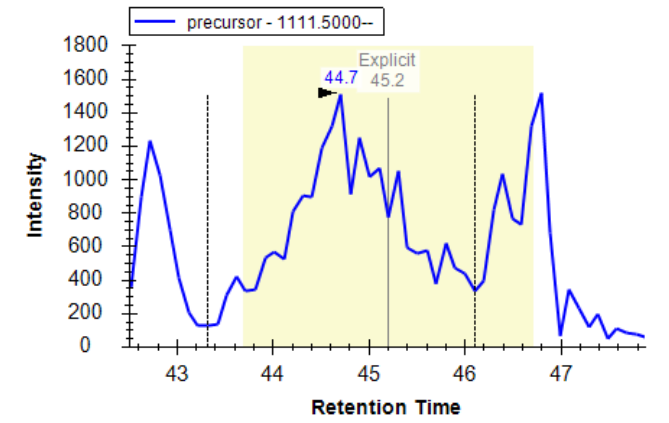
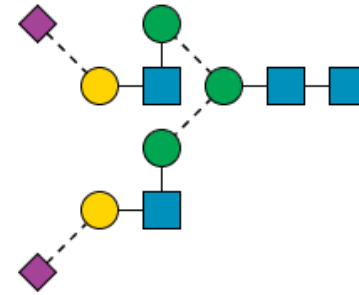
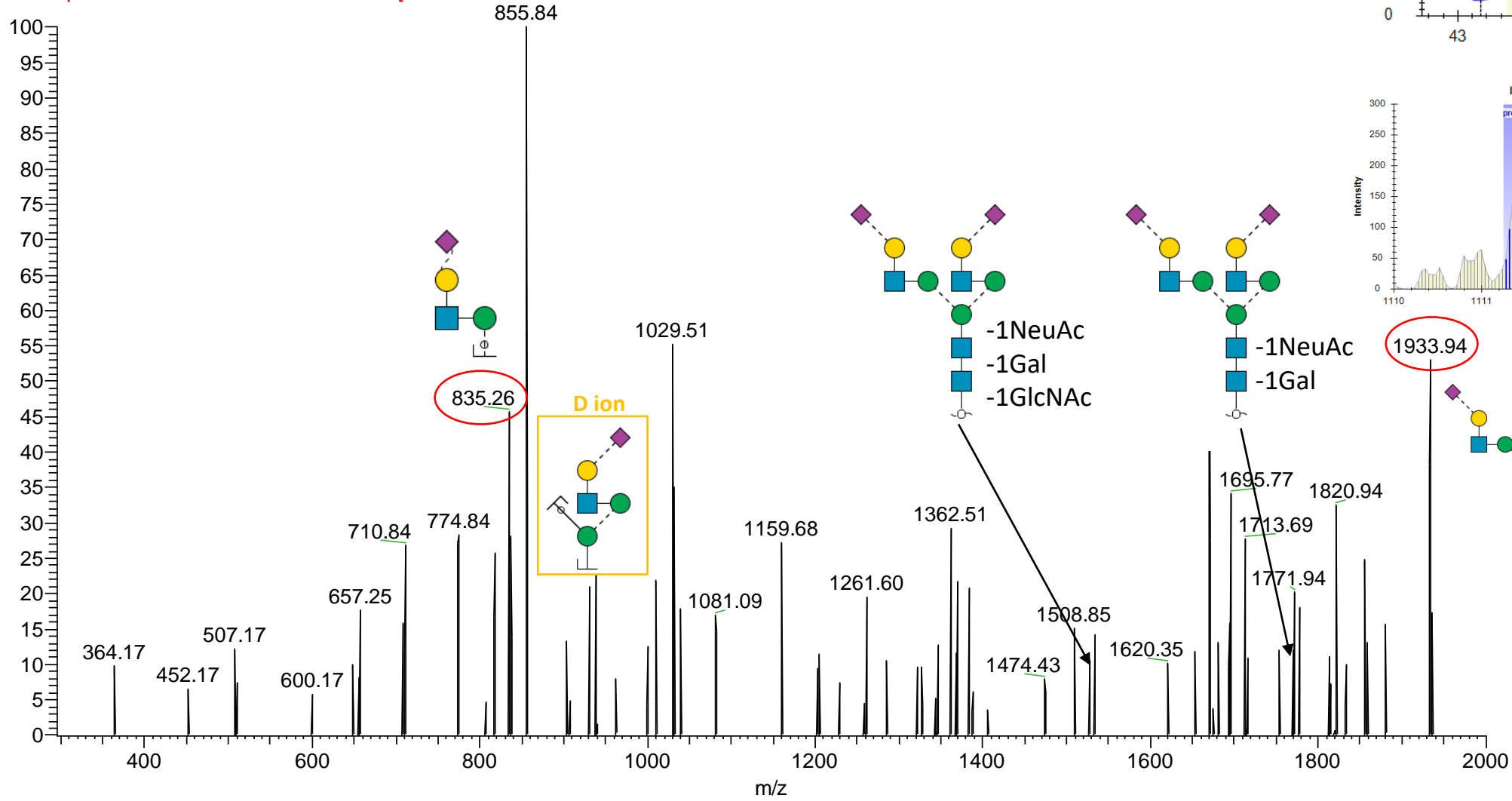
Complex

Hex₂HexNAc₂NeuAc₂ + Hex₃HexNAc₂

m/z: 1111.5⁽²⁻⁾

IL_VB_NG_260717 #4500 RT: 45.20 AV: 1 NL: 9.48

F: ITMS - p ESI d Full ms2 1111.45@cid35.00 [295.00-]



Note: Based on PGC-LC elution pattern, this glycan is annotated as the α 2,6- α 2,3-sialyl linkage isomer.

Glycan #34a

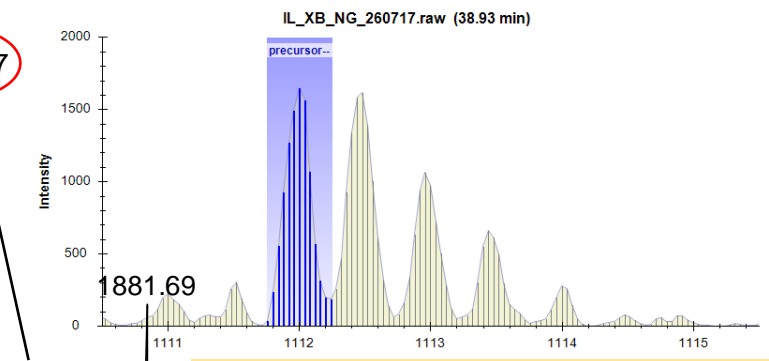
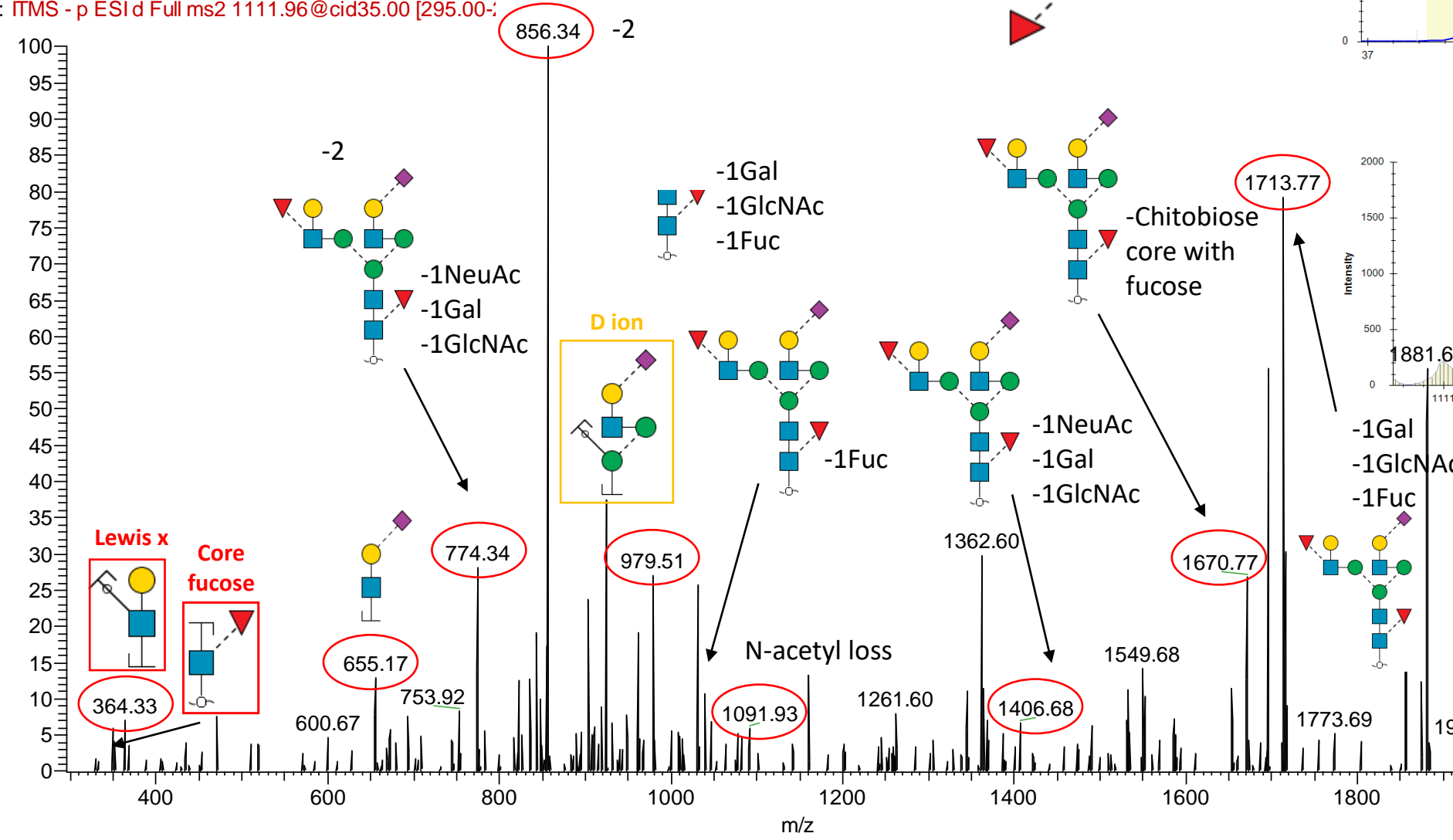
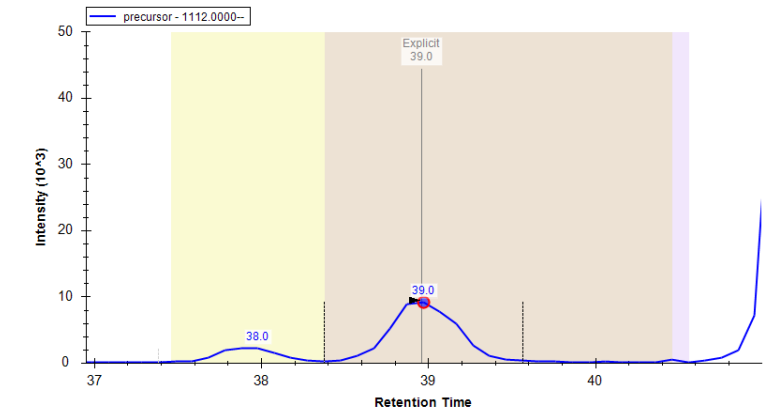
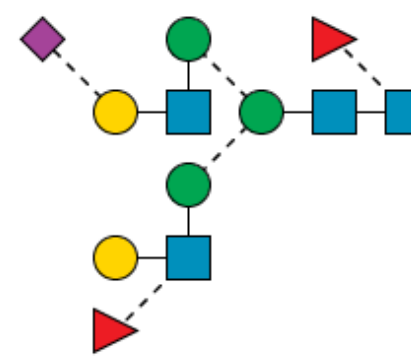
Complex

Hex₂HexNAc₂Fuc₁NeuAc₁ + Hex₃HexNAc₂Fuc₁

m/z: 1112.0⁽²⁻⁾

IL_XB_NG_260717 #3874 RT: 38.96 AV: 1 NL: 7.19E1

F: ITMS - p ESI d Full ms2 1111.96@cid35.00 [295.00-;



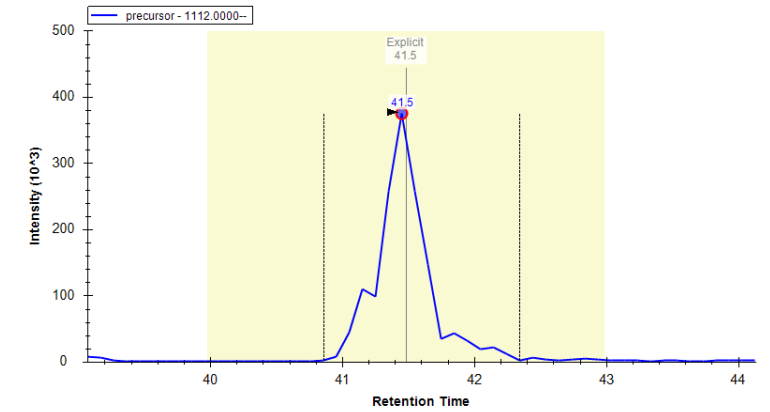
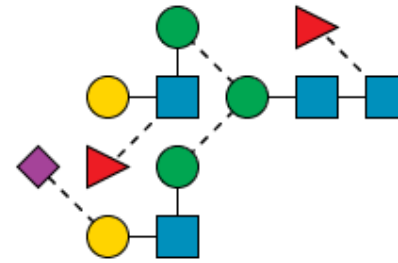
Note: Based on PGC-LC elution pattern, this glycan is annotated as the α 2,6-sialyl linkage isomer. Indication of both core and antenna fucose. The exact antennary fucosyl linkage(s) (here drawn as alpha1,3) remains undetermined. The exact antennary fucosyl linkage(s) (here drawn as alpha1,3) remains undetermined. The exact antennary fucosyl linkage(s) (here drawn as alpha1,3) remains undetermined.

Glycan #34b

Complex

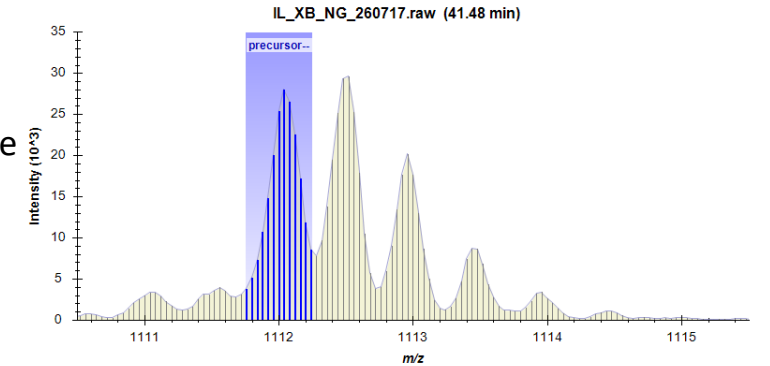
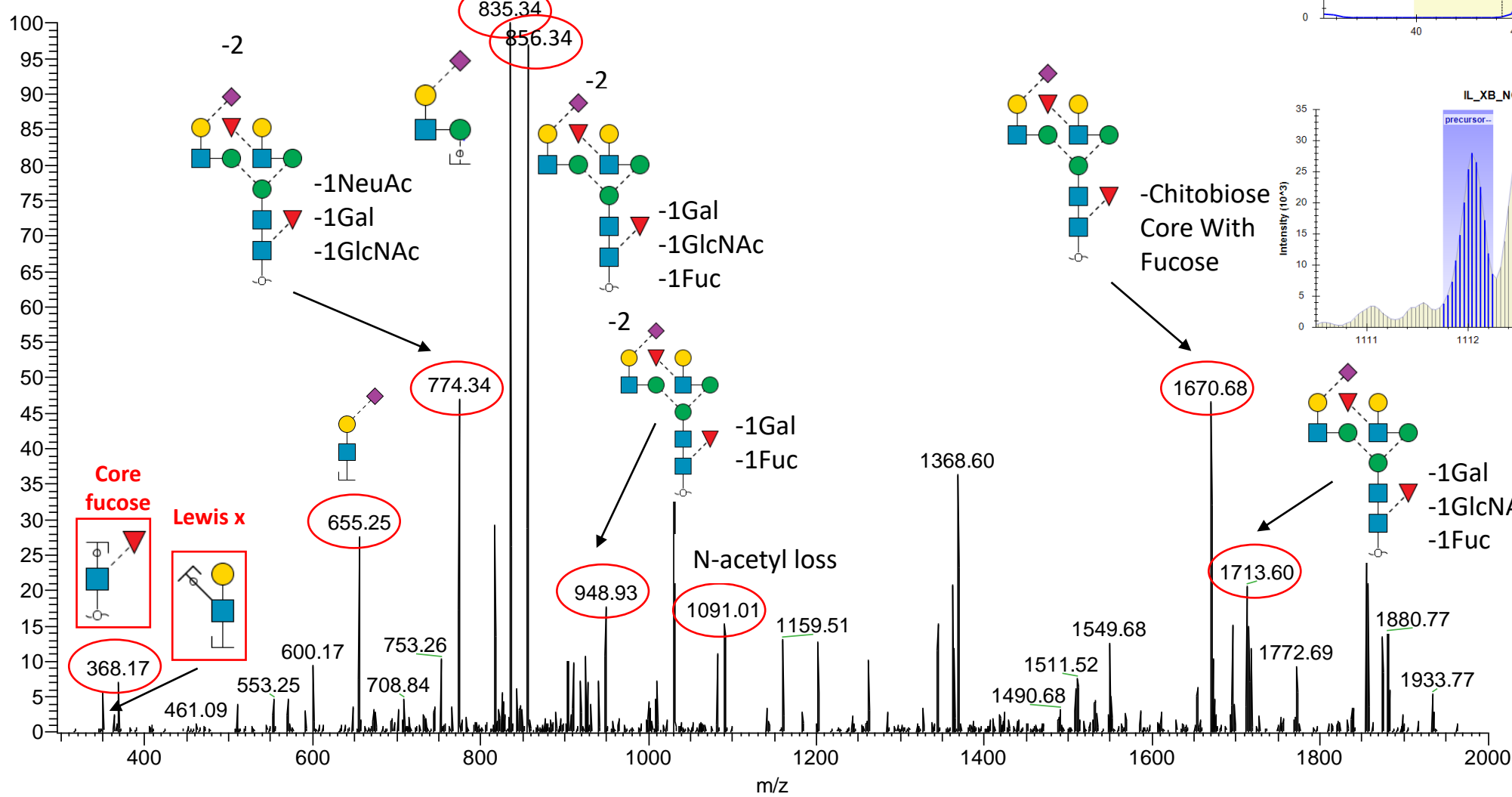
Hex₂HexNAc₂Fuc₁NeuAc₁ + Hex₃HexNAc₂Fuc₁

m/z: 1112.0⁽²⁻⁾



IL_XB_NG_260717 #4132 RT: 41.48 AV: 1 NL: 2.59E3

F: ITMS - p ESI d Full ms2 1111.96@cid35.00 [295.00-]



Note: Based on the early PGC-LC elution pattern, this glycan is annotated as the α 2,6-sialyl linkage isomer. Indication of both core and antenna fucose. The exact antennary fucosyl linkage(s) (here drawn as α 1,3) remains undetermined.

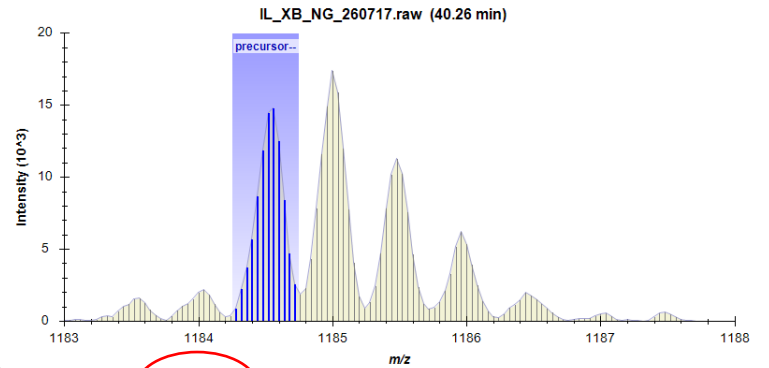
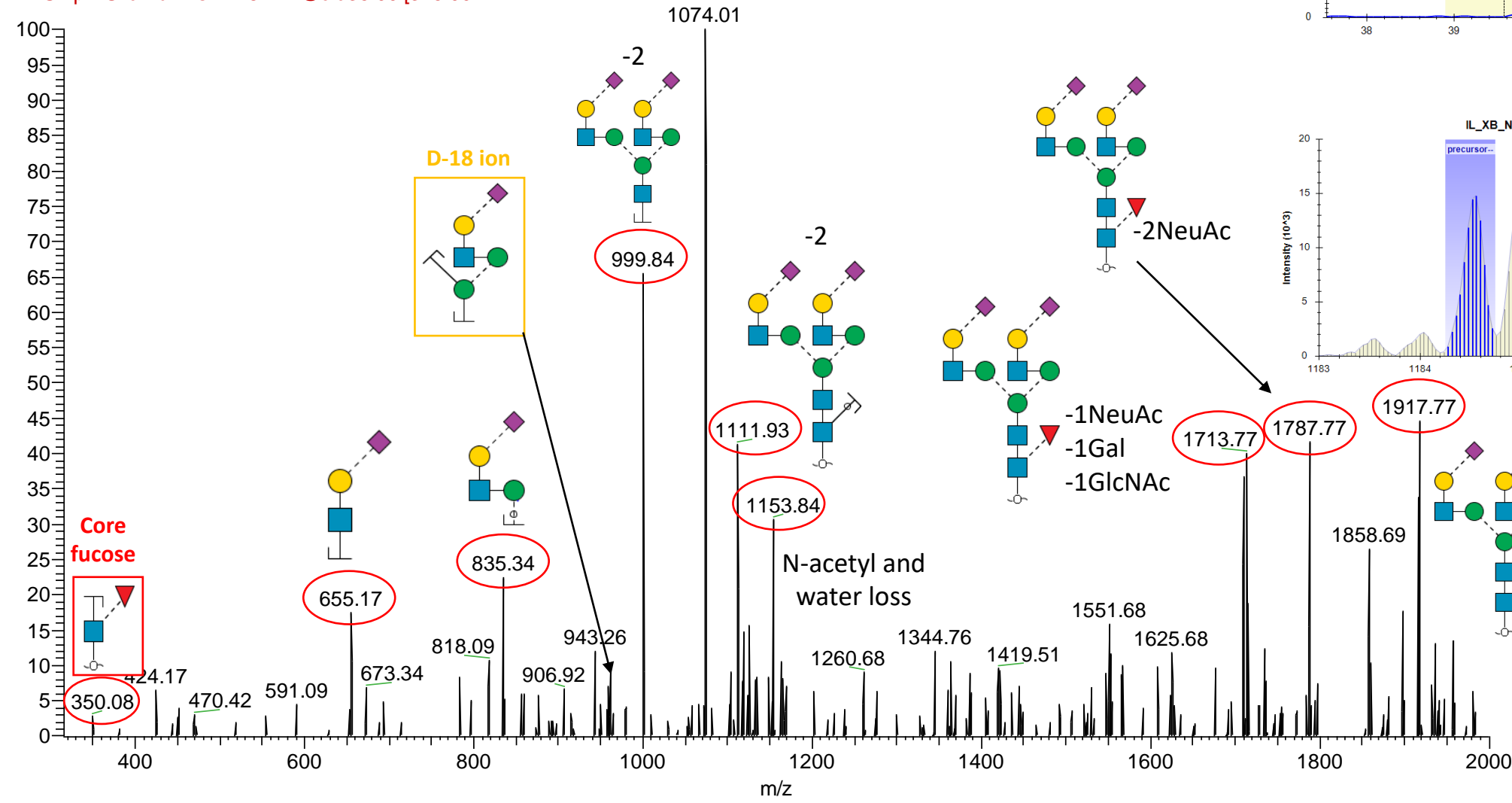
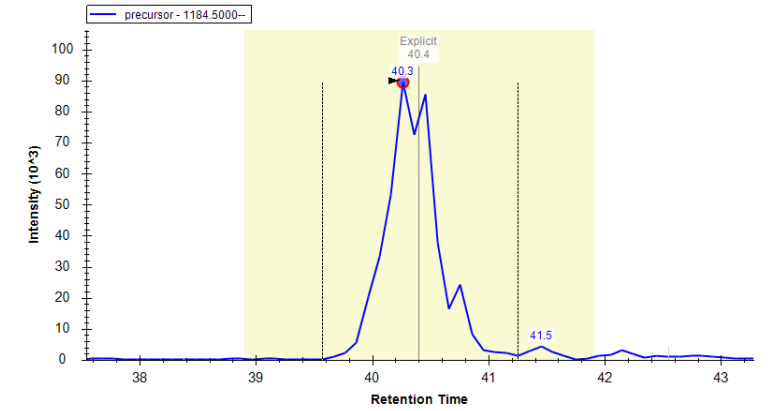
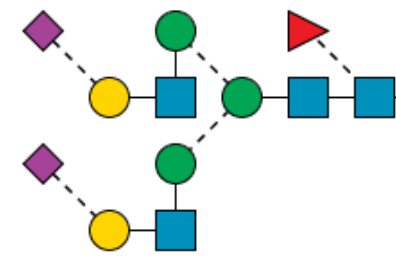
Glycan #35a

Complex

Hex₂HexNAc₂NeuAc₂ + Hex₃HexNAc₂Fuc₁

m/z: 1184.5 (2-)

IL_XB_NG_260717 #4022 RT: 40.45 AV: 1 NL: 1.57E2
F: ITMS - p ESI d Full ms2 1184.47@cid35.00 [315.00-]



Note: Based on PGC-LC elution pattern, this glycan is annotated as the α 2,6- α 2,6-sialyl linkage isomer. Indication of core fucose.

Glycan #35b

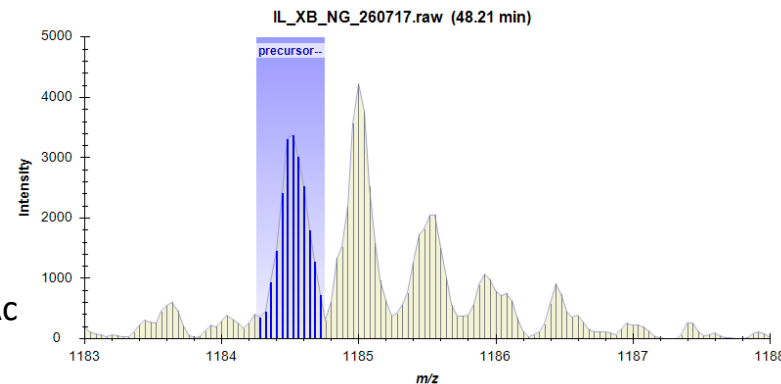
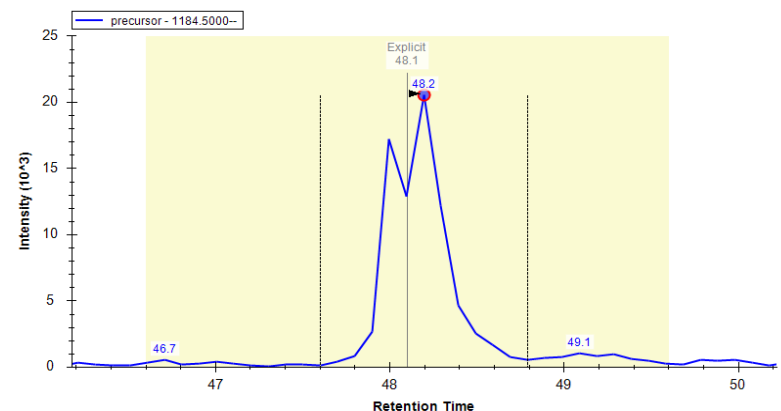
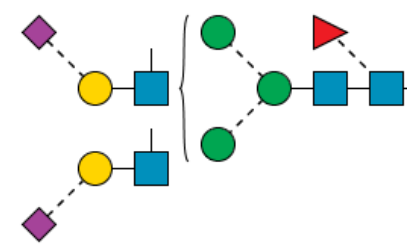
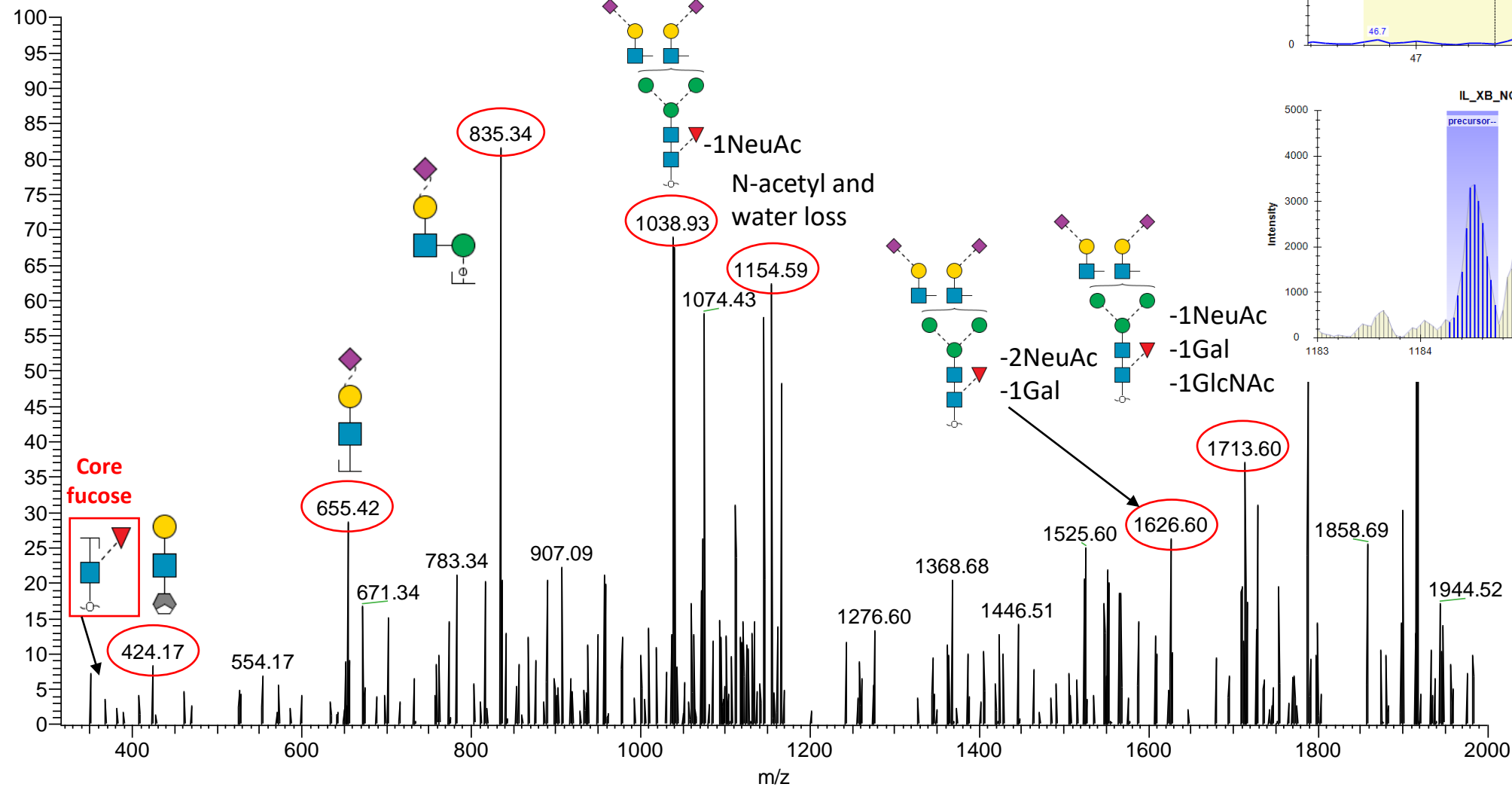
Complex

Hex₂HexNAc₂NeuAc₂ + Hex₃HexNAc₂Fuc₁

m/z: 1184.5⁽²⁻⁾

IL_XB_NG_260717 #4772 RT: 48.11 AV: 1 NL: 3.04E1

F: ITMS - p ESI d Full ms2 1184.47@cid35.00 [315.00-]



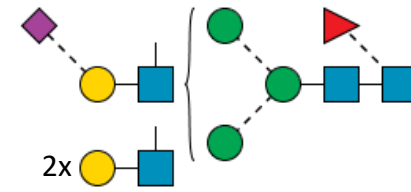
Note: Based on PGC-LC elution pattern, this glycan is annotated as the α2,6-α2,3-sialyl linkage isomer. Indication of core fucose.

Glycan #36a

Complex

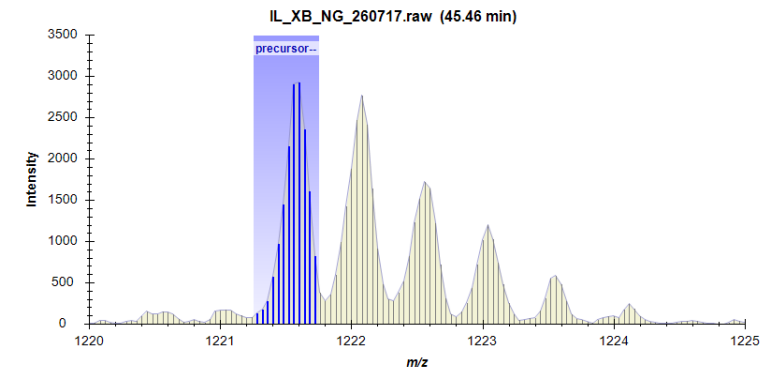
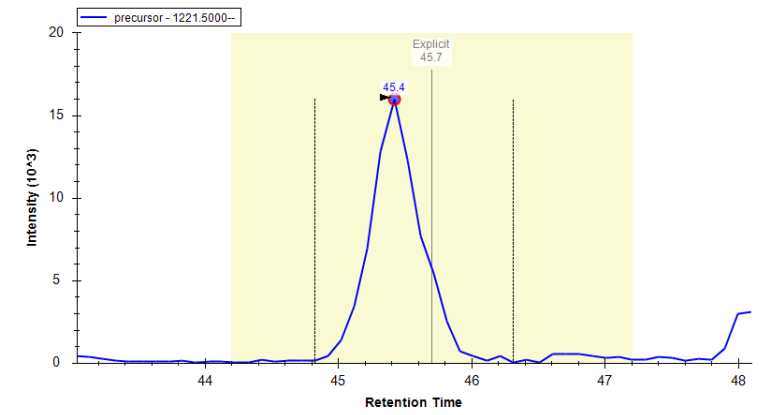
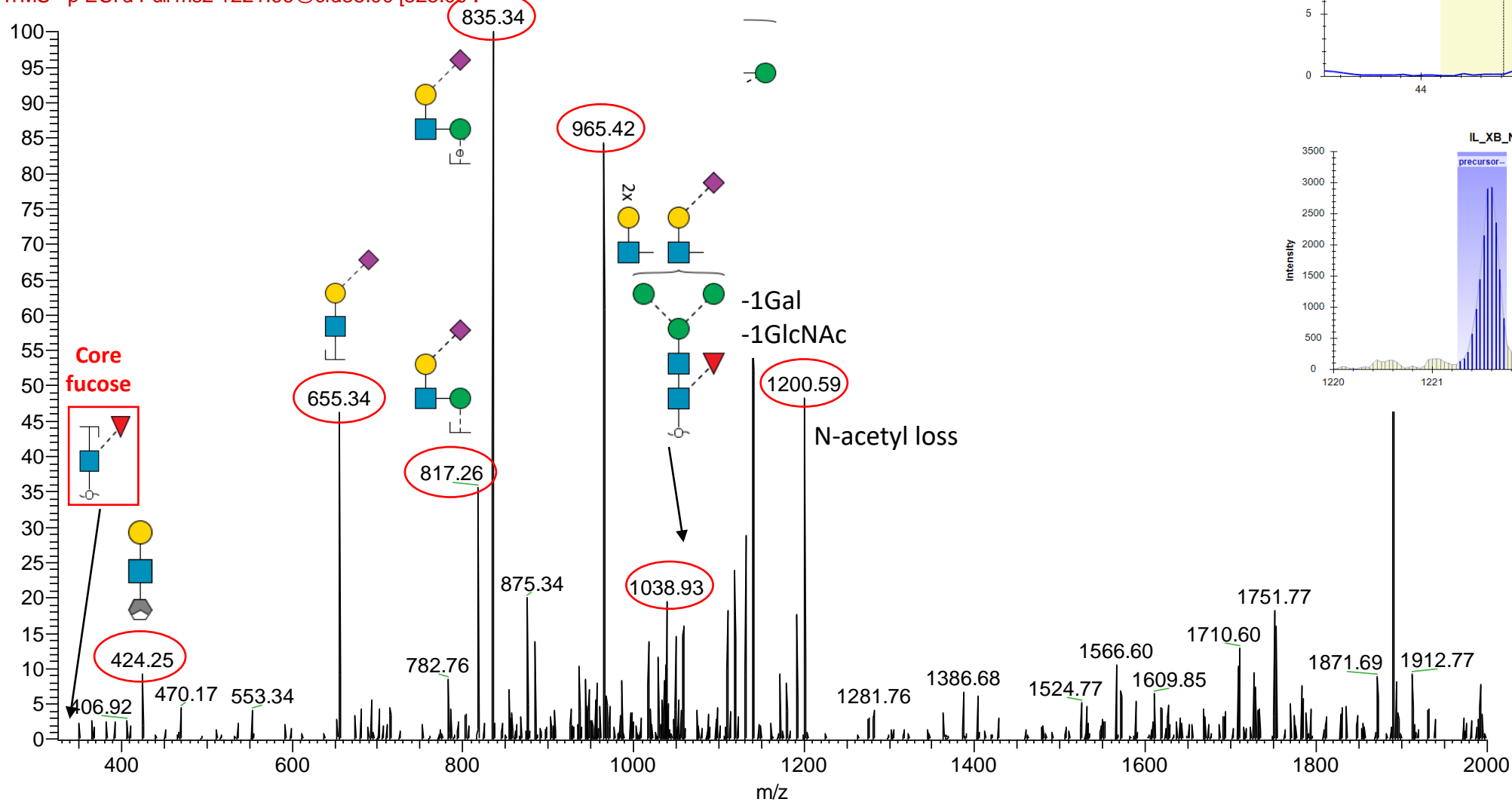
Hex₃HexNAc₃NeuAc₁ + Hex₃HexNAc₂Fuc₁

m/z: 1221.5 (2-)



IL_XB_NG_260717 #4512 RT: 45.37 AV: 1 NL: 1.00E2

F: ITMS - p ESI d Full ms2 1221.66@cid35.00 [325.00-]



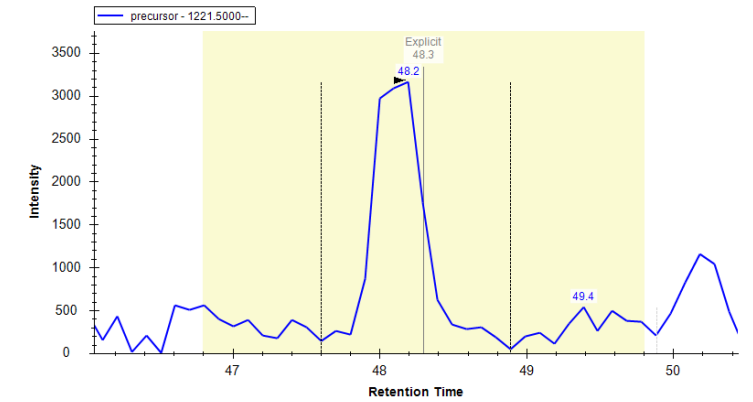
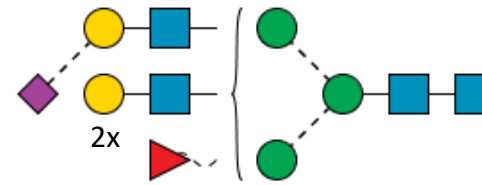
Note: Based on PGC-LC elution pattern, this glycan is annotated as the α 2,6-sialyl linkage isomer. Indication of core fucose.

Glycan #36b

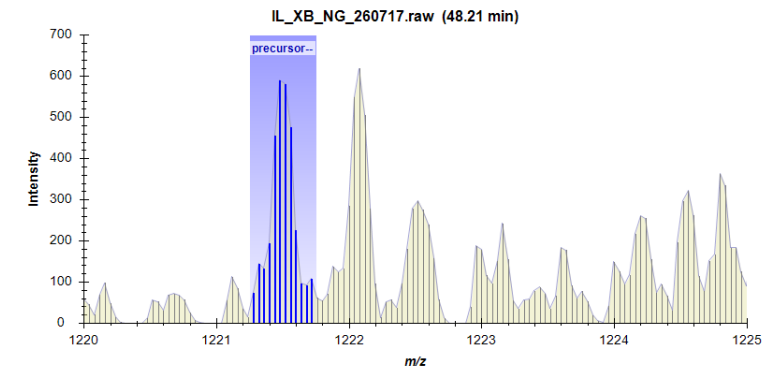
Complex

Hex₃HexNAc₃NeuAc₁ + Hex₃HexNAc₂Fuc₁

m/z: 1221.5 (2-)



No MS/MS available in glycomics data



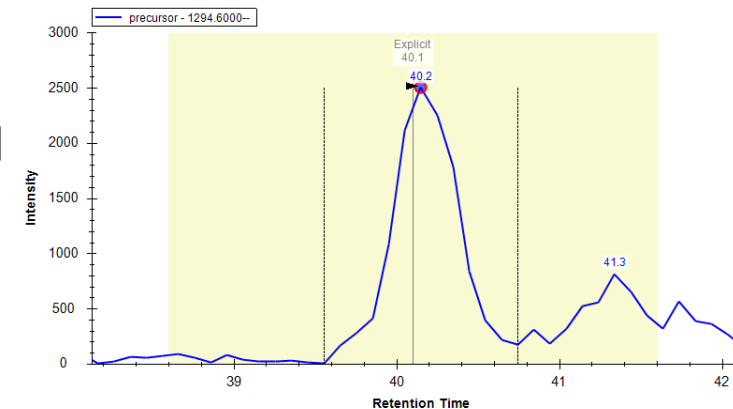
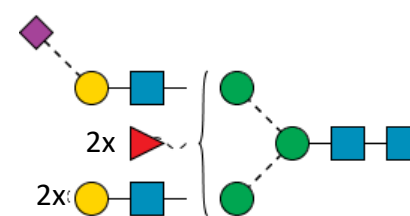
Note: Based on MS1 and retention time and the suspected biosynthetic relationship to Glycan #36a, this glycan has tentatively been annotated as the alpha2,3-sialyl isomer variant of Glycan #36a

Glycan #37a

Complex

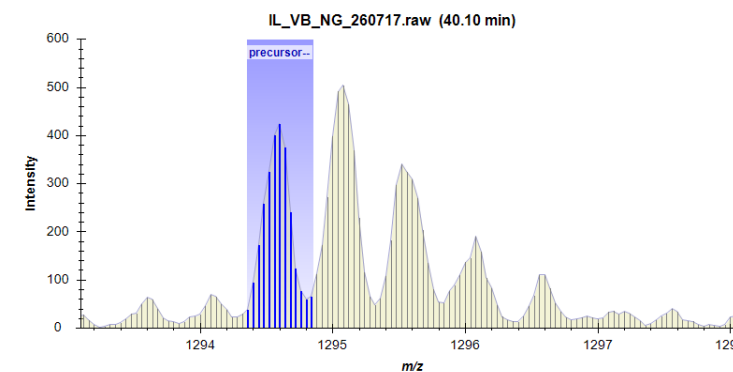
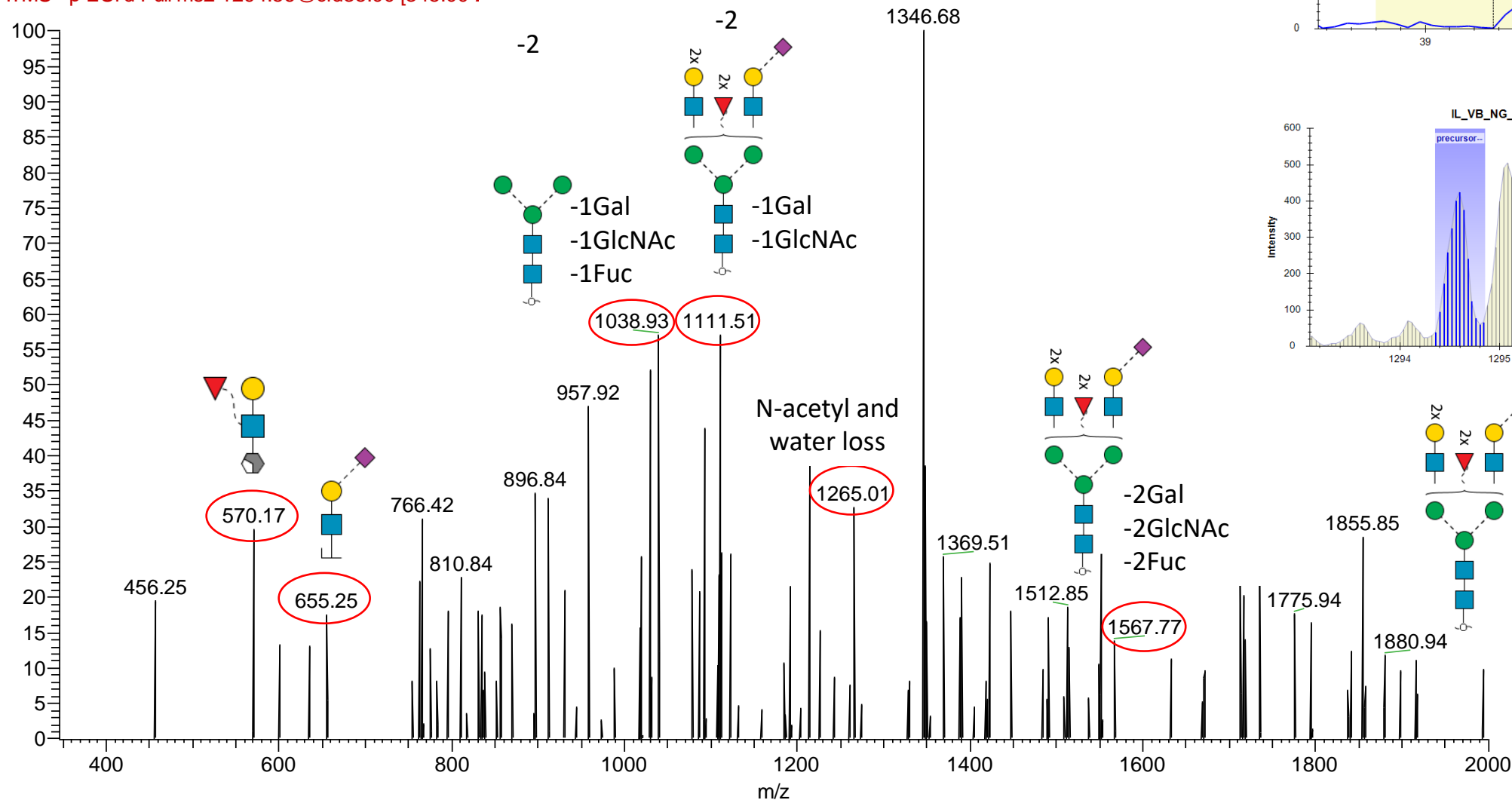
Hex₃HexNAc₃NeuAc₁Fuc₂ + Hex₃HexNAc₂

m/z: 1294.6⁽²⁻⁾



IL_VB_NG_260717 #4000 RT: 40.09 AV: 1 NL: 1.32E1

F: ITMS - p ESI d Full ms2 1294.56@cid35.00 [345.00-]



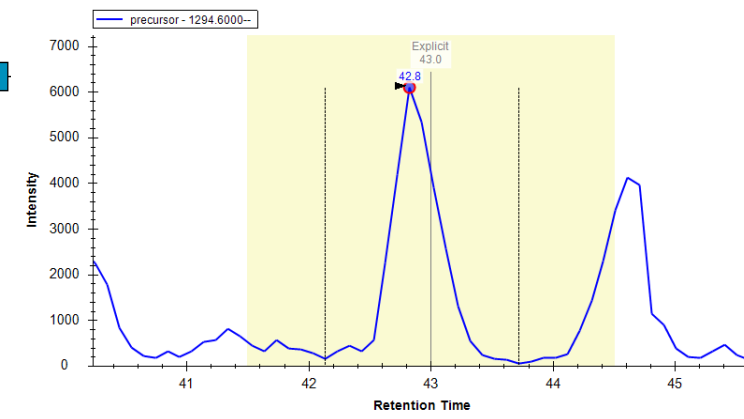
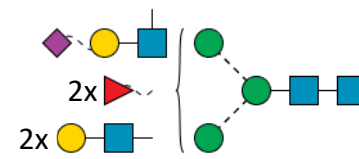
Note: Based on PGC-LC elution pattern, this glycan is annotated as the α 2,6-sialyl linkage isomer. Since there is no sign of core fucosylation, this structure has been annotated as being antenna fucosylated.

Glycan #37b

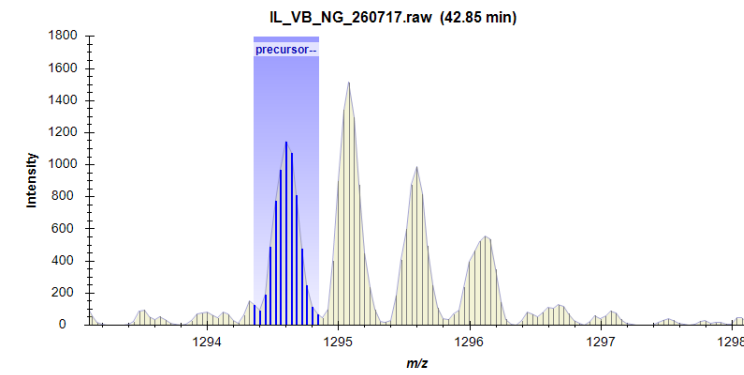
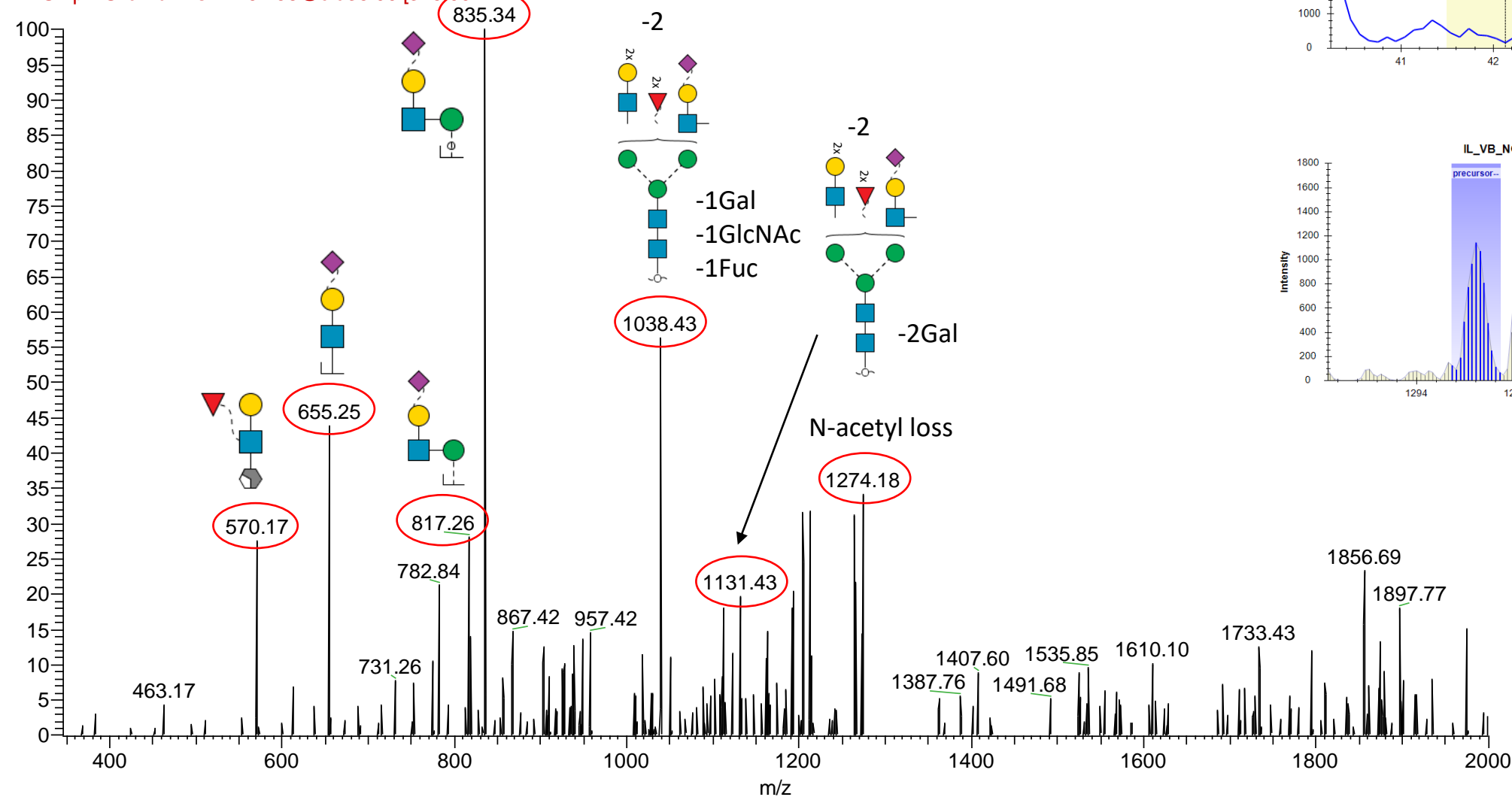
Complex

Hex₃HexNAc₃NeuAc₁Fuc₂ + Hex₃HexNAc₂

m/z: 1294.6⁽²⁻⁾



IL_VB_NG_260717 #4285 RT: 43.00 AV: 1 NL: 3.25E1
F: ITMS - p ESI d Full ms2 1294.56@cid35.00 [345.00-]



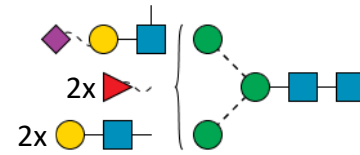
Note: Due to the lack of other isomers, this glycan is annotated with an unknown sialyl linkage isomer. Since there is no sign of core fucosylation, this structure has been annotated as being antenna fucosylated.

Glycan #37c

Complex

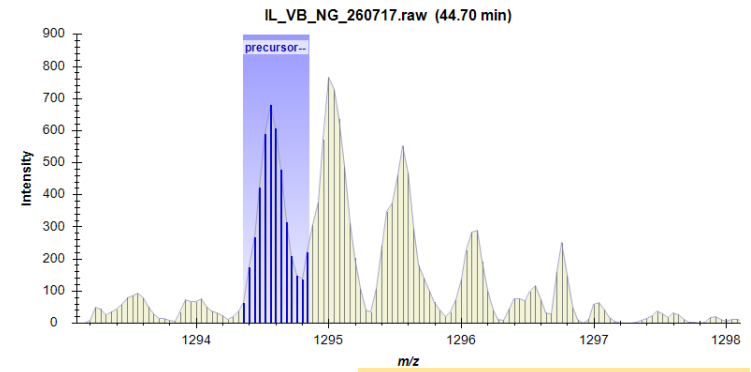
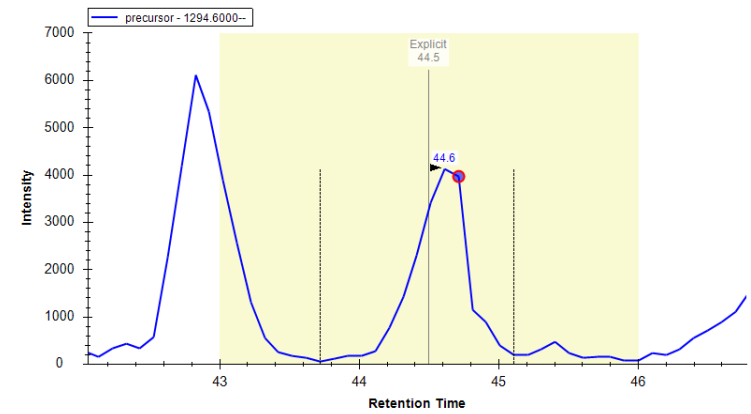
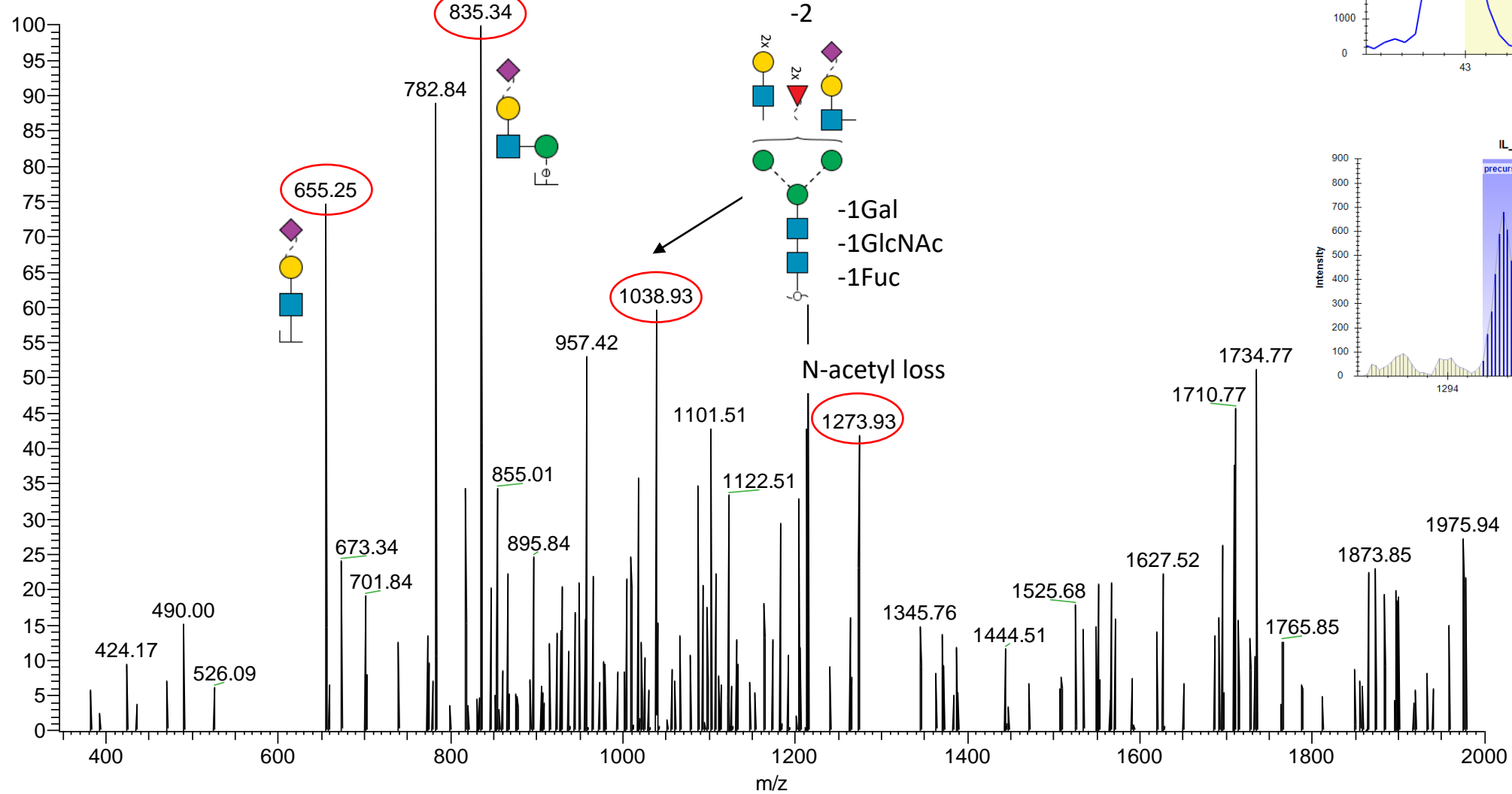
Hex₃HexNAc₃NeuAc₁Fuc₂ + Hex₃HexNAc₂

m/z: 1294.6⁽²⁻⁾



IL_VB_NG_260717 #4437 RT: 44.55 AV: 1 NL: 1.60E1

F: ITMS - p ESI d Full ms2 1294.56@cid35.00 [345.00-]



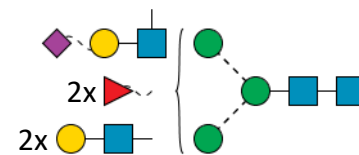
Note: Due to the lack of other isomers, this glycan is annotated with an unknown sialyl linkage isomer. Since there is no sign of core fucosylation, this structure has been annotated as being antenna fucosylated.

Glycan #37d

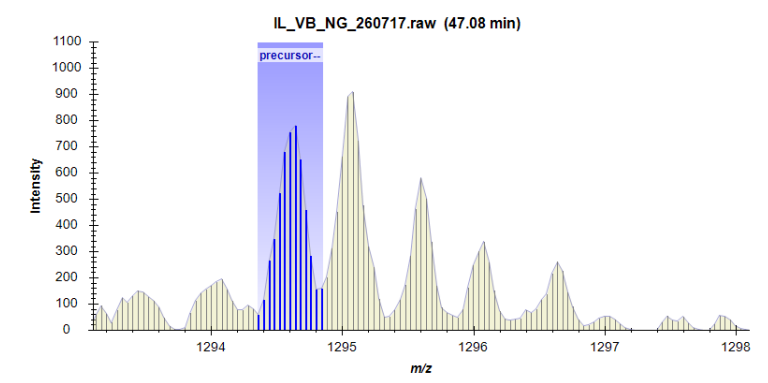
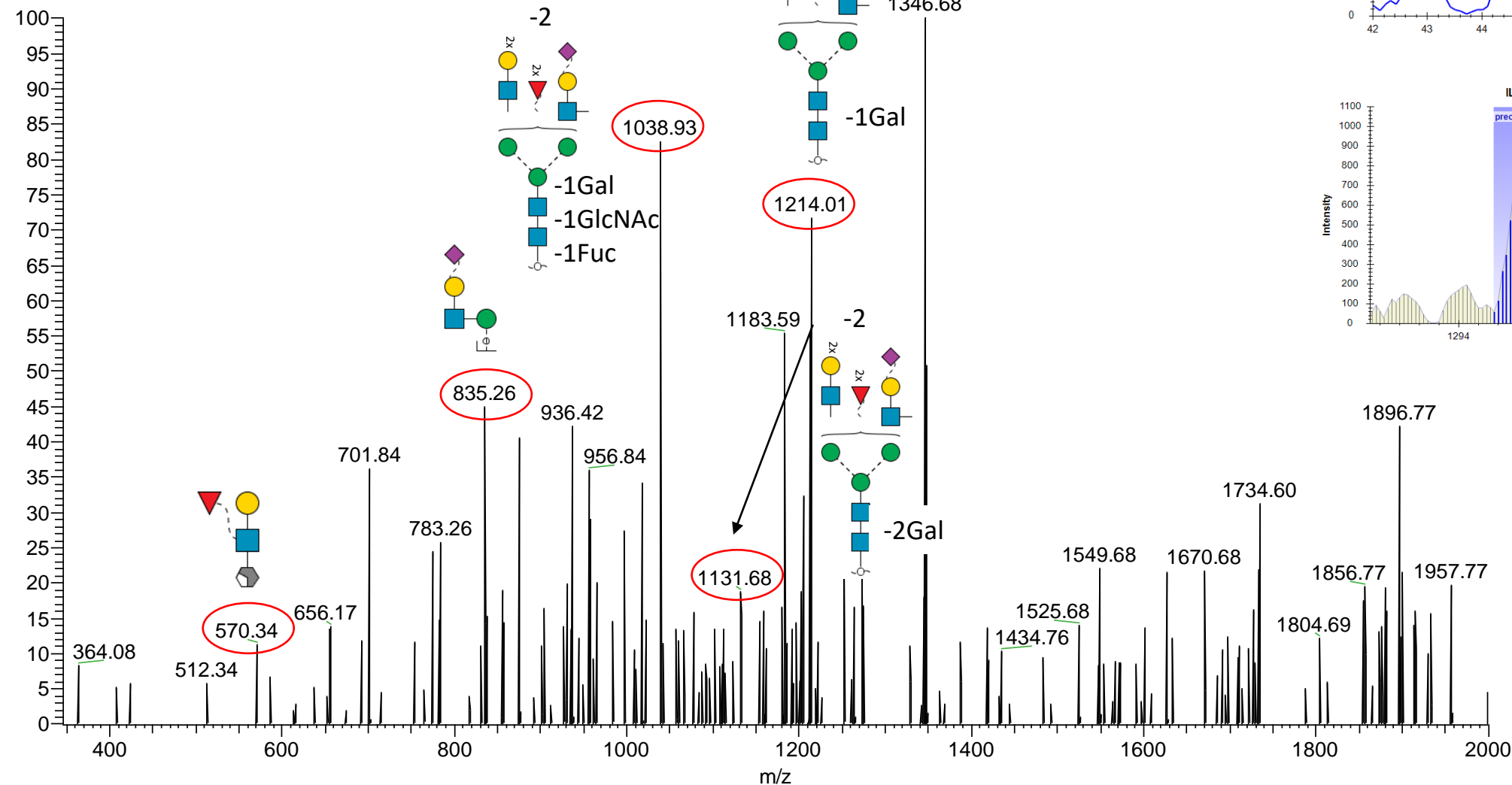
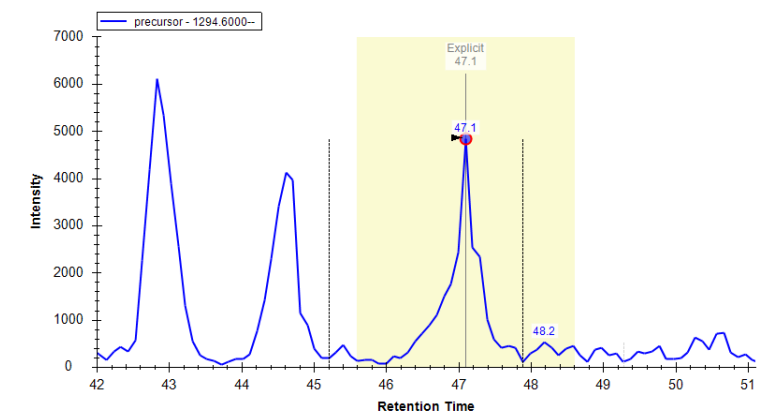
Complex

Hex₃HexNAc₃NeuAc₁Fuc₂ + Hex₃HexNAc₂

m/z: 1294.6 (2-)



IL_VB_NG_260717 #4678 RT: 47.05 AV: 1 NL: 1.54E1
F: ITMS - p ESI d Full ms2 1294.56@cid35.00 [345.00-]



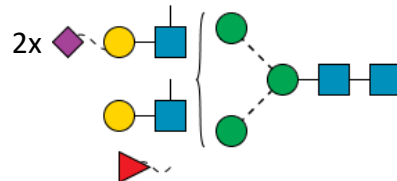
Note: Due to the lack of other isomers, this glycan is annotated with an unknown sialyl linkage isomer. Since there is no sign of core fucosylation, this structure has been annotated as being antenna fucosylated.

Glycan #38

Complex

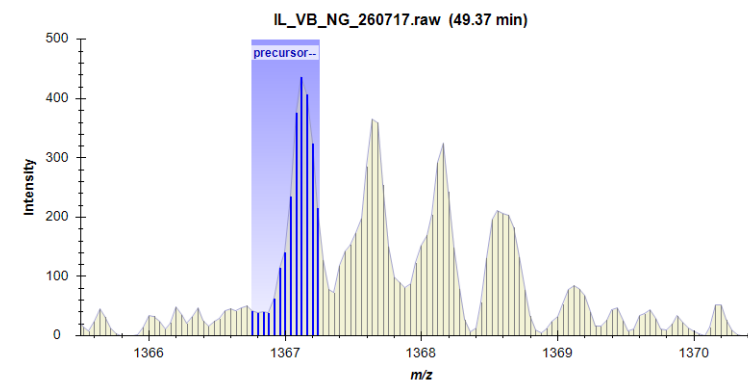
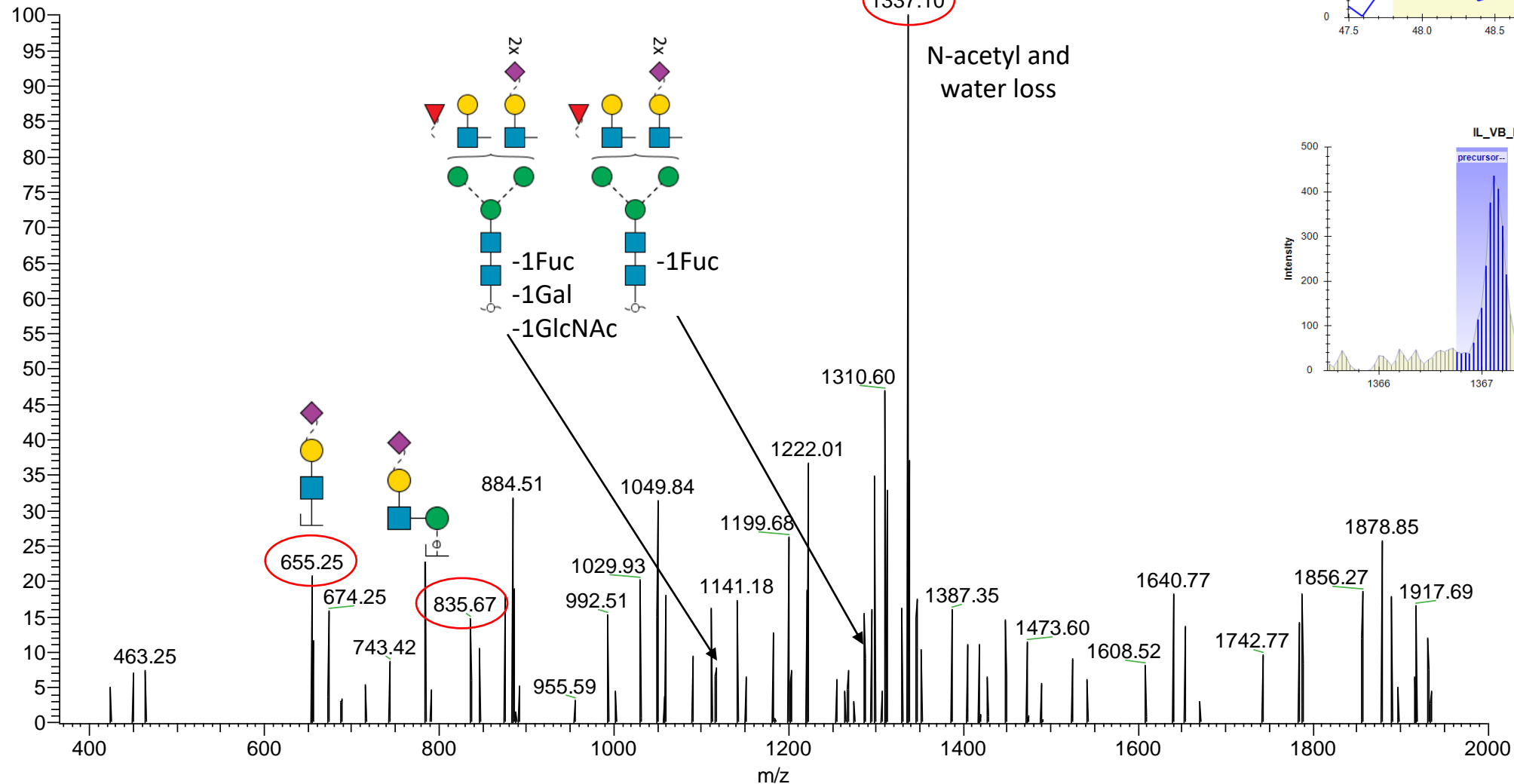
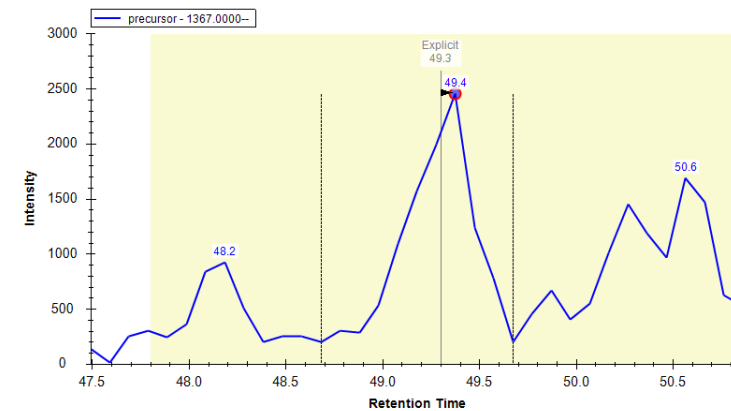
Hex₃HexNAc₃NeuAc₂Fuc₁ + Hex₃HexNAc₂

m/z: 1367.0⁽²⁻⁾



IL_VB_NG_260717 #4897 RT: 49.33 AV: 1 NL: 1.16E1

F: ITMS - p ESI d Full ms2 1367.08@cid35.00 [365.00-]



Note: Due to the lack of robust fragment ions, this glycan is annotated without sialyl linkage isomer information. No indication of core fucose.

Glycan #39a

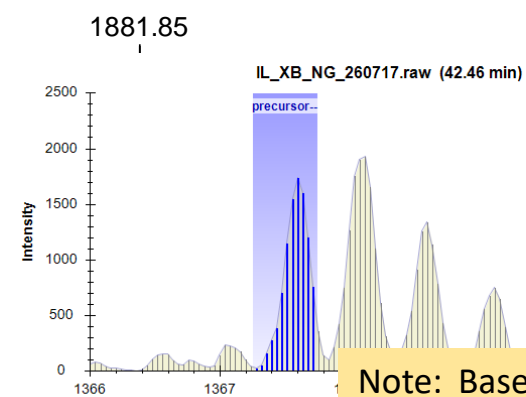
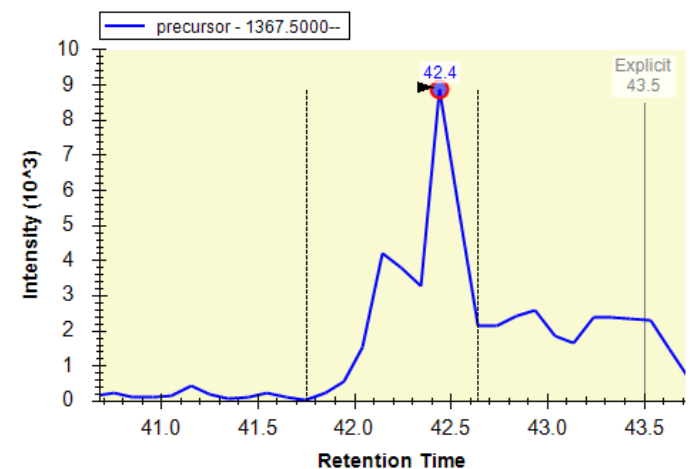
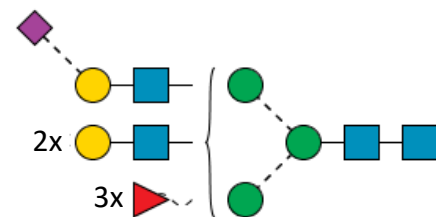
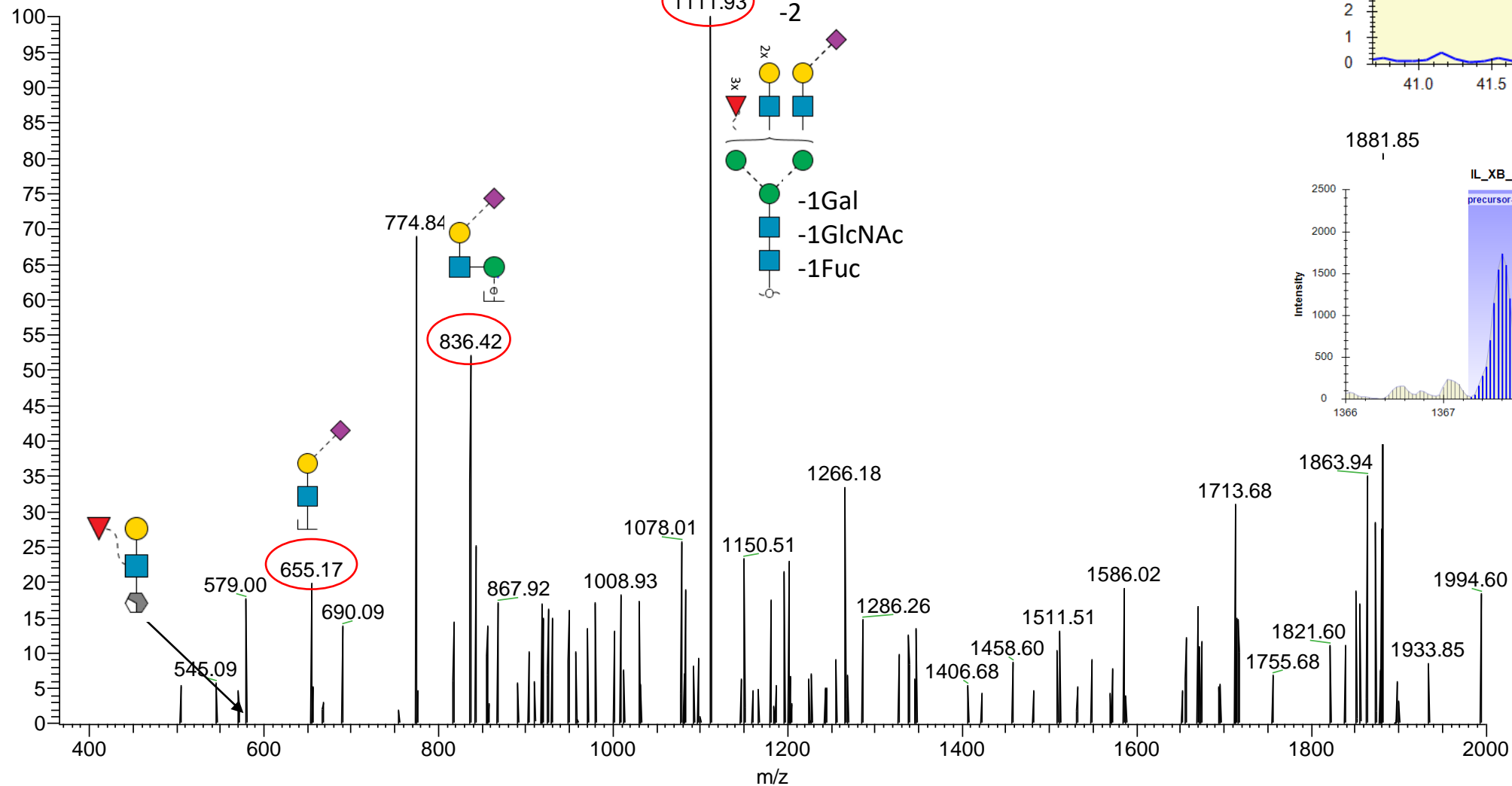
Complex

Hex₃HexNAc₃NeuAc₁Fuc₃ + Hex₃HexNAc₂

m/z: 1367.5 (2-)

IL_XB_NG_260717 #4334 RT: 43.52 AV: 1 NL: 1.82E1

F: ITMS - p ESI d Full ms2 1367.59@cid35.00 [365.00-;



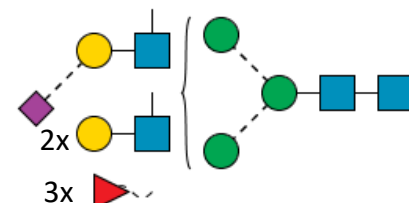
Note: Based on the early PGC-LC elution pattern, this glycan is annotated as the α 2,6-sialyl linkage isomer. Due to the lack of robust fragment ions, this glycan is otherwise annotated without sialyl linkage isomer information.

Glycan #39b

Complex

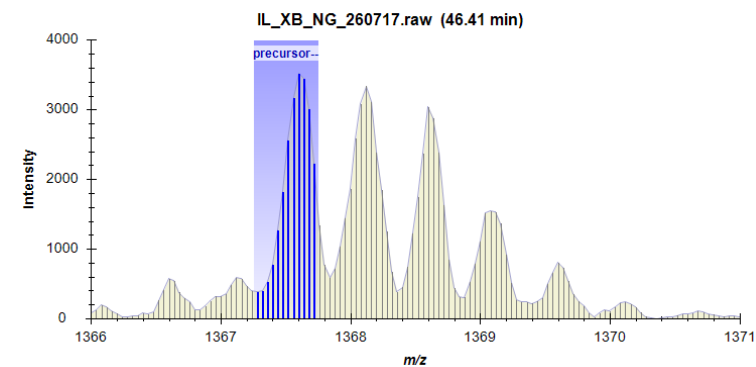
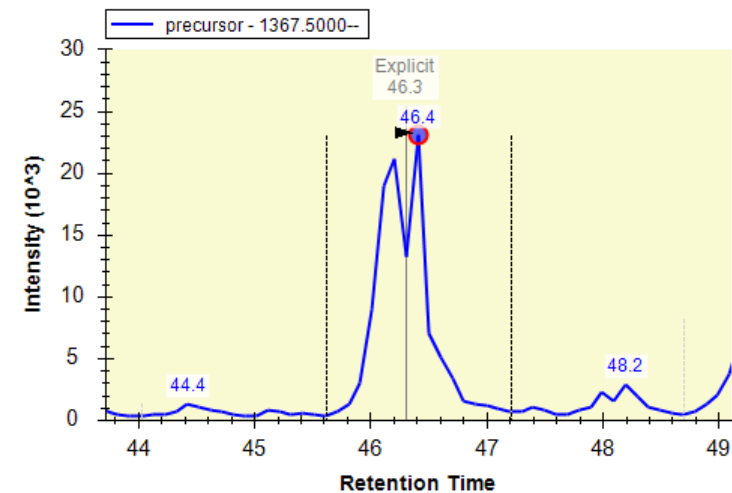
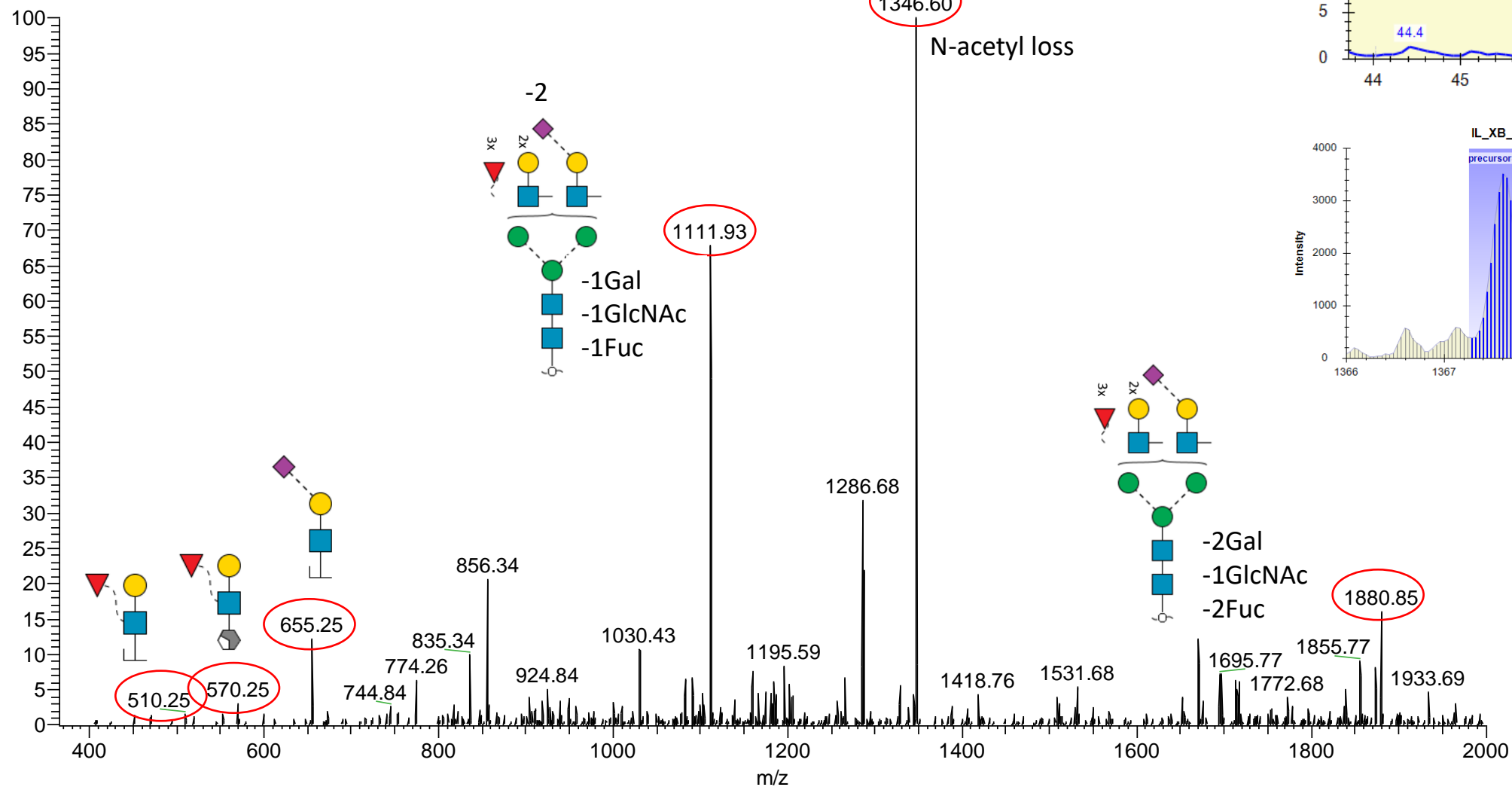
Hex₃HexNAc₃NeuAc₁Fuc₃ + Hex₃HexNAc₂

m/z: 1367.5 (2-)



IL_XB_NG_260717 #4602 RT: 46.31 AV: 1 NL: 3.02E2

F: ITMS - p ESI d Full ms2 1367.59@cid35.00 [365.00-]



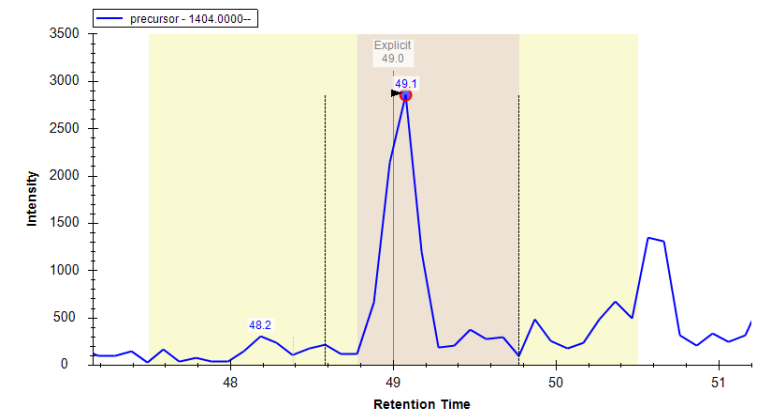
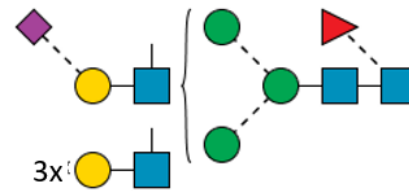
Note: Based on the PGC-LC elution pattern, this glycan is annotated as the α 2,3-sialyl linkage isomer. Due to the lack of robust fragment ions, this glycan is otherwise annotated without sialyl linkage isomer information.

Glycan #40a

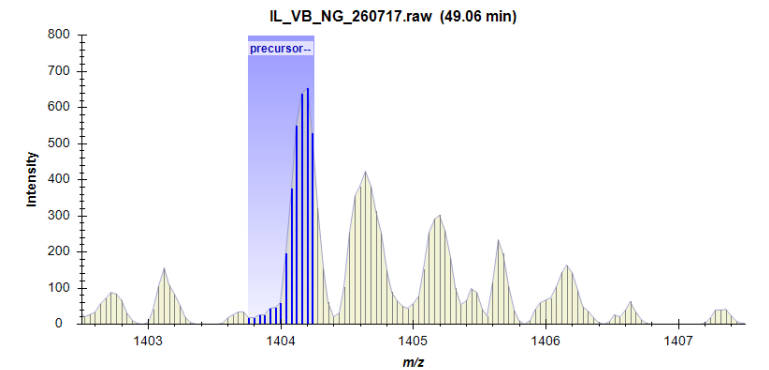
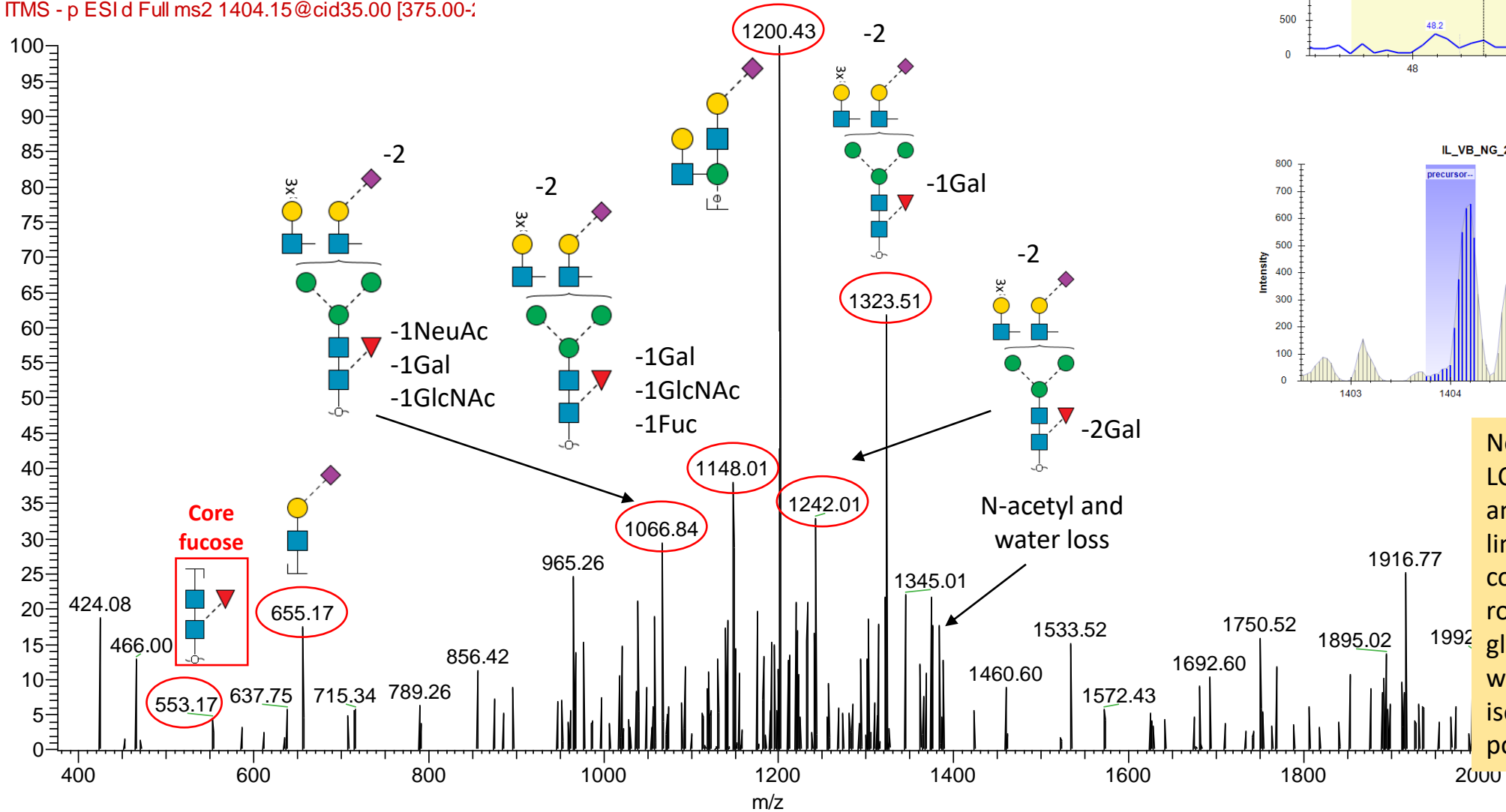
Complex

Hex₄HexNAc₄NeuAc₁ + Hex₃HexNAc₂Fuc₁

m/z: 1404.0⁽²⁻⁾



IL_VB_NG_260717 #4876 RT: 49.11 AV: 1 NL: 3.07E1
F: ITMS - p ESI d Full ms2 1404.15@cid35.00 [375.00-;



Note: Based on the early PGC-LC elution, this glycan is annotated as the α 2,6-sialyl linkage isomer. Indication of core fucose. Due to the lack of robust fragment ions, this glycan is otherwise annotated without known sialyl linkage isomer information and fucose position.

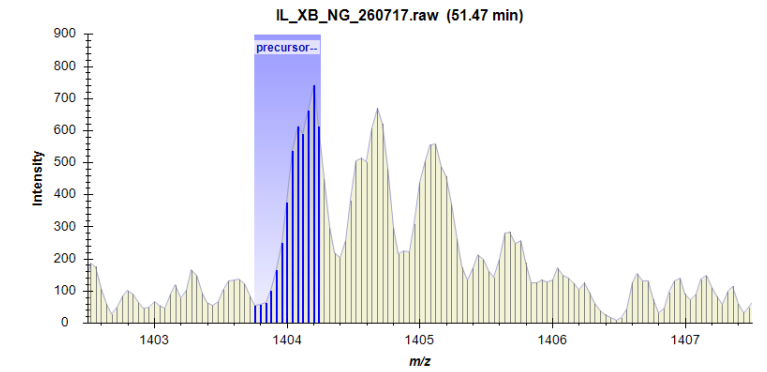
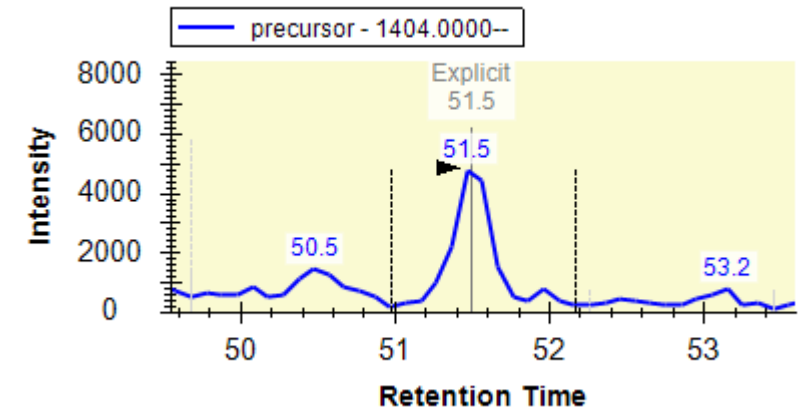
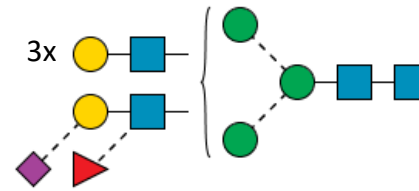
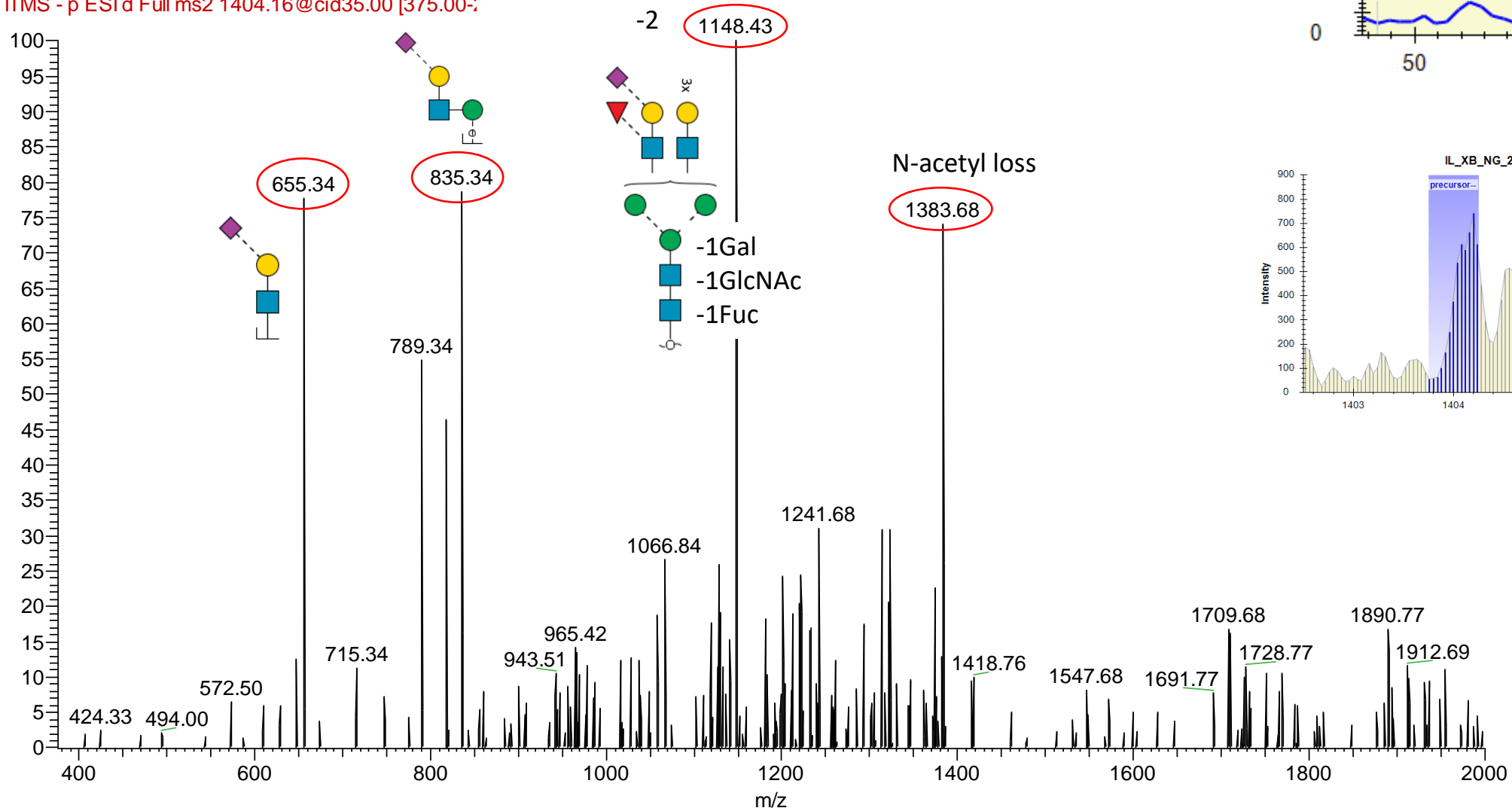
Glycan #40b

Complex

Hex₄HexNAc₄NeuAc₁ + Hex₃HexNAc₂Fuc₁

m/z: 1404.0 (2-)

IL_XB_NG_260717 #5093 RT: 51.49 AV: 1 NL: 2.94E1
F: ITMS - p ESI d Full ms2 1404.16@cid35.00 [375.00-:



Note: No indication of core fucose. Based on retention time this structure is therefore annotated as antenna fucosylated with alpha2,3-sialylated. The exact antennary fucosyl linkage(s) (here drawn as alpha1,3) remains undetermined.

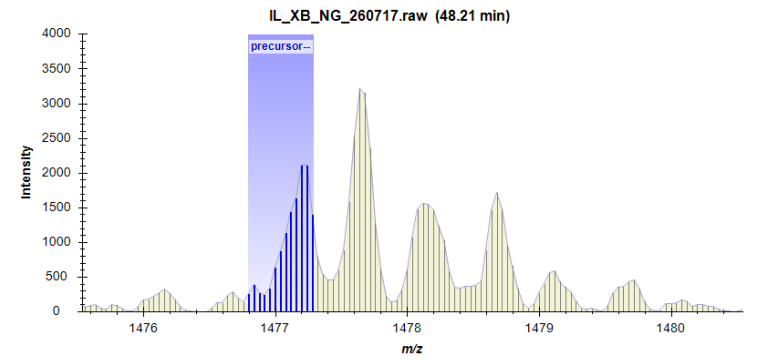
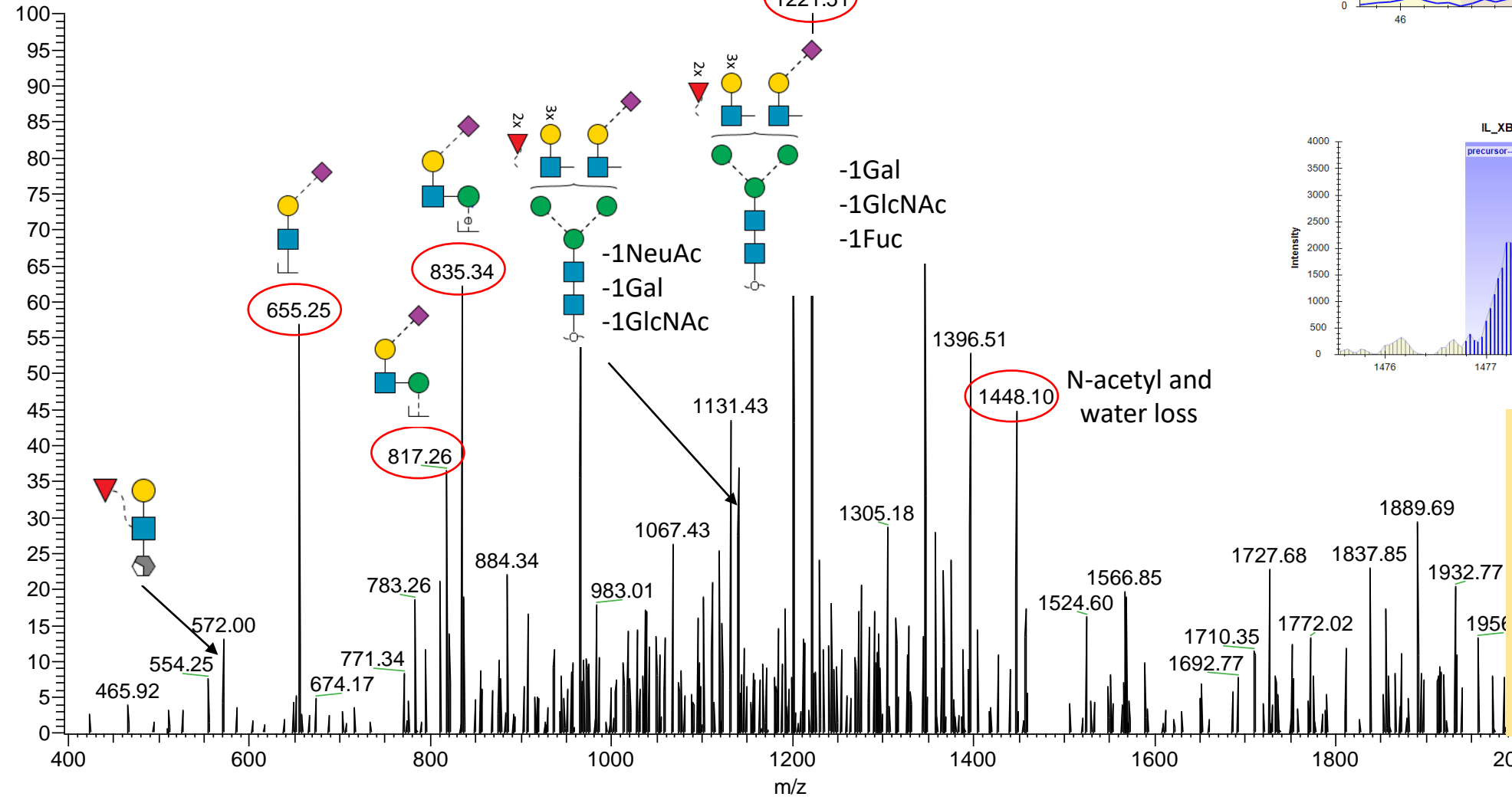
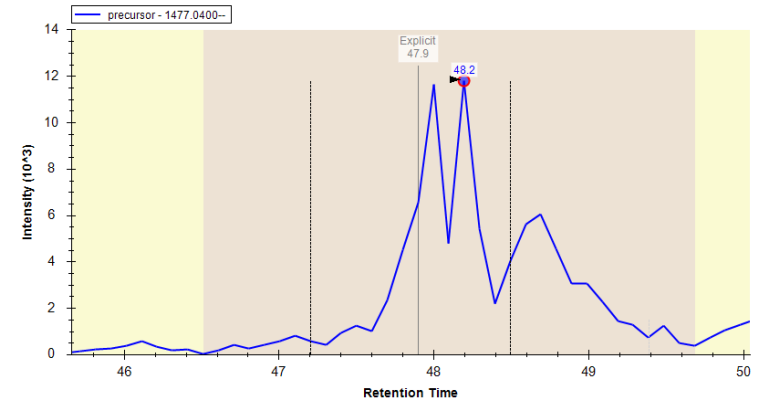
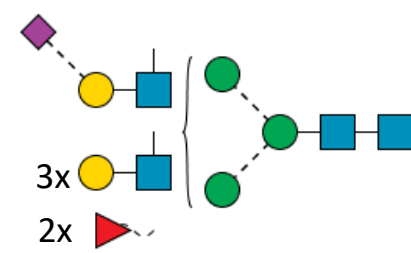
Glycan #41a

Complex

Hex₄HexNAc₄NeuAc₁Fuc₂ + Hex₃HexNAc₂

m/z: 1477.0 (2-)

IL_XB_NG_260717 #4755 RT: 47.93 AV: 1 NL: 2.99E1
 F: ITMS - p ESI d Full ms2 1477.15@cid35.00 [395.00-;



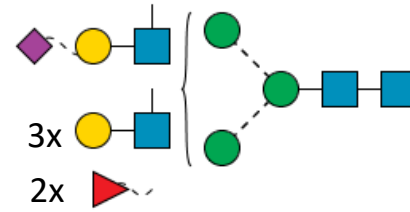
Note: Based on PGC-LC elution pattern, this glycan is annotated as the α2,6-sialyl linkage isomer. Due to the lack of robust fragment ions, this glycan is otherwise annotated without known sialyl linkage isomer information and fucose position.

Glycan #41b

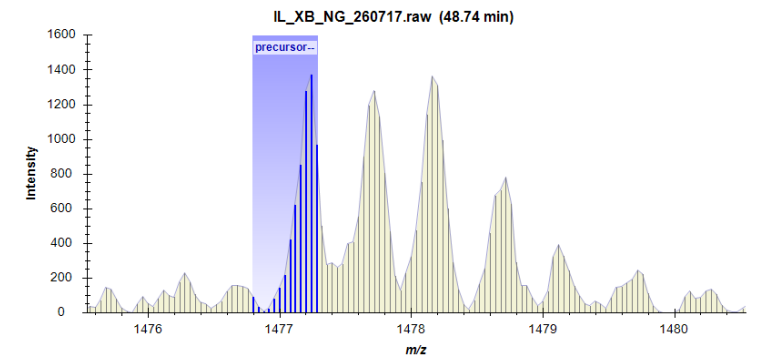
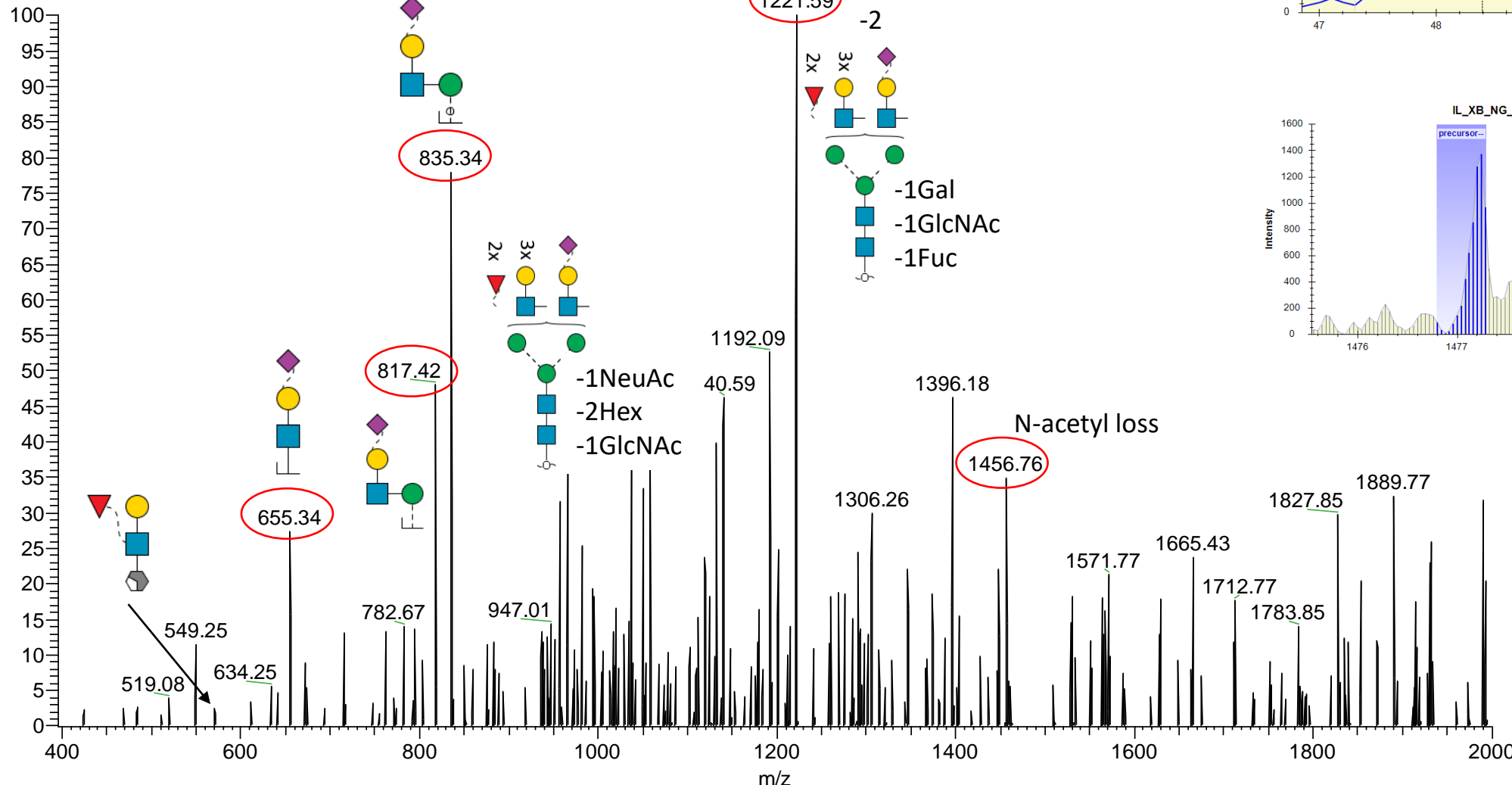
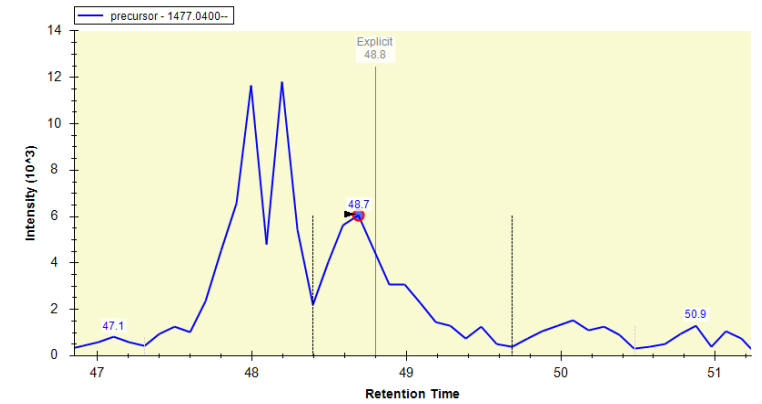
Complex

Hex₄HexNAc₄NeuAc₁Fuc₂ + Hex₃HexNAc₂

m/z: 1477.0⁽²⁻⁾



IL_XB_NG_260717 #4810 RT: 48.52 AV: 1 NL: 2.22E1
F: ITMS - p ESI d Full ms2 1477.15@cid35.00 [395.00-;



Note: Due to the lack of robust fragment ions, this glycan is annotated without known sialyl linkage isomer information and fucose position.

Glycan #42

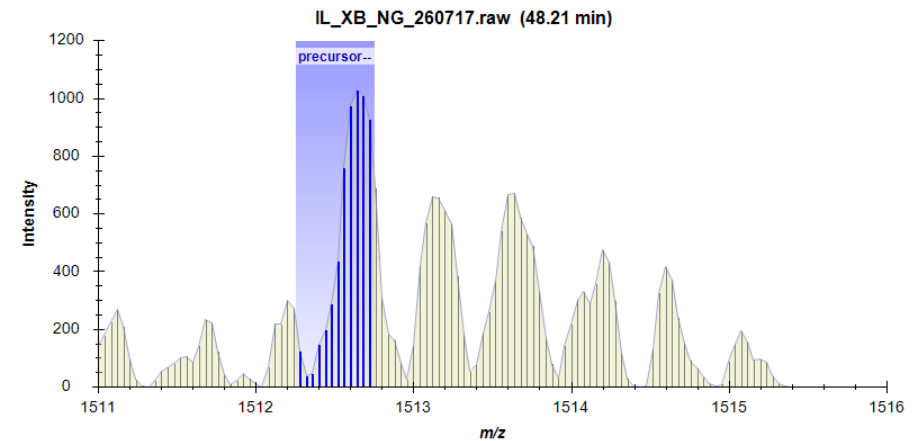
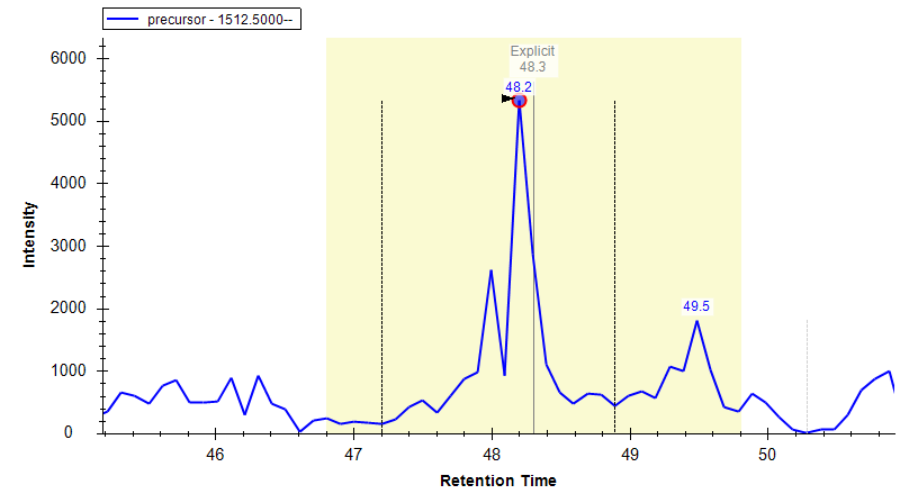
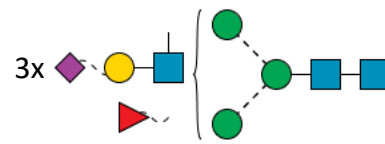
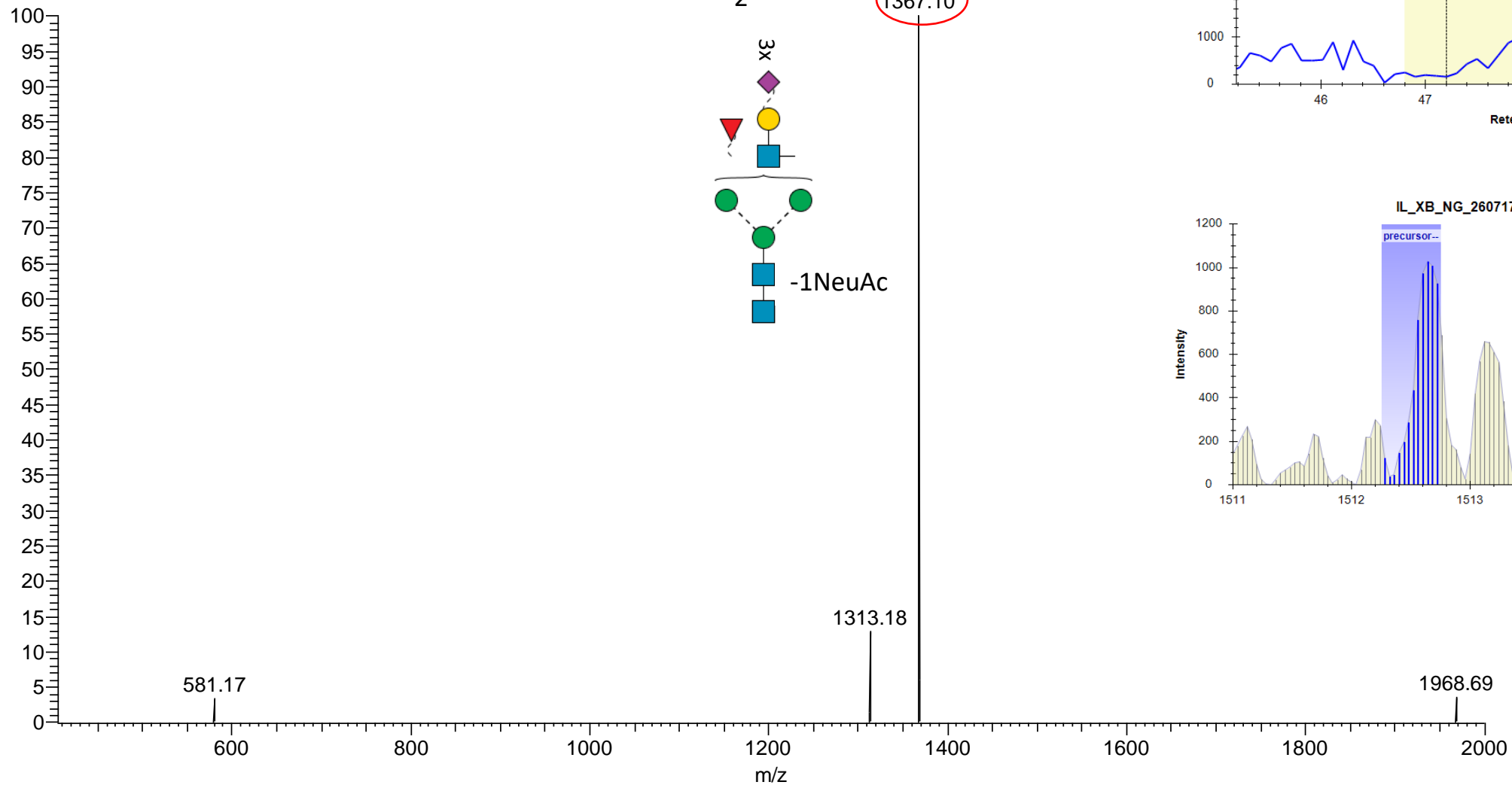
Complex

Hex₃HexNAc₃ NeuAc₃Fuc₁+ Hex₃HexNAc₂

m/z: 1512.5 (2-)

IL_XB_NG_260717 #4790 RT: 48.31 AV: 1 NL: 2.55E1

F: ITMS - p ESI d Full ms2 1512.66@cid35.00 [405.00-;



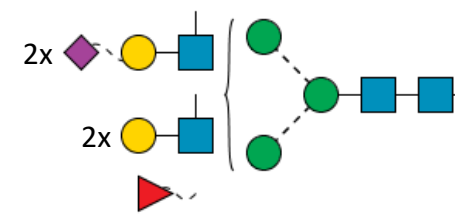
Note: Due to the lack of robust fragment ions, this glycan is annotated without known sialyl linkage isomer information and fucose position.

Glycan #43a

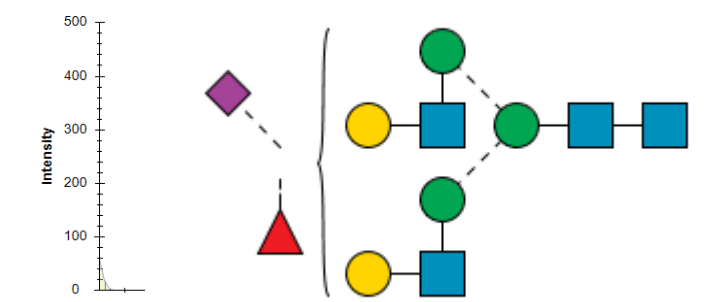
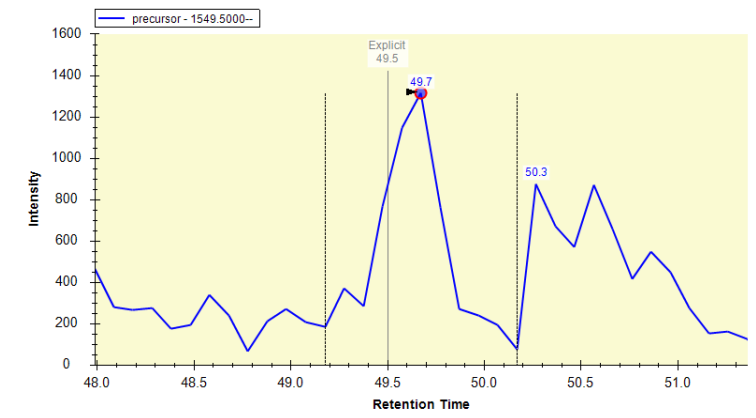
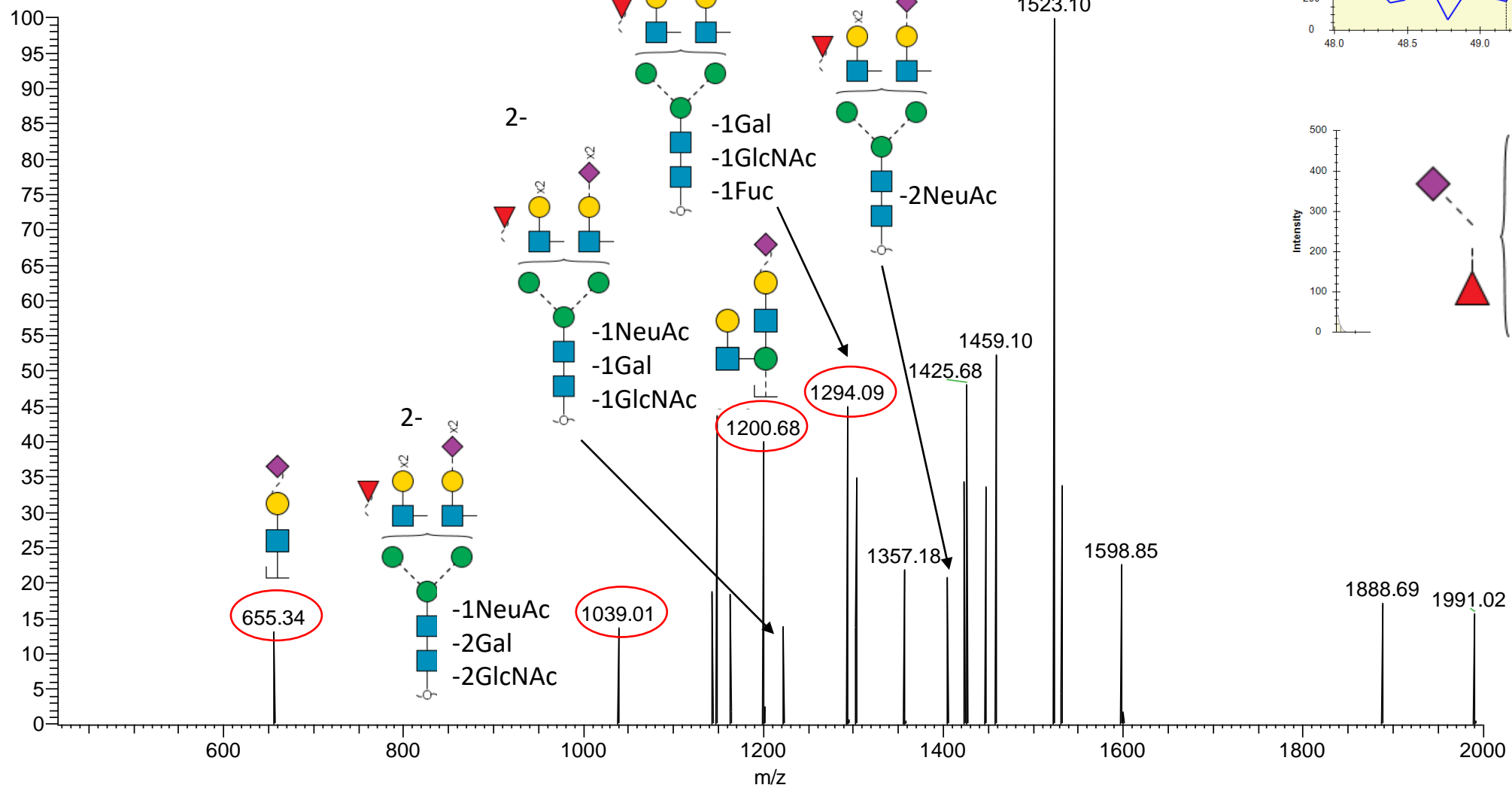
Complex

Hex₄HexNAc₄NeuAc₂Fuc₁+ Hex₃HexNAc₂

m/z: 1549.7⁽²⁻⁾



IL_VB_NG_260717 #4938 RT: 49.75 AV: 1 NL: 3.50
F: ITMS - p ESI d Full ms2 1549.69@cid35.00 [415.00-]



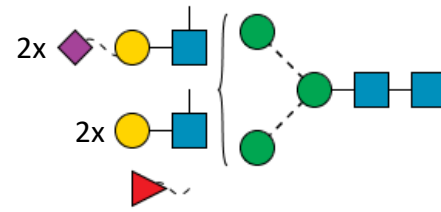
Note: Due to the lack of robust fragment ions, this glycan is annotated without known sialyl linkage isomer information and fucose position.

Glycan #43b

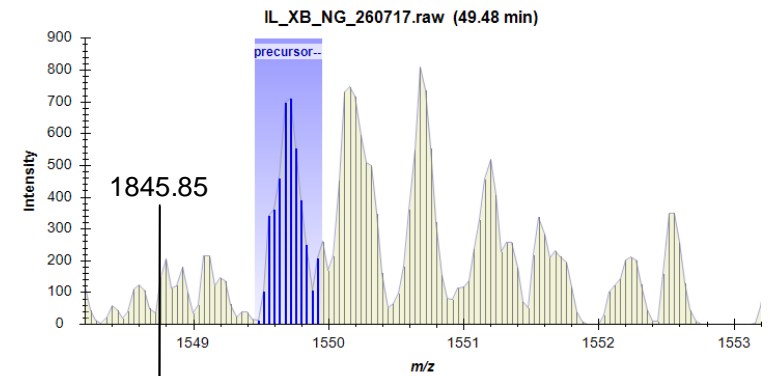
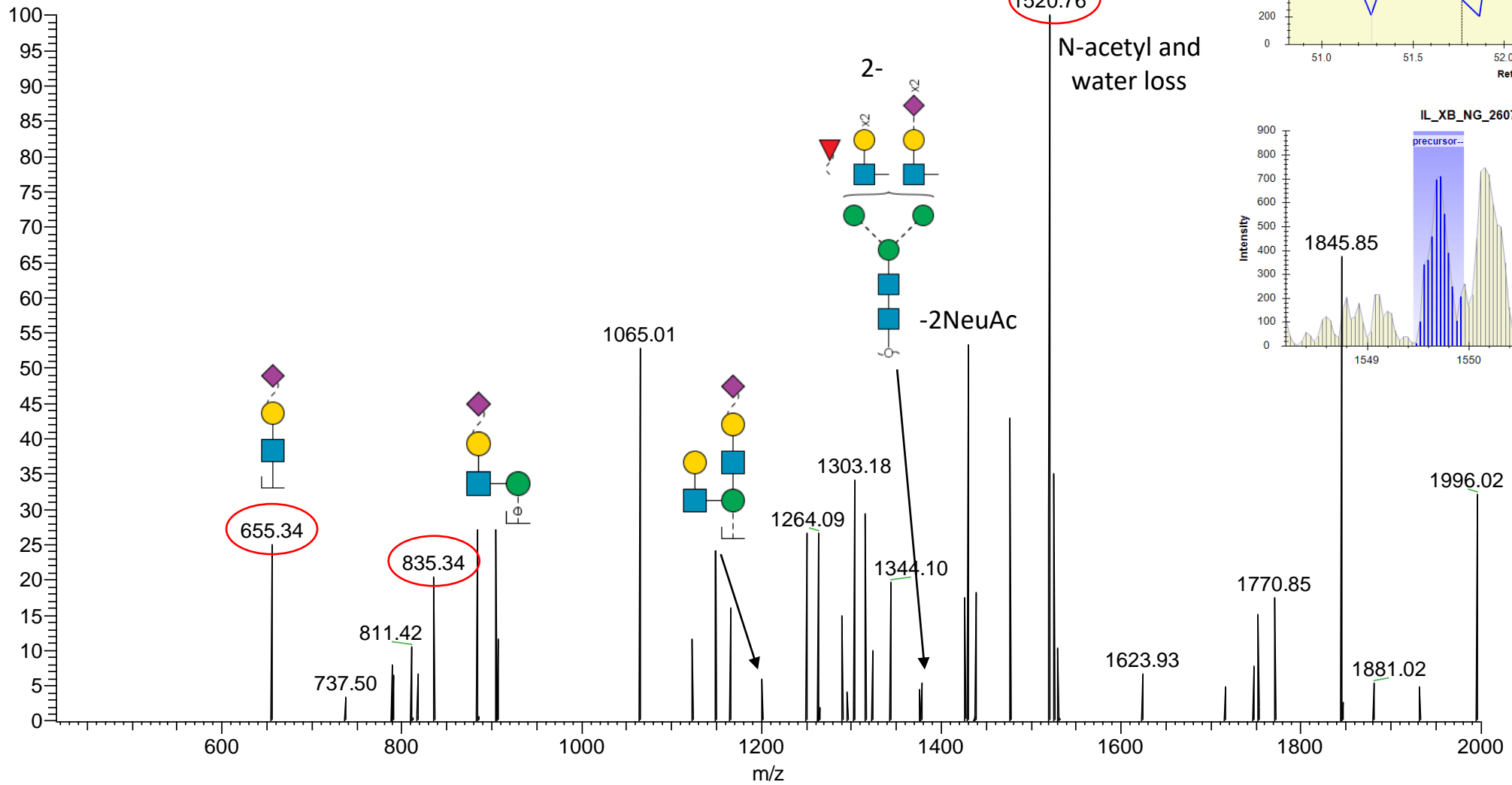
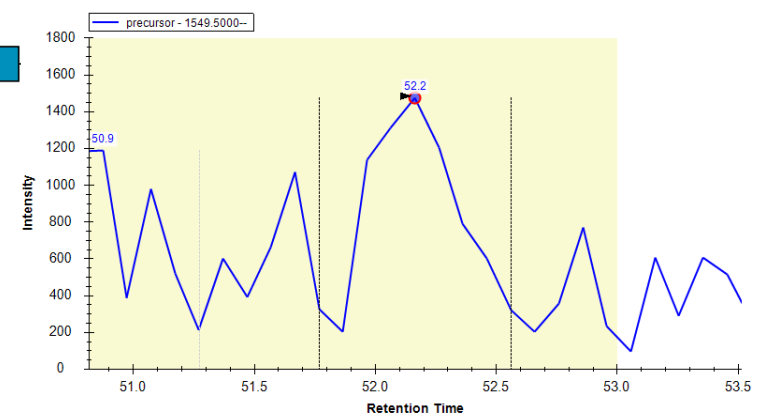
Complex

Hex₄HexNAc₄NeuAc₂Fuc₁+ Hex₃HexNAc₂

m/z: 1549.7 (2-)



IL_XB_NG_260717 #5160 RT: 52.20 AV: 1 NL: 9.20
F: ITMS - p ESI d Full ms2 1550.17@cid35.00 [415.00-;



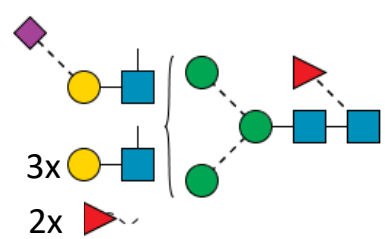
Note: Due to the lack of robust fragment ions, this glycan is annotated without known sialyl linkage isomer information and fucose position.

Glycan #44a

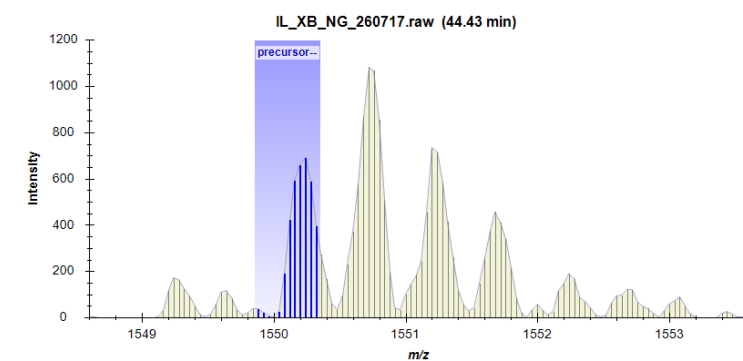
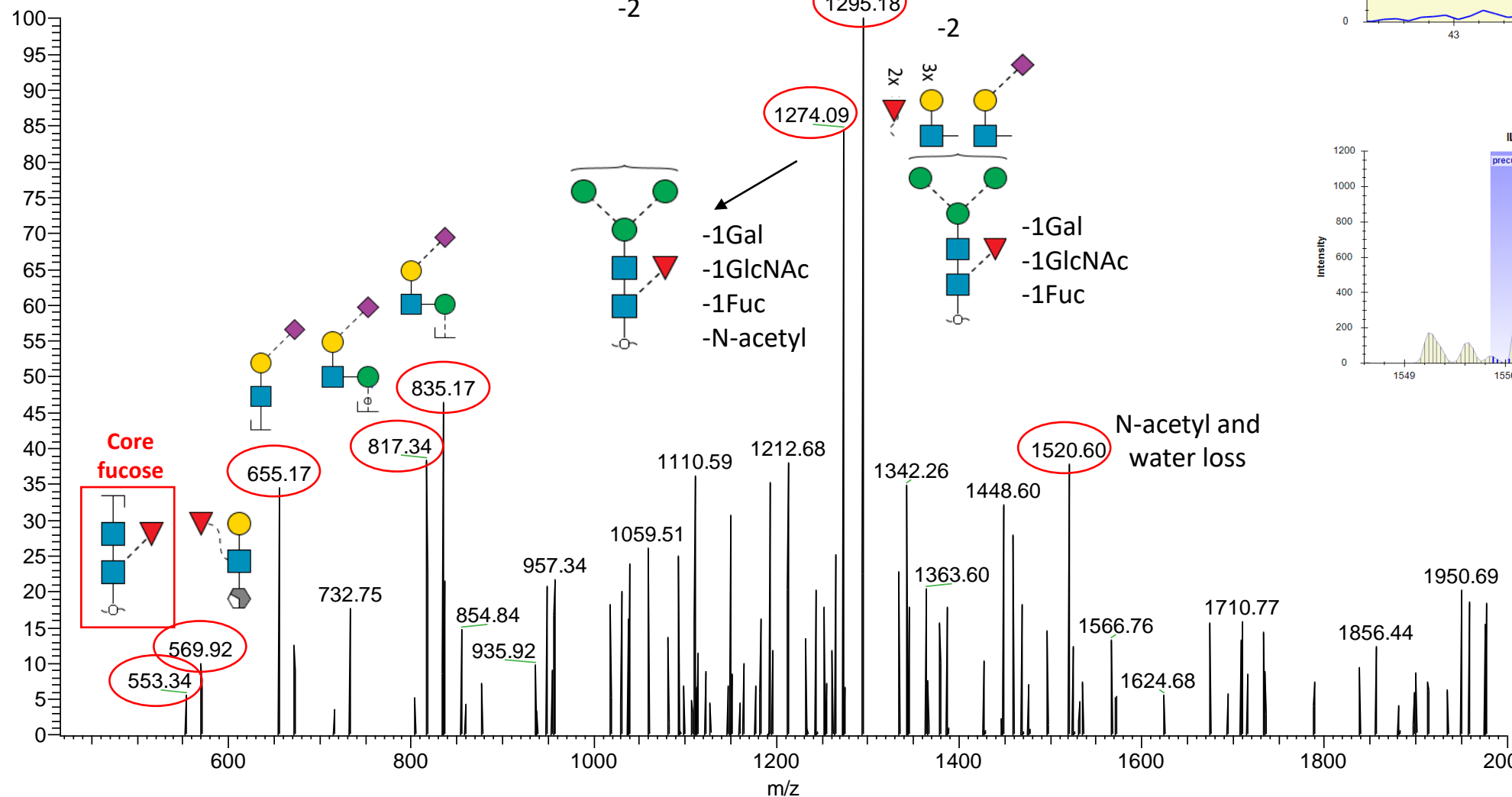
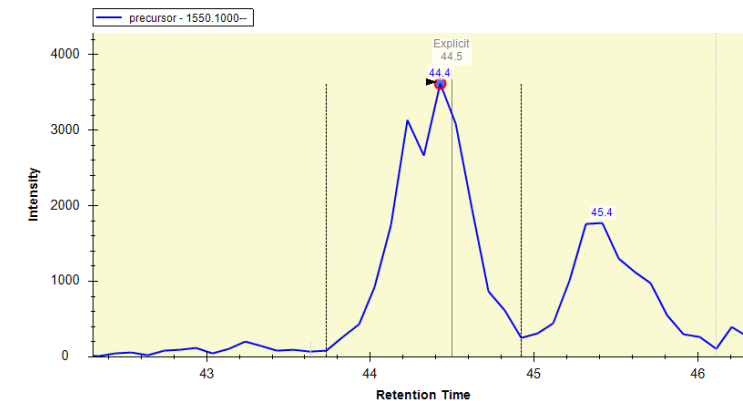
Complex

Hex₄HexNAc₄NeuAc₁Fuc₂+ Hex₃HexNAc₂Fuc₁

m/z: 1550.1⁽²⁻⁾



IL_XB_NG_260717 #4429 RT: 44.51 AV: 1 NL: 1.32E1
F: ITMS -p ESI d Full ms2 1550.17@cid35.00 [415.00-]



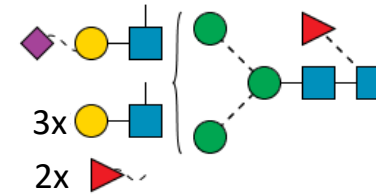
Note: Based on the early PGC-LC elution, this glycan is annotated as the α 2,6-sialyl linkage isomer. Indication of core fucose. Due to the lack of robust fragment ions, this glycan is otherwise annotated without known sialyl linkage isomer information and fucose position.

Glycan #44b

Complex

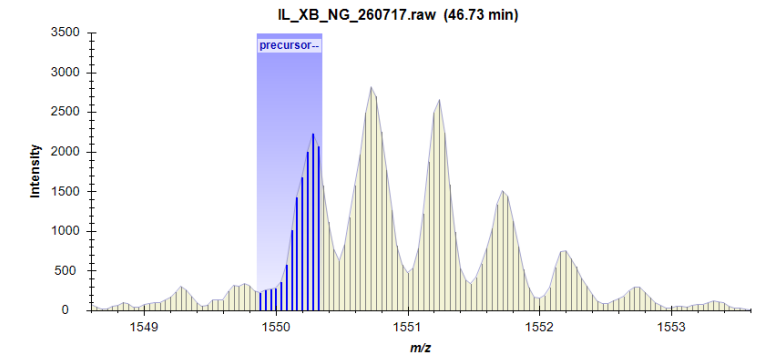
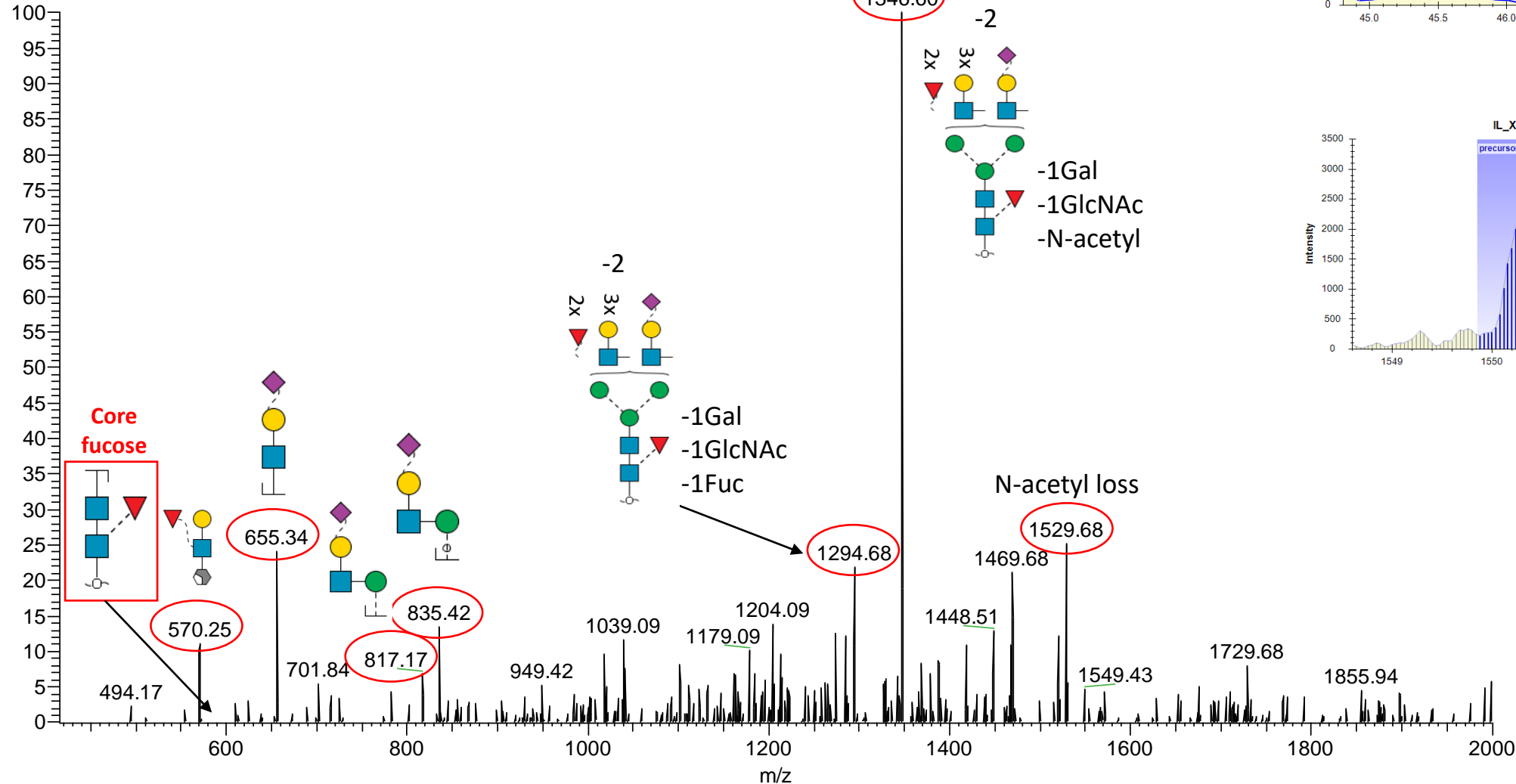
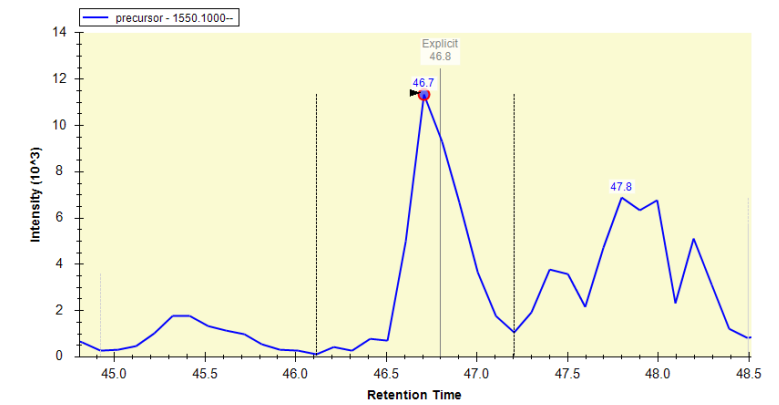
Hex₄HexNAc₄NeuAc₁Fuc₂+ Hex₃HexNAc₂Fuc₁

m/z: 1550.1⁽²⁻⁾



IL_XB_NG_260717 #4652 RT: 46.84 AV: 1 NL: 7.88E1

F: ITMS - p ESI d Full ms2 1550.17@cid35.00 [415.00-;



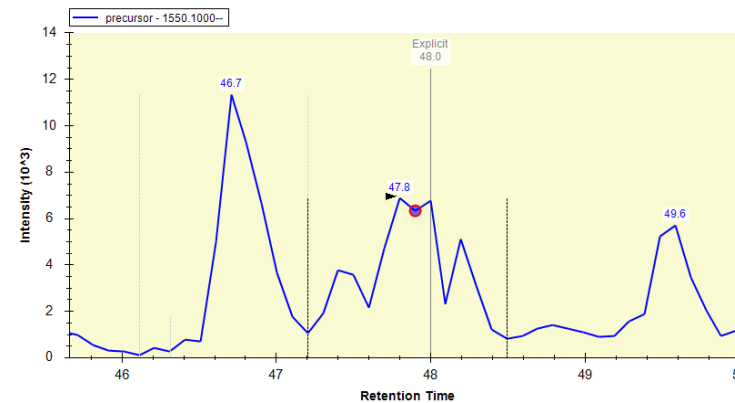
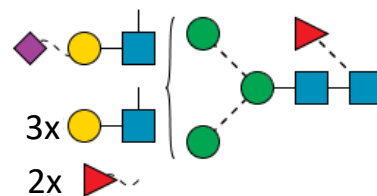
Note: Indication of core fucose. Due to the lack of robust fragment ions, this glycan is otherwise annotated without known sialyl linkage isomer information and fucose position.

Glycan #44c

Complex

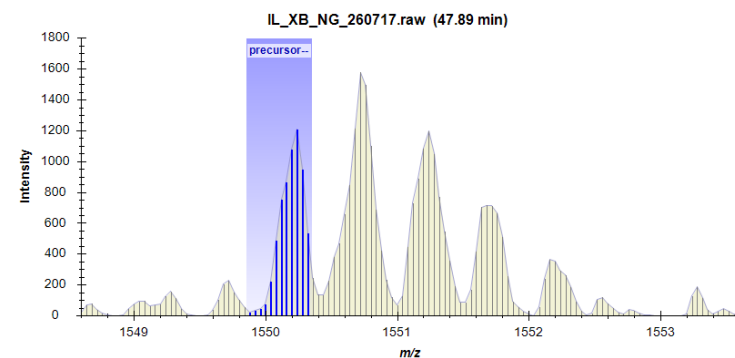
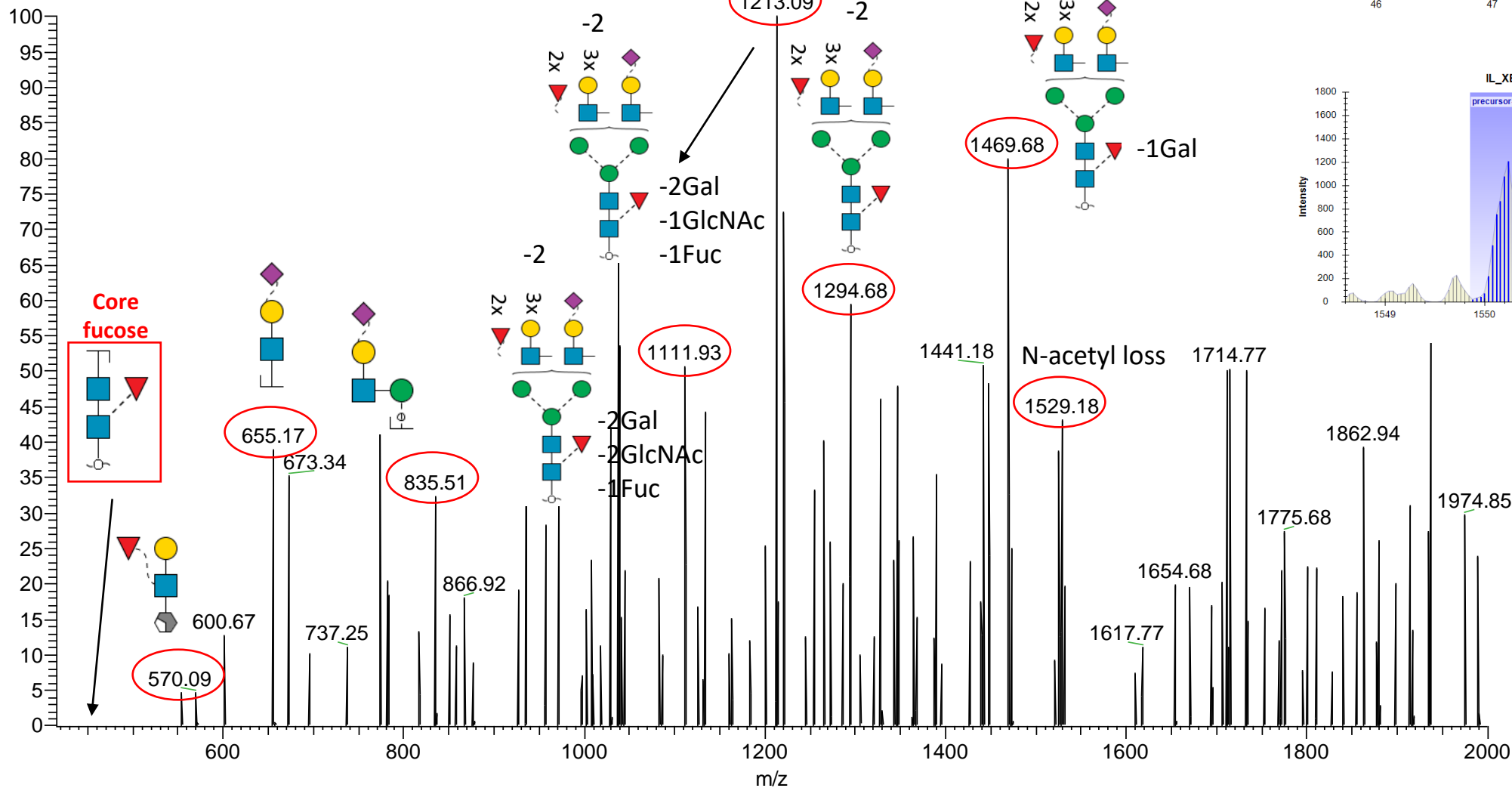
Hex₄HexNAc₄NeuAc₁Fuc₂+ Hex₃HexNAc₂Fuc₁

m/z: 1550.1⁽²⁻⁾



IL_XB_NG_260717 #4769 RT: 48.08 AV: 1 NL: 7.28

F: ITMS - p ESI d Full ms2 1550.17@cid35.00 [415.00-]



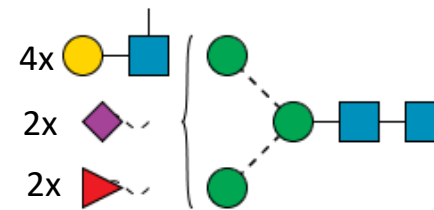
Note: Indication of core fucose. Due to the lack of robust fragment ions, this glycan is otherwise annotated without known sialyl linkage isomer information and fucose position.

Glycan #45

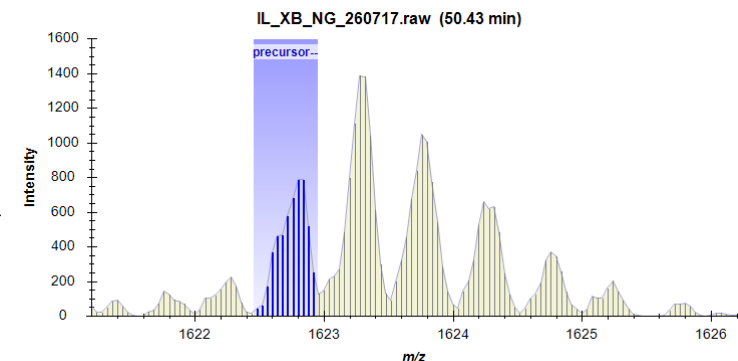
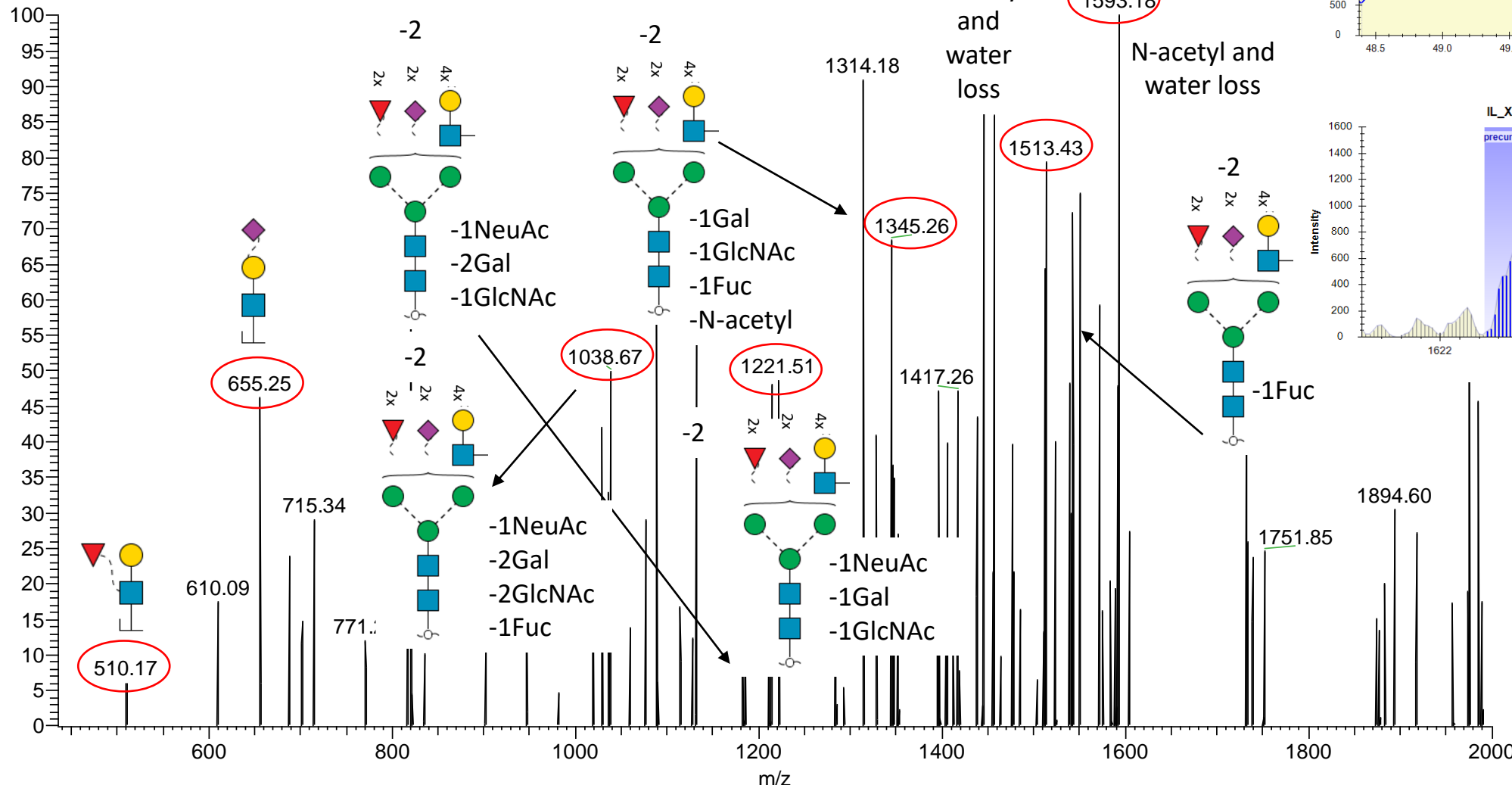
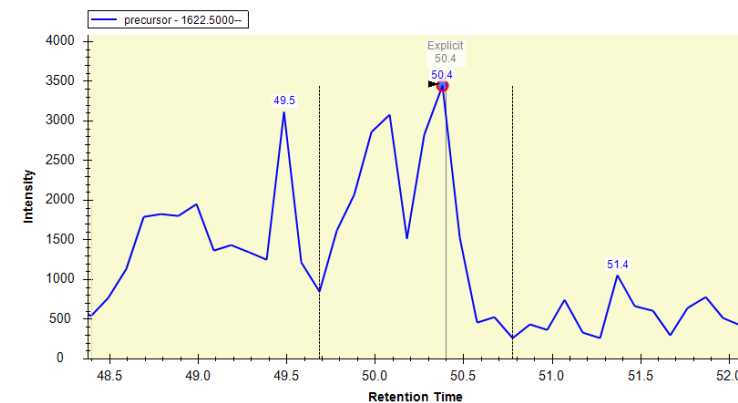
Complex

Hex₄HexNAc₄NeuAc₂Fuc₂ + Hex₃HexNAc₂

m/z: 1622.7⁽²⁻⁾



IL_XB_NG_260717 #4995 RT: 50.47 AV: 1 NL: 5.97
F: ITMS - p ESI d Full ms2 1622.79@cid35.00 [435.00-;



Note: Due to the lack of robust fragment ions, this glycan is otherwise annotated without known sialyl linkage isomer information and fucose position.

Glycan #46a

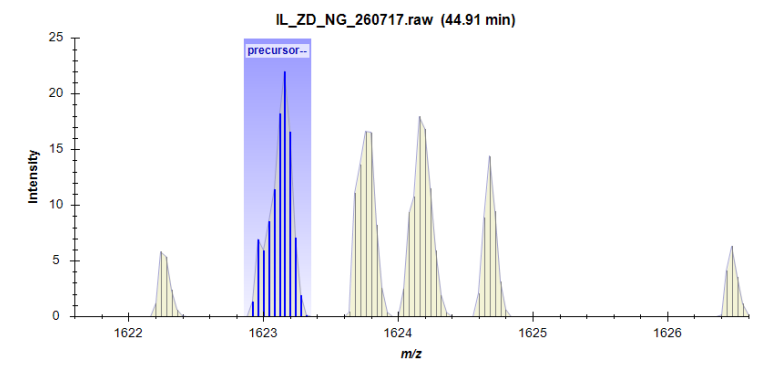
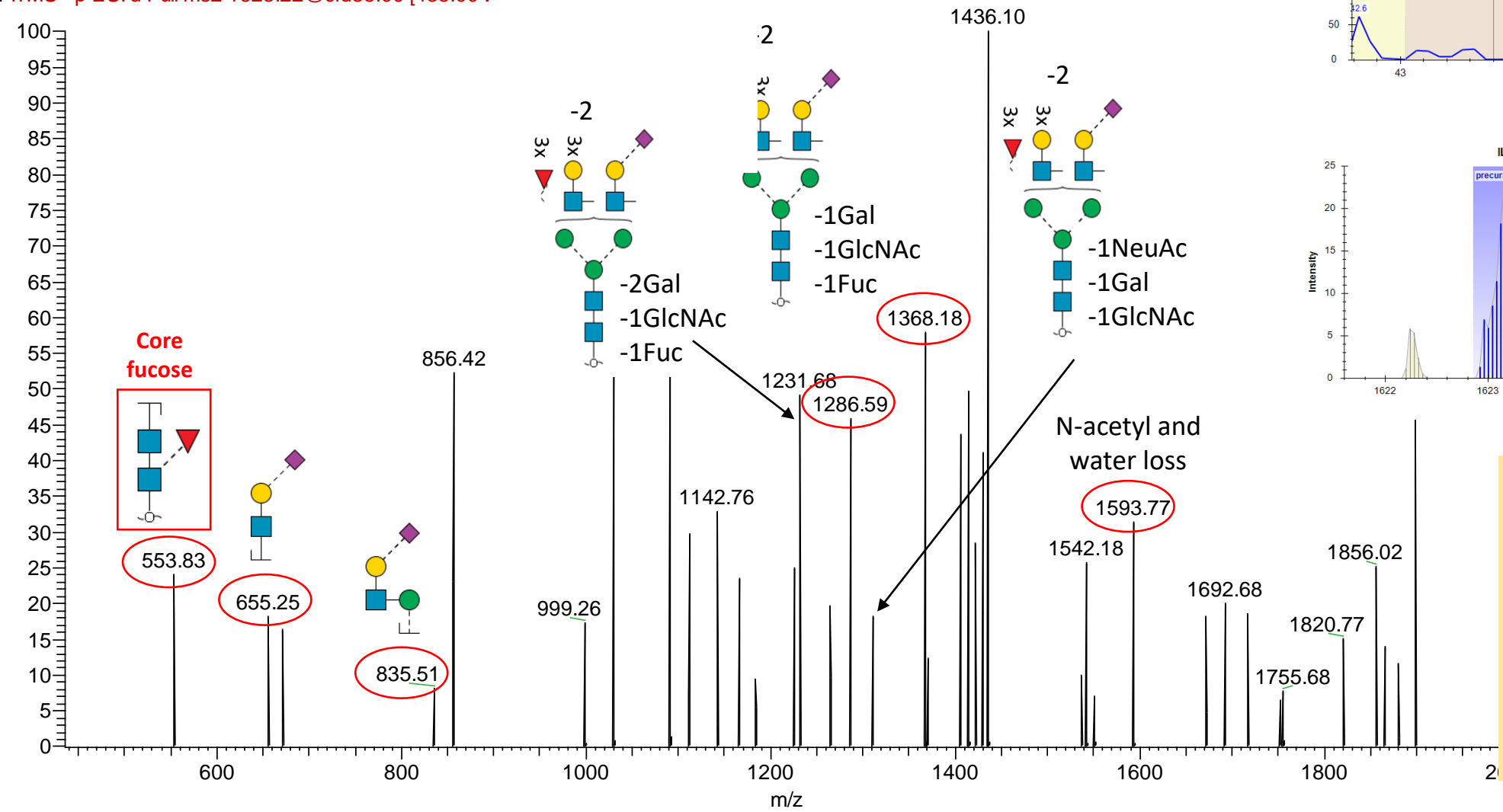
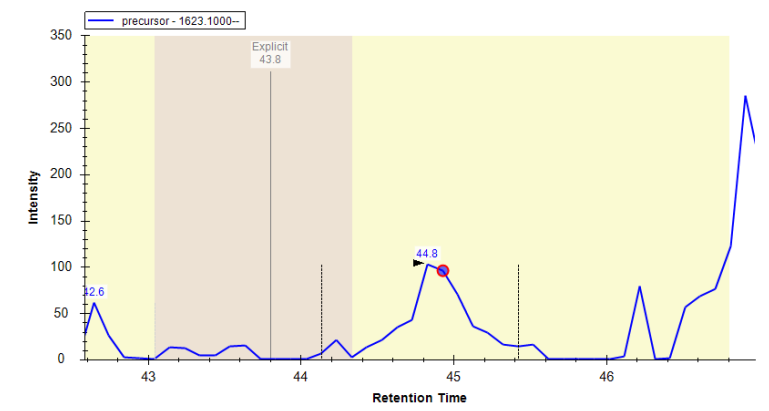
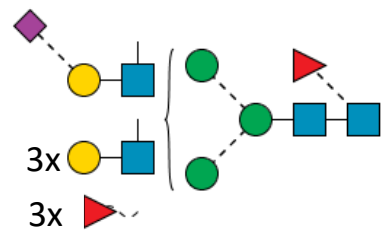
Complex

Hex₄HexNAc₄NeuAc₁Fuc₃ + Hex₃HexNAc₂Fuc₁

m/z: 1623.1 (2-)

IL_ZB_NG_260717 #4390 RT: 44.02 AV: 1 NL: 5.78

F: ITMS - p ESI d Full ms2 1623.22@cid35.00 [435.00-]



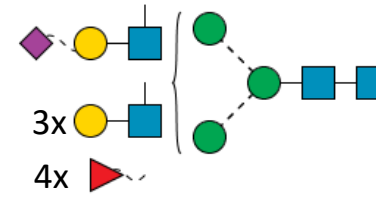
Note: Based on the early PGC-LC elution, this glycan is annotated as the α 2,6-sialyl linkage isomer. Due to the lack of robust fragment ions, this glycan is otherwise annotated without known sialyl linkage isomer information and fucose position.

Glycan #46b

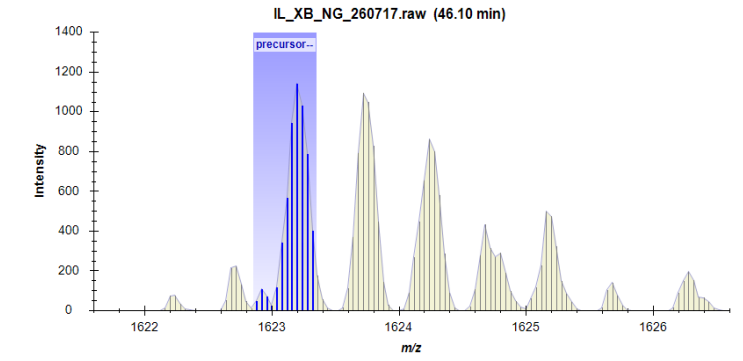
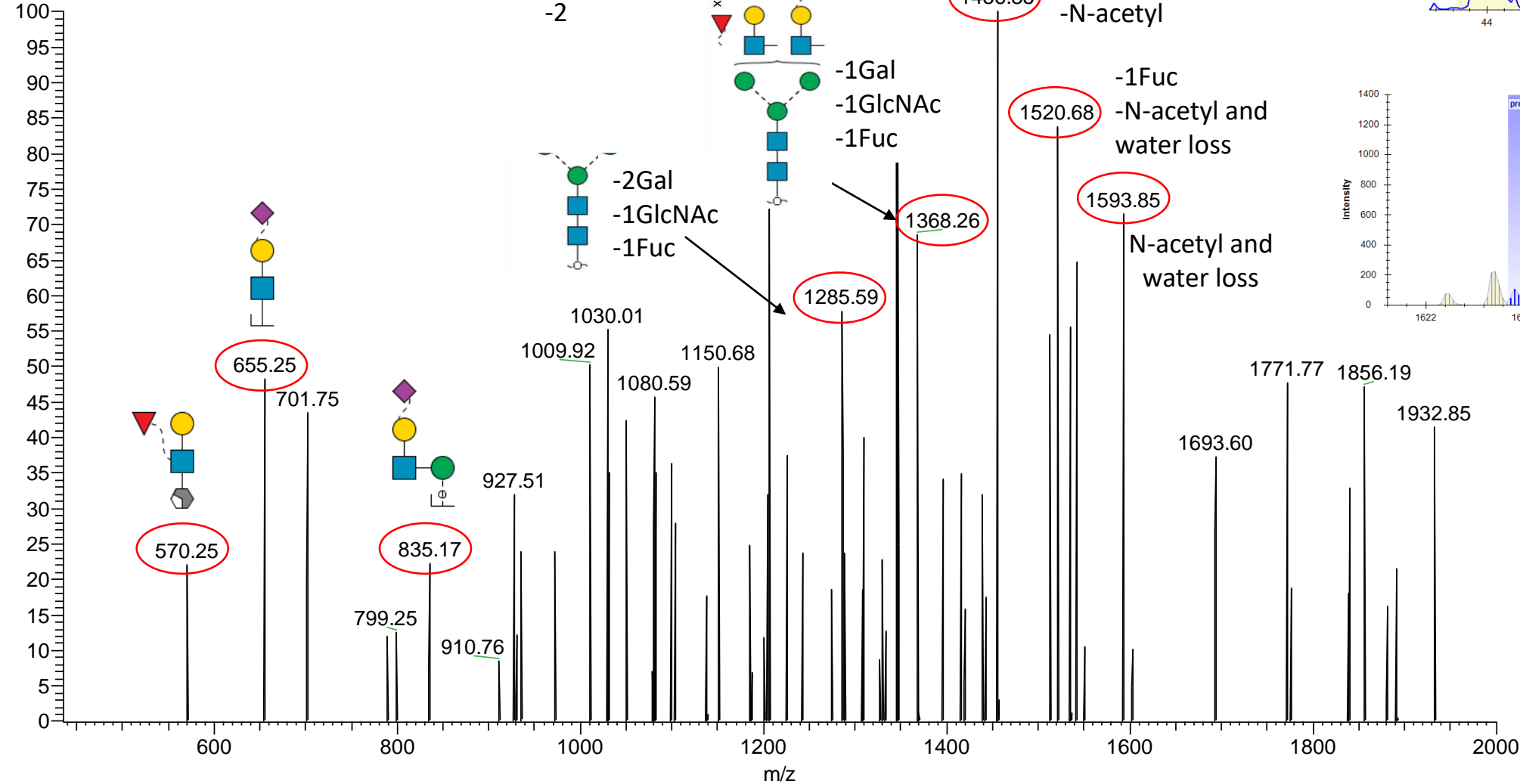
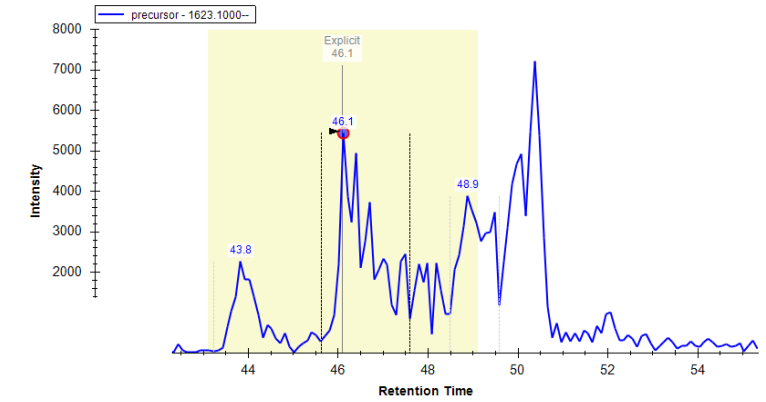
Complex

Hex₄HexNAc₄NeuAc₁Fuc₄ + Hex₃HexNAc₂

m/z: 1623.1 (2-)



IL_XB_NG_260717 #4626 RT: 46.57 AV: 1 NL: 4.21
F: ITMS - p ESI d Full ms2 1623.23@cid35.00 [435.00-;



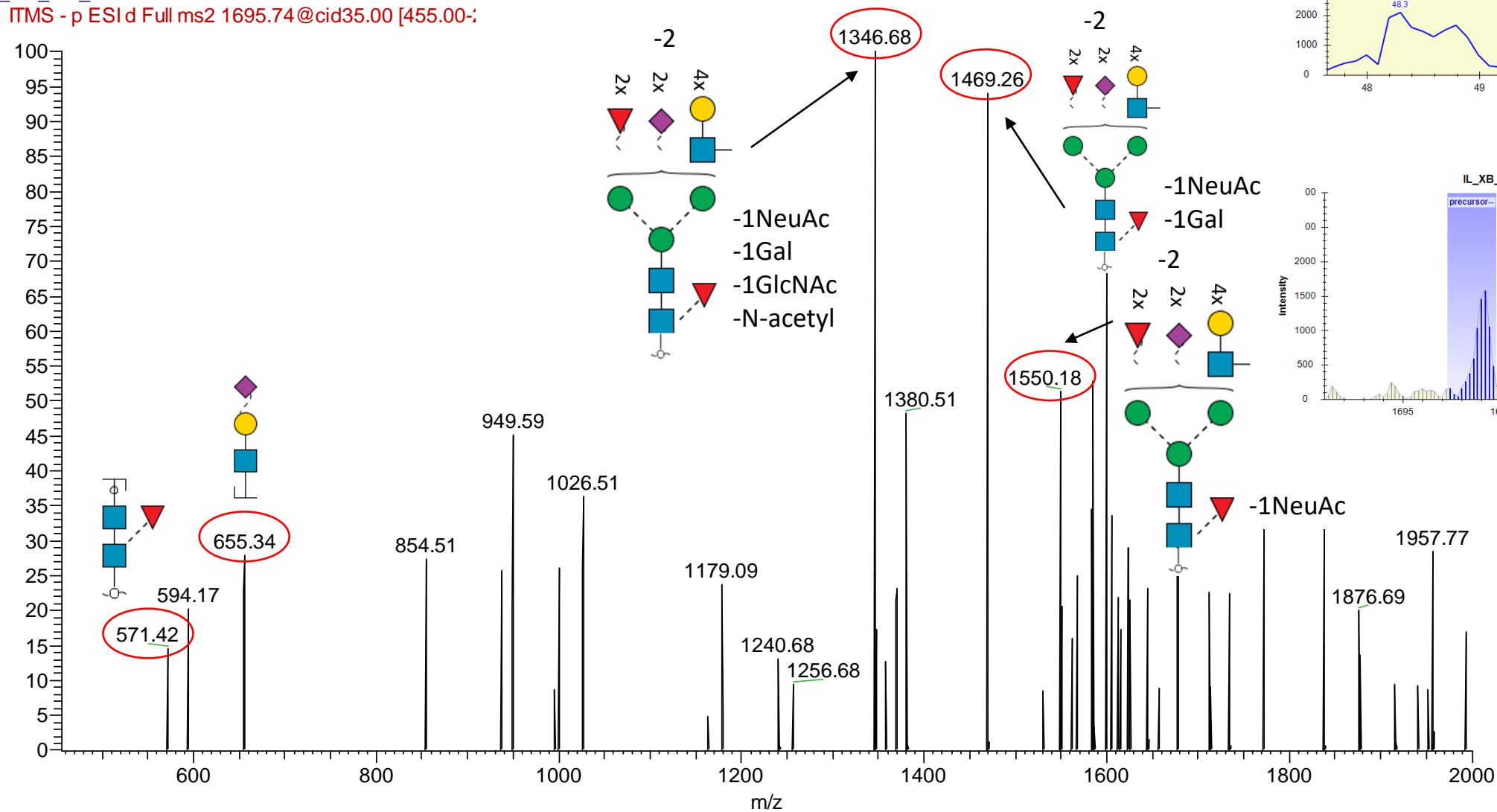
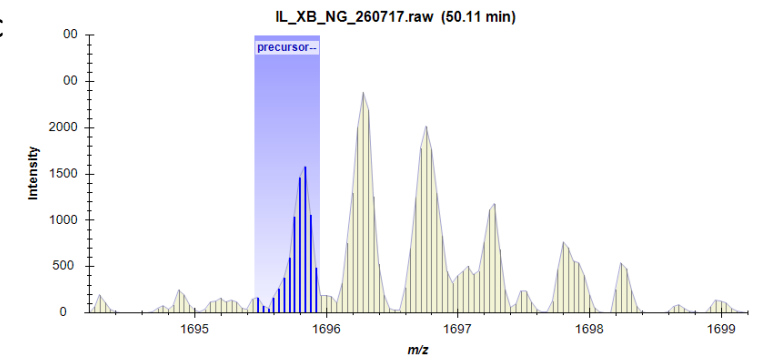
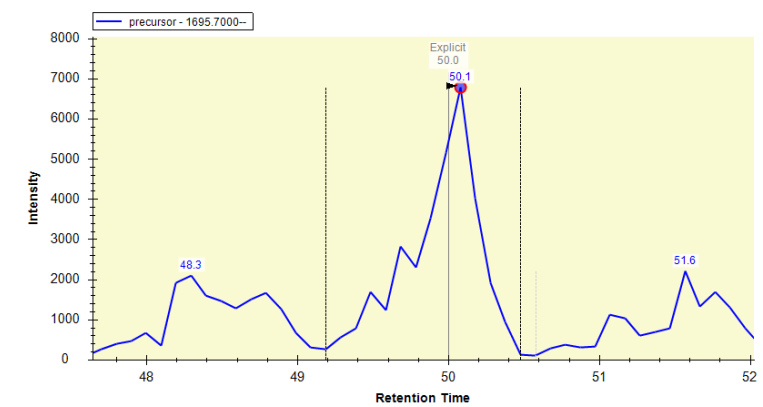
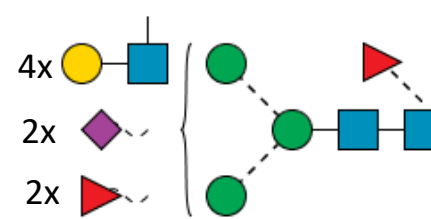
Note: Due to the lack of robust fragment ions, this glycan is annotated without known sialyl linkage isomer information and fucose position.

Glycan #47

Complex

Hex₄HexNAc₄NeuAc₂Fuc₃ + Hex₃HexNAc₂

m/z: 1695.7 (2-)



Note: Indication of core fucosylation. Due to the lack of robust fragment ions, this glycan is otherwise annotated without known sialyl linkage isomer information and fucose position.