

# Supplementary Information 1

## N-Glycomics – Structural Elucidation

### Integrated N- and O-Glycomics of Acute Myeloid Leukemia (AML) Cell Lines

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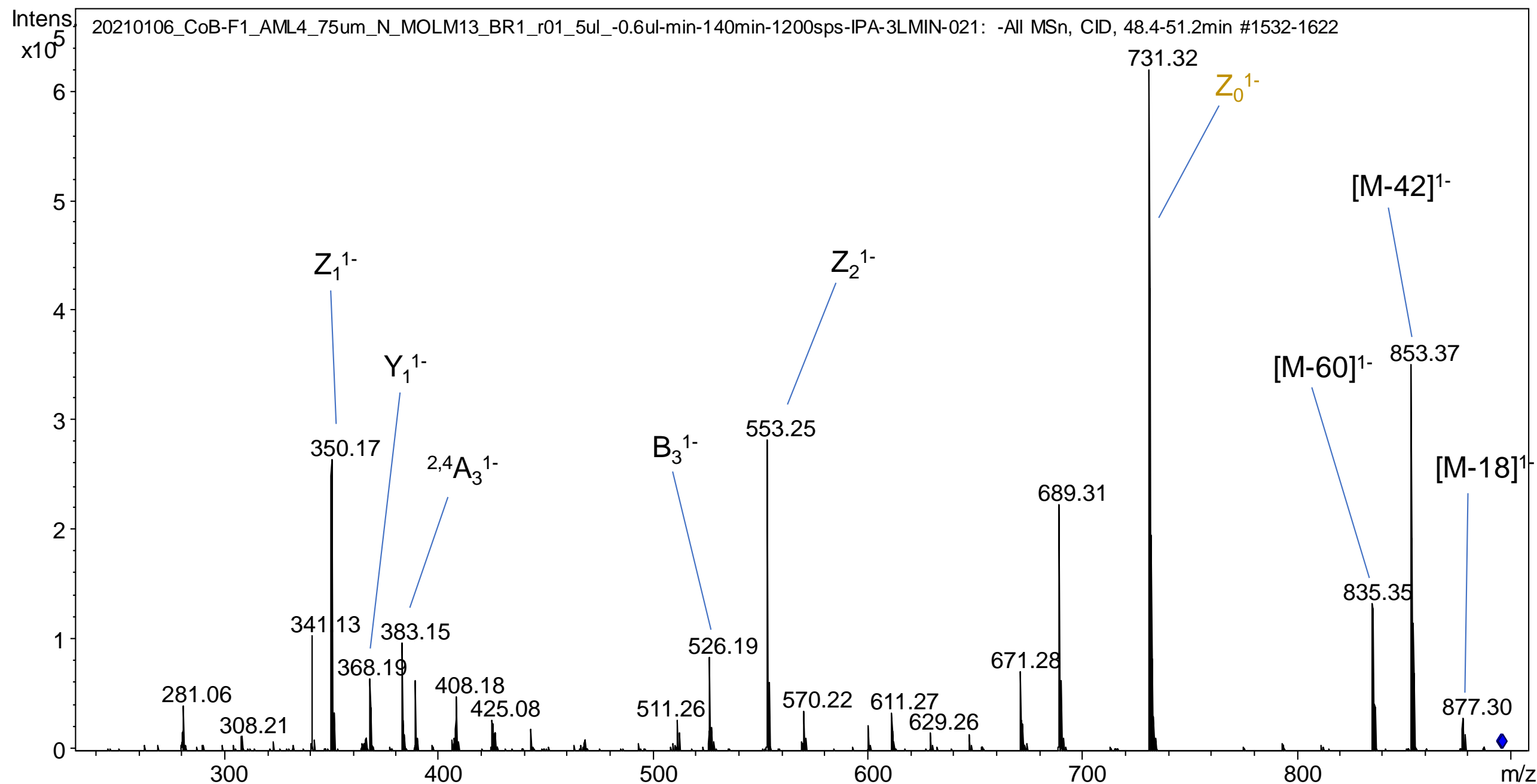
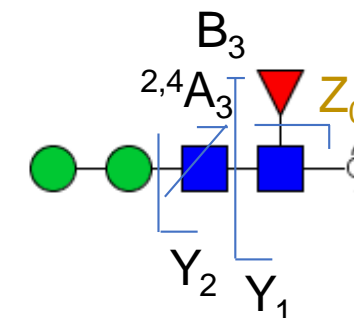
# Glycan 1

H2N2F1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 896.35 Da  
Charge observed: 1-  
Theoretical ion: *m/z* 895.34  
Observed ion: *m/z* 895.38  
Mass deviation: *m/z* 0.04  
Retention time: 49.0 min

UniCarb-DB: #2223



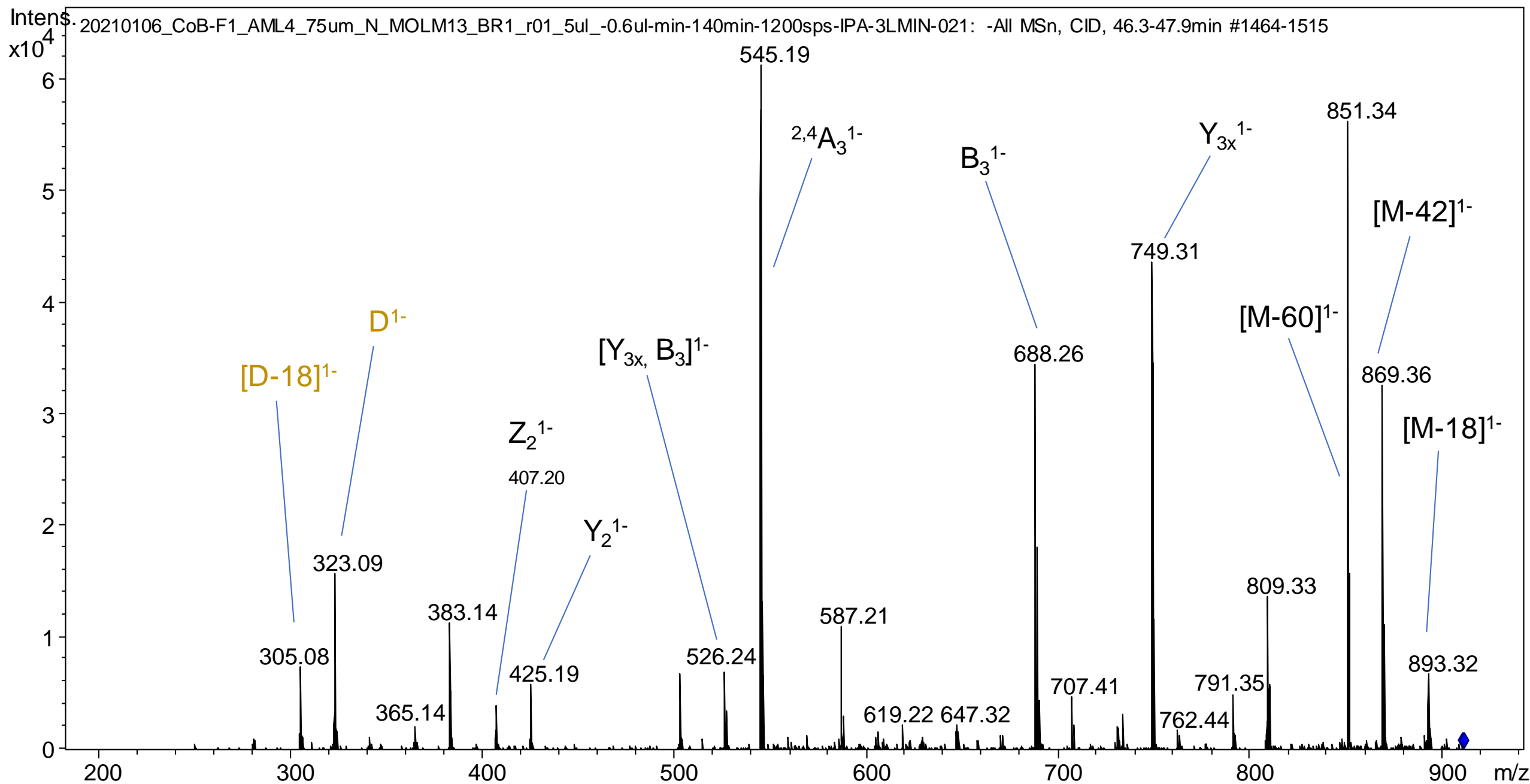
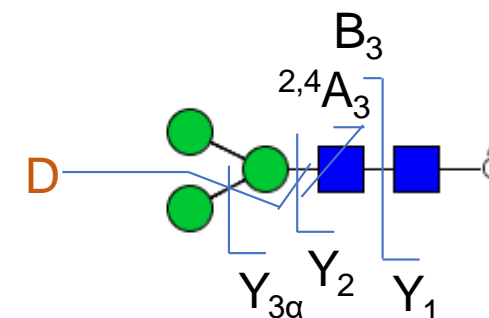
# Glycan 2

## H3N2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 912.35 Da  
Charge observed: 1-  
Theoretical ion: *m/z* 911.34  
Observed ion: *m/z* 911.36  
Mass deviation: *m/z* 0.02  
Retention time: 47.1 min

UniCarb-DB: #610



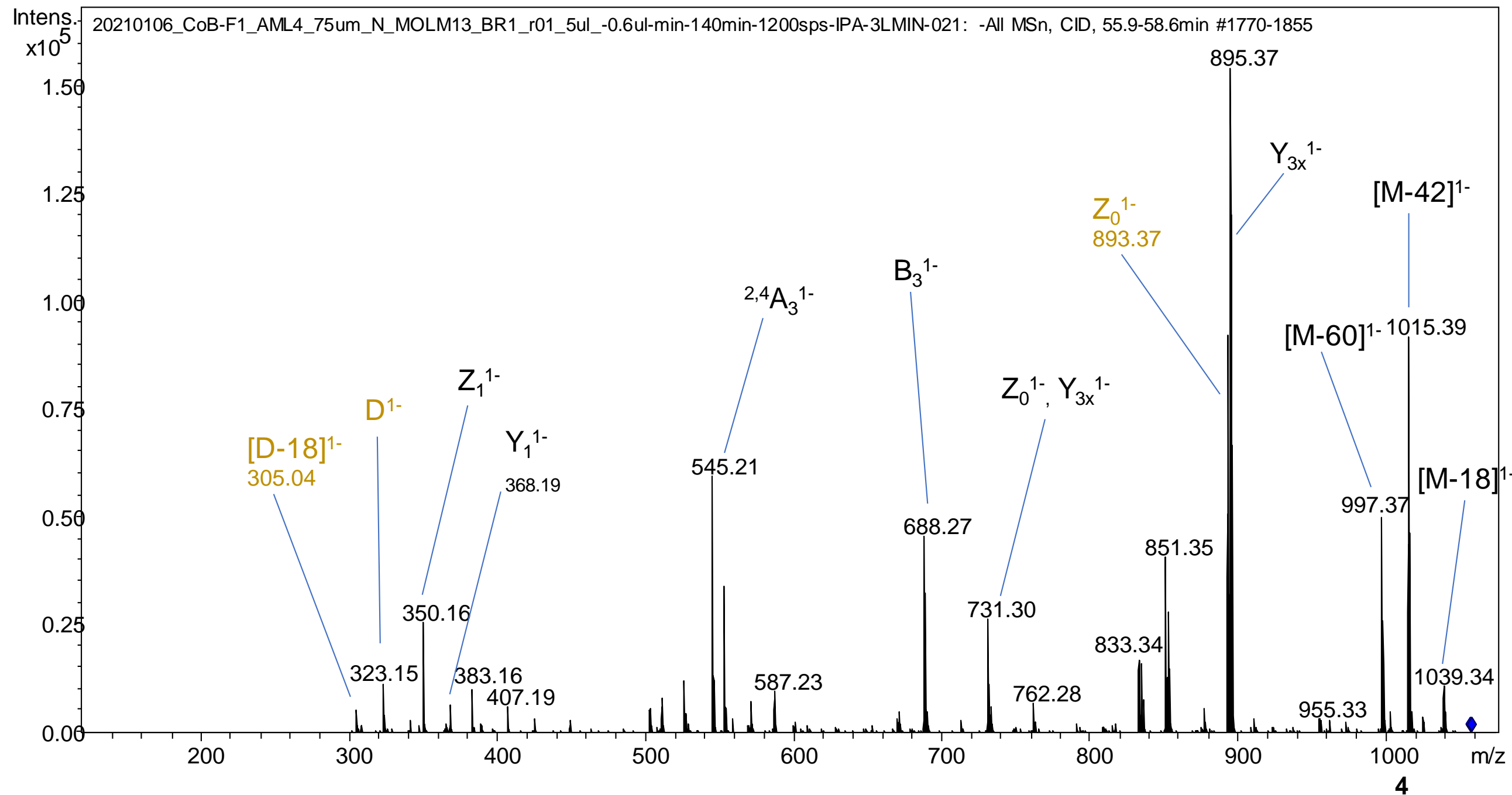
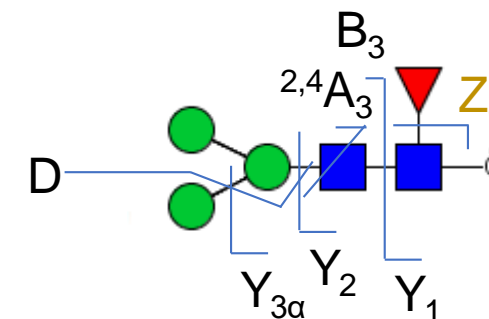
# Glycan 3

H3N2F1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 1058.40 Da  
Charge observed: 1-  
Theoretical ion: *m/z* 1057.39  
Observed ion: *m/z* 1057.40  
Mass deviation: *m/z* 0.01  
Retention time: 56.4 min

UniCarb-DB: #441

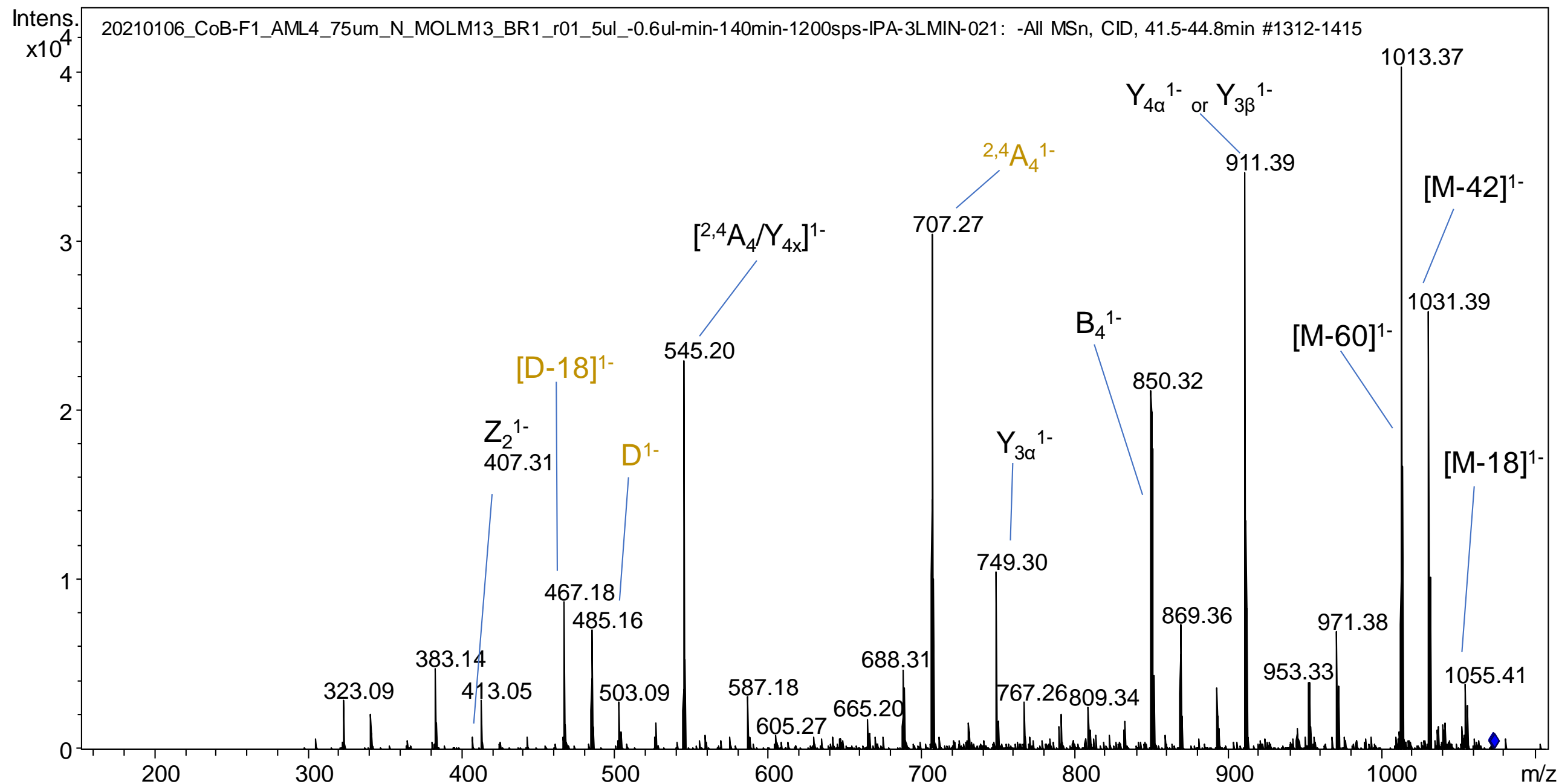
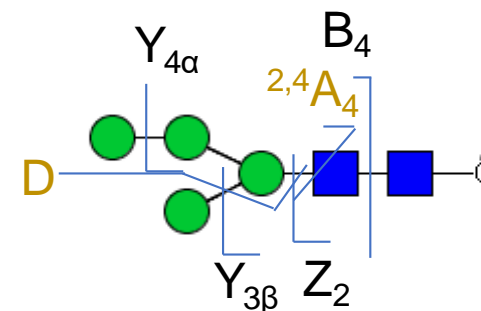


# Glycan 4

H4N2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 1074.40 Da  
Charge observed: 1-  
Theoretical ion: *m/z* 1073.39  
Observed ion: *m/z* 1073.39  
Mass deviation: *m/z* 0.00  
Retention time: 43.3 min

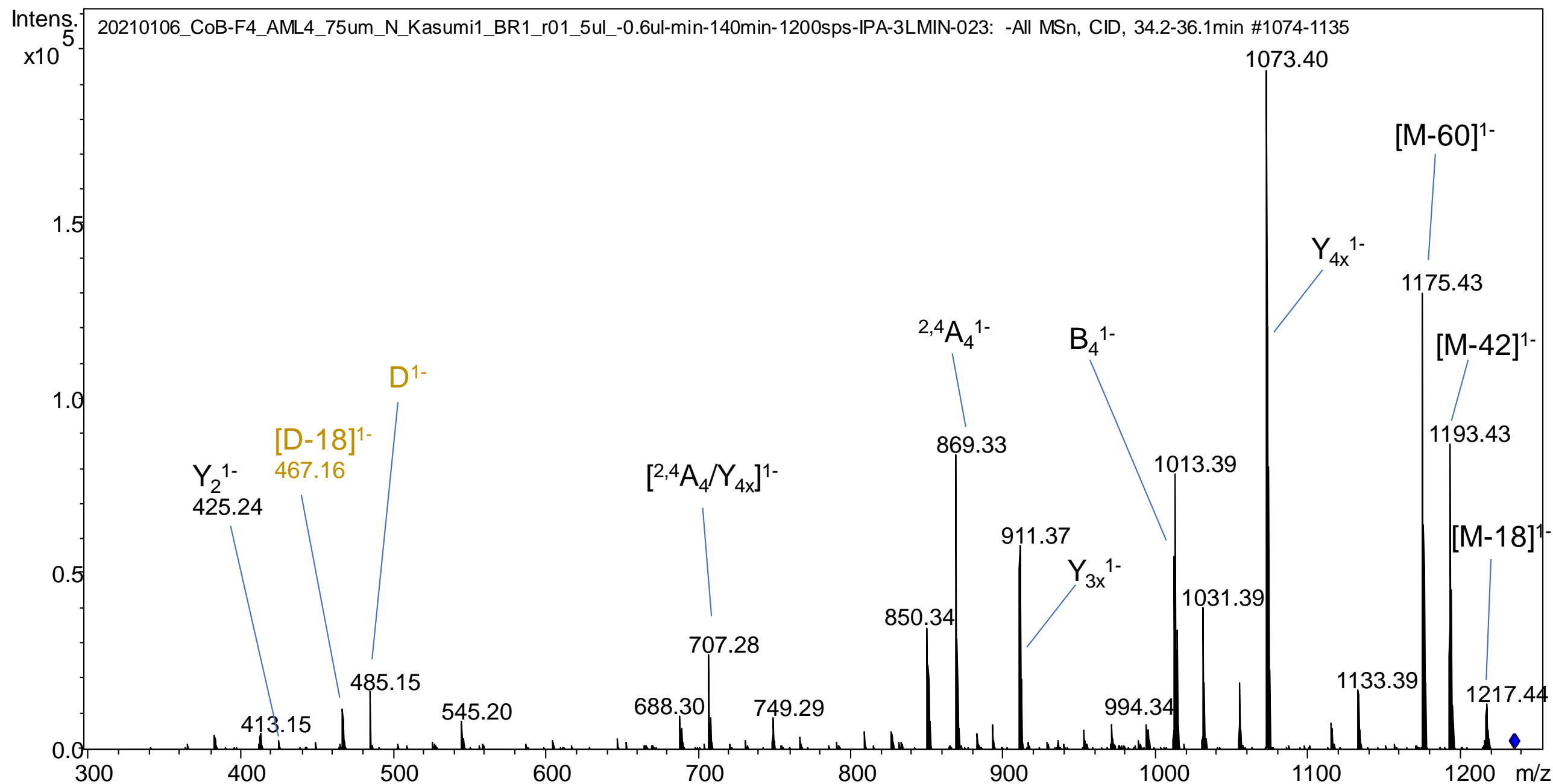
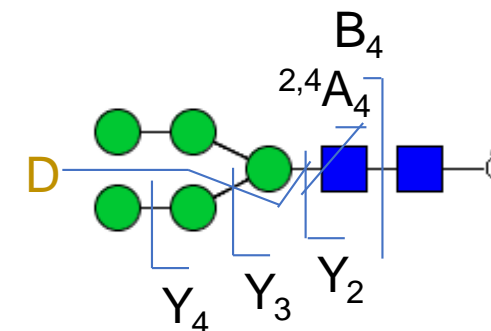


# H5N2

**Depicted MS<sup>2</sup> was obtained from analysis of cell line: Kasumi-1**

<b>Monoisotopic mass:</b>	<b>1236.45 Da</b>
<b>Charge observed:</b>	<b>1-</b>
<b>Theoretical ion:</b>	<b><i>m/z</i> 1235.44</b>
<b>Observed ion:</b>	<b><i>m/z</i> 1235.47</b>
<b>Mass deviation:</b>	<b><i>m/z</i> 0.03</b>
<b>Retention time:</b>	<b>34.7 min</b>

**UniCarb-DB: #2213**



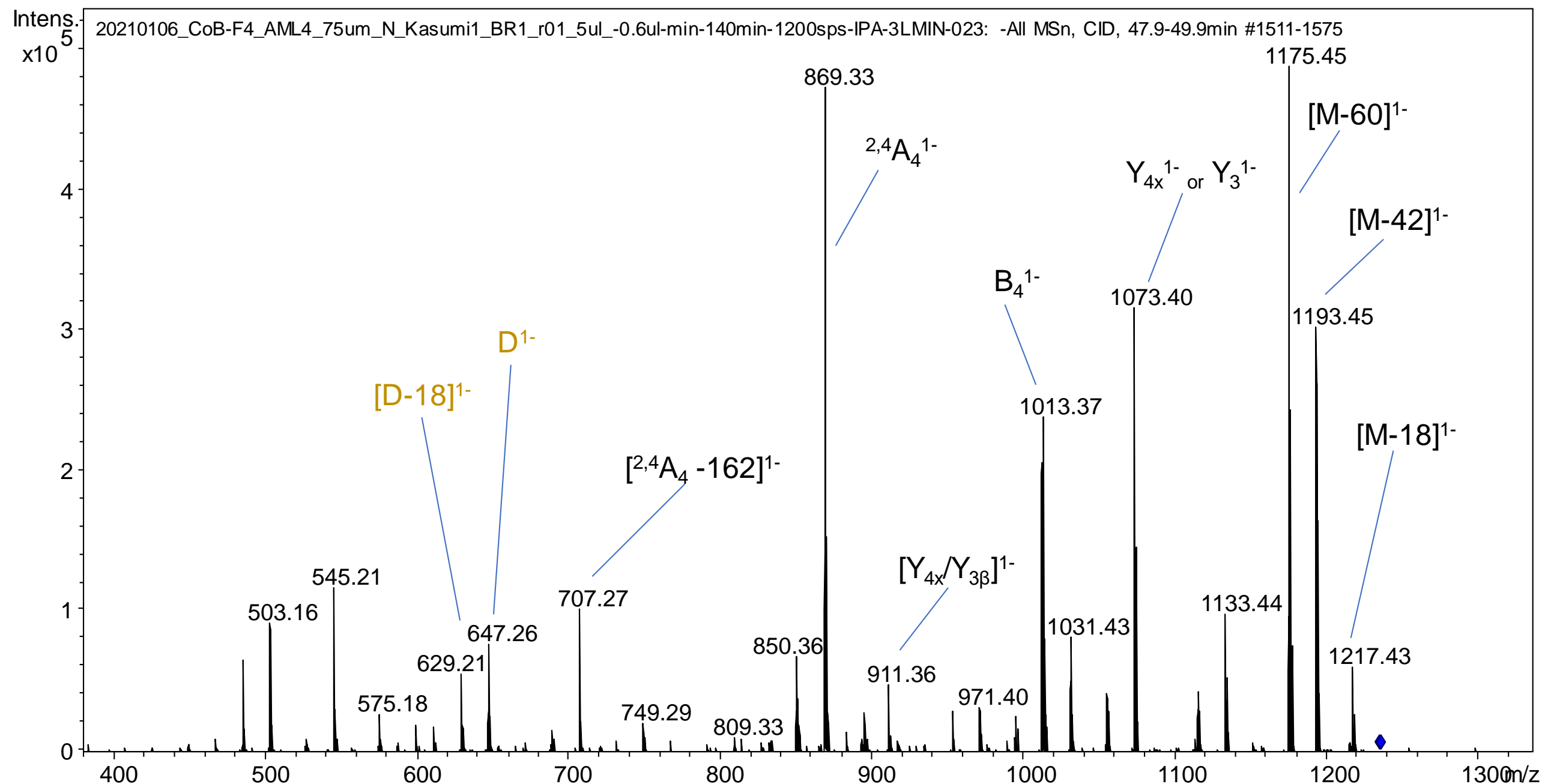
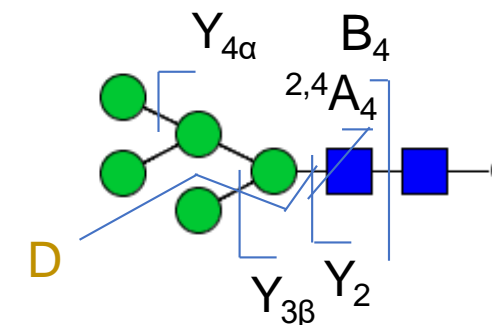
# Glycan 5b

## H5N2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: Kasumi-1

Monoisotopic mass: 1236.45 Da  
Charge observed: 1-  
Theoretical ion: *m/z* 1235.44  
Observed ion: *m/z* 1235.46  
Mass deviation: *m/z* 0.02  
Retention time: 48.4 min

UniCarb-DB: #395



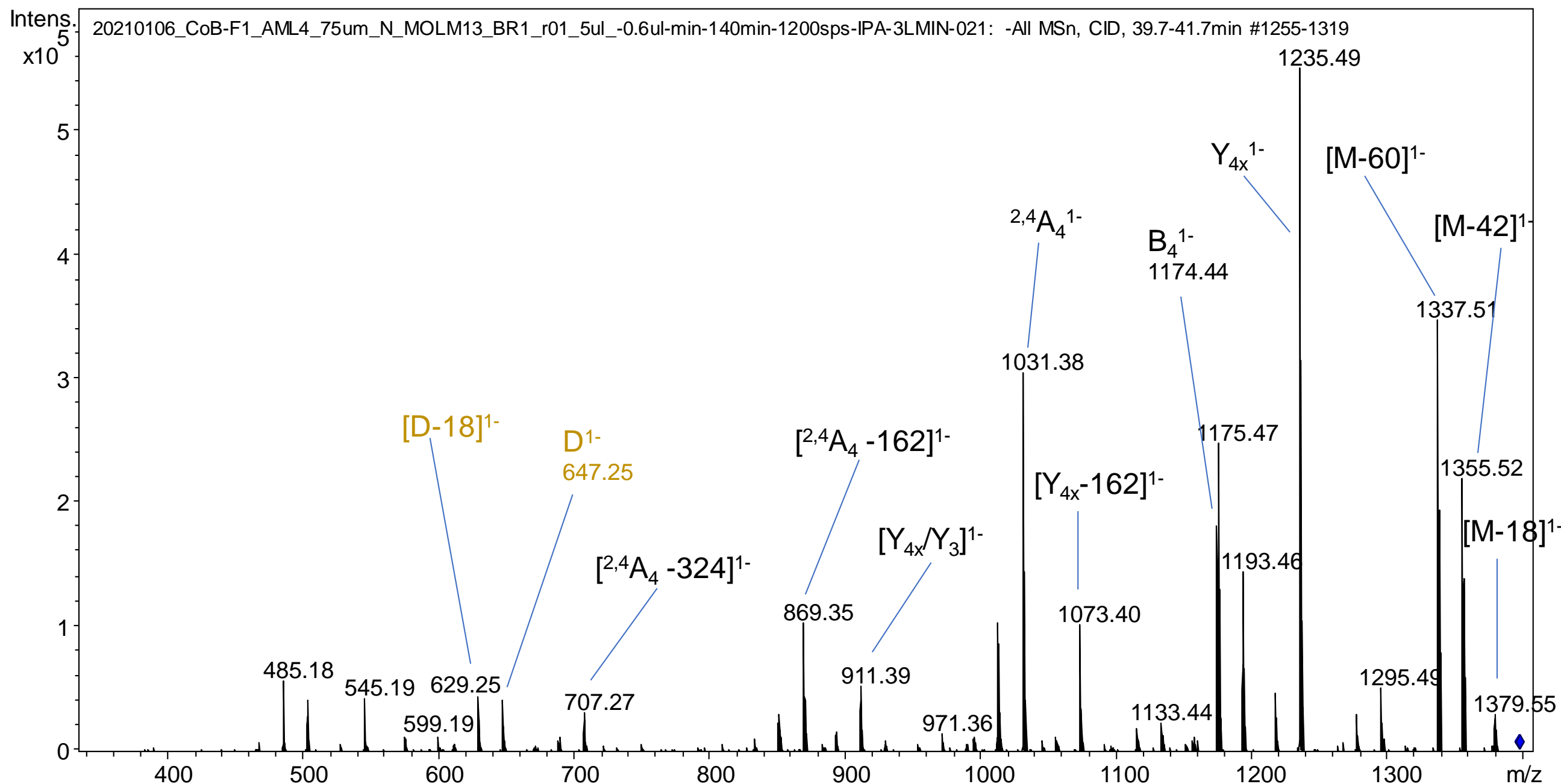
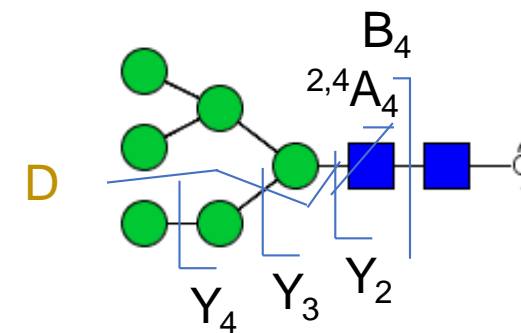
# Glycan 6

## H6N2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 1398.51 Da  
Charge observed: 1-  
Theoretical ion: *m/z* 1397.50  
Observed ion: *m/z* 1397.54  
Mass deviation: *m/z* 0.04  
Retention time: 39.9 min

UniCarb-DB: #613





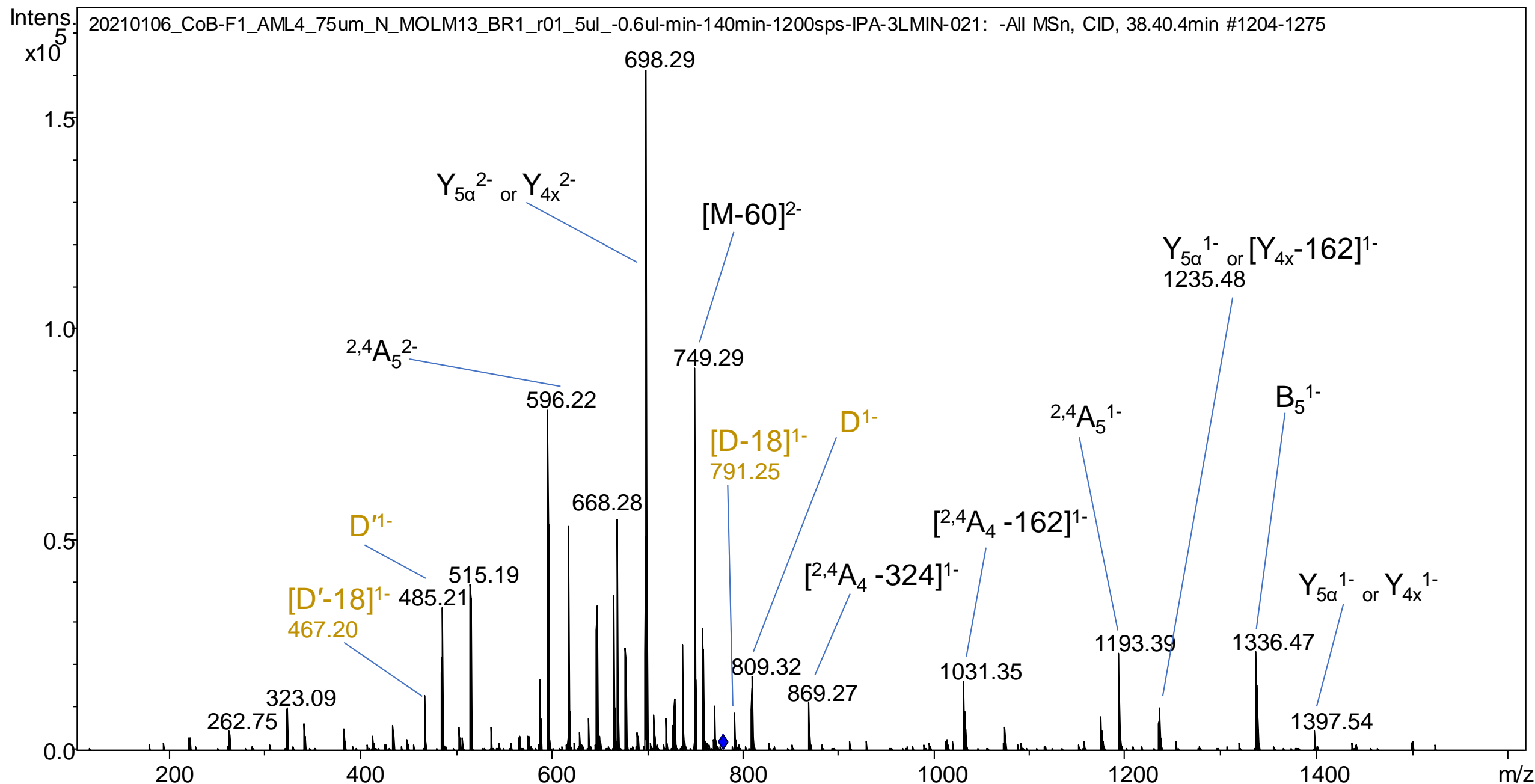
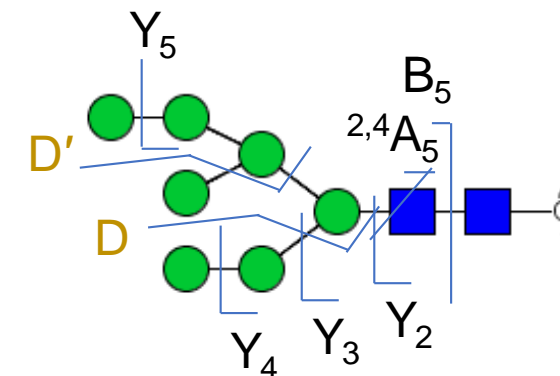
# Glycan 7

## H7N2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 1560.55 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 779.27  
Observed ion: *m/z* 779.31  
Mass deviation: *m/z* 0.04  
Retention time: 38.4 min

UniCarb-DB: #403



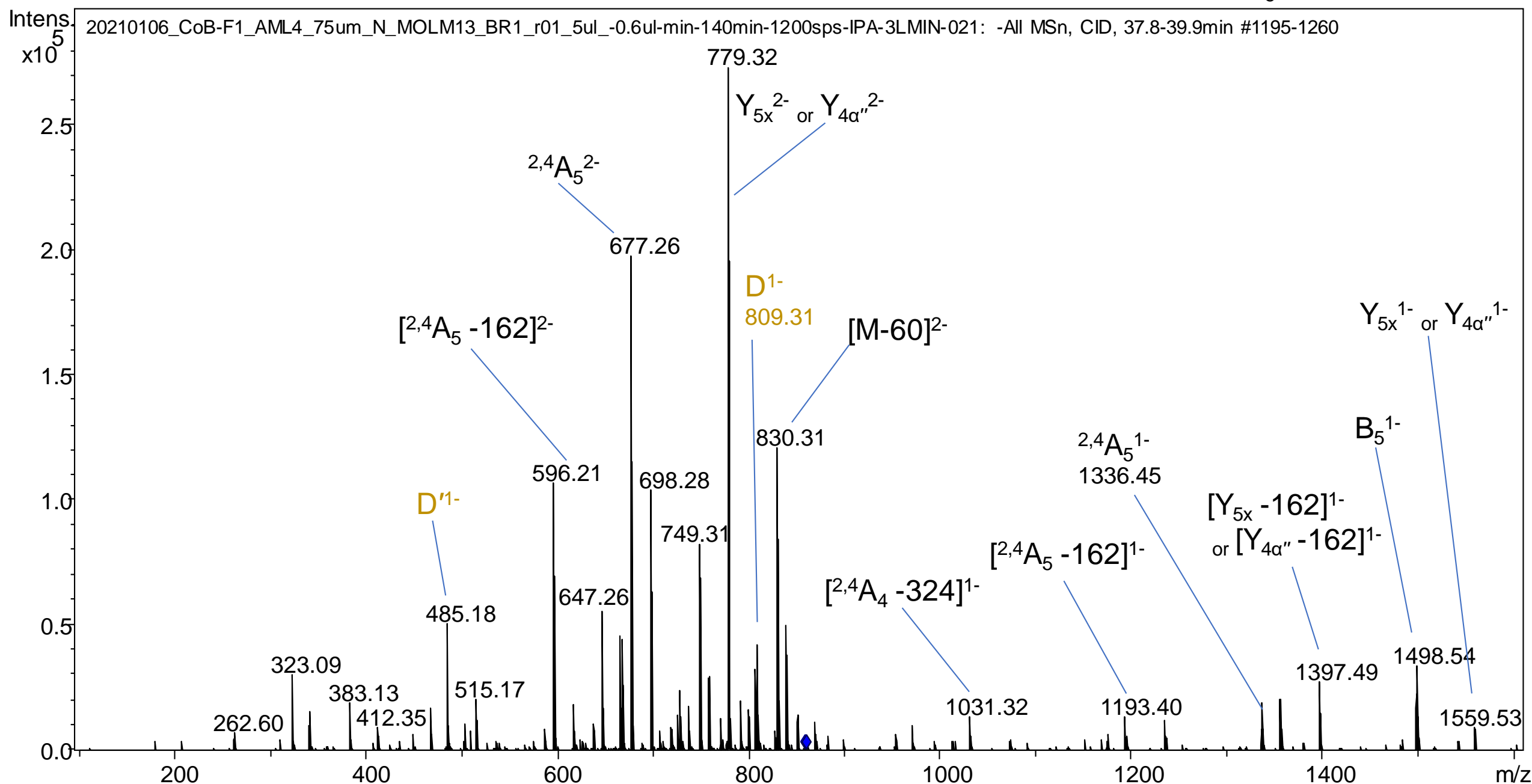
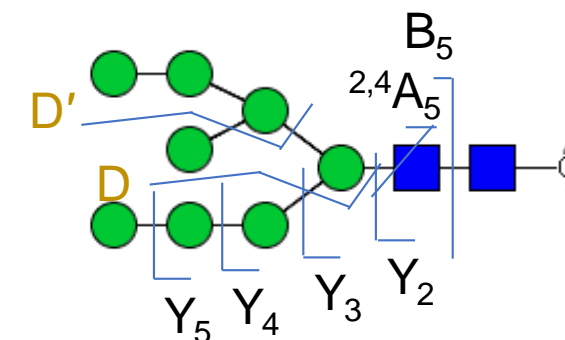
# Glycan 8

## H8N2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 1722.61 Da  
Charge observed: 2-  
Theoretical ion:  $m/z$  860.30  
Observed ion:  $m/z$  860.34  
Mass deviation:  $m/z$  0.04  
Retention time: 38.4 min

UniCarb-DB: #2296



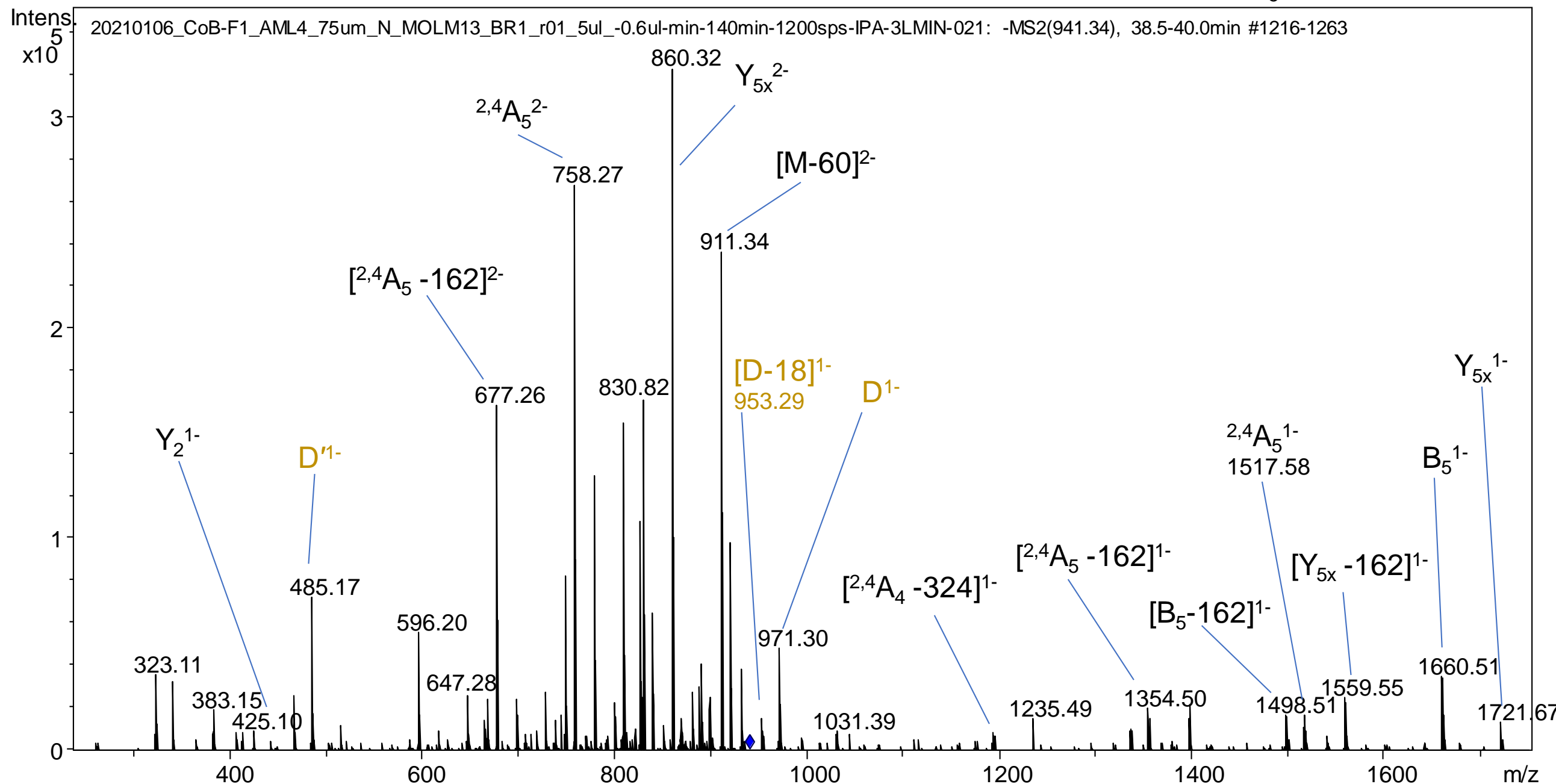
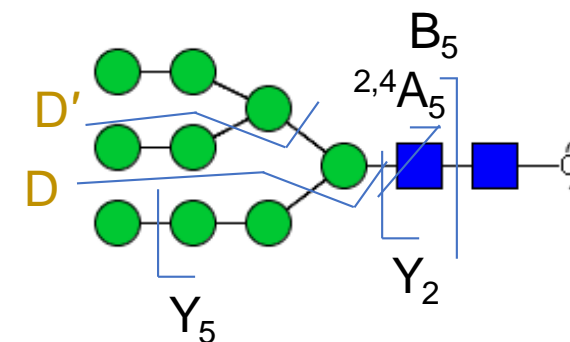
# Glycan 9

## H9N2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 1884.66 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 941.32  
Observed ion: *m/z* 941.34  
Mass deviation: *m/z* 0.02  
Retention time: 38.8 min

UniCarb-DB: #429

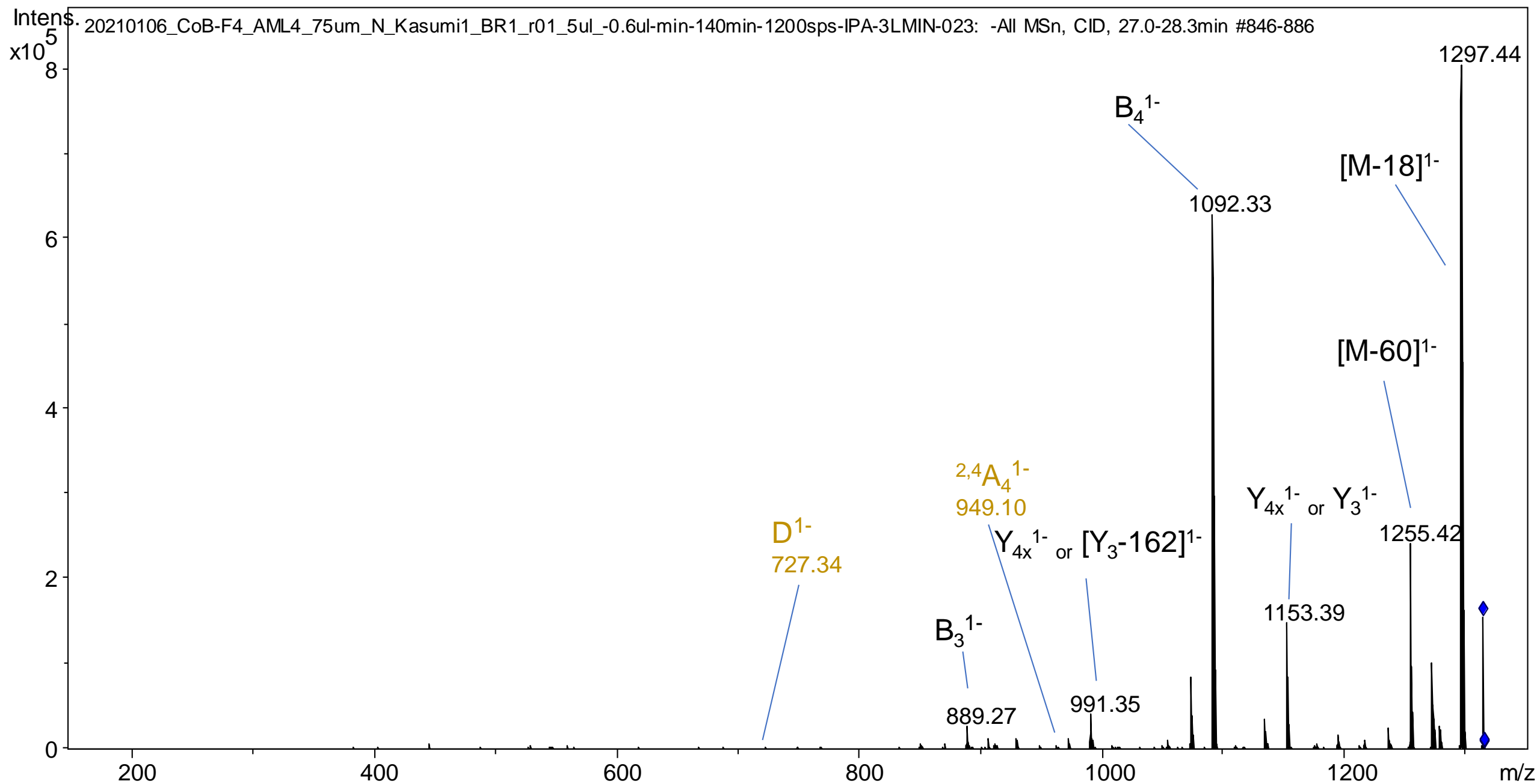
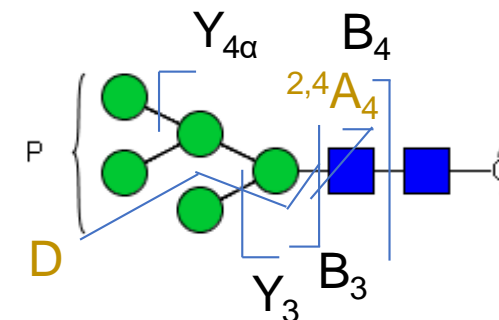


# Glycan 10a

H5N2P1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: Kasumi-1

Monoisotopic mass: 1316.42 Da  
Charge observed: 1-  
Theoretical ion: *m/z* 1315.41  
Observed ion: *m/z* 1315.42  
Mass deviation: *m/z* 0.01  
Retention time: 27.2 min

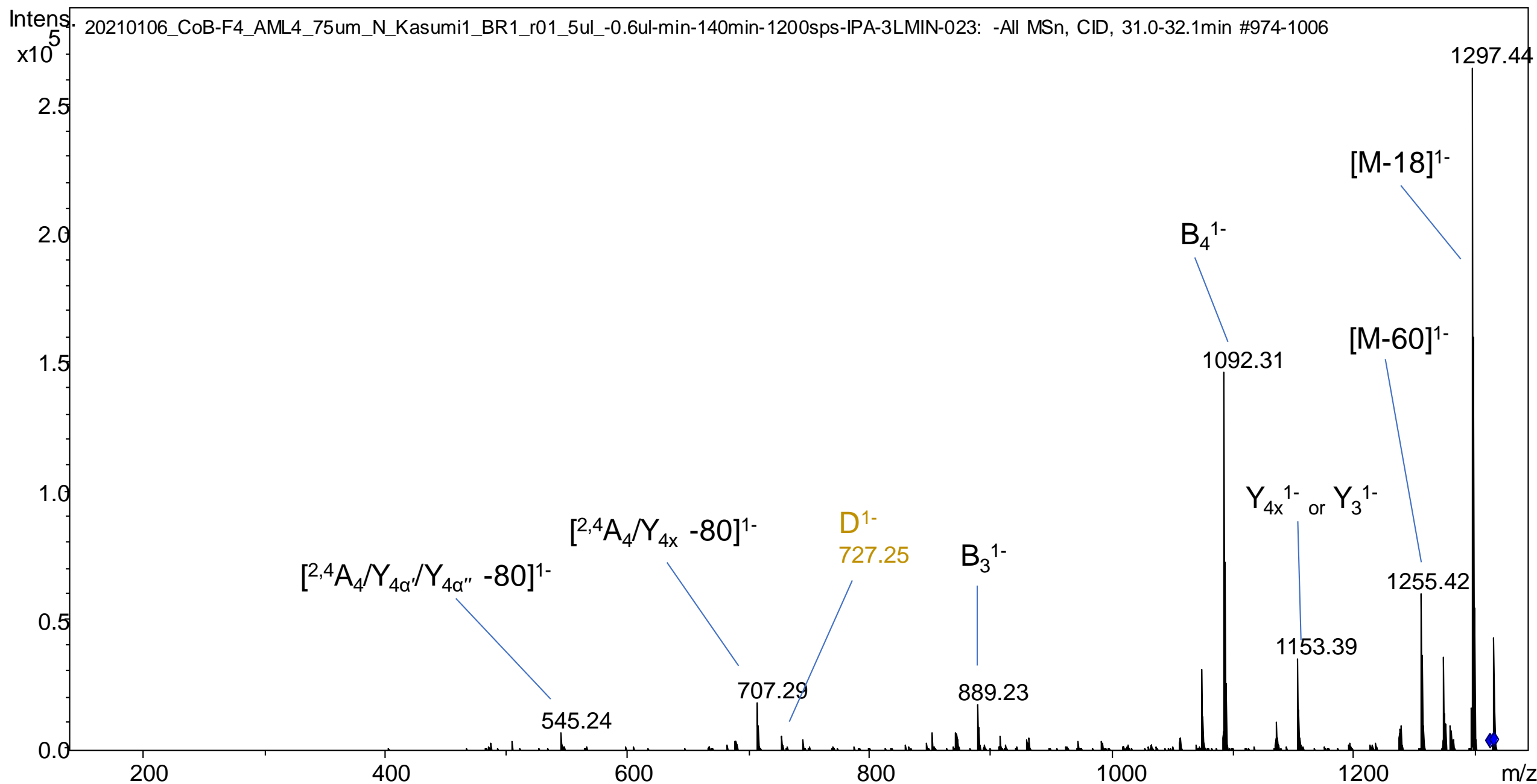
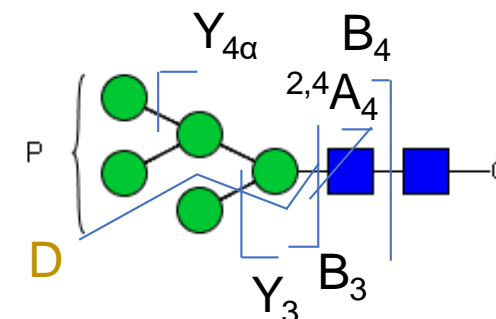


# Glycan 10b

H5N2P1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: Kasumi-1

Monoisotopic mass: 1316.42 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1315.41  
Observed ion: *m/z* 1315.44  
Mass deviation: *m/z* 0.03  
Retention time: 31.1 min

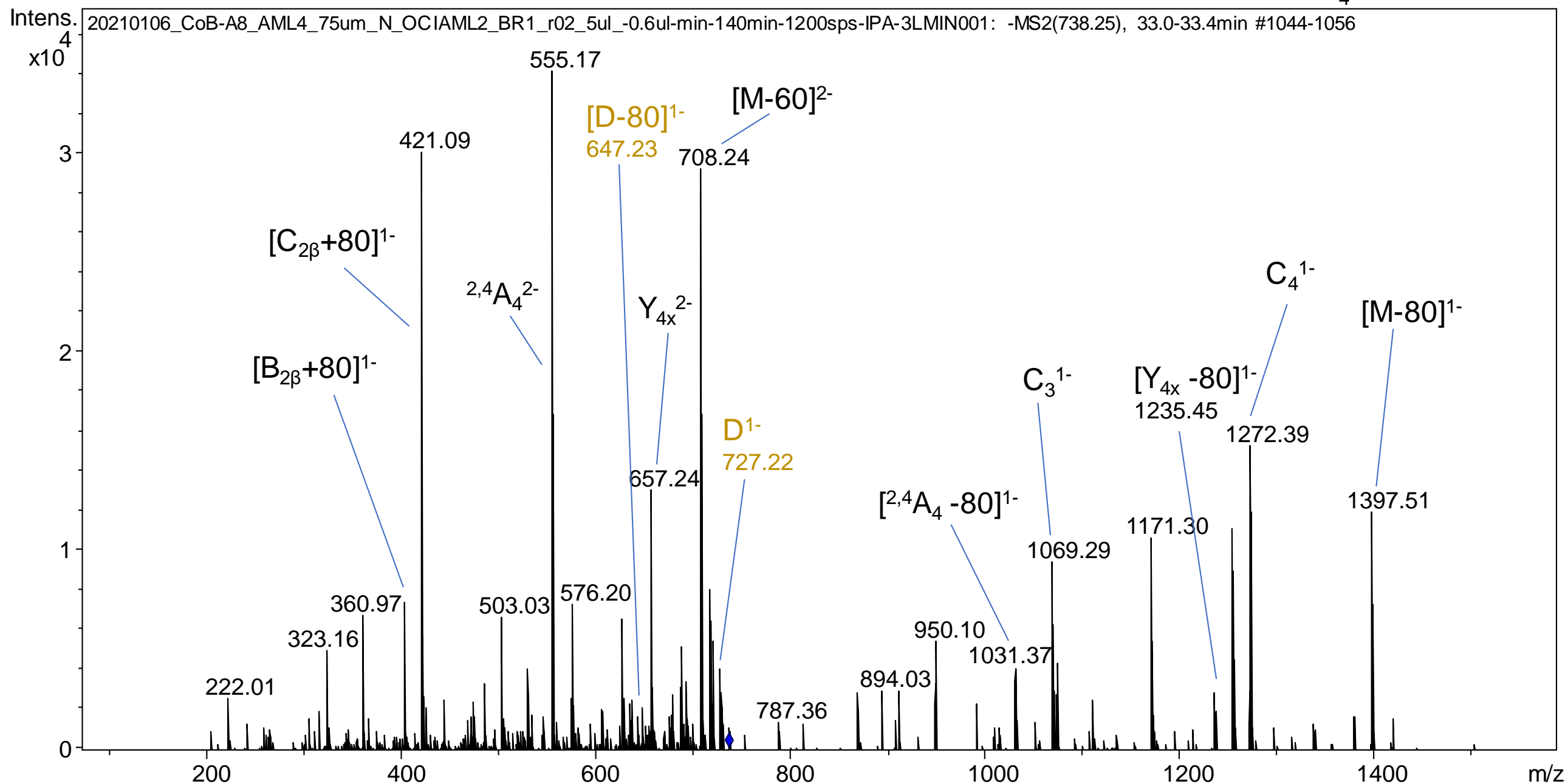
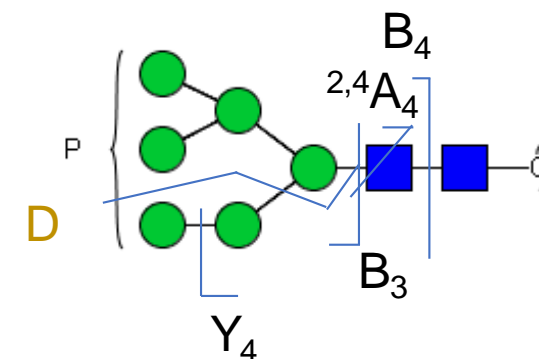


# Glycan 11a

H6N2P1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: OCI-AML-2

Monoisotopic mass: 1478.47 Da  
Charge observed: 2-  
Theoretical ion:  $m/z$  738.23  
Observed ion:  $m/z$  738.25  
Mass deviation:  $m/z$  0.02  
Retention time: 32.6 min

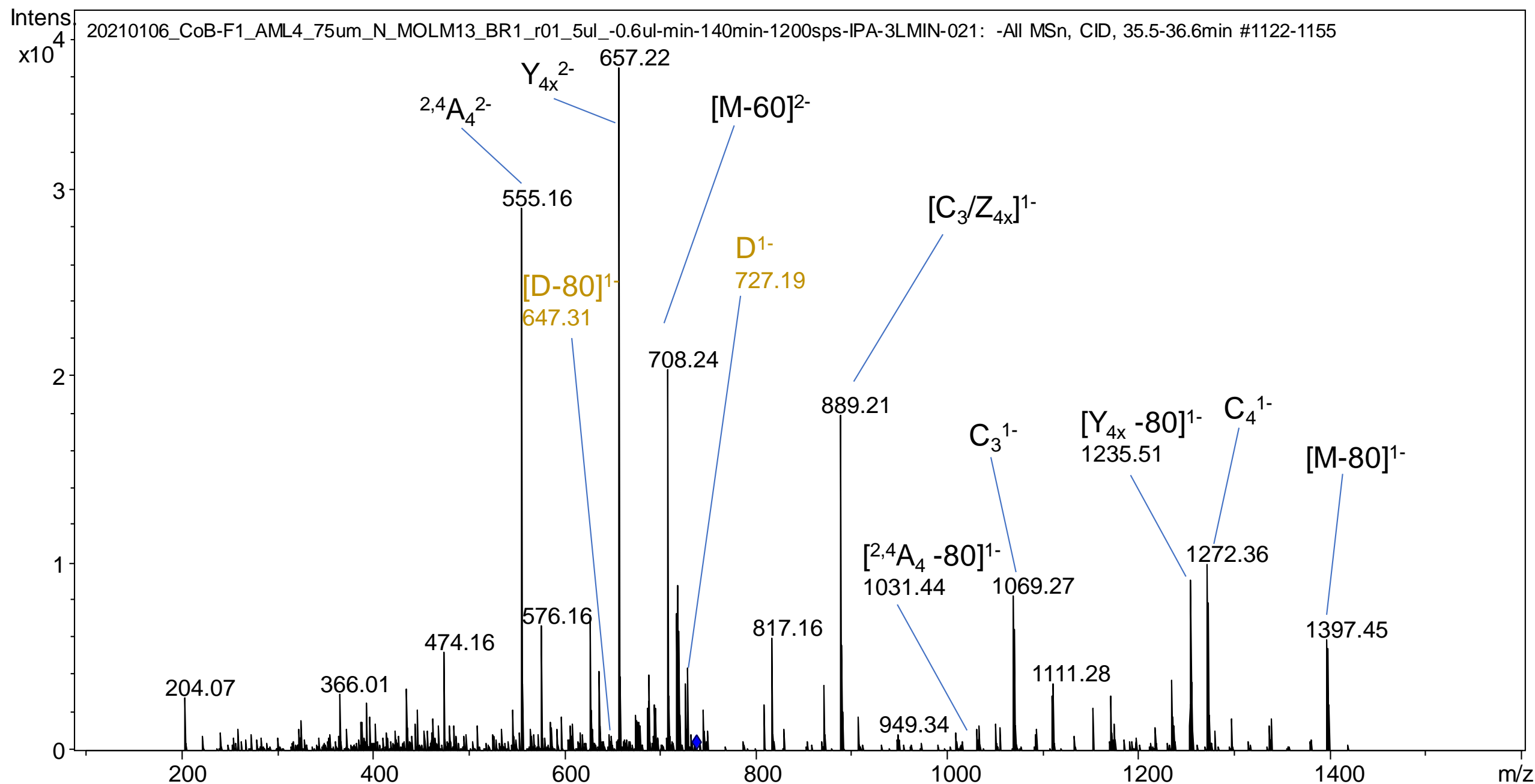
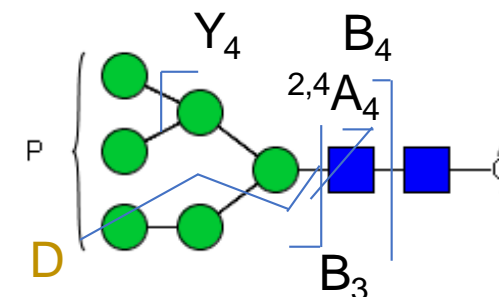


# Glycan 11b

H6N2P1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 1478.47 Da  
Charge observed: 2-  
Theoretical ion:  $m/z$  738.23  
Observed ion:  $m/z$  738.25  
Mass deviation:  $m/z$  0.02  
Retention time: 35.6 min

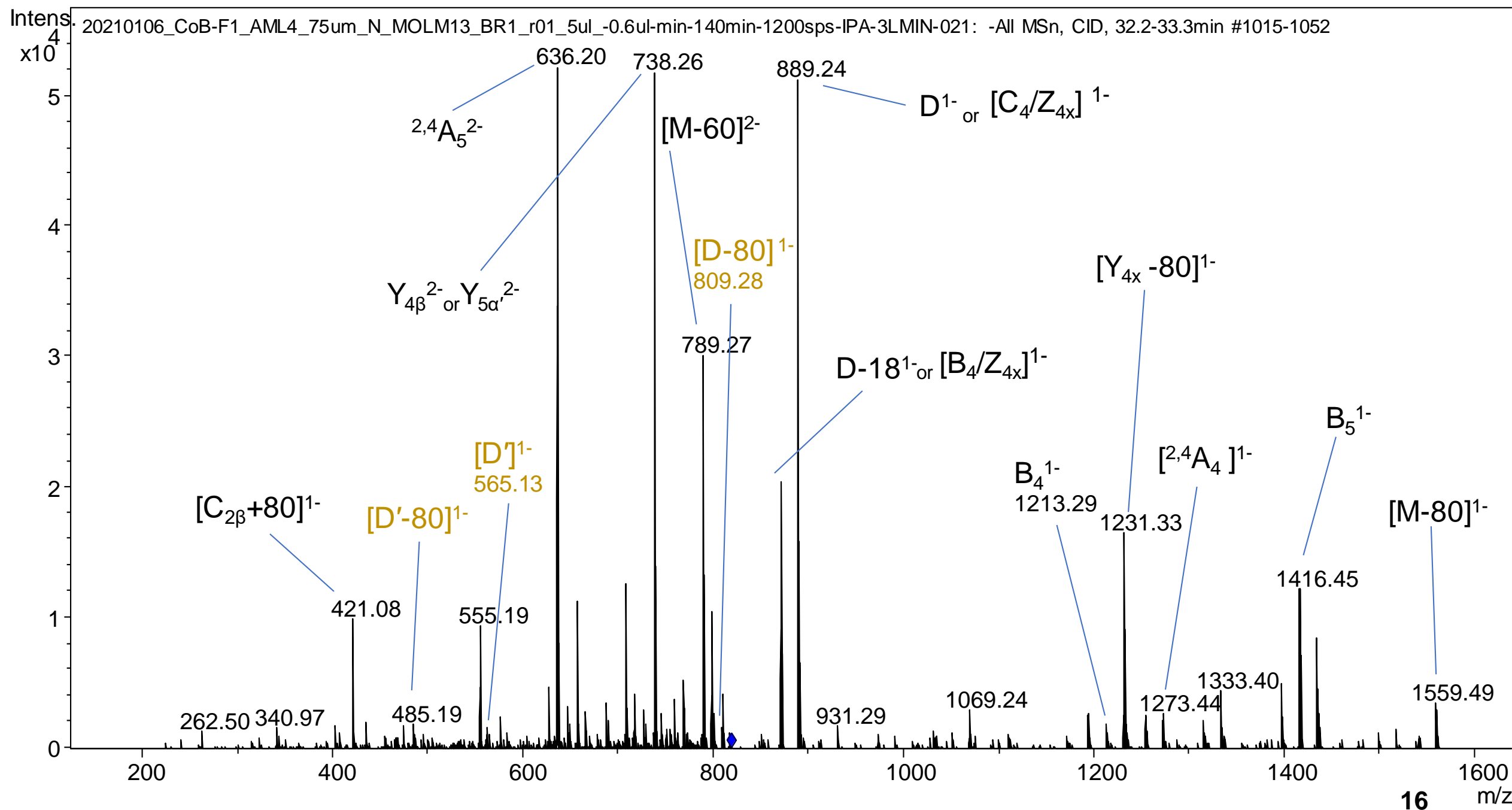
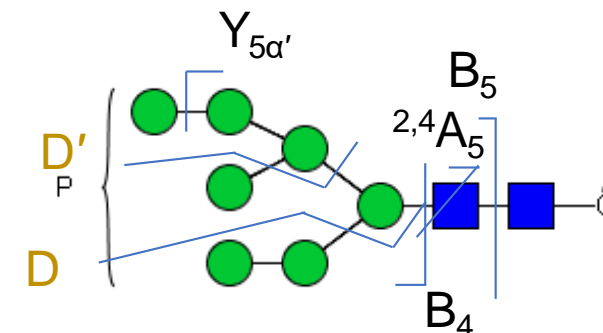


# Glycan 12

H7N2P1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 1640.52 Da  
Charge observed: 2-  
Theoretical ion:  $m/z$  819.25  
Observed ion:  $m/z$  819.28  
Mass deviation:  $m/z$  0.03  
Retention time: 32.4 min



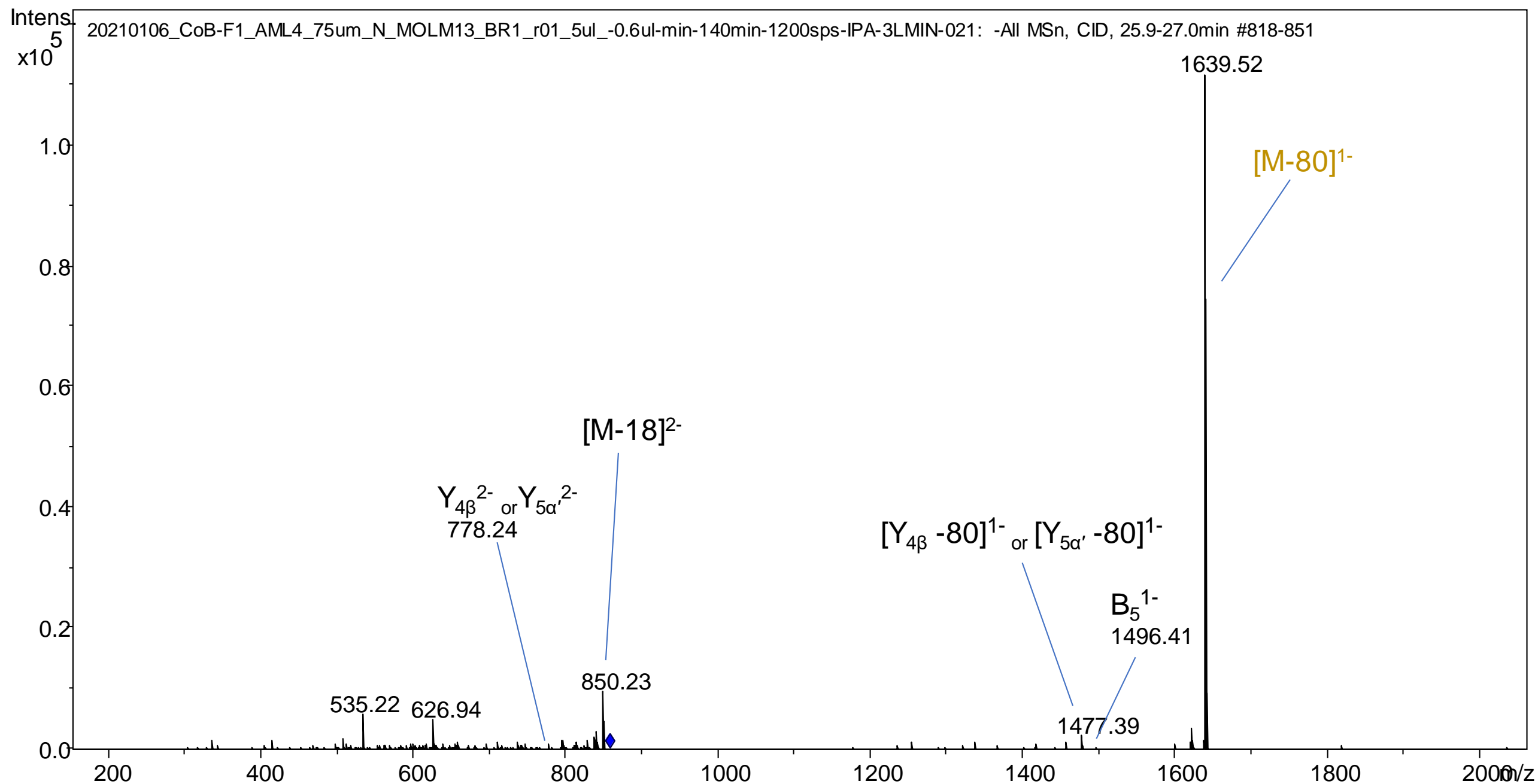
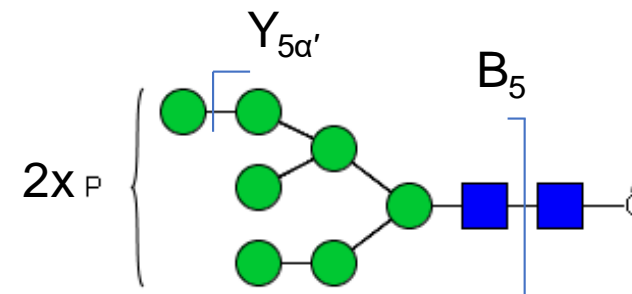


# Glycan 13

H7N2P2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 1720.49 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 859.24  
Observed ion: *m/z* 859.26  
Mass deviation: *m/z* 0.02  
Retention time: 26.2 min



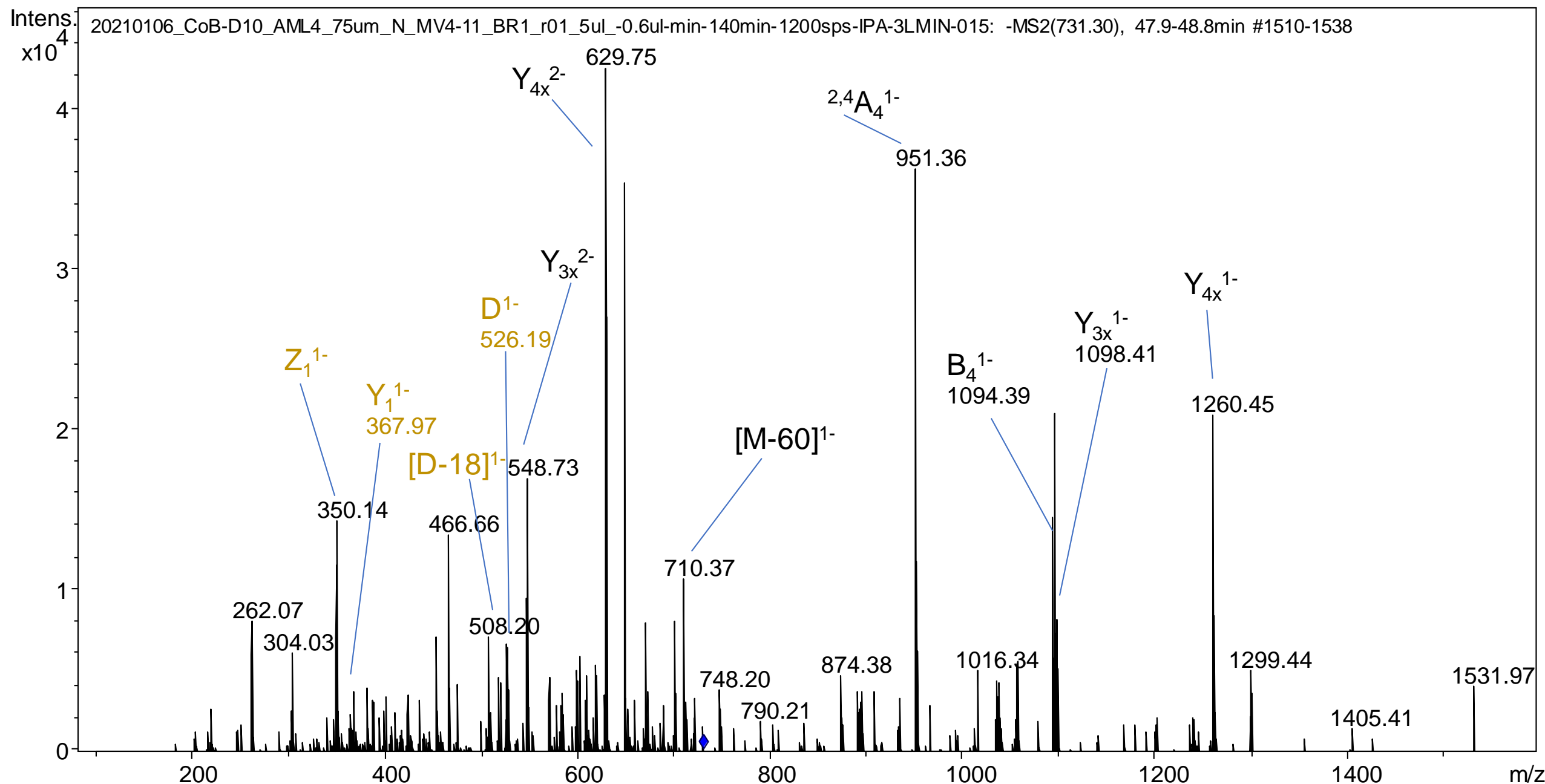
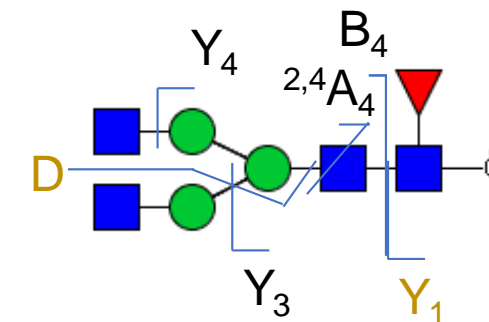
# Glycan 14

H3N4F1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MV4-11

Monoisotopic mass: 1464.56 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 731.28  
Observed ion: *m/z* 731.32  
Mass deviation: *m/z* 0.04  
Retention time: 48.4 min

UniCarb-DB: #399



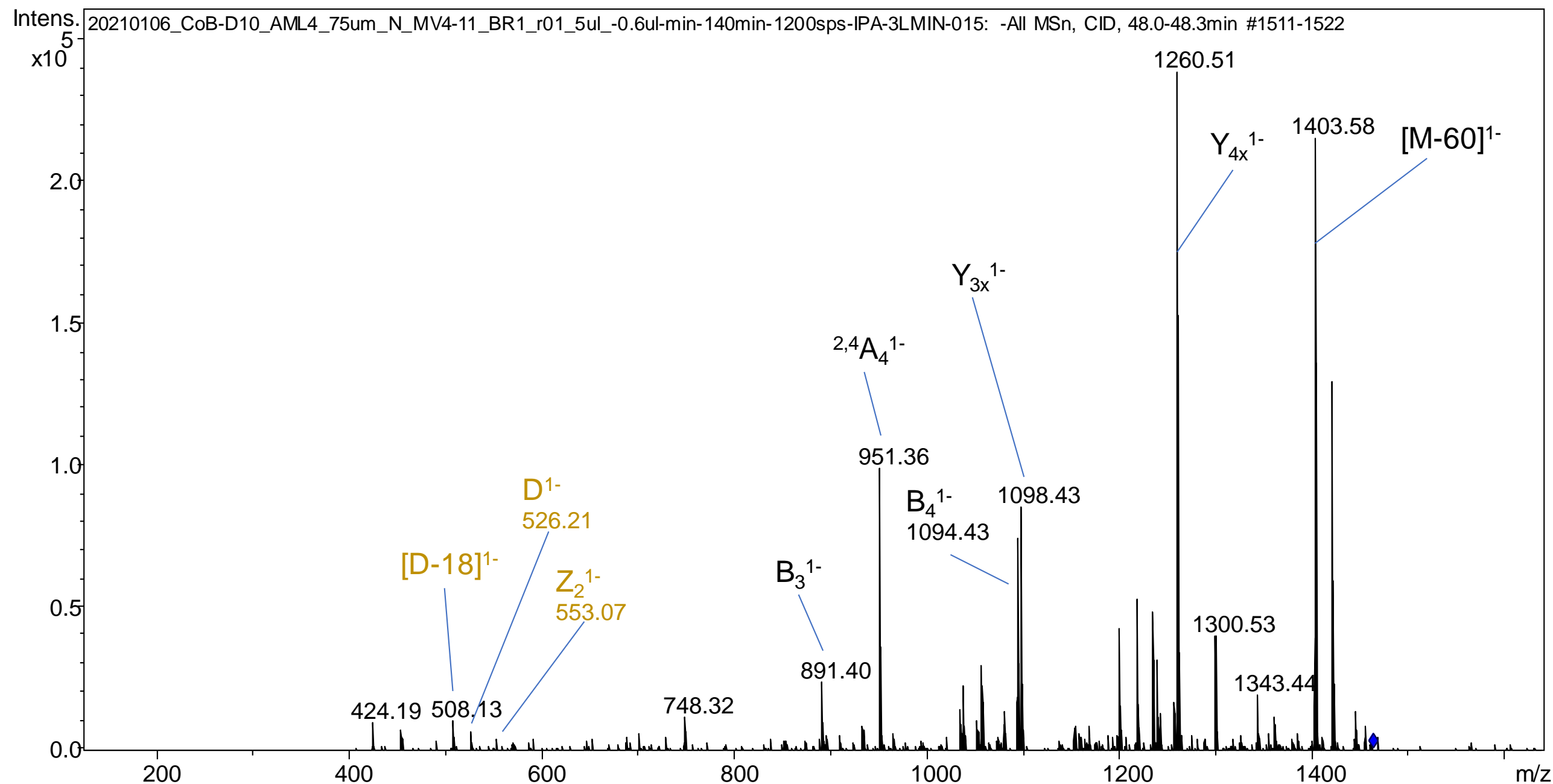
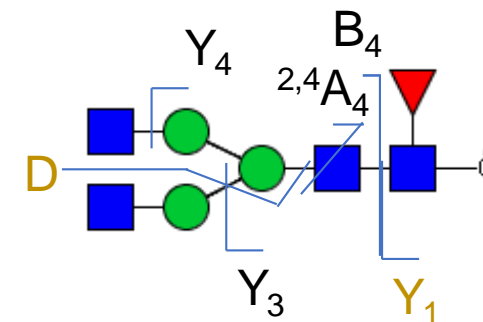
# Glycan 14

H3N4F1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MV4-11

Monoisotopic mass: 1464.56 Da  
Charge observed: 1-  
Theoretical ion: *m/z* 1463.55  
Observed ion: *m/z* 1463.60  
Mass deviation: *m/z* 0.05  
Retention time: 48.4 min

UniCarb-DB: #399

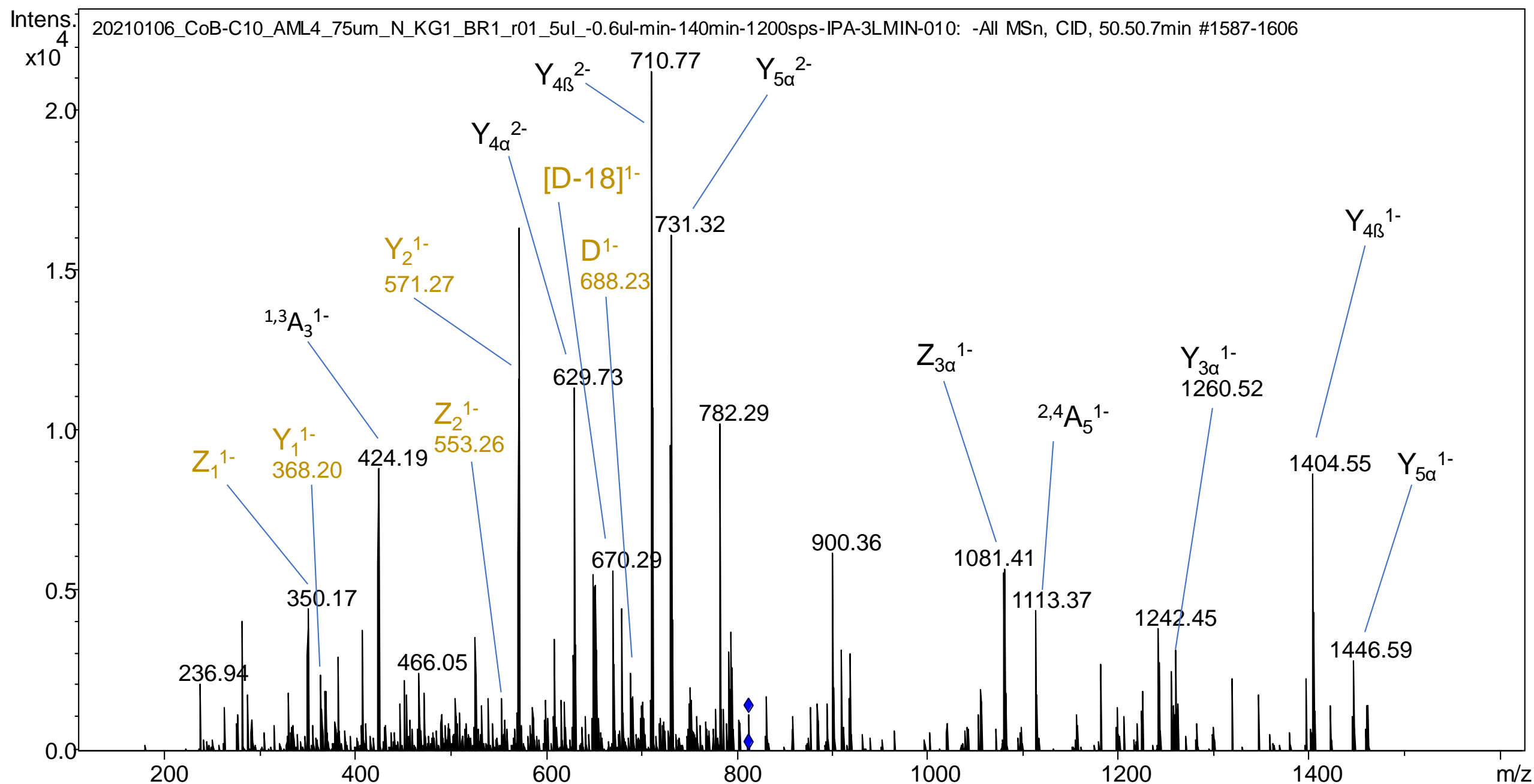
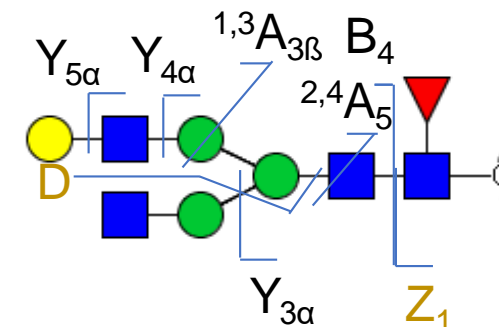


# Glycan 15

H4N4F1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: KG-1

Monoisotopic mass: 1626.61 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 812.30  
Observed ion: *m/z* 812.32  
Mass deviation: *m/z* 0.02  
Retention time: 50.3 min

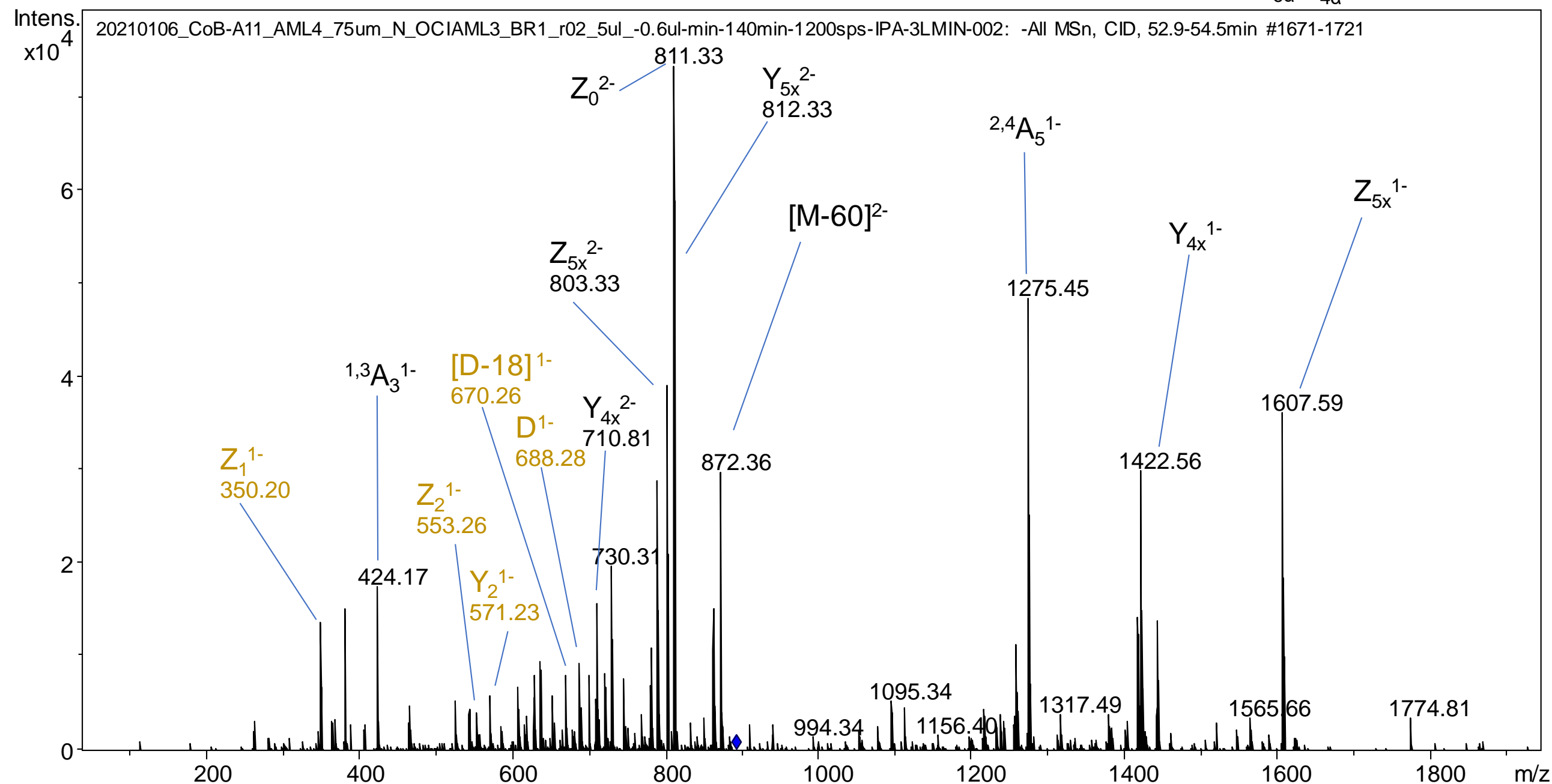
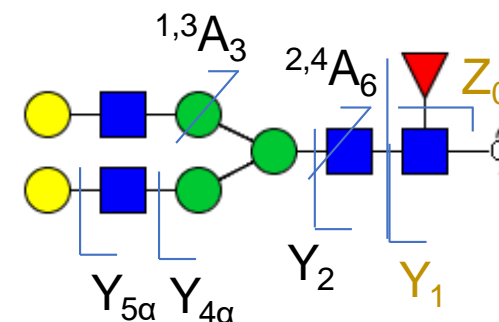


# H5N4F1

Depicted MS<sup>2</sup> was obtained from analysis of cell line: OCI-AML-3

<b>Monoisotopic mass:</b>	<b>1788.67 Da</b>
<b>Charge observed:</b>	<b>2-</b>
<b>Theoretical ion:</b>	<b><i>m/z</i> 893.33</b>
<b>Observed ion:</b>	<b><i>m/z</i> 893.36</b>
<b>Mass deviation:</b>	<b><i>m/z</i> 0.03</b>
<b>Retention time:</b>	<b>53.6 min</b>

**UniCarb-DB: #425**



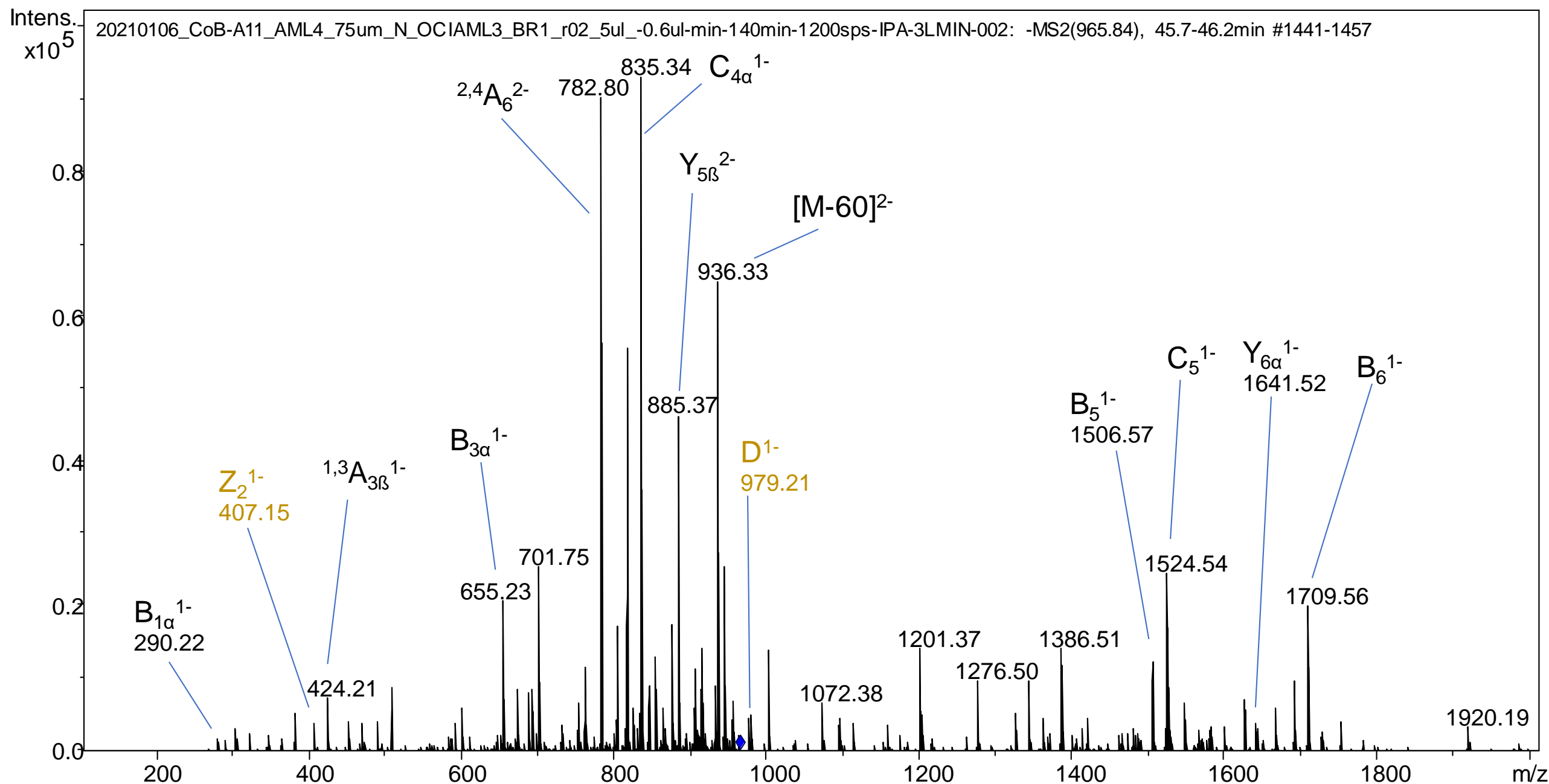
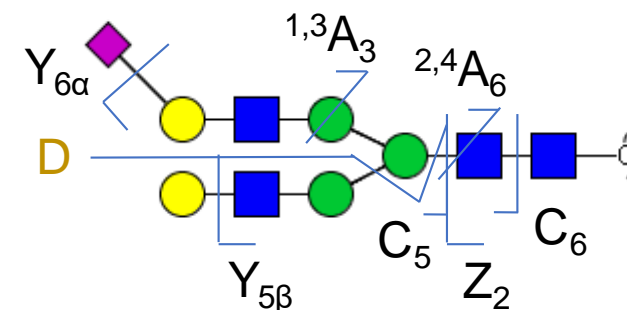
# Glycan 17a

## H5N4S1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: OCI-AML-3

Monoisotopic mass: 1933.70 Da  
Charge observed: 2-  
Theoretical ion:  $m/z$  965.84  
Observed ion:  $m/z$  965.84  
Mass deviation:  $m/z$  0.00  
Retention time: 45.7 min  
Note:  $\alpha$ -2,6 sialic acid linkage confirmed by  
neuraminidase S and A treatment

UniCarb-DB: #2338

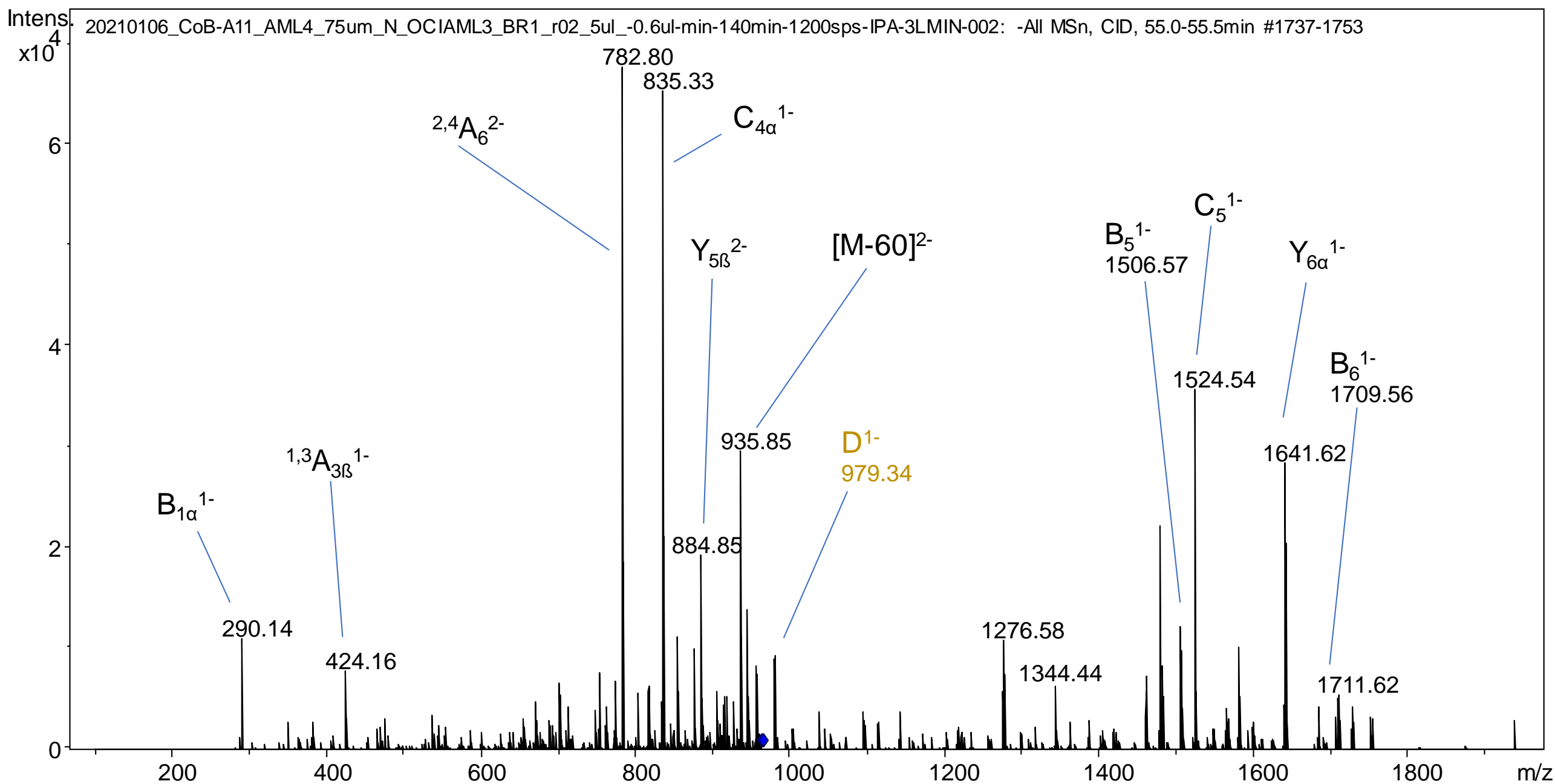
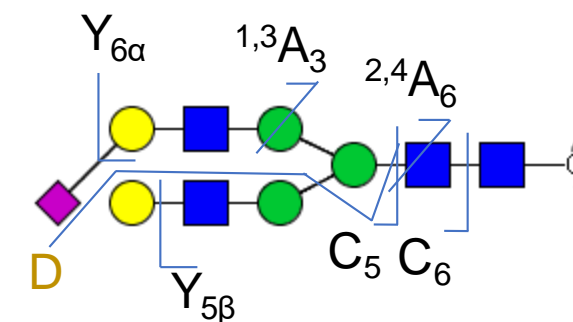


# H5N4S1

Depicted MS<sup>2</sup> was obtained from analysis of cell line: OCI-AML-3

<b>Monoisotopic mass:</b>	<b>1933.70 Da</b>
<b>Charge observed:</b>	<b>2-</b>
<b>Theoretical ion:</b>	<b><i>m/z</i> 965.84</b>
<b>Observed ion:</b>	<b><i>m/z</i> 965.88</b>
<b>Mass deviation:</b>	<b><i>m/z</i> 0.04</b>
<b>Retention time:</b>	<b>55.2 min</b>
<b>Note: <math>\alpha</math>-2,3 sialic acid linkage confirmed by neuraminidase S and A treatment</b>	

**UniCarb-DB: #2338**



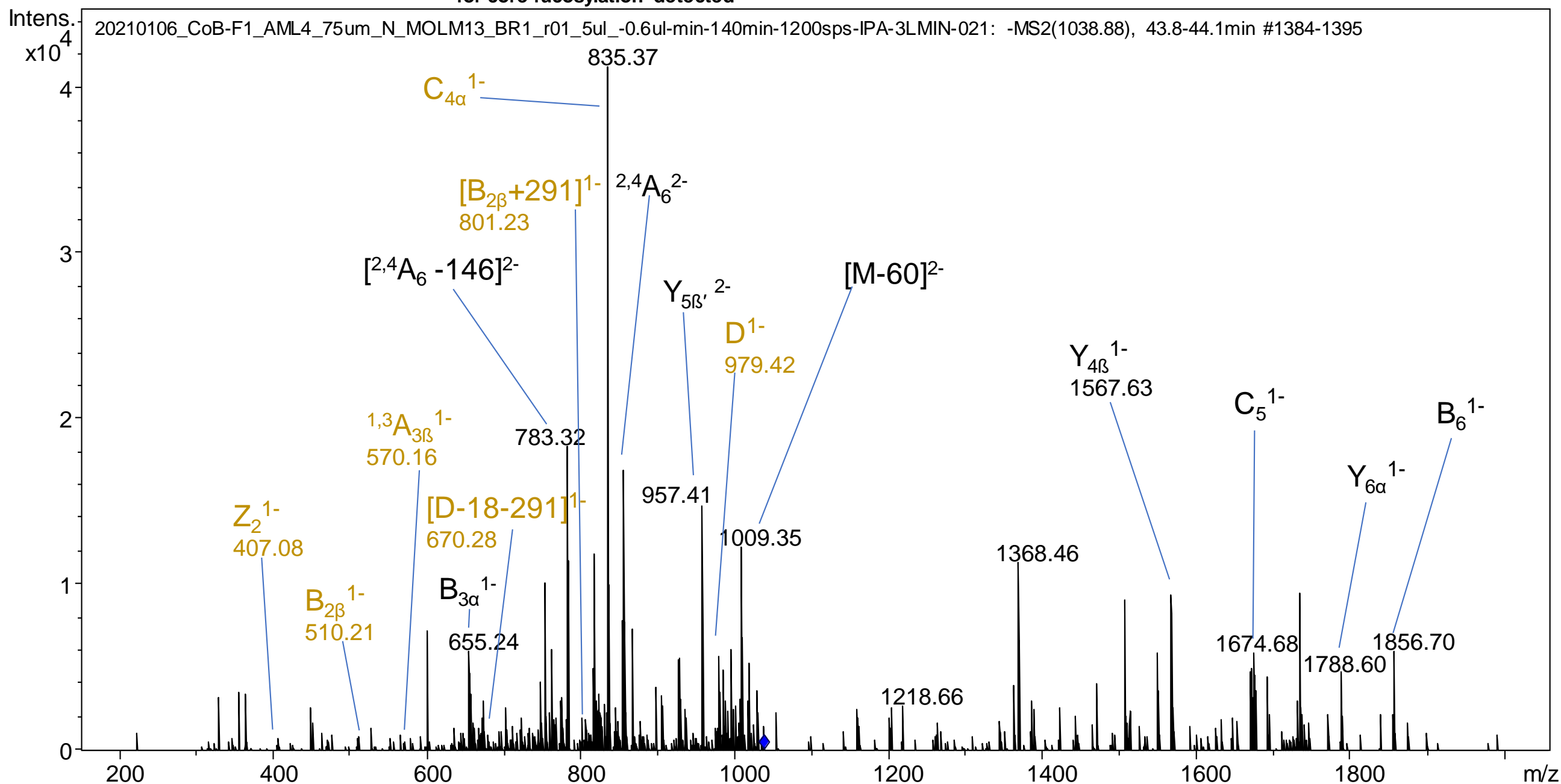
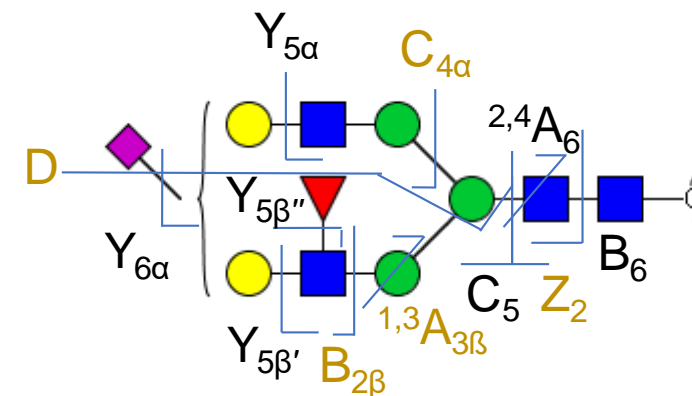
# Glycan 18a

H5N4F1S1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 2079.76 Da  
Charge observed: 2-  
Theoretical ion:  $m/z$  1038.87  
Observed ion:  $m/z$  1038.88  
Mass deviation:  $m/z$  0.01  
Retention time: 43.9 min

Note:  $\alpha$ -2,6 sialic acid linkage confirmed by  
neuraminidase S and A treatment; no diagnostic ions  
for core fucosylation detected





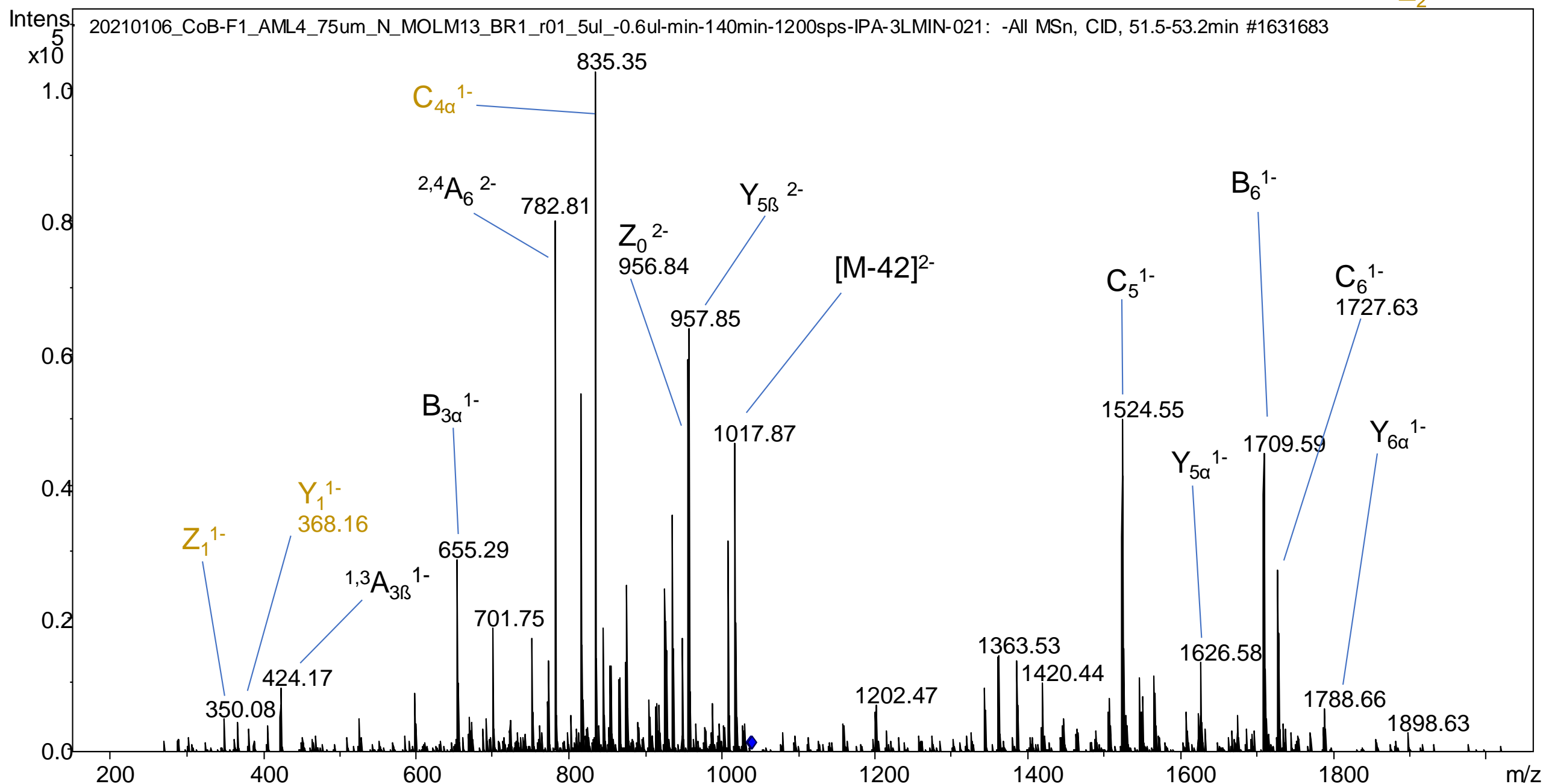
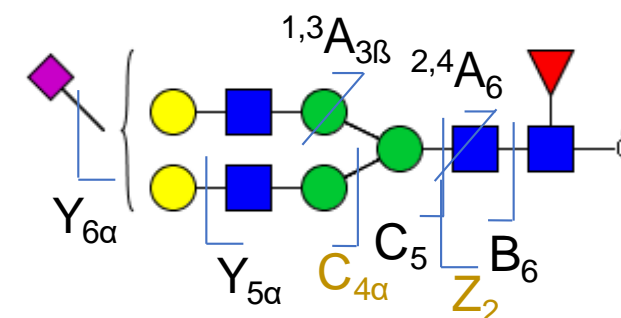
# Glycan 18b

H5N4F1S1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 2079.76 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1038.87  
Observed ion: *m/z* 1038.88  
Mass deviation: *m/z* 0.01  
Retention time: 51.8 min  
Note:  $\alpha$ -2,6 sialic acid linkage confirmed by  
neuraminidase S and A treatment

UniCarb-DB: #2364

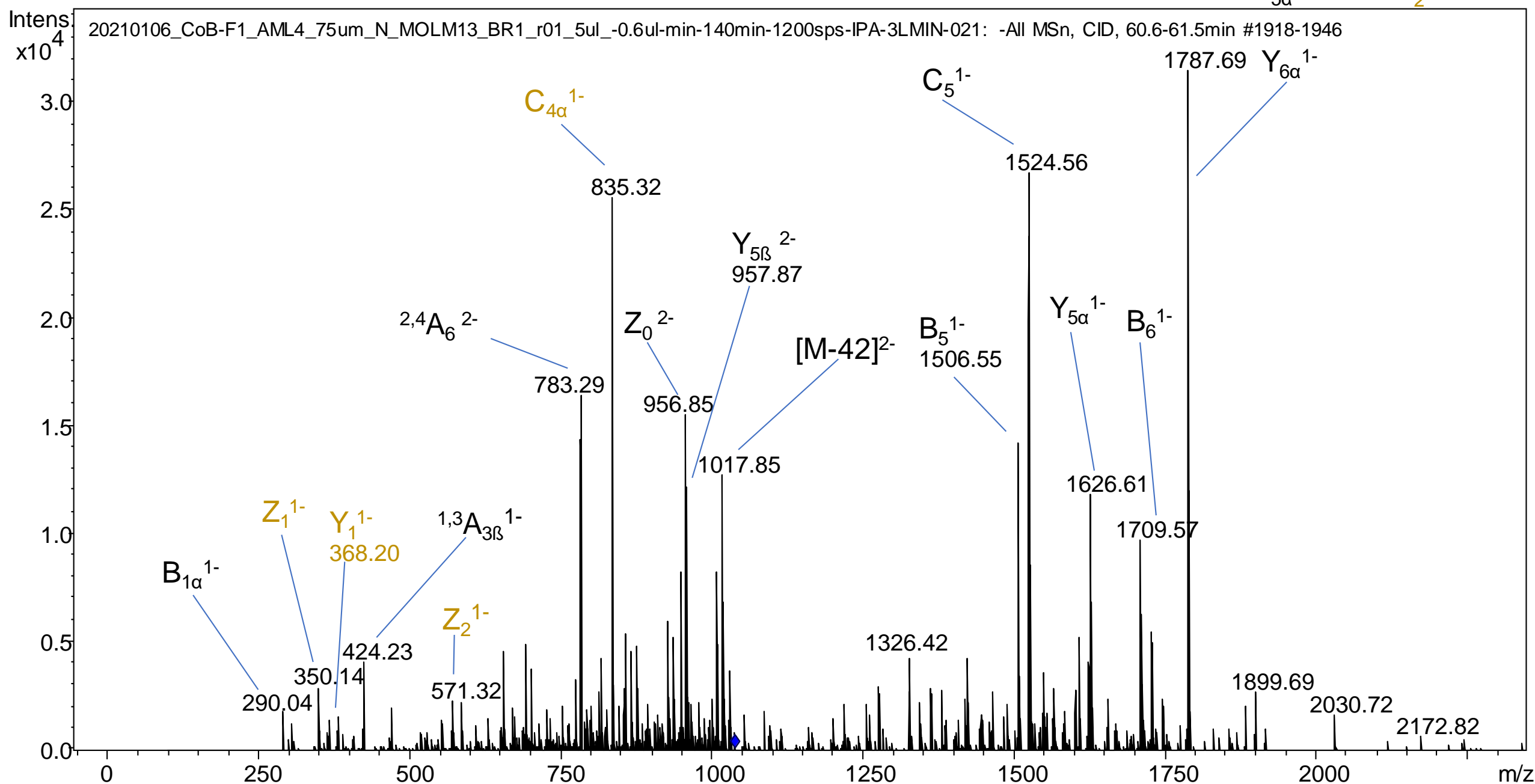
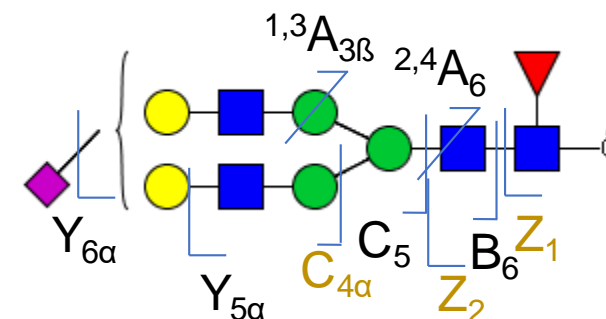


H5N4F1S1

**Depicted MS<sup>2</sup> was obtained from analysis of cell line: MOLM-13**

**Monoisotopic mass:** 2079.76 Da  
**Charge observed:** 2-  
**Theoretical ion:** *m/z* 1038.87  
**Observed ion:** *m/z* 1038.88  
**Mass deviation:** *m/z* 0.01  
**Retention time:** 60.8 min  
**Note:** α-2,3 sialic acid linkage confirmed by neuraminidase S and A treatment

**UniCarb-DB: #2364**

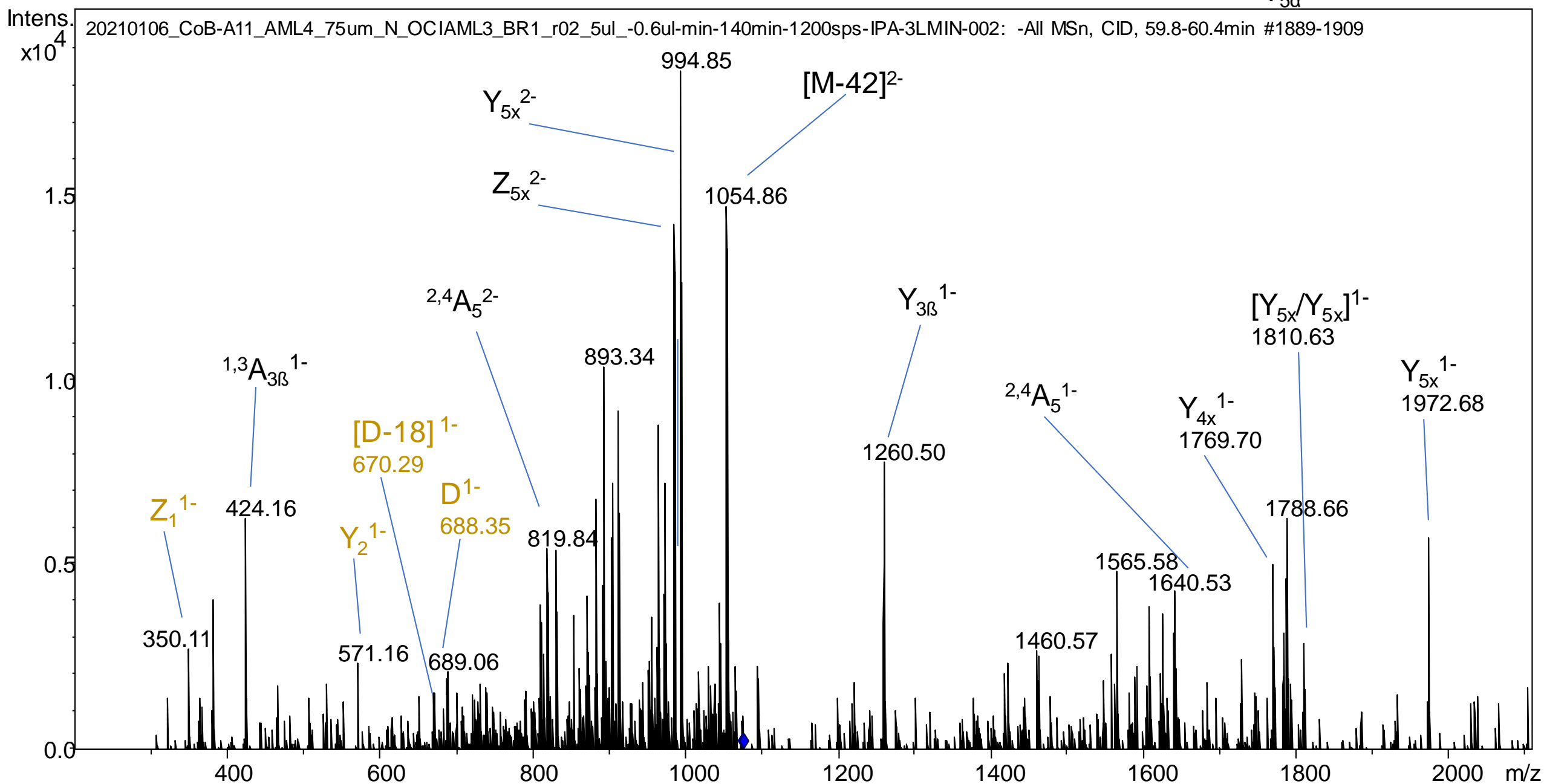
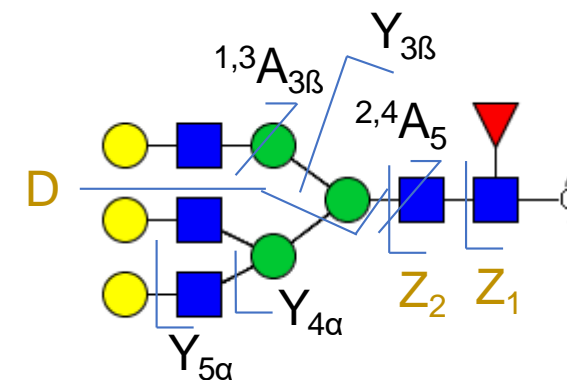


# H6N5F1

Depicted MS<sup>2</sup> was obtained from analysis of cell line: OCI-AML-3

<b>Monoisotopic mass:</b>	<b>2153.80 Da</b>
<b>Charge observed:</b>	<b>2-</b>
<b>Theoretical ion:</b>	<b><i>m/z</i> 1075.89</b>
<b>Observed ion:</b>	<b><i>m/z</i> 1075.88</b>
<b>Mass deviation:</b>	<b><i>m/z</i> 0.01</b>
<b>Retention time:</b>	<b>60.8 min</b>

UniCarb-DB: #2549



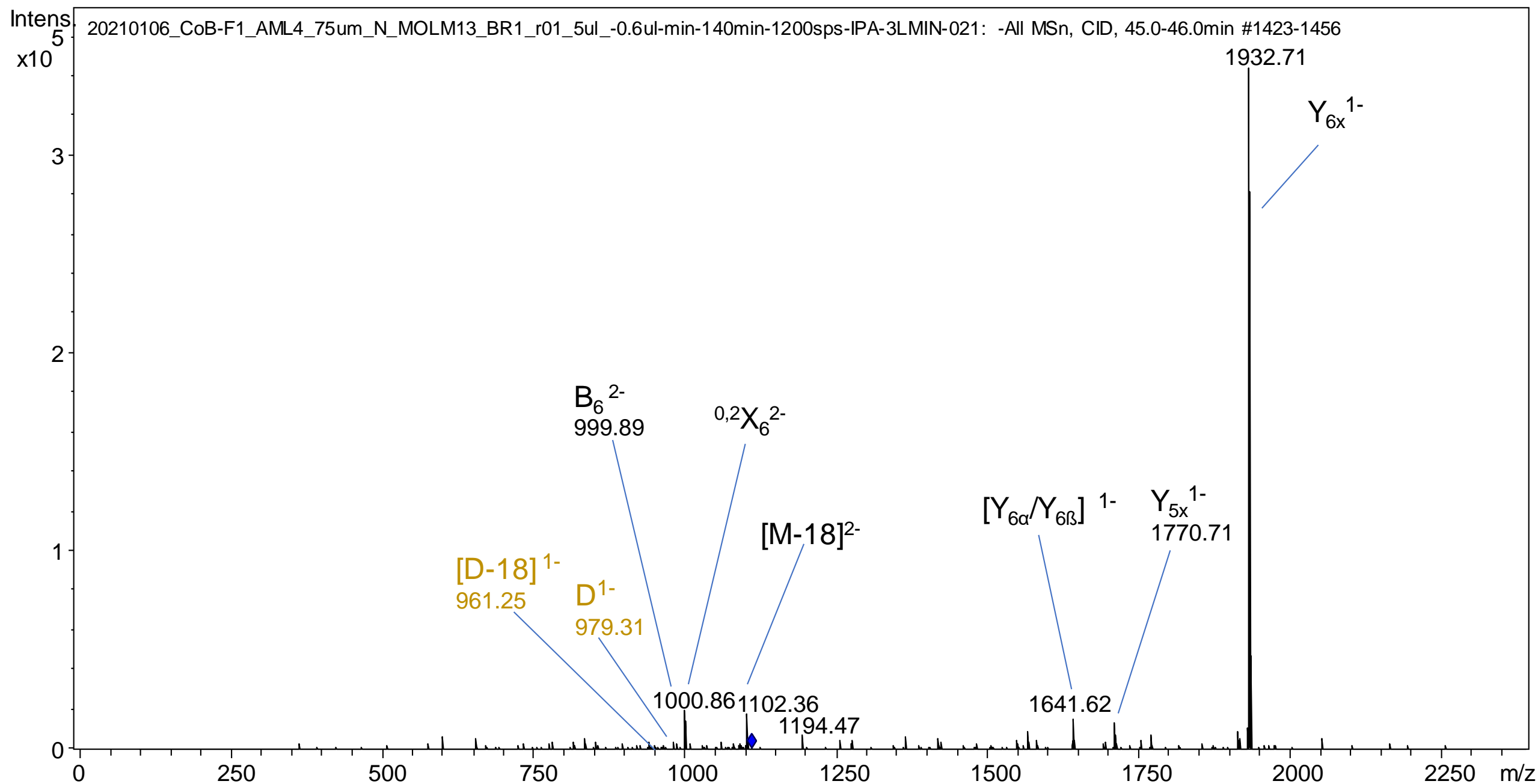
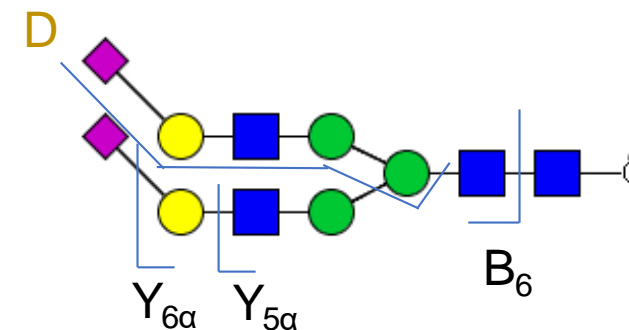
# Glycan 20a

H5N4S2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 2224.80 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1111.39  
Observed ion: *m/z* 1111.38  
Mass deviation: *m/z* 0.01  
Retention time: 45.2 min  
Note:  $\alpha$ -2,6 sialic acid linkages confirmed by  
neuraminidase S and A treatment

UniCarb-DB: #378

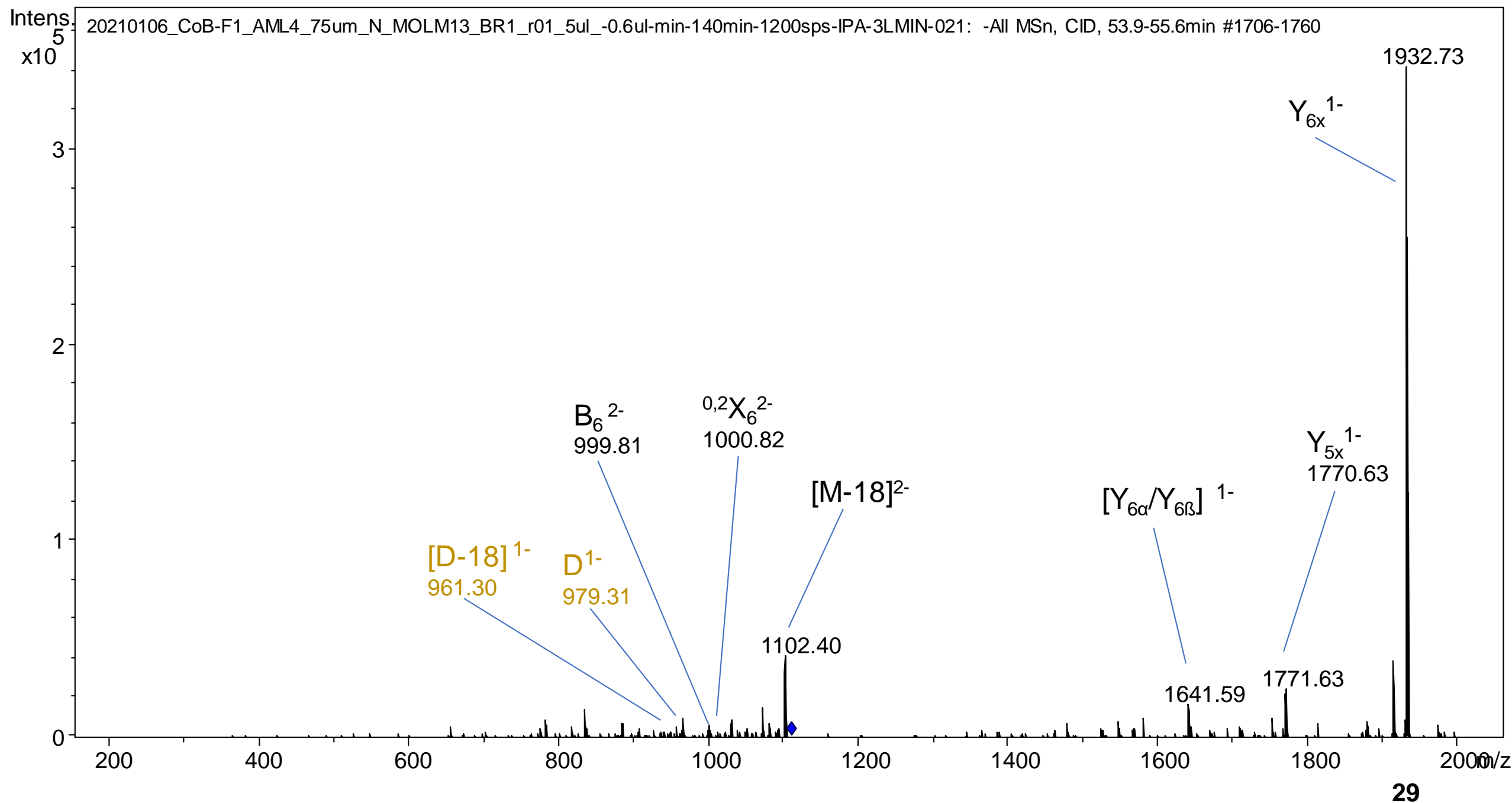
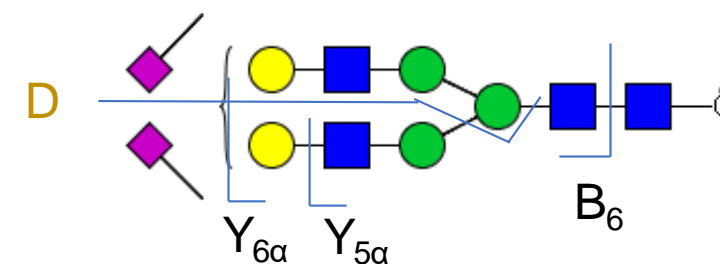


# Glycan 20b

## H5N4S2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

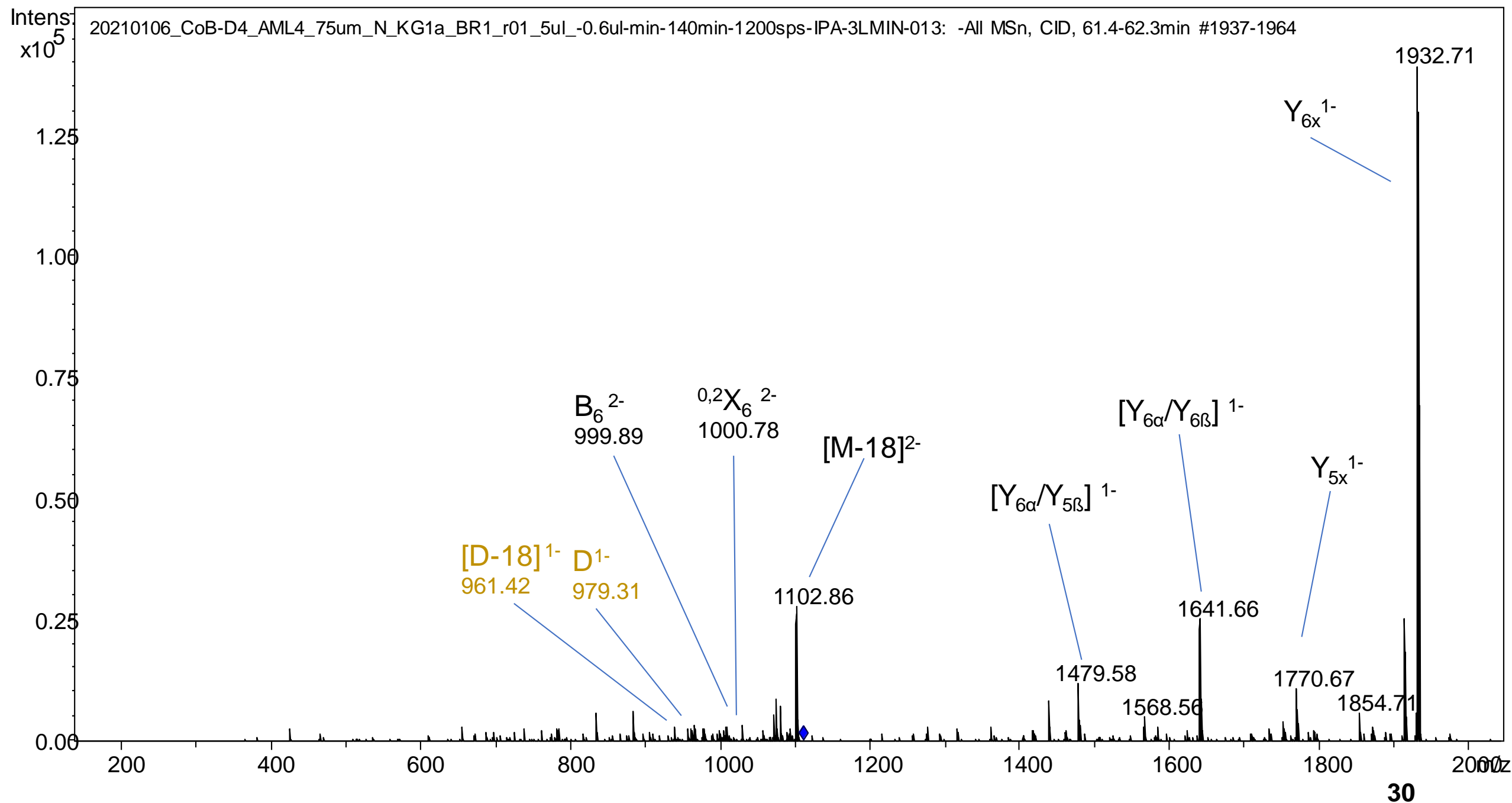
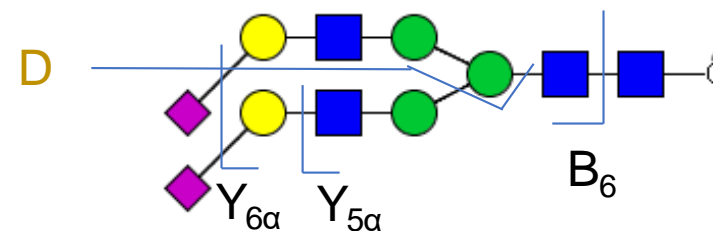
Monoisotopic mass: 2224.80 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1111.39  
Observed ion: *m/z* 1111.40  
Mass deviation: *m/z* 0.01  
Retention time: 54.1 min  
Note: Sialic acid linkages confirmed by  
neuraminidase S and A treatment



# H5N4S2

Depicted MS<sup>2</sup> was obtained from analysis of cell line: KG-1a

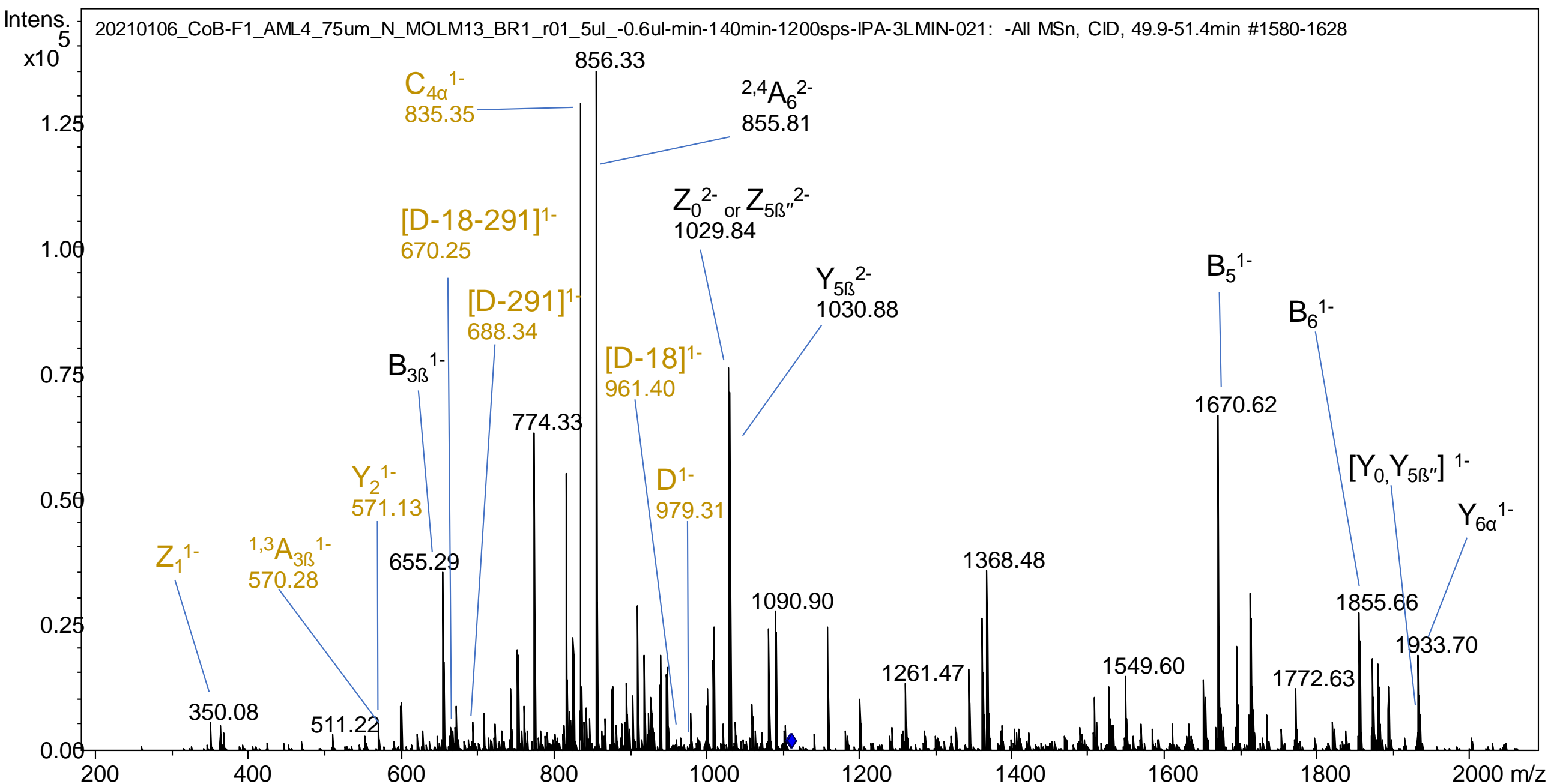
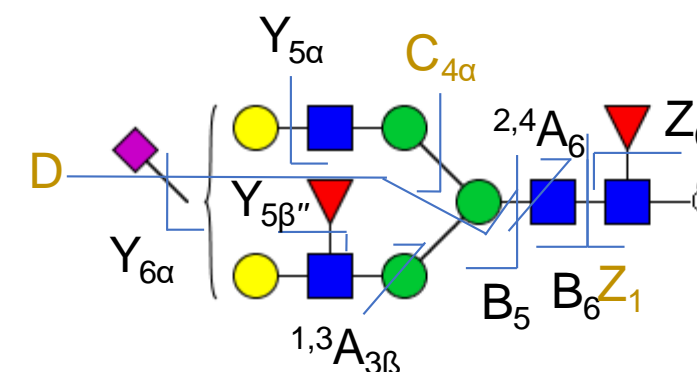
**Monoisotopic mass:** 2224.80 Da  
**Charge observed:** 2-  
**Theoretical ion:** *m/z* 1111.42  
**Observed ion:** *m/z* 1111.39  
**Mass deviation:** *m/z* 0.01  
**Retention time:** 61.7 min  
**Note:** α-2,6 sialic acid linkages confirmed by neuraminidase S and A treatment



H5N4F2S1

**Depicted MS<sup>2</sup> was obtained from analysis of cell line: MOLM-13**

**Monoisotopic mass:** 2225.82 Da  
**Charge observed:** 2-  
**Theoretical ion:** *m/z* 1111.90  
**Observed ion:** *m/z* 1111.90  
**Mass deviation:** *m/z* 0.00  
**Retention time:** 50.1 min  
**Note:** α-2,6 sialic acid linkages confirmed by neuraminidase S and A treatment



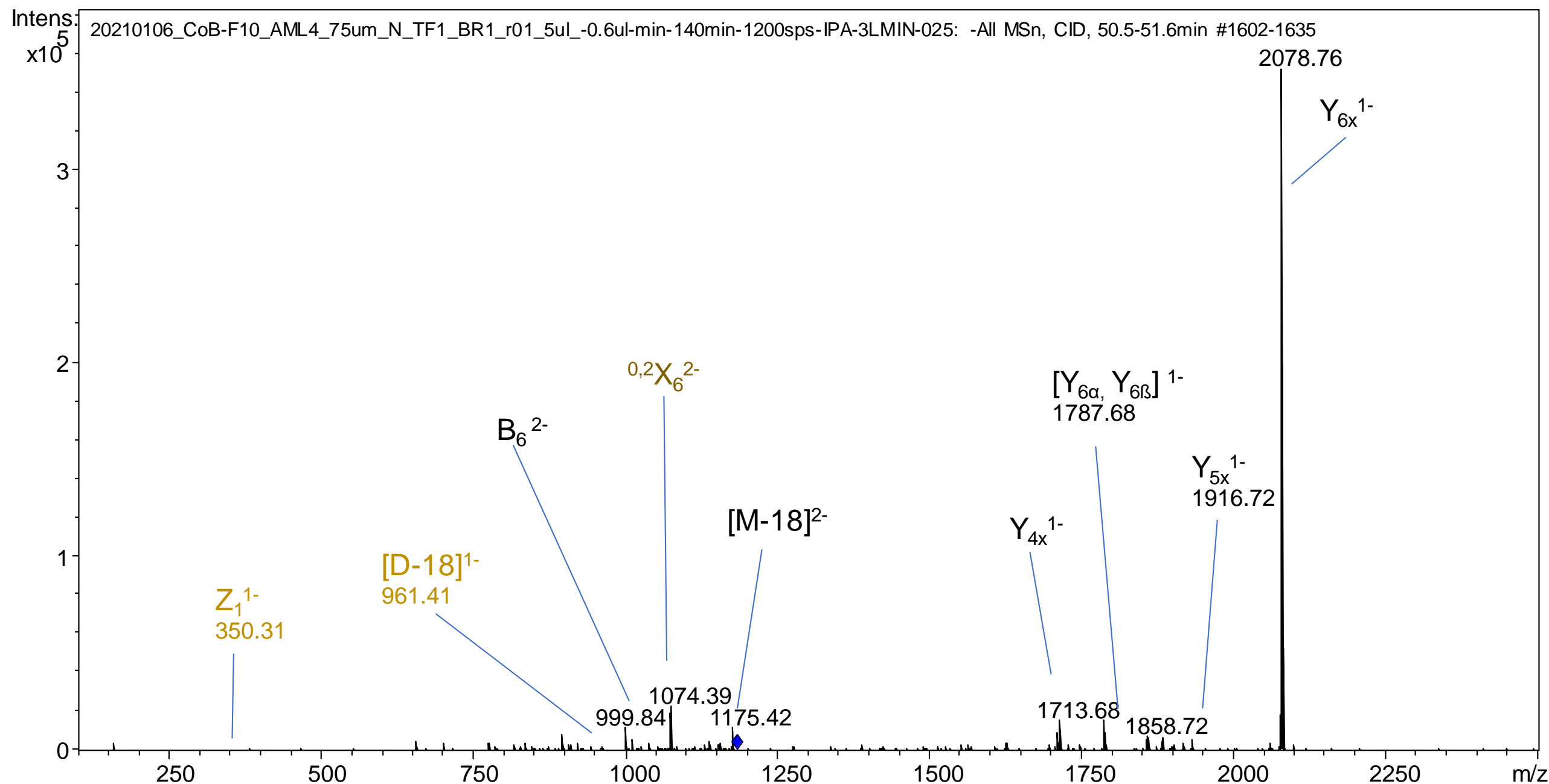
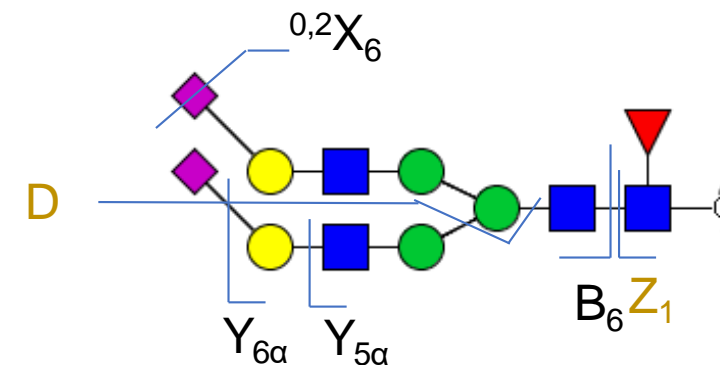
# Glycan 22a

H5N4S2F1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: TF-1

Monoisotopic mass: 2370.86 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1184.42  
Observed ion: *m/z* 1184.43  
Mass deviation: *m/z* 0.01  
Retention time: 50.8 min  
Note:  $\alpha$ -2,6 sialic acid linkages confirmed by  
neuraminidase S and A treatment

UniCarb-DB: #389



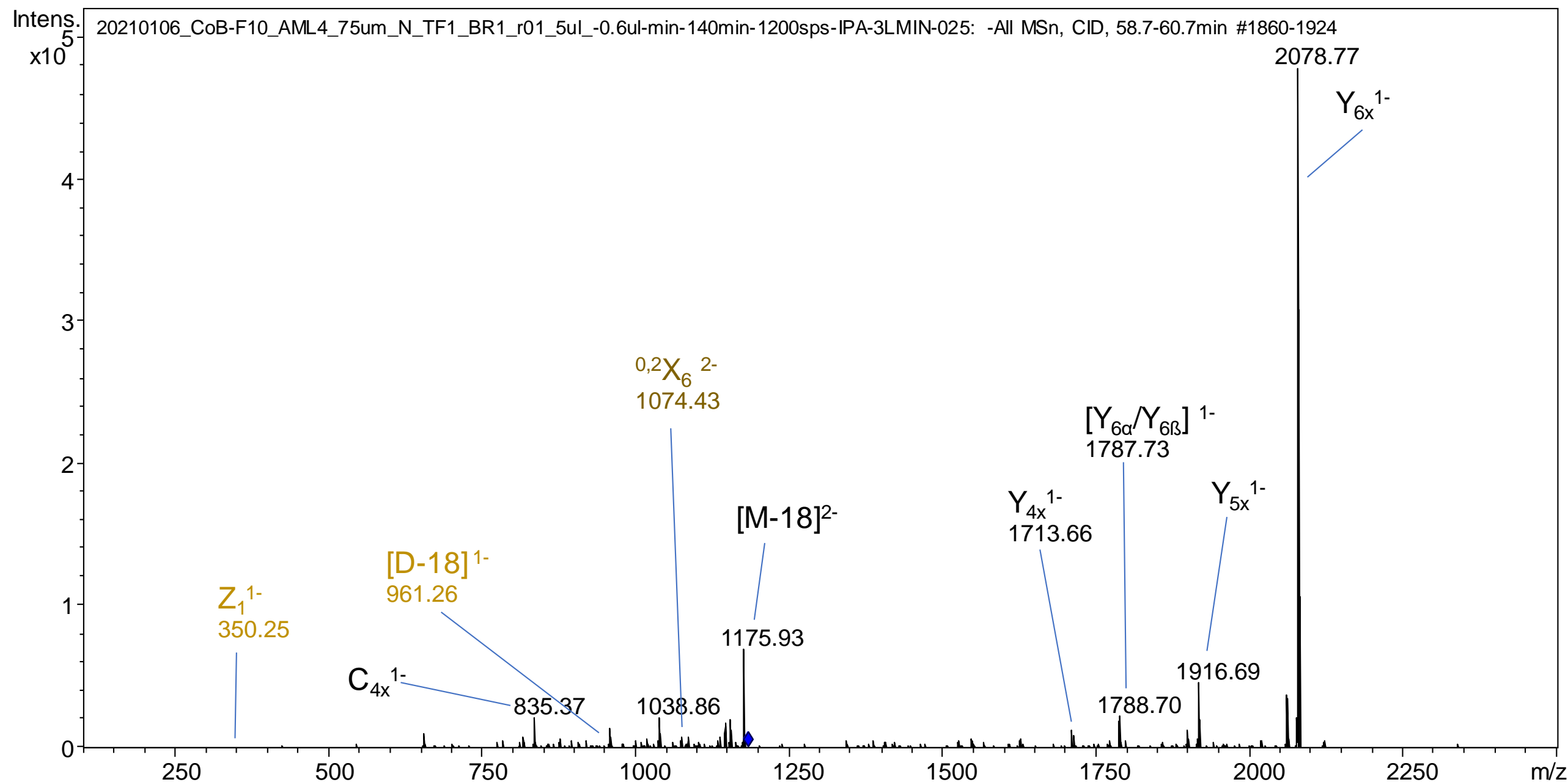
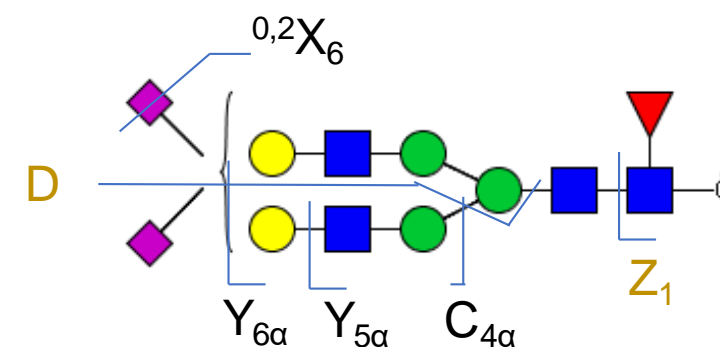


# Glycan 22b

H5N4S2F1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: TF-1

Monoisotopic mass: 2370.86 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1184.42  
Observed ion: *m/z* 1184.44  
Mass deviation: *m/z* 0.02  
Retention time: 59.4 min  
Note: Sialic acid linkages confirmed by  
neuraminidase S and A treatment



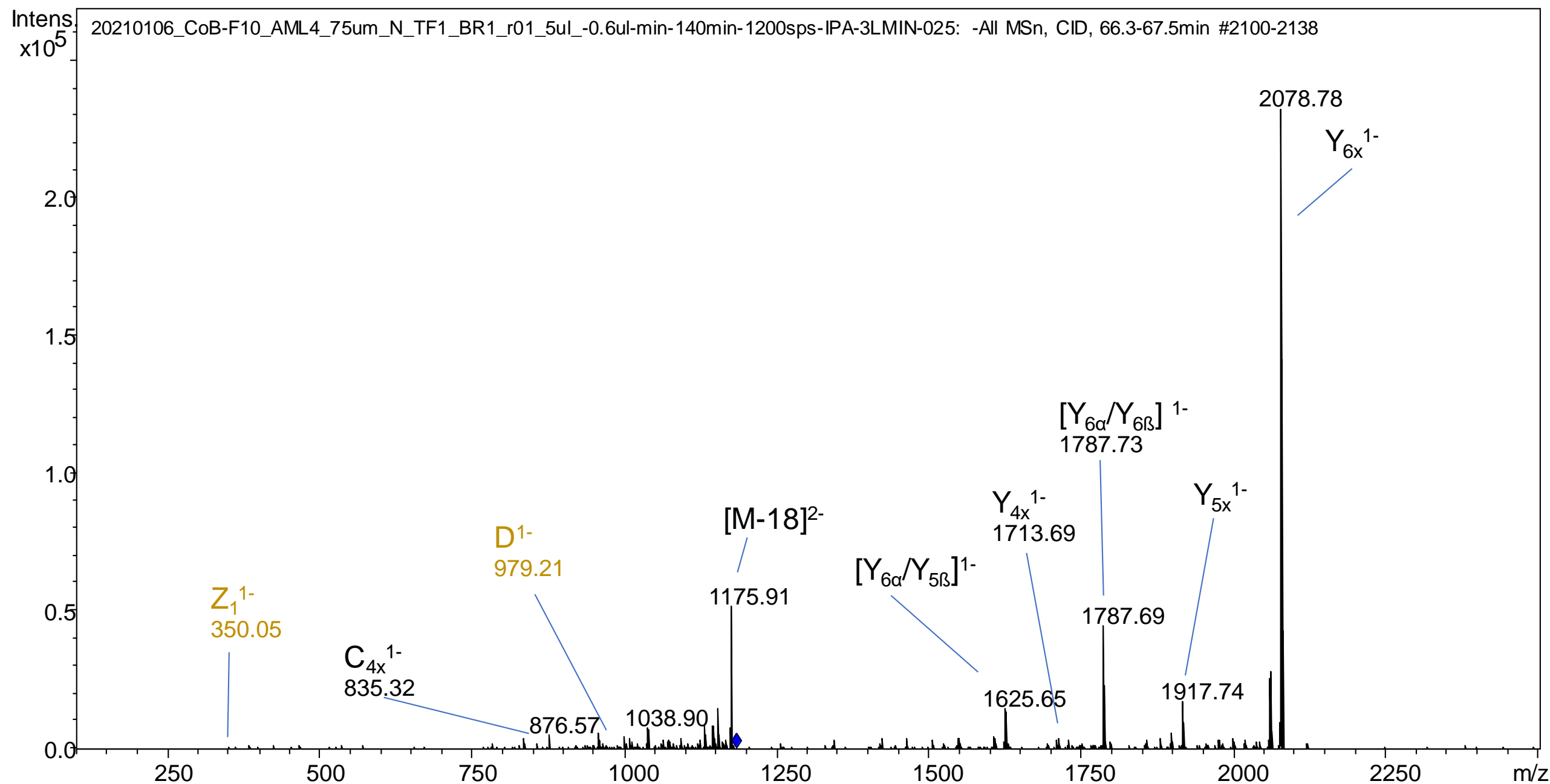
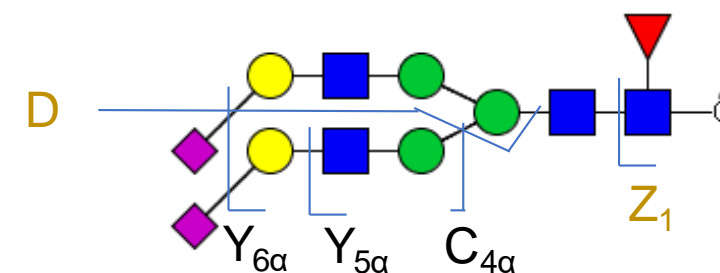
# Glycan 22c

H5N4S2F1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: TF-1

Monoisotopic mass: 2370.86 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1184.42  
Observed ion: *m/z* 1184.44  
Mass deviation: *m/z* 0.02  
Retention time: 66.6 min  
Note: Sialic acid linkages confirmed by  
neuraminidase S and A treatment

UniCarb-DB: #2563



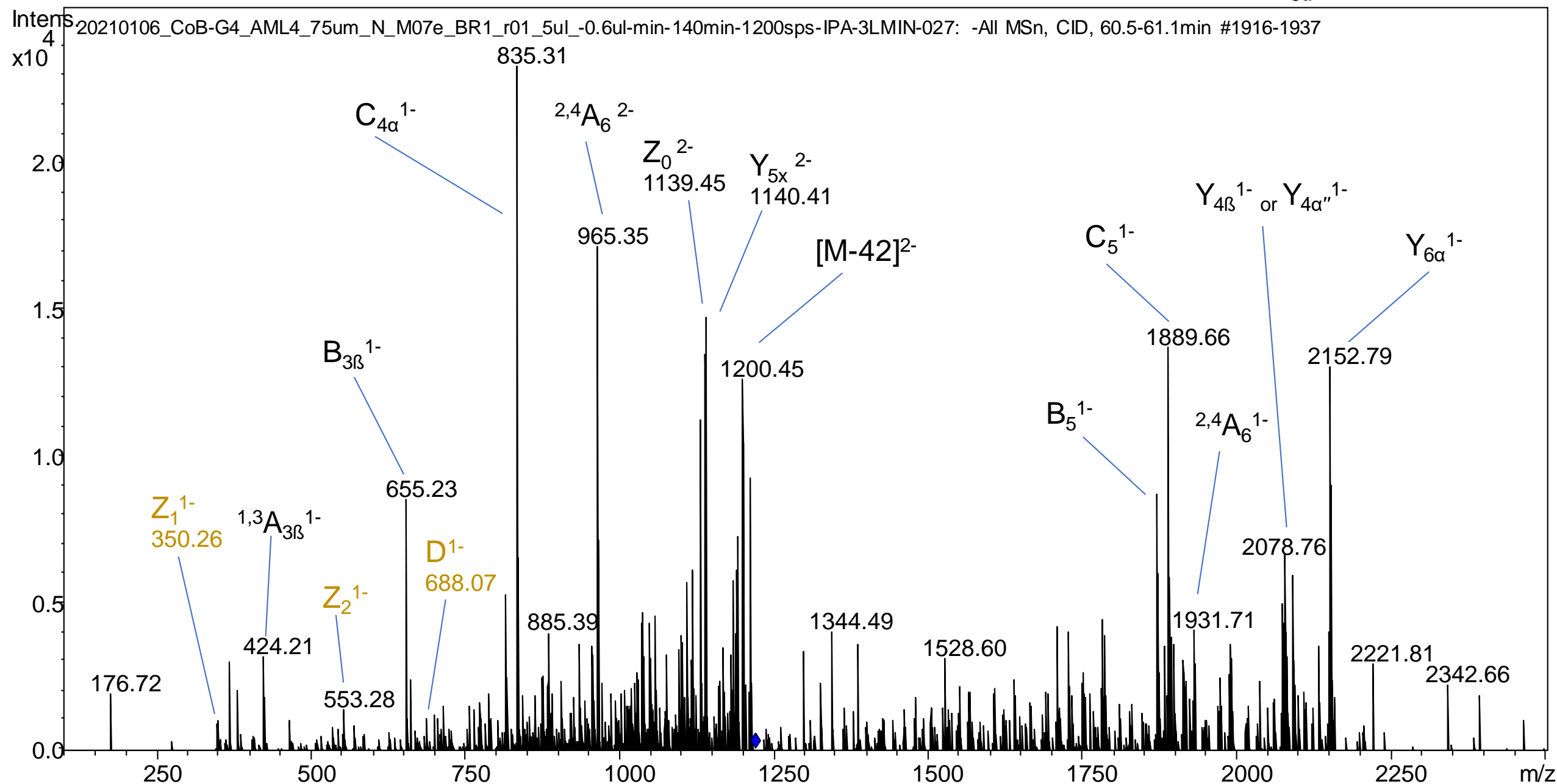
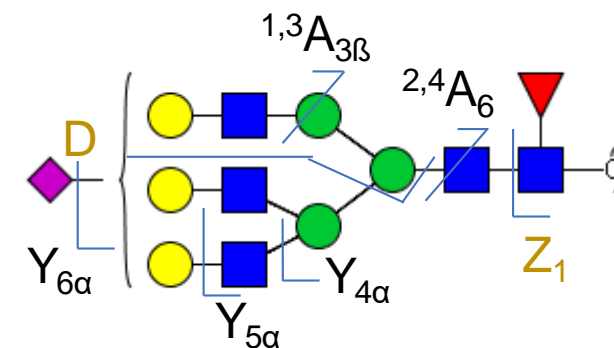
# Glycan 23

H6N5F1S1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: M-07e

Monoisotopic mass: 2444.89 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1221.45  
Observed ion: *m/z* 1221.45  
Mass deviation: *m/z* 0.00  
Retention time: 60.9 min  
Note:  $\alpha$ -2,6 sialic acid linkage confirmed by  
neuraminidase S and A treatment

UniCarb-DB: #2566

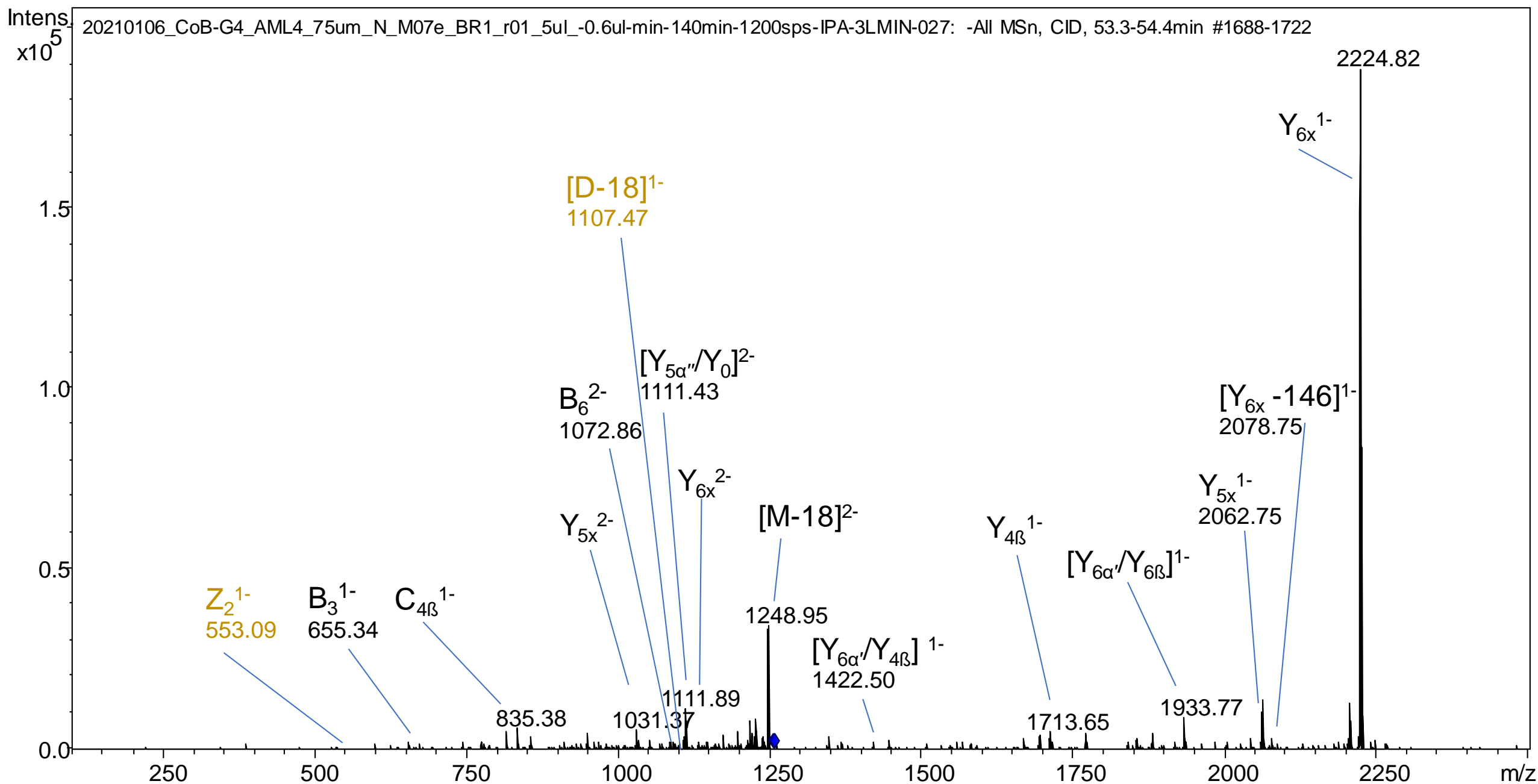
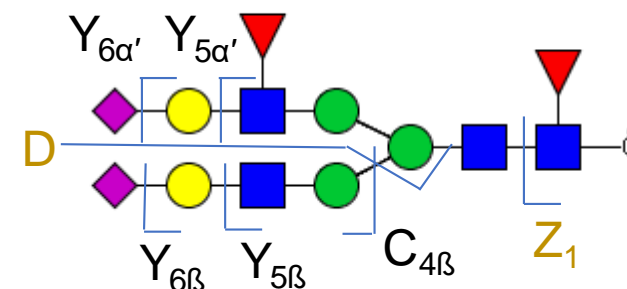


# Glycan 24a

H5N4S2F2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: M-07e

Monoisotopic mass: 2516.92 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1257.45  
Observed ion: *m/z* 1257.46  
Mass deviation: *m/z* 0.01  
Retention time: 53.4 min

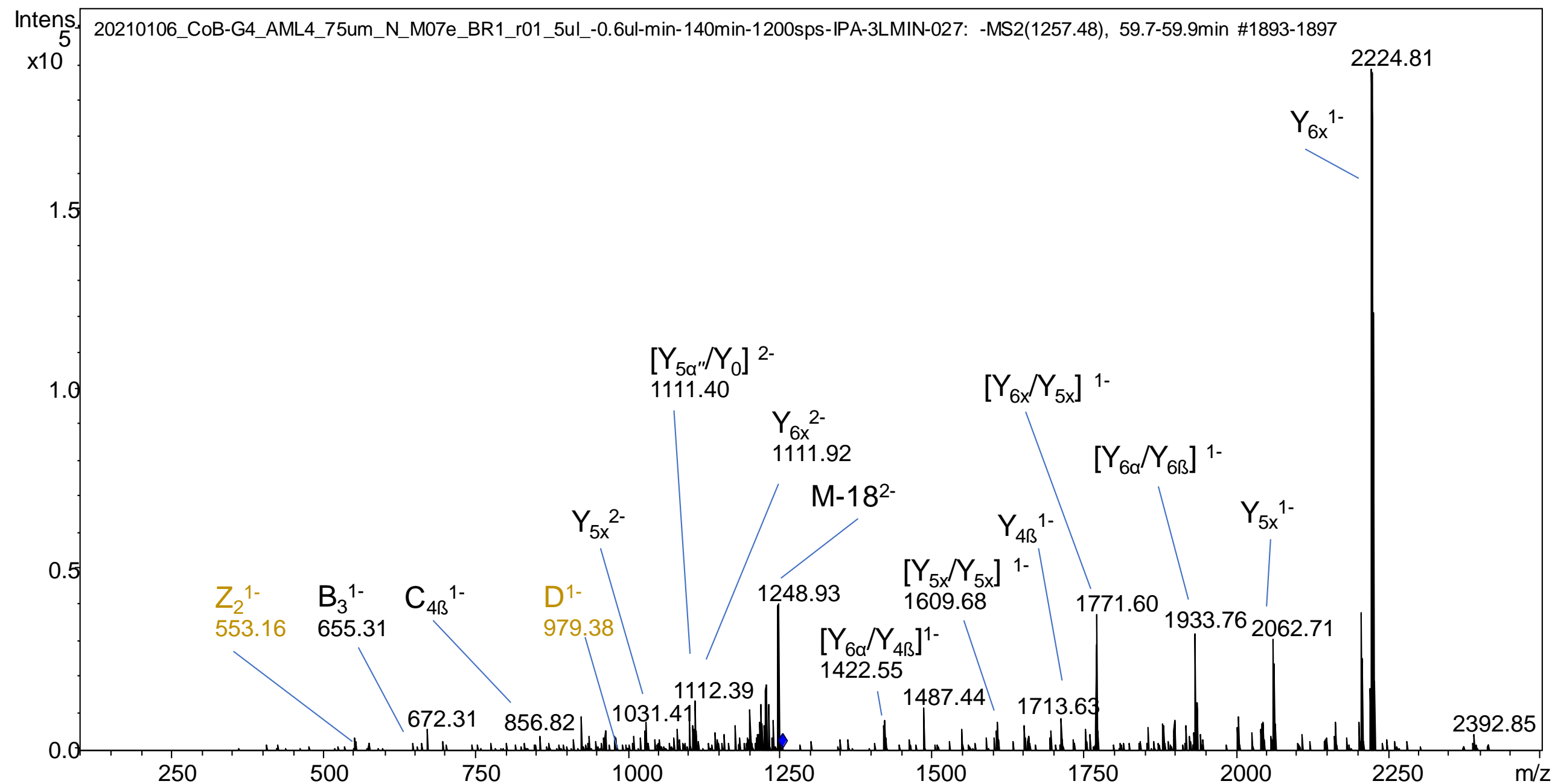
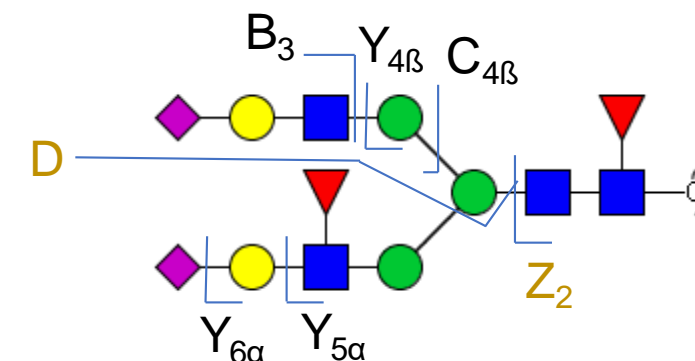


H5N4S2F2

Depicted MS<sup>2</sup> was obtained from analysis of cell line: M-07e

<b>Monoisotopic mass:</b>	<b>2516.92 Da</b>
<b>Charge observed:</b>	<b>2-</b>
<b>Theoretical ion:</b>	<b><i>m/z</i> 1257.45</b>
<b>Observed ion:</b>	<b><i>m/z</i> 1257.48</b>
<b>Mass deviation:</b>	<b><i>m/z</i> 0.03</b>
<b>Retention time:</b>	<b>59.9 min</b>

**UniCarb-DB: #2254**

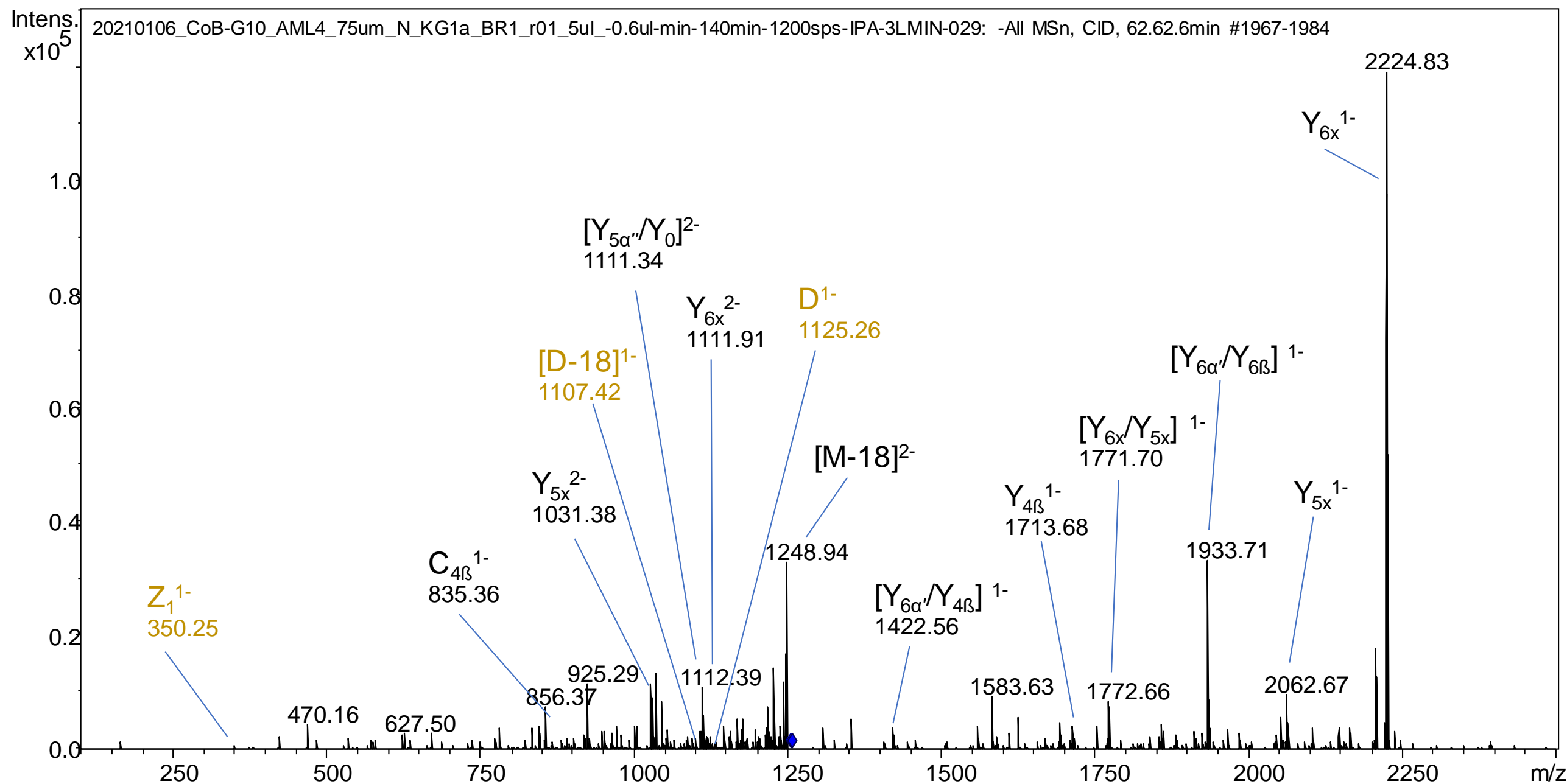
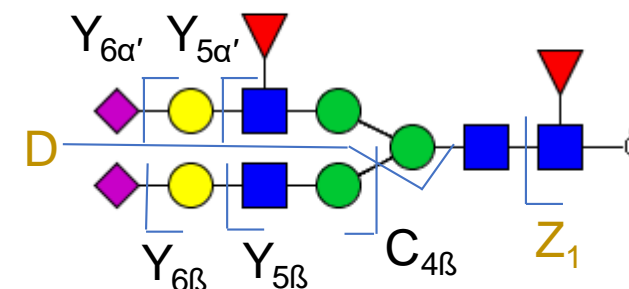


# Glycan 24c

H5N4S2F2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: KG-1a

Monoisotopic mass: 2516.92 Da  
Charge observed: 2-  
Theoretical ion:  $m/z$  1257.45  
Observed ion:  $m/z$  1257.46  
Mass deviation:  $m/z$  0.01  
Retention time: 62.1 min

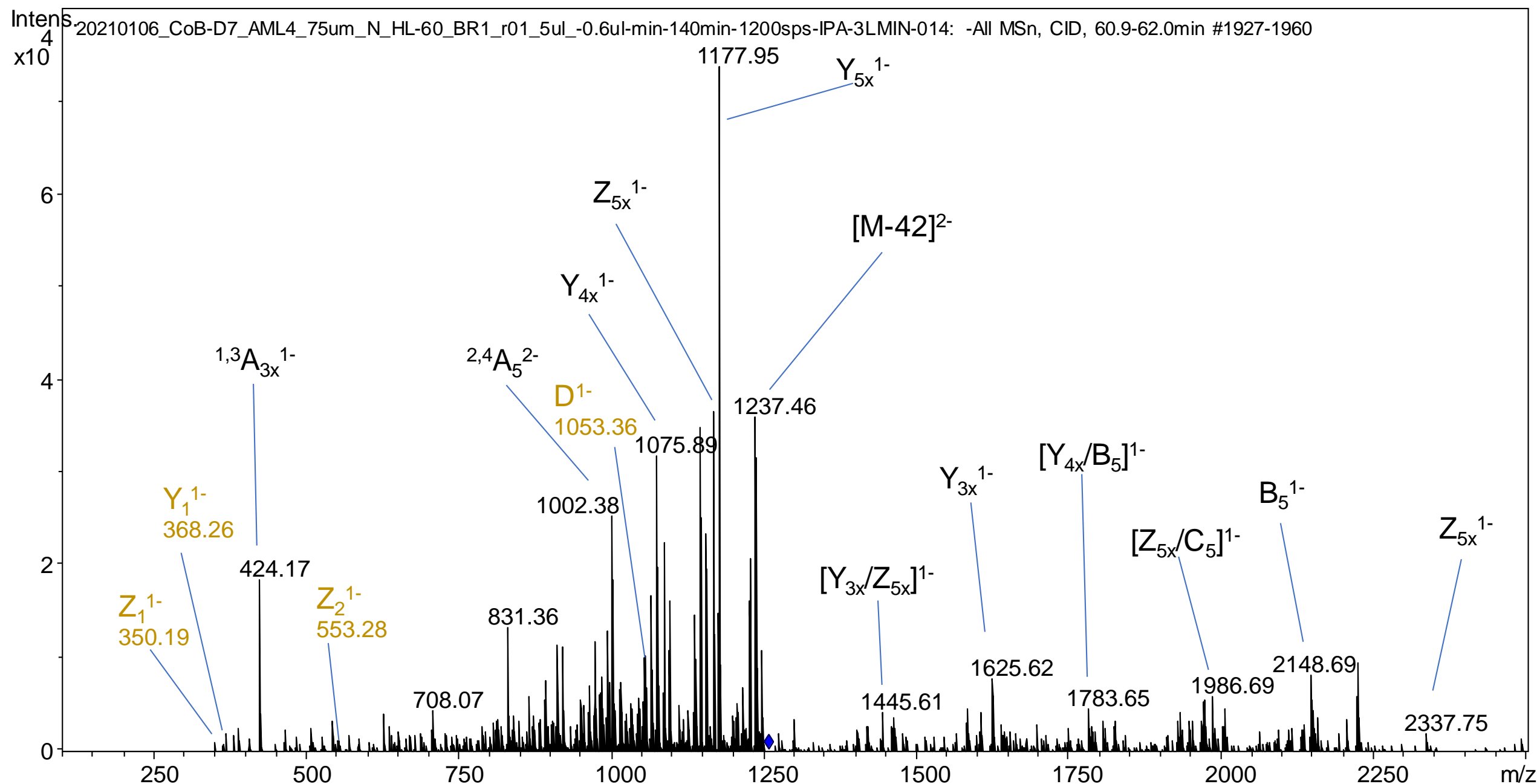
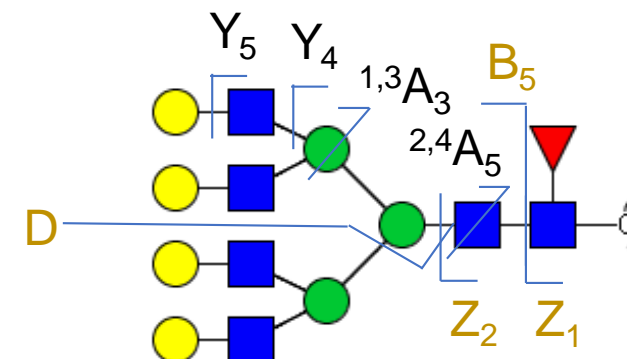


# H7N6F1

Depicted MS<sup>2</sup> was obtained from analysis of cell line: HL-60

<b>Monoisotopic mass:</b>	<b>2518.93 Da</b>
<b>Charge observed:</b>	<b>2-</b>
<b>Theoretical ion:</b>	<b><i>m/z</i> 1258.46</b>
<b>Observed ion:</b>	<b><i>m/z</i> 1258.45</b>
<b>Mass deviation:</b>	<b><i>m/z</i> 0.01</b>
<b>Retention time:</b>	<b>61.7 min</b>

**UniCarb-DB: #2417**



# Glycan 26a

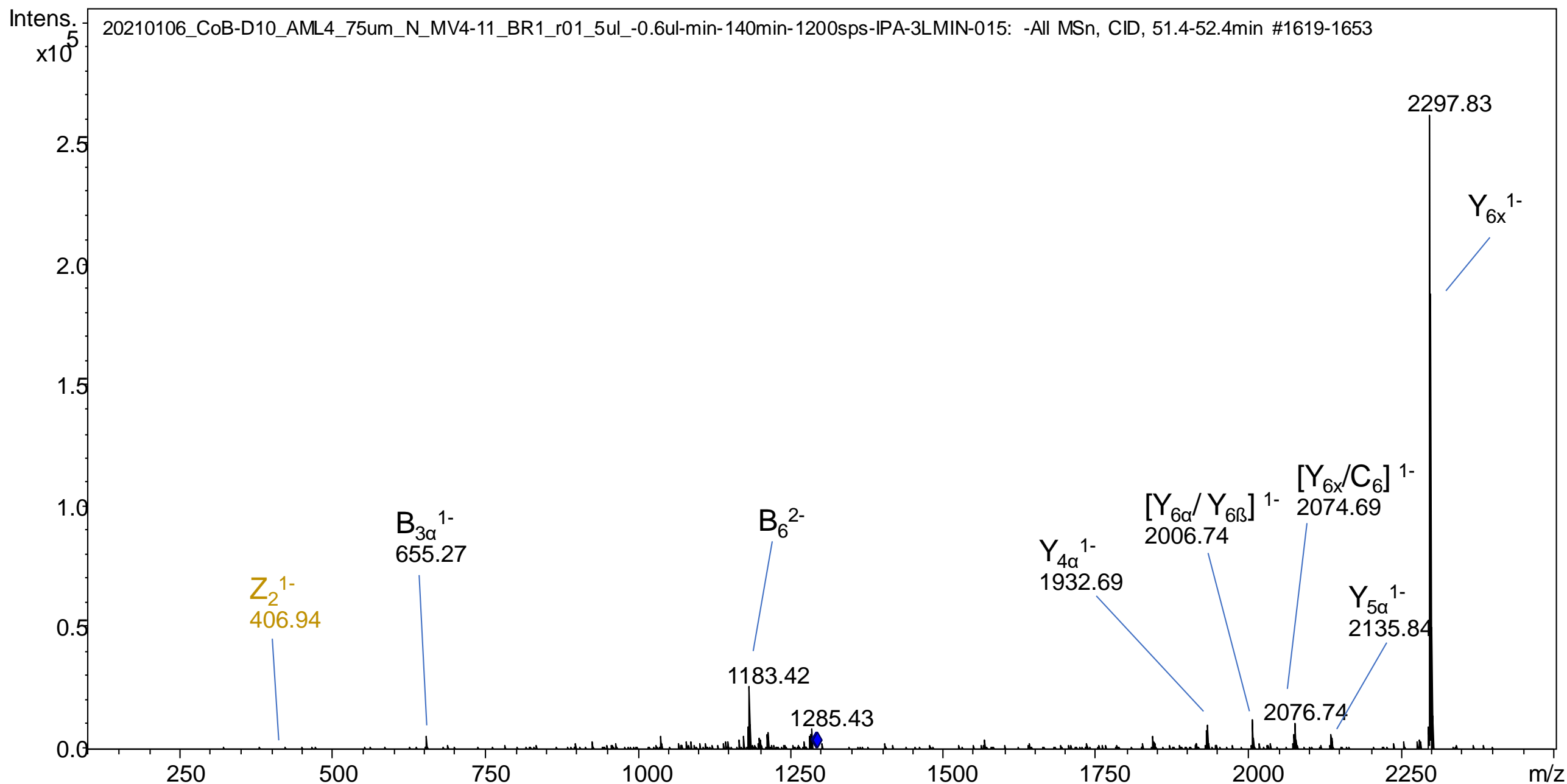
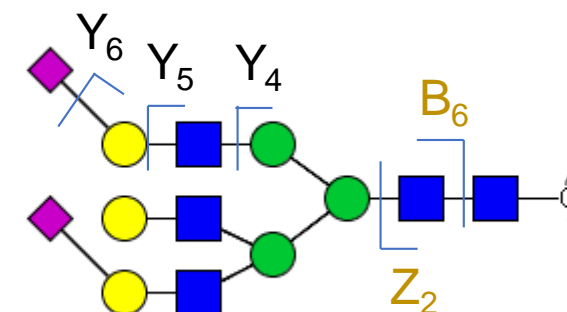
## H6N5S2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MV4-11

Monoisotopic mass: 2589.93 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1293.96  
Observed ion: *m/z* 1293.96  
Mass deviation: *m/z* 0.00  
Retention time: 51.4 min  
Note:  $\alpha$ -2,6 sialic acid linkages confirmed by  
neuraminidase S and A treatment

UniCarb-DB: #2420

*Retention time fits to  
glycan isomer identified in  
Fetuin standard (G.  
Palmisano et al. Rsc Adv,  
2013, 3, 22706-22726).*





# Glycan 26b

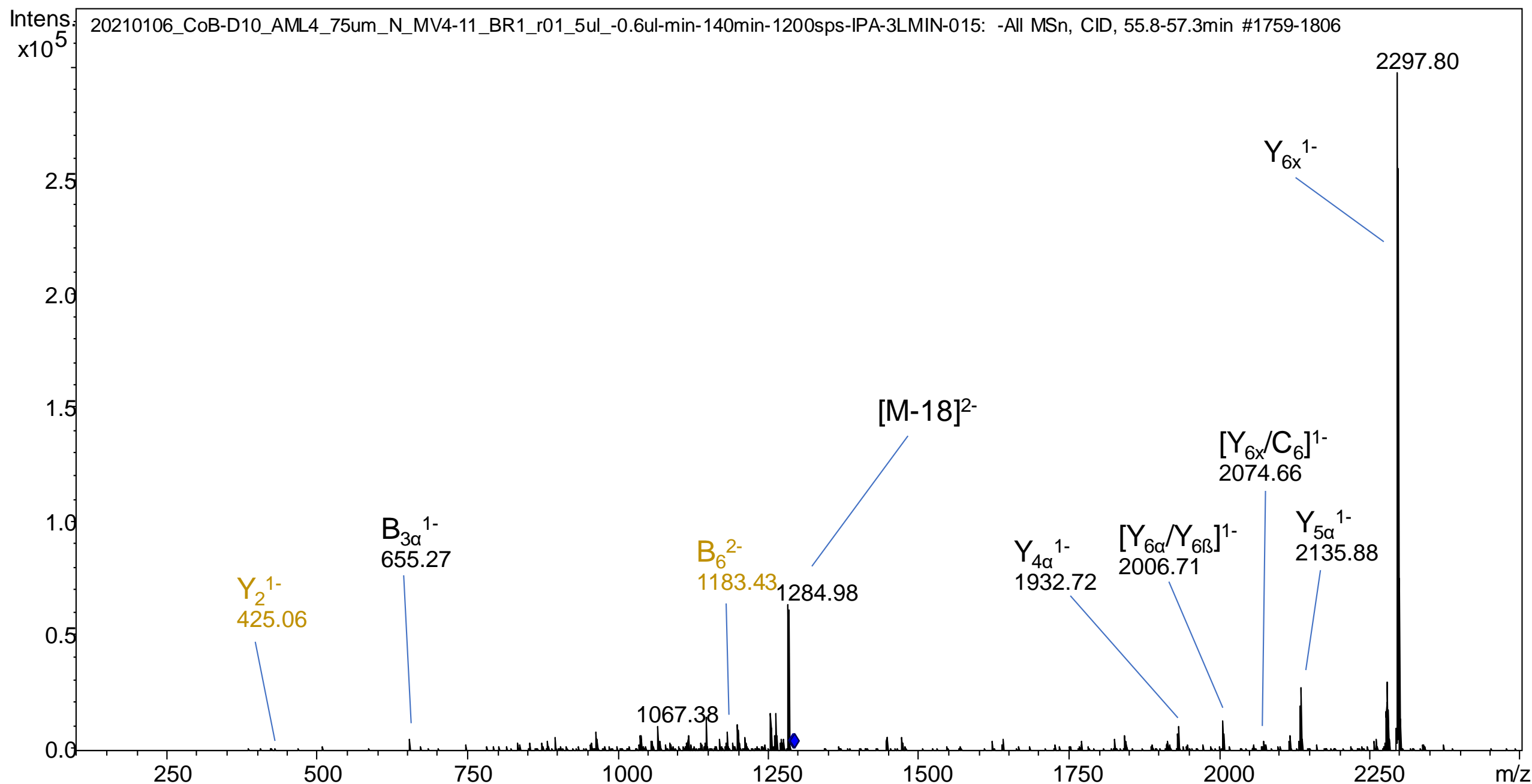
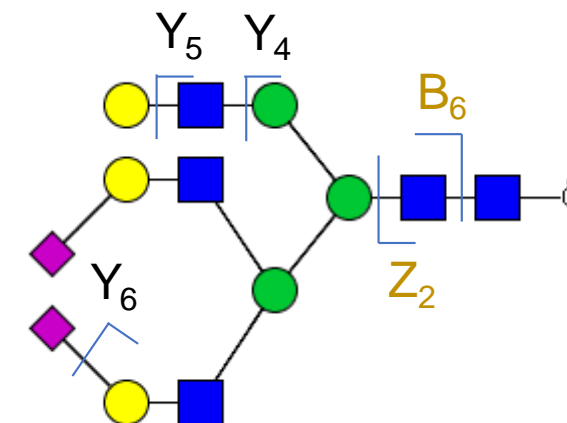
## H6N5S2

Depicted MS<sup>2</sup> was obtained from analysis of cell line: MV4-11

Monoisotopic mass: 2589.93 Da  
Charge observed: 2-  
Theoretical ion:  $m/z$  1293.96  
Observed ion:  $m/z$  1293.96  
Mass deviation:  $m/z$  0.00  
Retention time: 56.1 min  
Note: Sialic acid linkages confirmed by neuraminidase S and A treatment

UniCarb-DB: #2420

Retention time fits to glycan isomer identified in Fetuin standard (G. Palmisano et al. Rsc Adv, 2013, 3, 22706-22726).

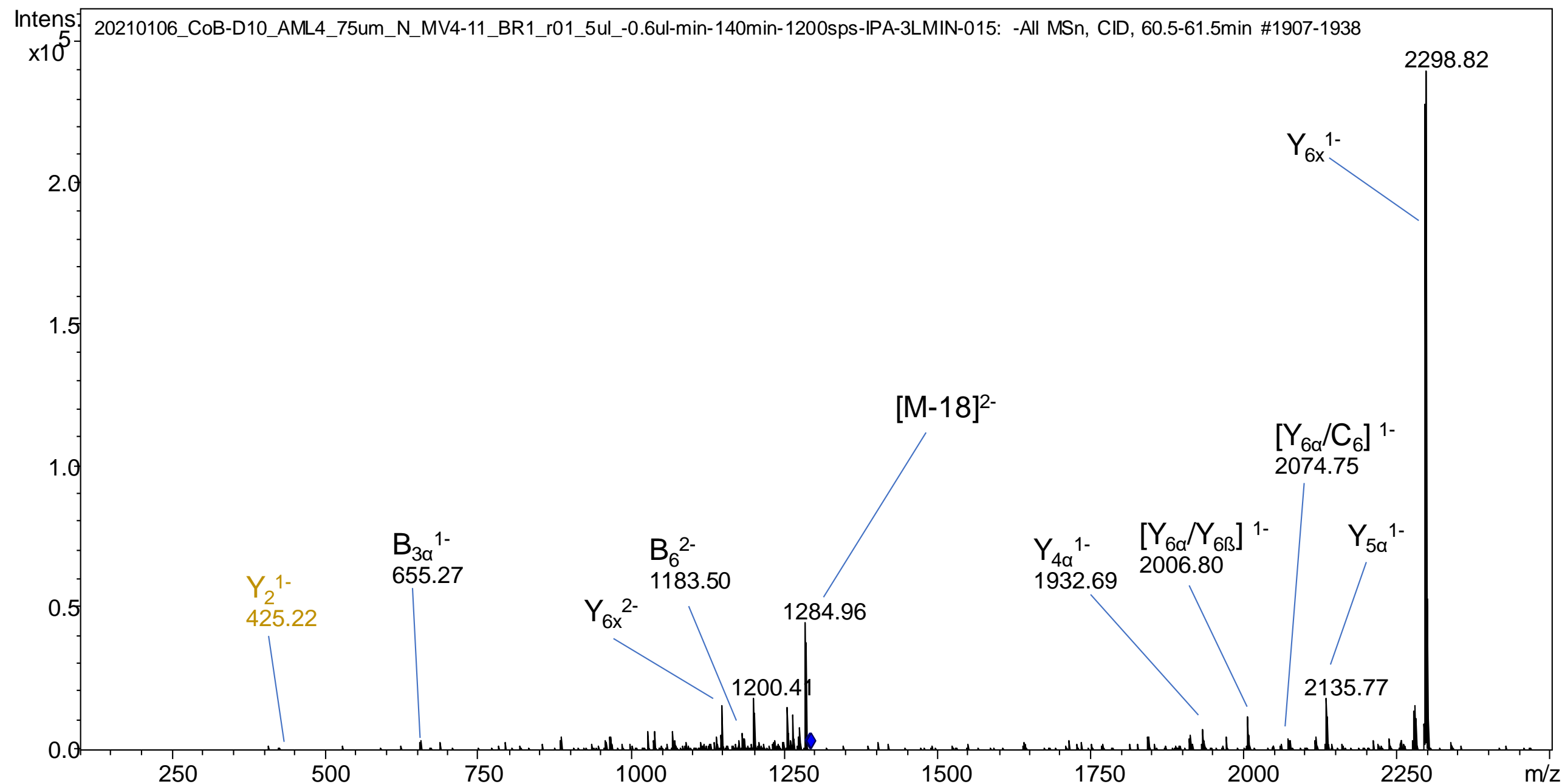
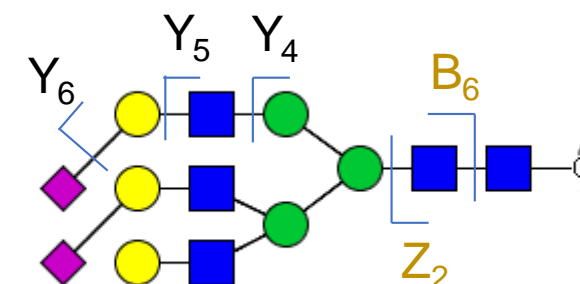


## H6N5S2

**Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MV4-11**

**Monoisotopic mass:** 2589.93 Da  
**Charge observed:** 2-  
**Theoretical ion:** *m/z* 1293.96  
**Observed ion:** *m/z* 1293.95  
**Mass deviation:** *m/z* 0.01  
**Retention time:** 60.5 min  
**Note:** α-2,3 sialic acid linkages confirmed by neuraminidase S and A treatment

***Retention time fits to glycan isomer identified in Fetuin standard (G. Palmisano et al. Rsc Adv, 2013, 3, 22706-22726).***

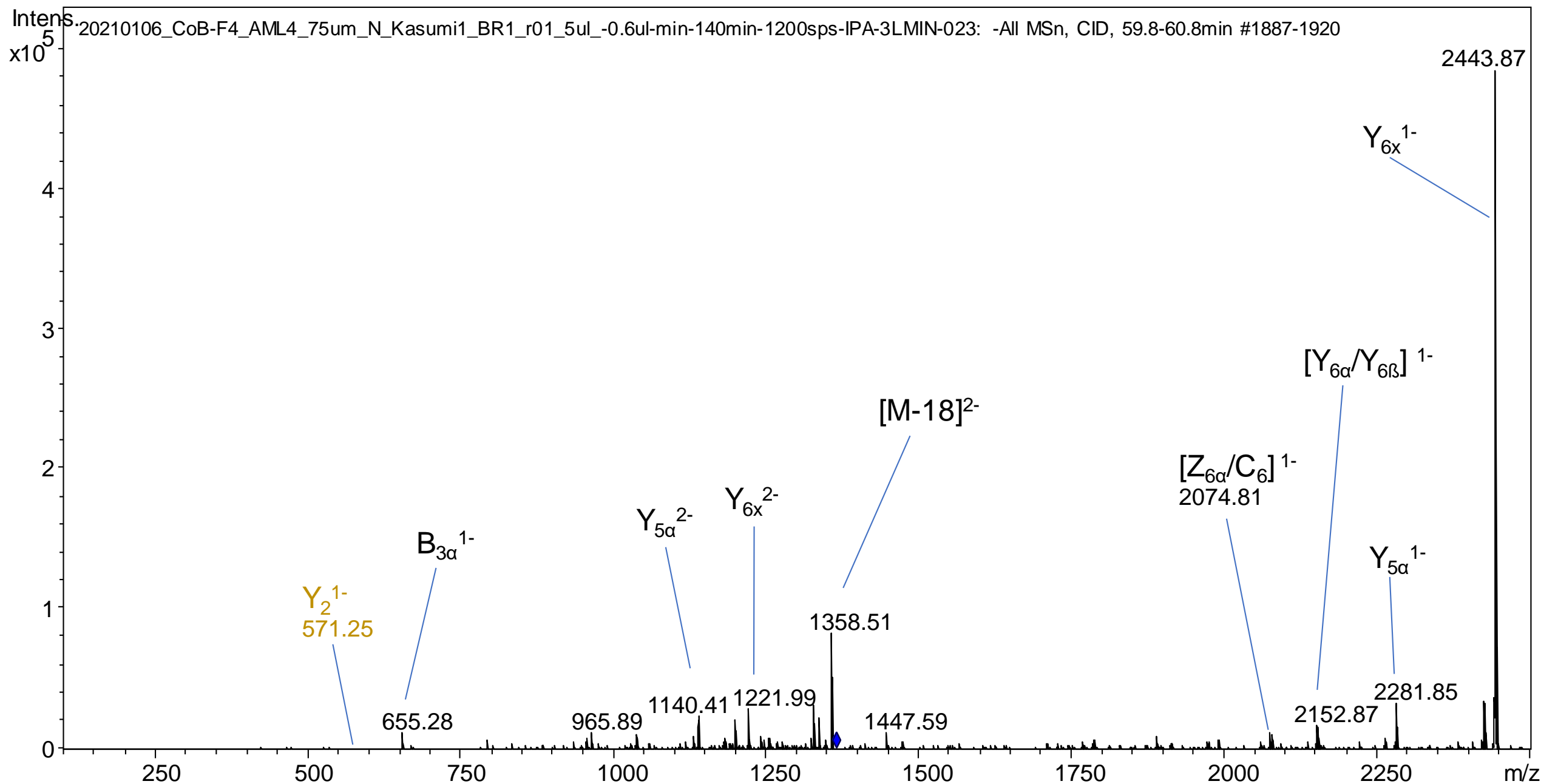
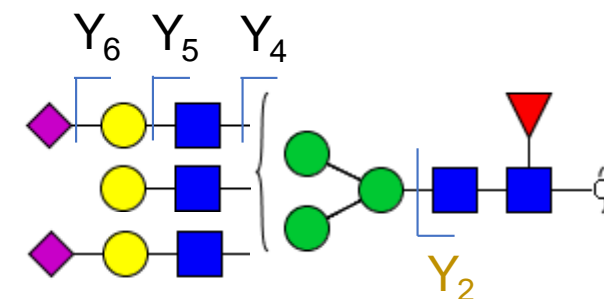


# Glycan 27a

H6N5F1S2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: Kasumi-1

Monoisotopic mass: 2589.93 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1366.99  
Observed ion: *m/z* 1366.98  
Mass deviation: *m/z* 0.01  
Retention time: 60.0 min

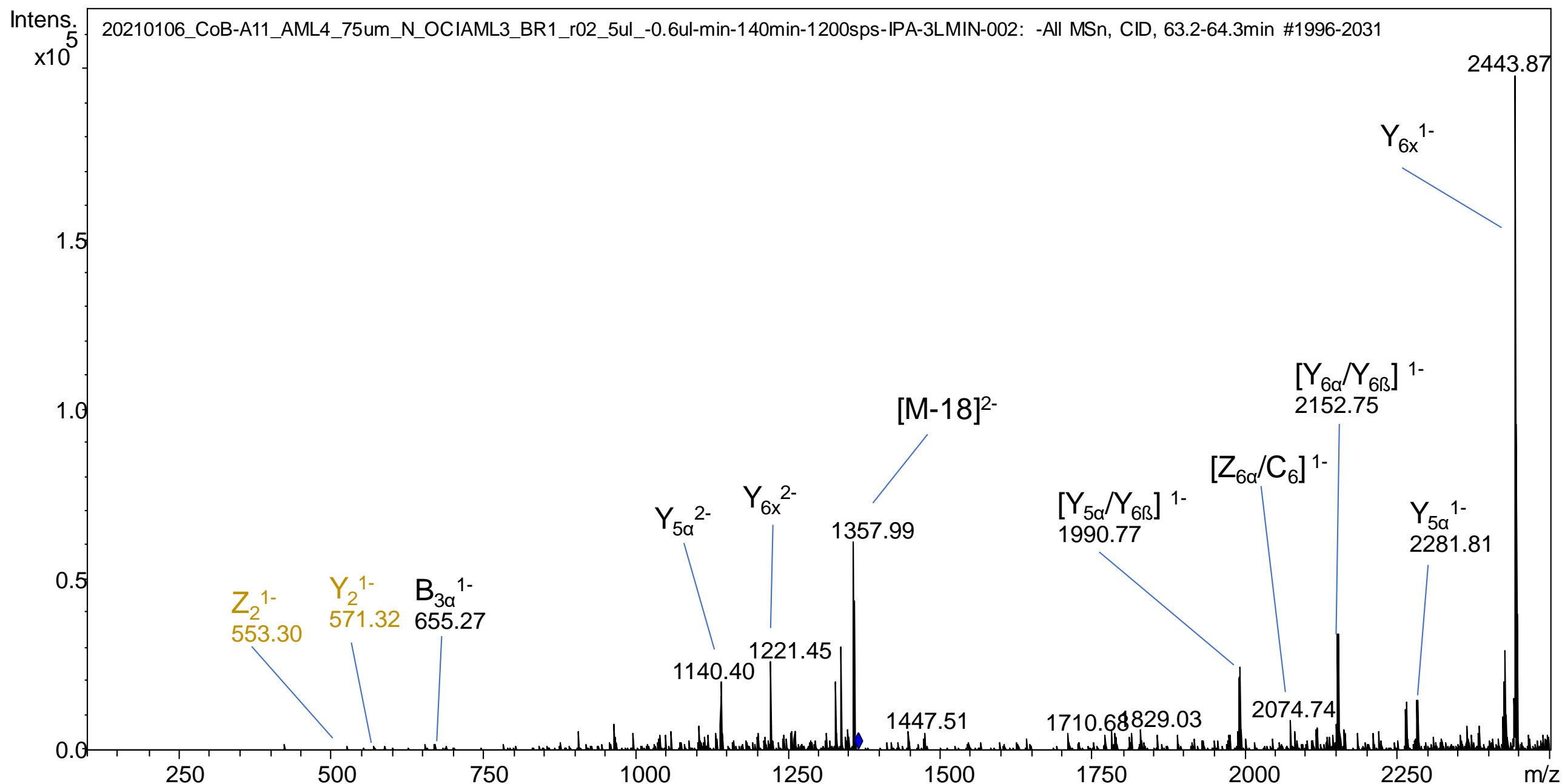
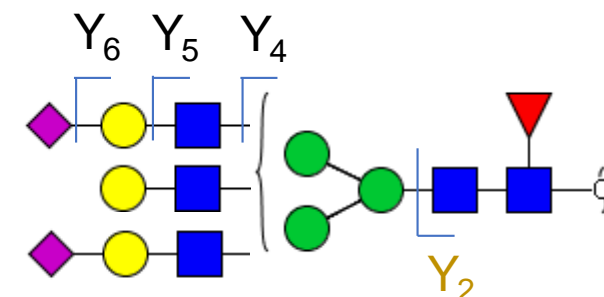


# Glycan 27b

H6N5F1S2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: OCI-AML-3

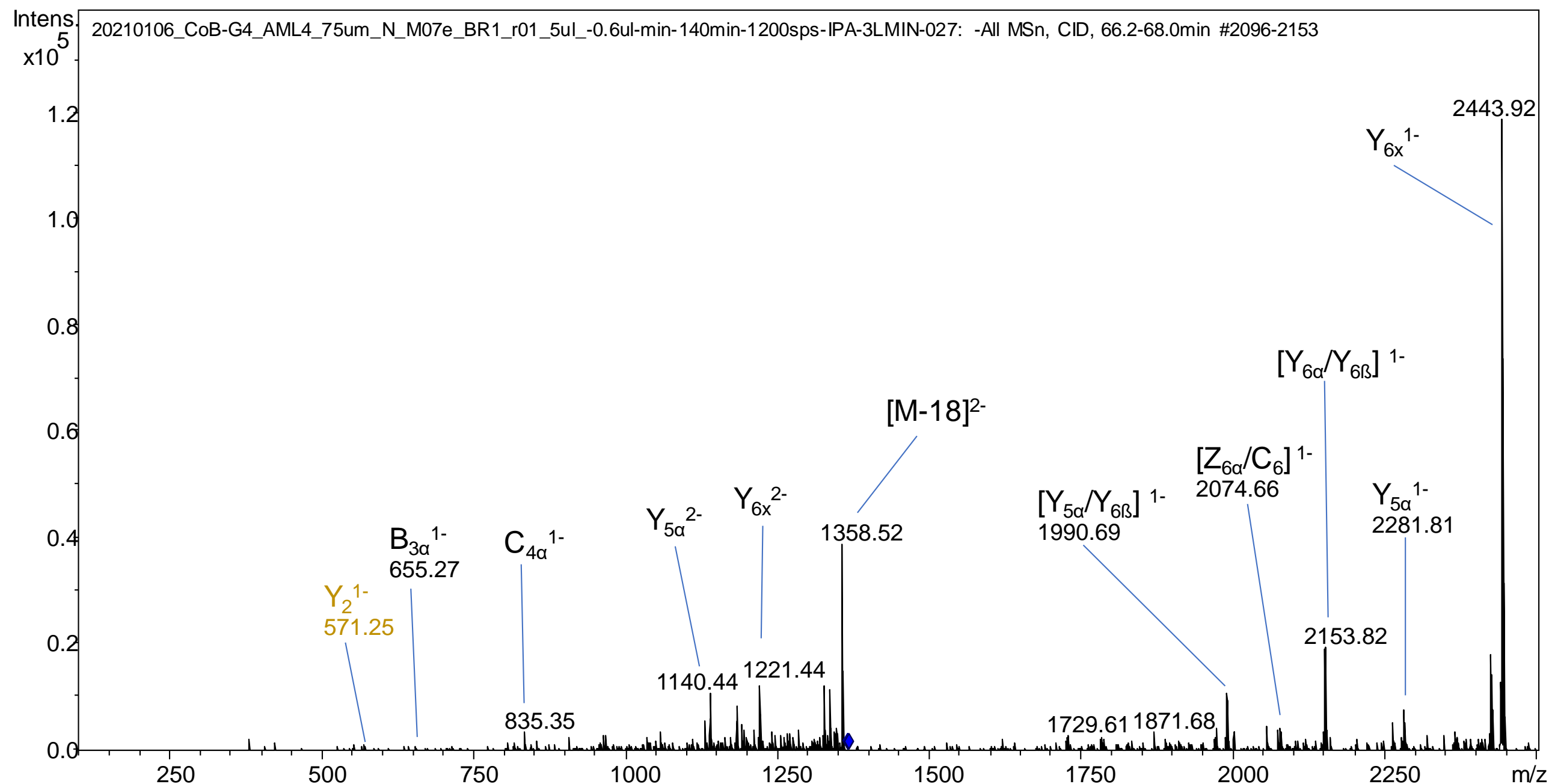
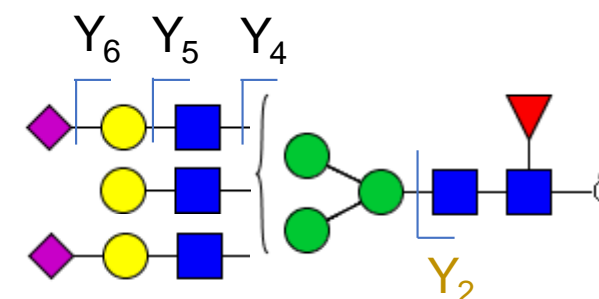
Monoisotopic mass: 2589.93 Da  
Charge observed: 2-  
Theoretical ion:  $m/z$  1366.99  
Observed ion:  $m/z$  1367.00  
Mass deviation:  $m/z$  0.01  
Retention time: 63.4 min



H6N5F1S2

Depicted MS<sup>2</sup> was obtained from analysis of cell line: M-07e

<b>Monoisotopic mass:</b>	<b>2735.99 Da</b>
<b>Charge observed:</b>	<b>2-</b>
<b>Theoretical ion:</b>	<b><i>m/z</i> 1366.99</b>
<b>Observed ion:</b>	<b><i>m/z</i> 1366.98</b>
<b>Mass deviation:</b>	<b><i>m/z</i> 0.02</b>
<b>Retention time:</b>	<b>66.5 min</b>



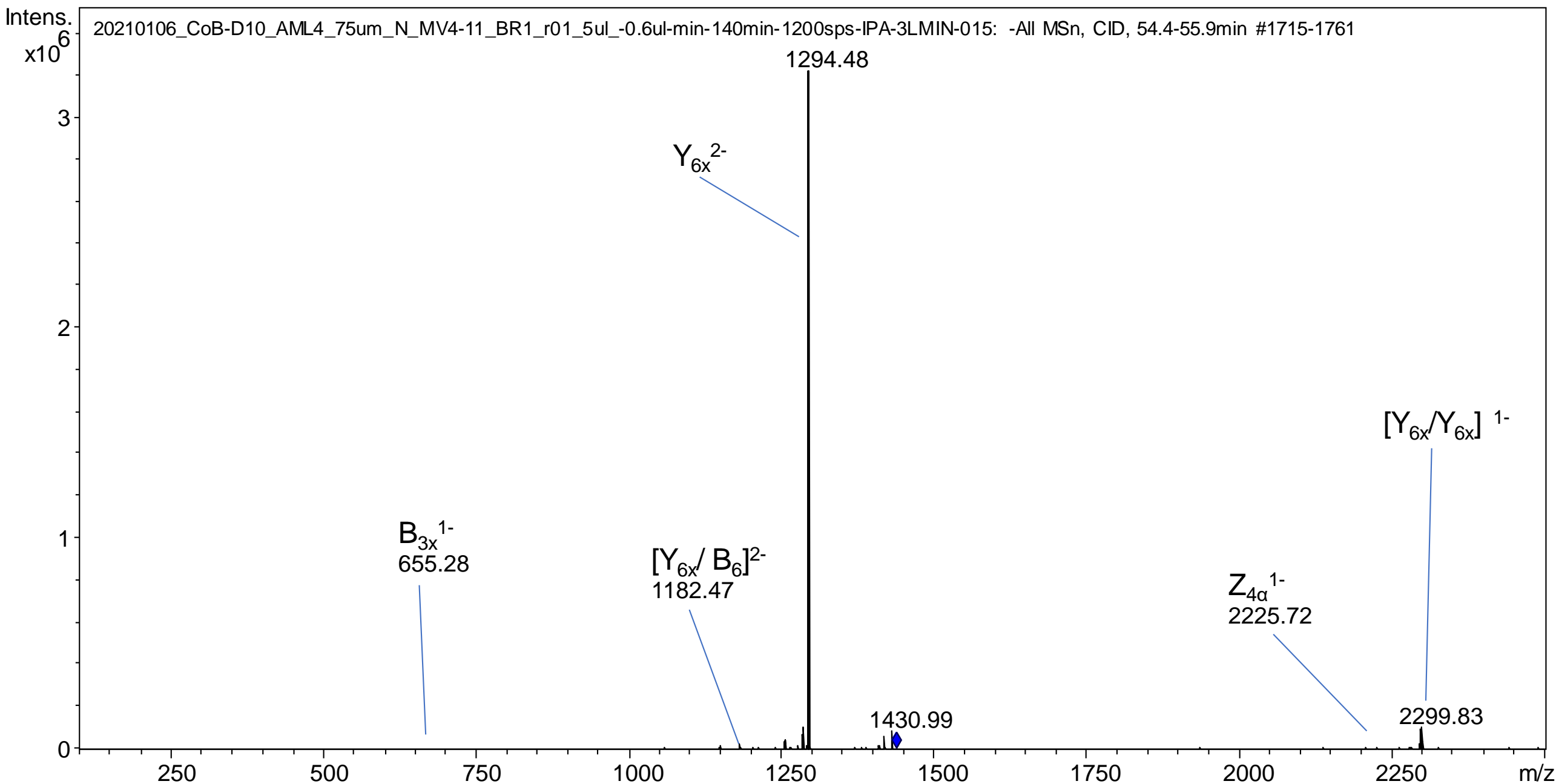
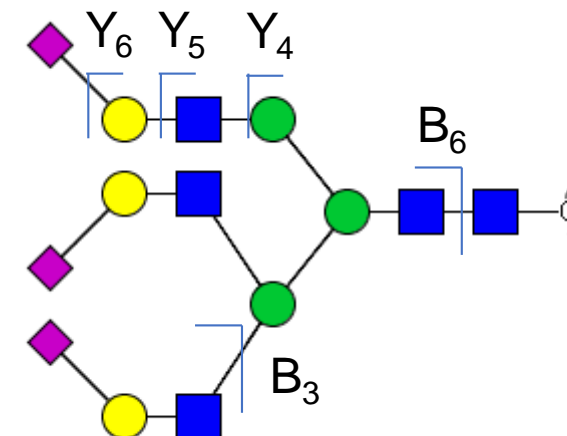
# Glycan 28a

H6N5S3

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MV4-11

Monoisotopic mass: 2881.03 Da  
Charge observed: 2-  
Theoretical ion:  $m/z$  1439.51  
Observed ion:  $m/z$  1439.51  
Mass deviation:  $m/z$  0.00  
Retention time: 54.7 min

Retention time fits to  
glycan isomer identified in  
Fetuin standard (G.  
Palmisano et al. Rsc Adv,  
2013, 3, 22706-22726).



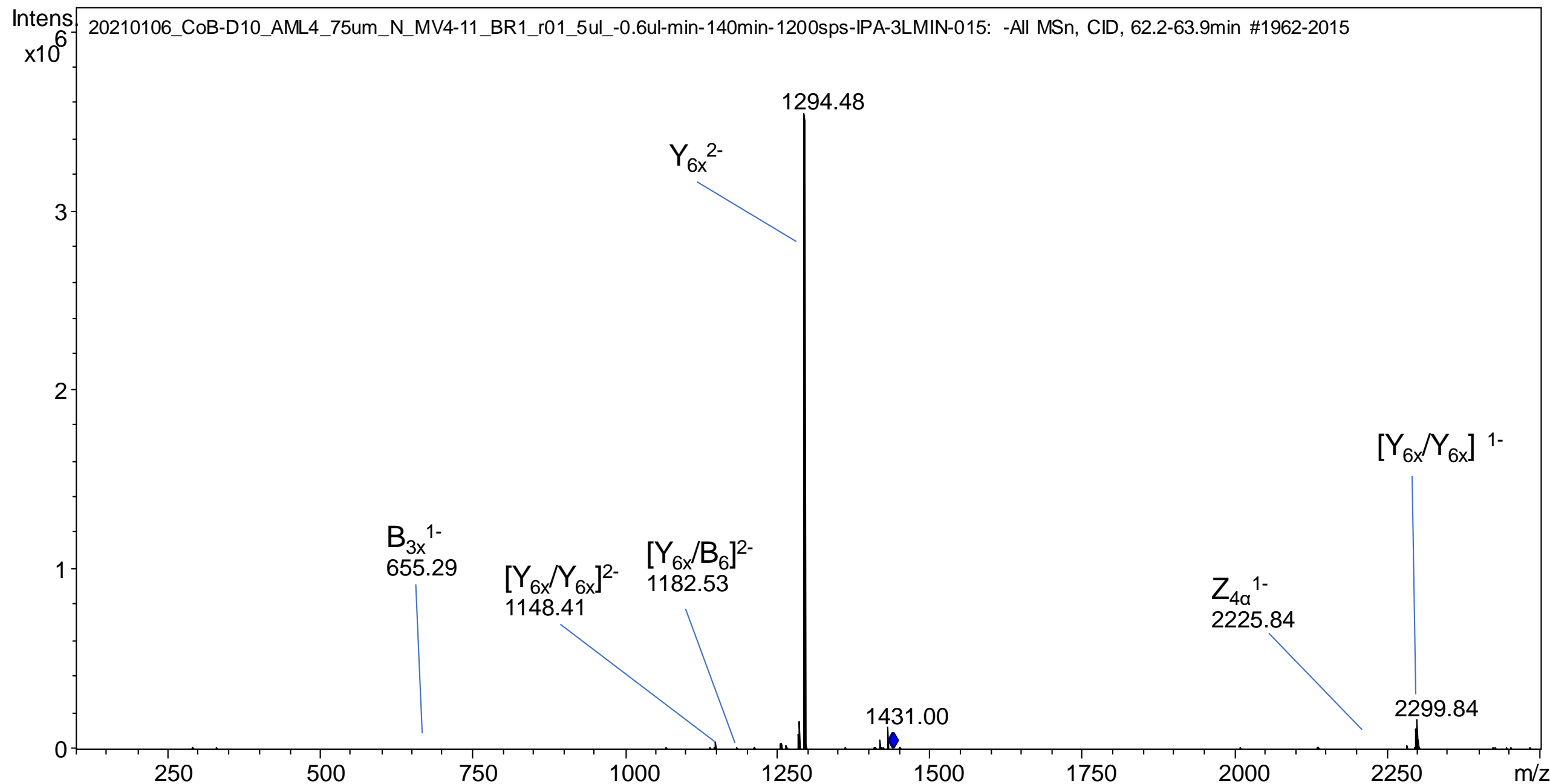
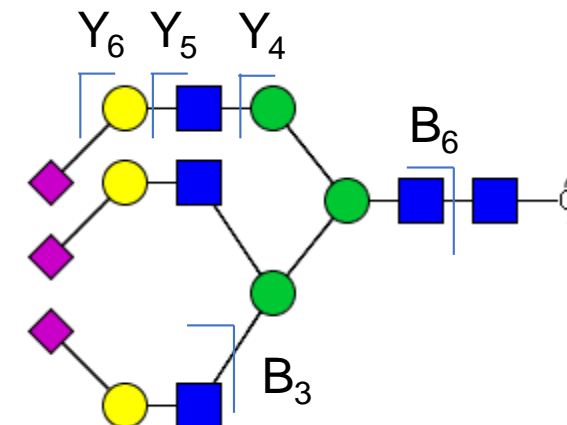
# Glycan 28b

H6N5S3

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MV4-11

Monoisotopic mass: 2881.03 Da  
Charge observed: 2-  
Theoretical ion:  $m/z$  1439.51  
Observed ion:  $m/z$  1439.51  
Mass deviation:  $m/z$  0.00  
Retention time: 62.8 min

Retention time fits to  
glycan isomer identified in  
Fetuin standard (G.  
Palmisano et al. Rsc Adv,  
2013, 3, 22706-22726).

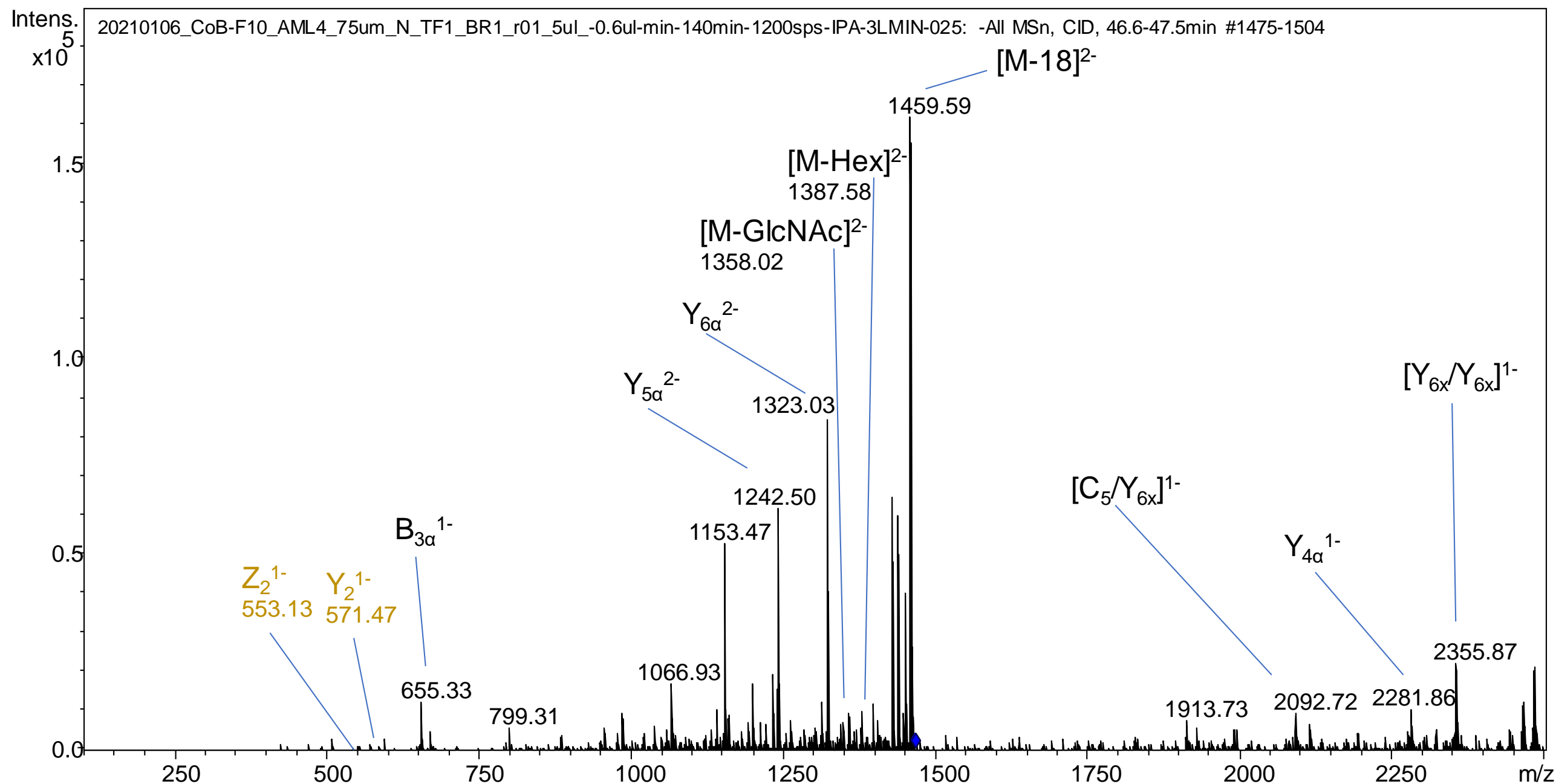
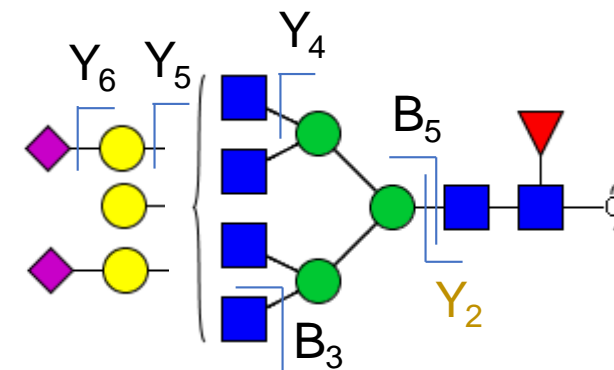


# Glycan 29a

H6N6F1S2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: TF-1

Monoisotopic mass: 2939.07 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1468.53  
Observed ion: *m/z* 1468.53  
Mass deviation: *m/z* 0.00  
Retention time: 46.6 min



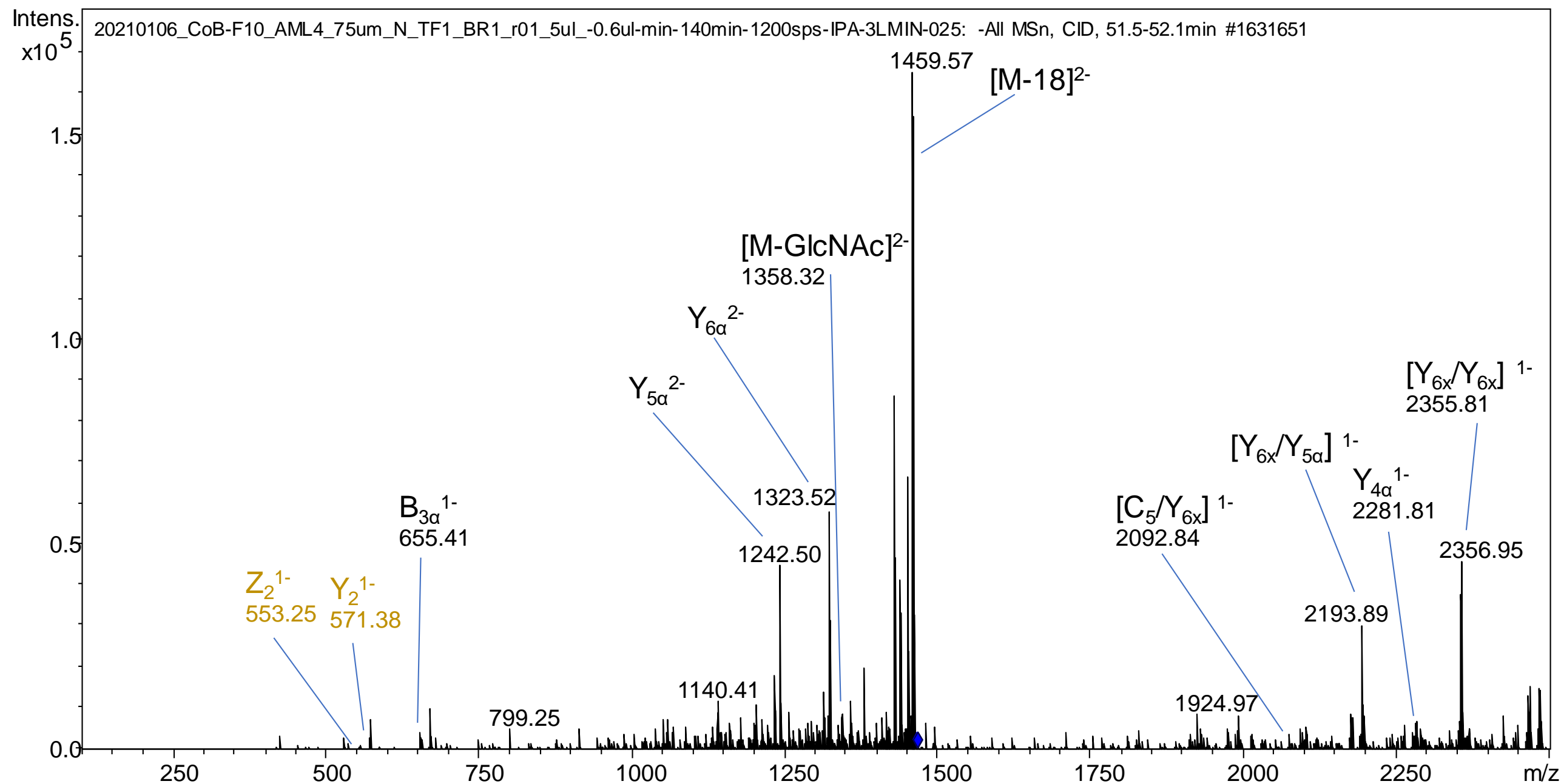
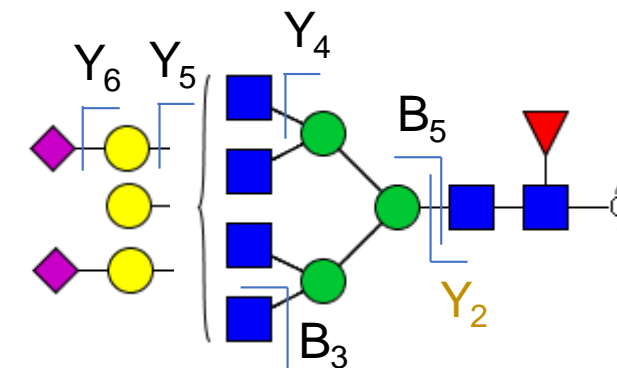


# Glycan 29b

H6N6F1S2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: TF-1

Monoisotopic mass: 2939.07 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1468.53  
Observed ion: *m/z* 1468.53  
Mass deviation: *m/z* 0.00  
Retention time: 51.5 min

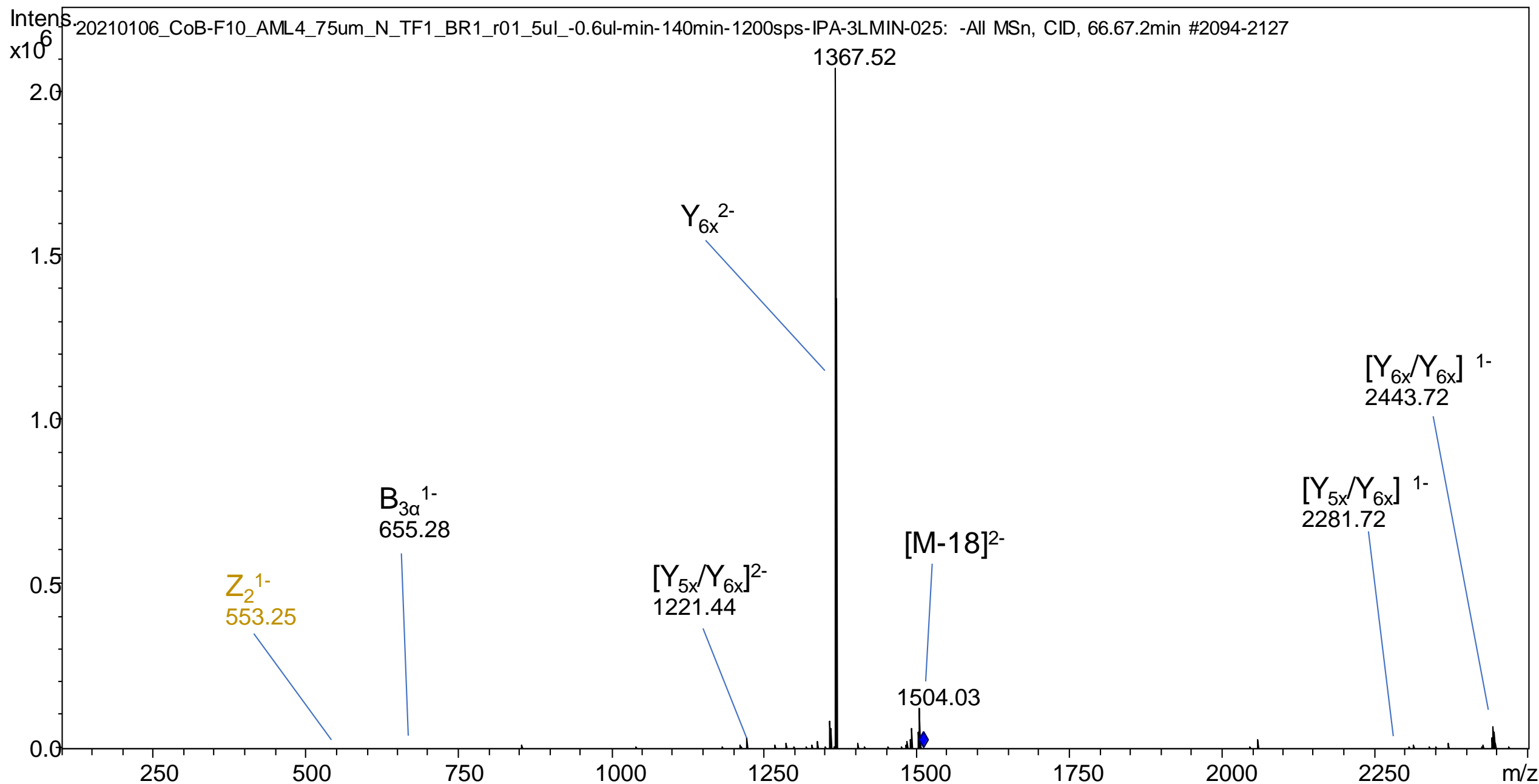
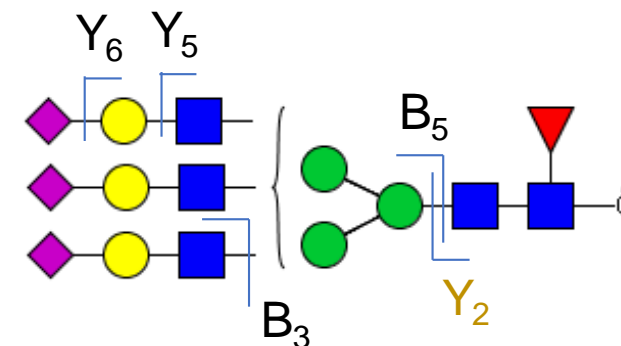


# Glycan 30a

H6N5F1S3

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: TF-1

Monoisotopic mass: 3027.08 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1512.54  
Observed ion: *m/z* 1512.52  
Mass deviation: *m/z* 0.02  
Retention time: 66.5 min

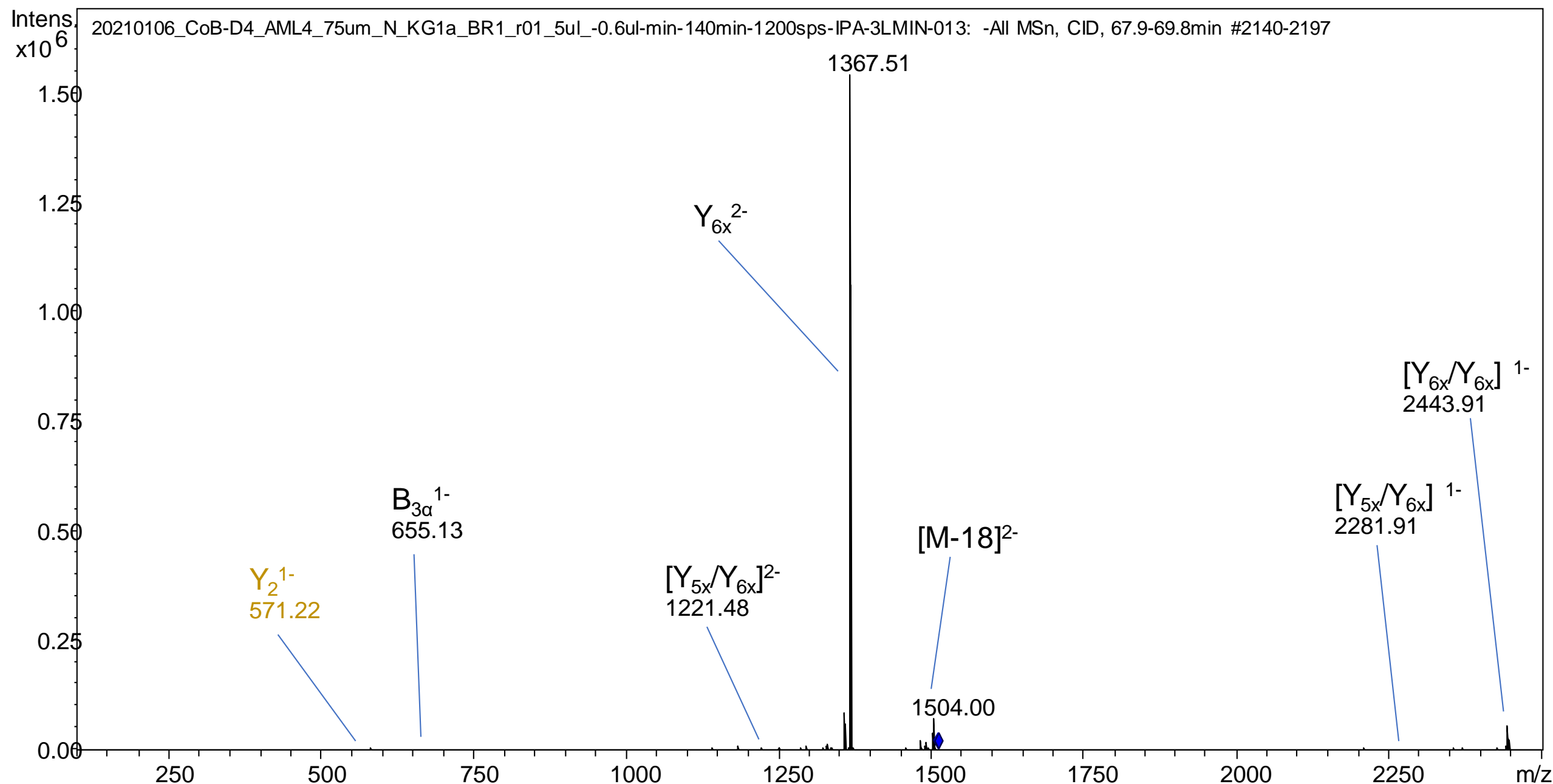
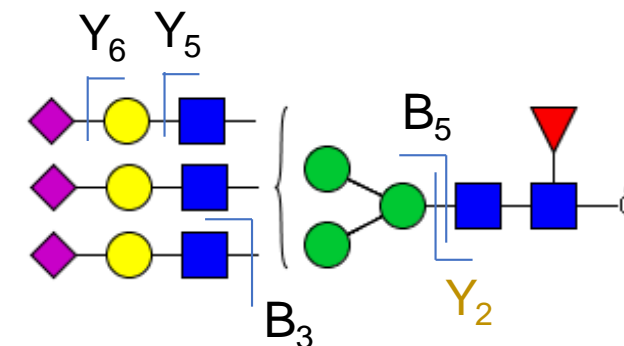


# Glycan 30b

H6N5F1S3

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: KG-1a

Monoisotopic mass: 3027.08 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1512.54  
Observed ion: *m/z* 1512.53  
Mass deviation: *m/z* 0.01  
Retention time: 68.1 min



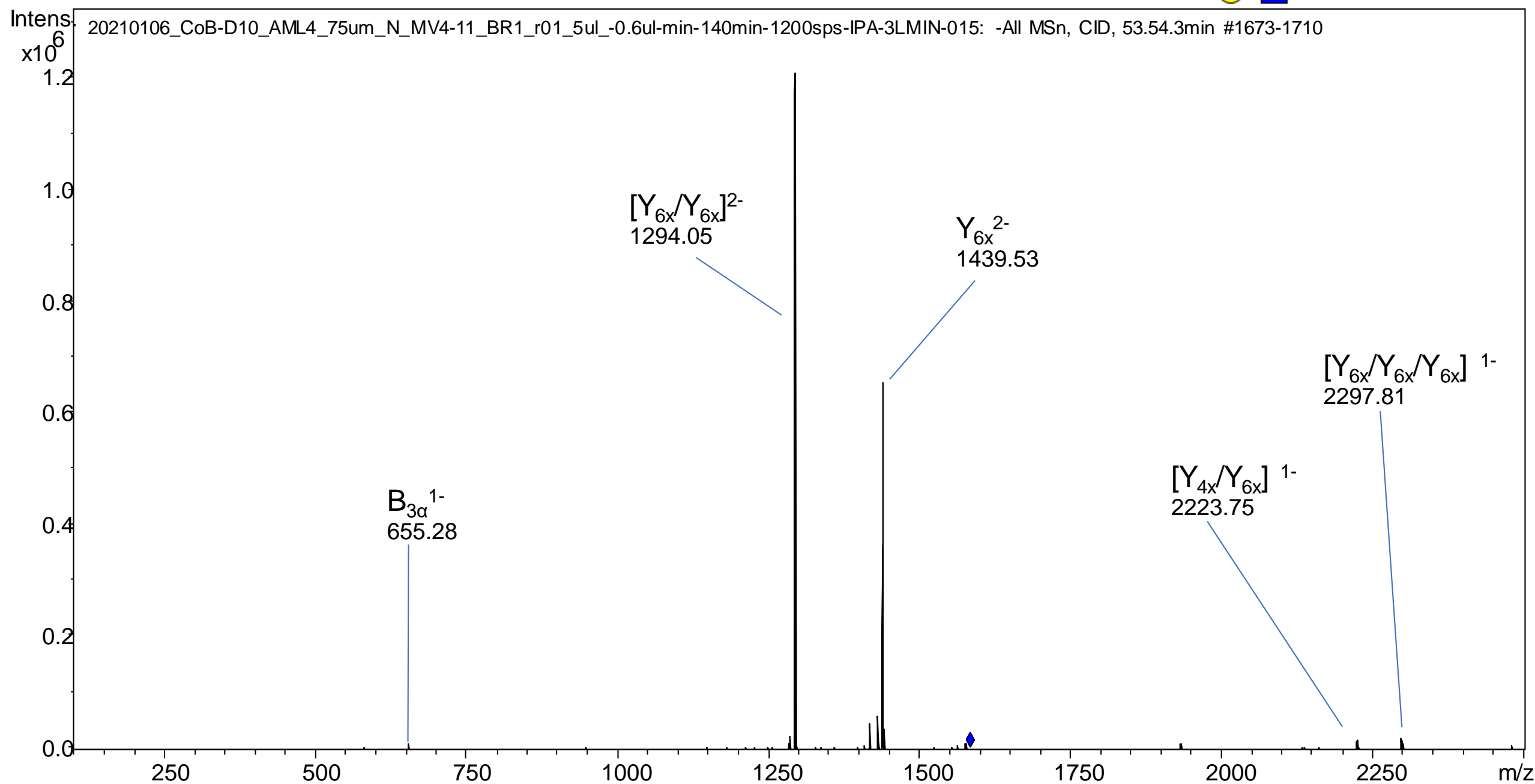
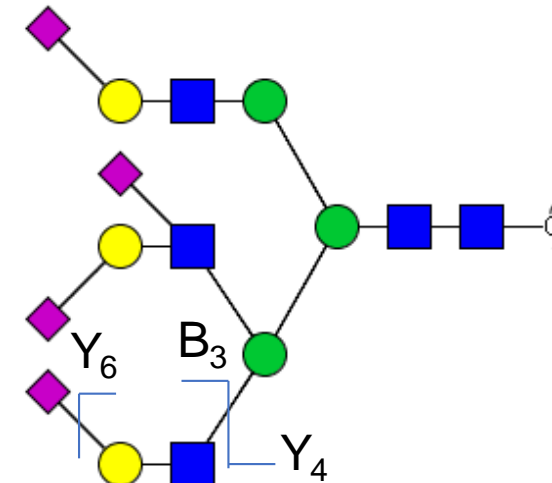
# Glycan 31a

H6N5S4

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MV4-11

Monoisotopic mass: 3172.12 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1585.05  
Observed ion: *m/z* 1585.05  
Mass deviation: *m/z* 0.00  
Retention time: 53.4 min

*Retention time fits to  
glycan isomer identified in  
Fetuin standard (G.  
Palmisano et al. Rsc Adv,  
2013, 3, 22706-22726).*



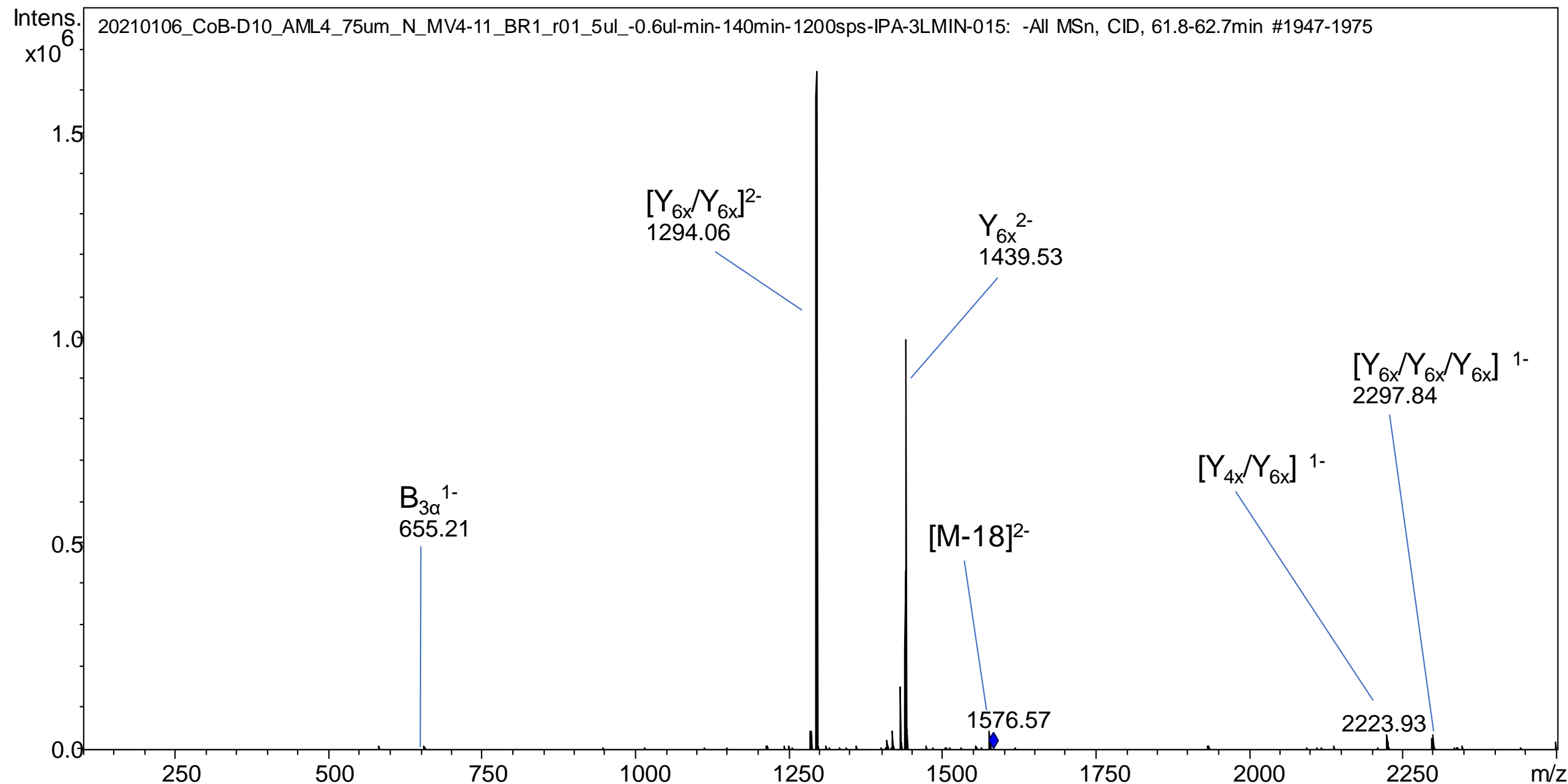
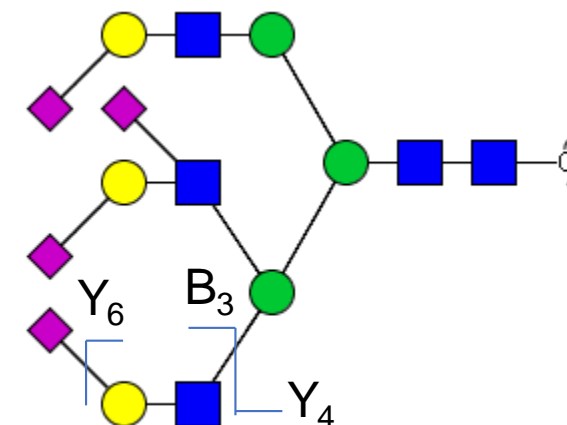
# Glycan 31b

H6N5S4

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MV4-11

Monoisotopic mass: 3172.12 Da  
Charge observed: 2-  
Theoretical ion:  $m/z$  1585.05  
Observed ion:  $m/z$  1585.04  
Mass deviation:  $m/z$  0.01  
Retention time: 62.0 min

Retention time fits to  
glycan isomer identified in  
Fetuin standard (G.  
Palmisano et al. *Rsc Adv*,  
2013, 3, 22706-22726).



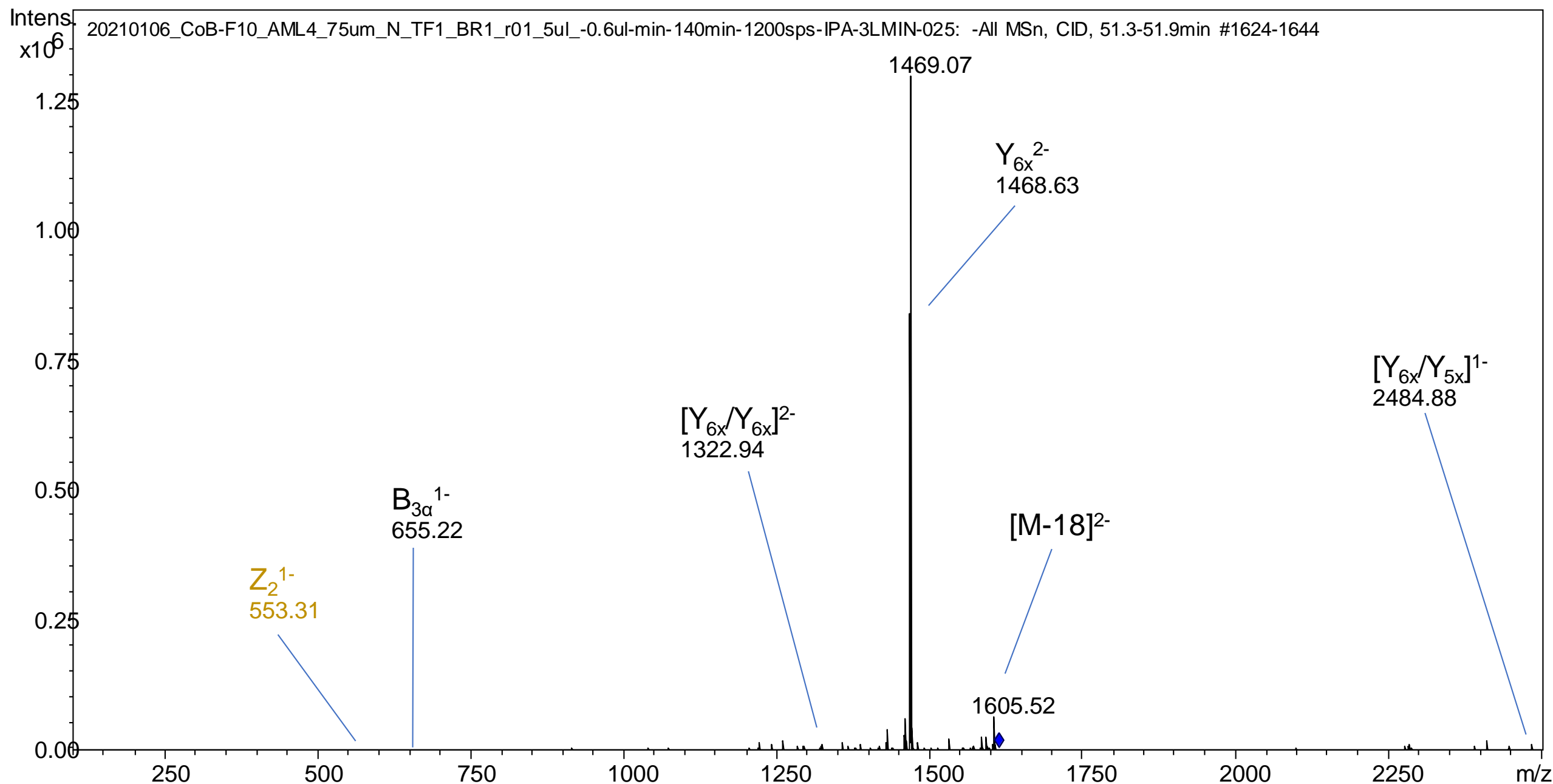
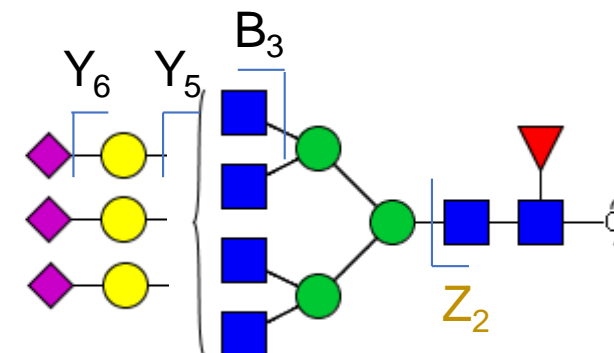
# Glycan 32

H6N6F1S3

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: TF-1

Monoisotopic mass: 3230.17 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1614.08  
Observed ion: *m/z* 1614.06  
Mass deviation: *m/z* 0.02  
Retention time: 51.1 min

UniCarb-DB: #

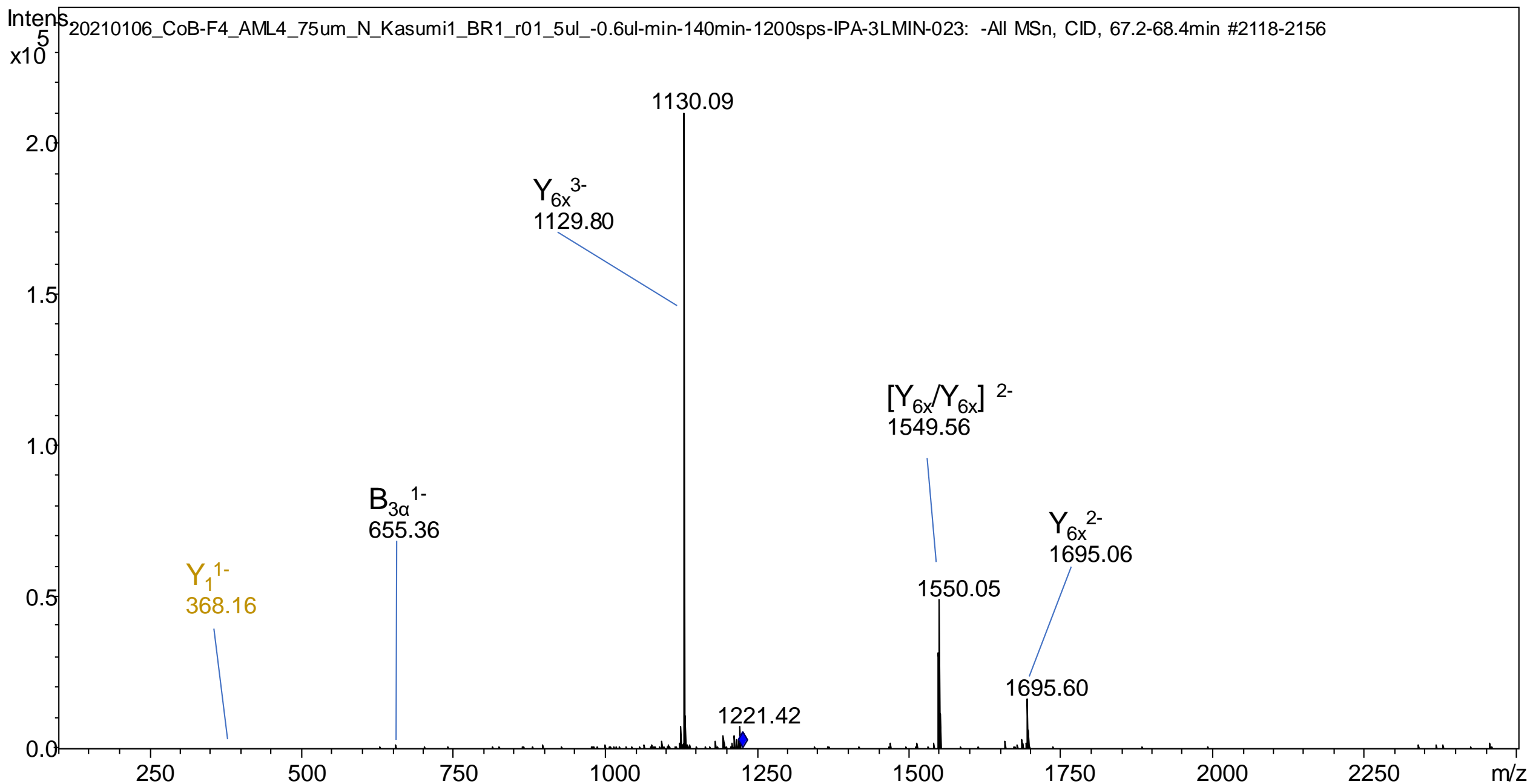
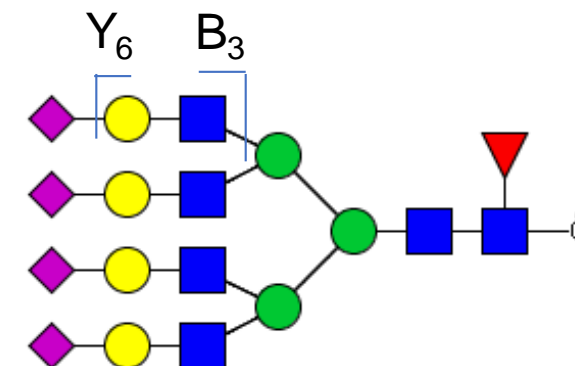


# Glycan 33a

H7N6F1S4

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: Kasumi-1

Monoisotopic mass: 3683.31 Da  
Charge observed: 3-  
Theoretical ion: *m/z* 1226.76  
Observed ion: *m/z* 1226.76  
Mass deviation: *m/z* 0.00  
Retention time: 67.8 min

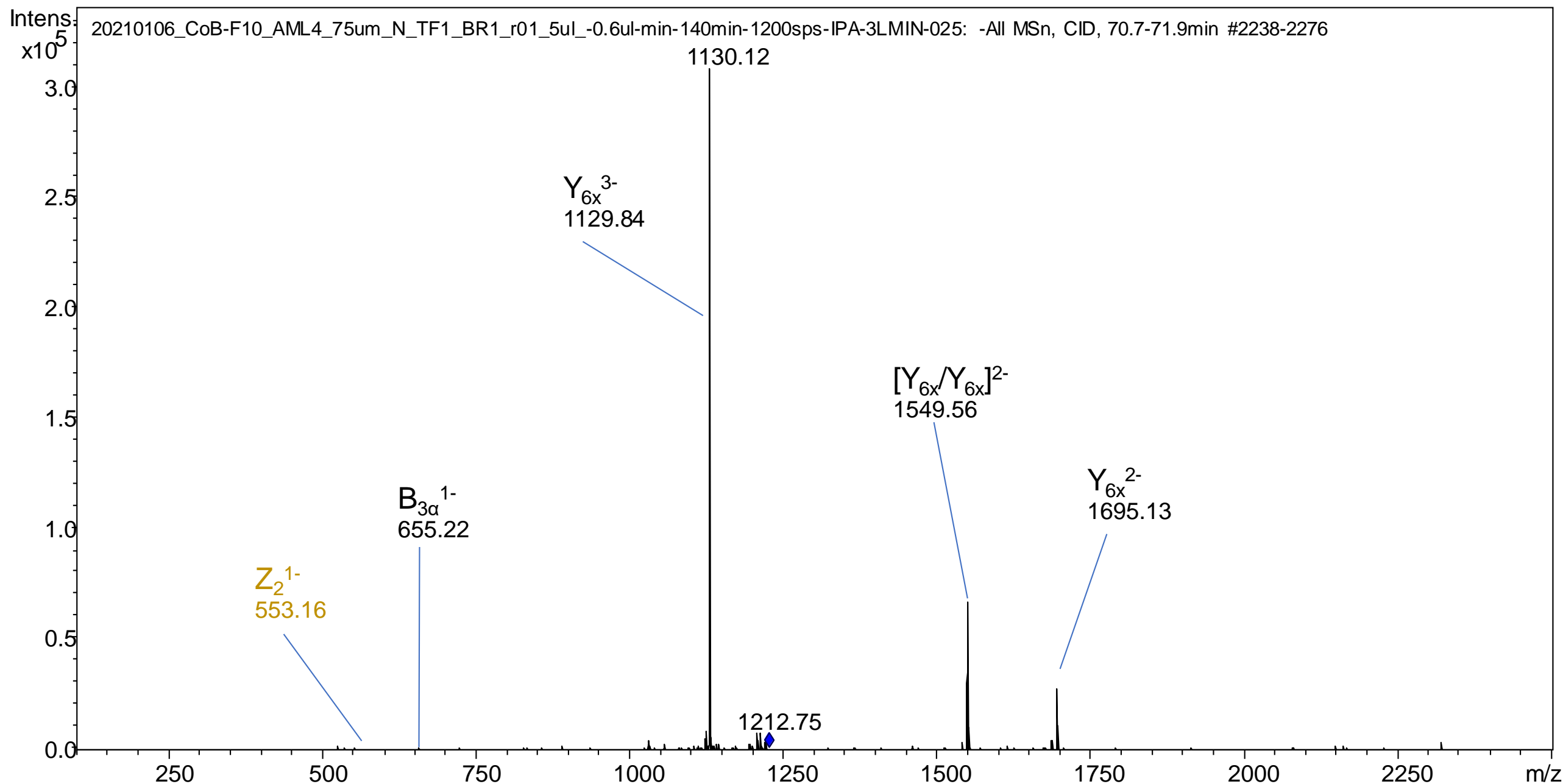
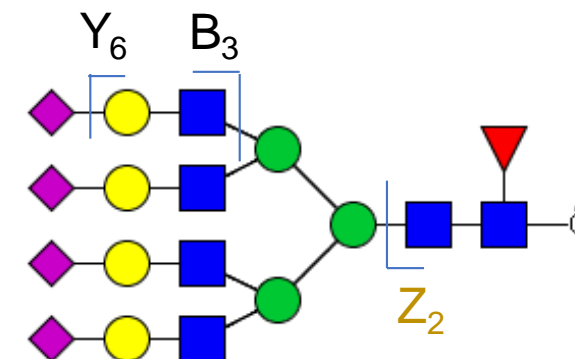


# Glycan 33b

H7N6F1S4

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: TF-1

Monoisotopic mass: 3683.31 Da  
Charge observed: 3-  
Theoretical ion: *m/z* 1226.76  
Observed ion: *m/z* 1226.76  
Mass deviation: *m/z* 0.00  
Retention time: 71.0 min





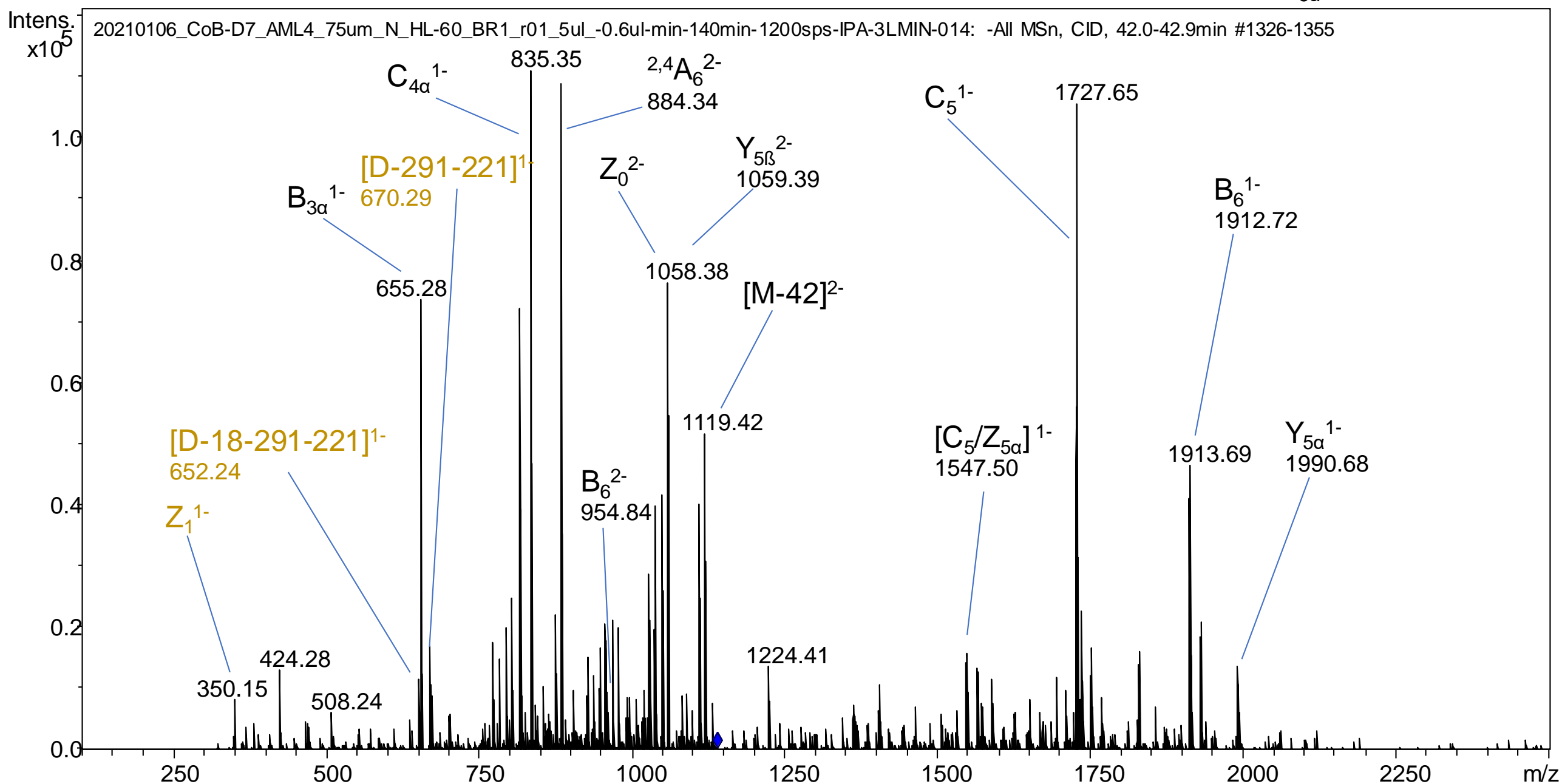
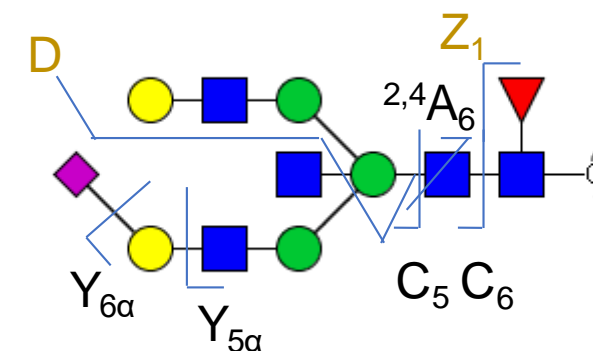
# Glycan 34a

H5N5F1S1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: HL-60

Monoisotopic mass: 2282.85 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1140.41  
Observed ion: *m/z* 1140.42  
Mass deviation: *m/z* 0.01  
Retention time: 42.2 min  
Note:  $\alpha$ -2,6 sialic acid linkage confirmed by  
neuraminidase S and A treatment

UniCarb-DB: #2395



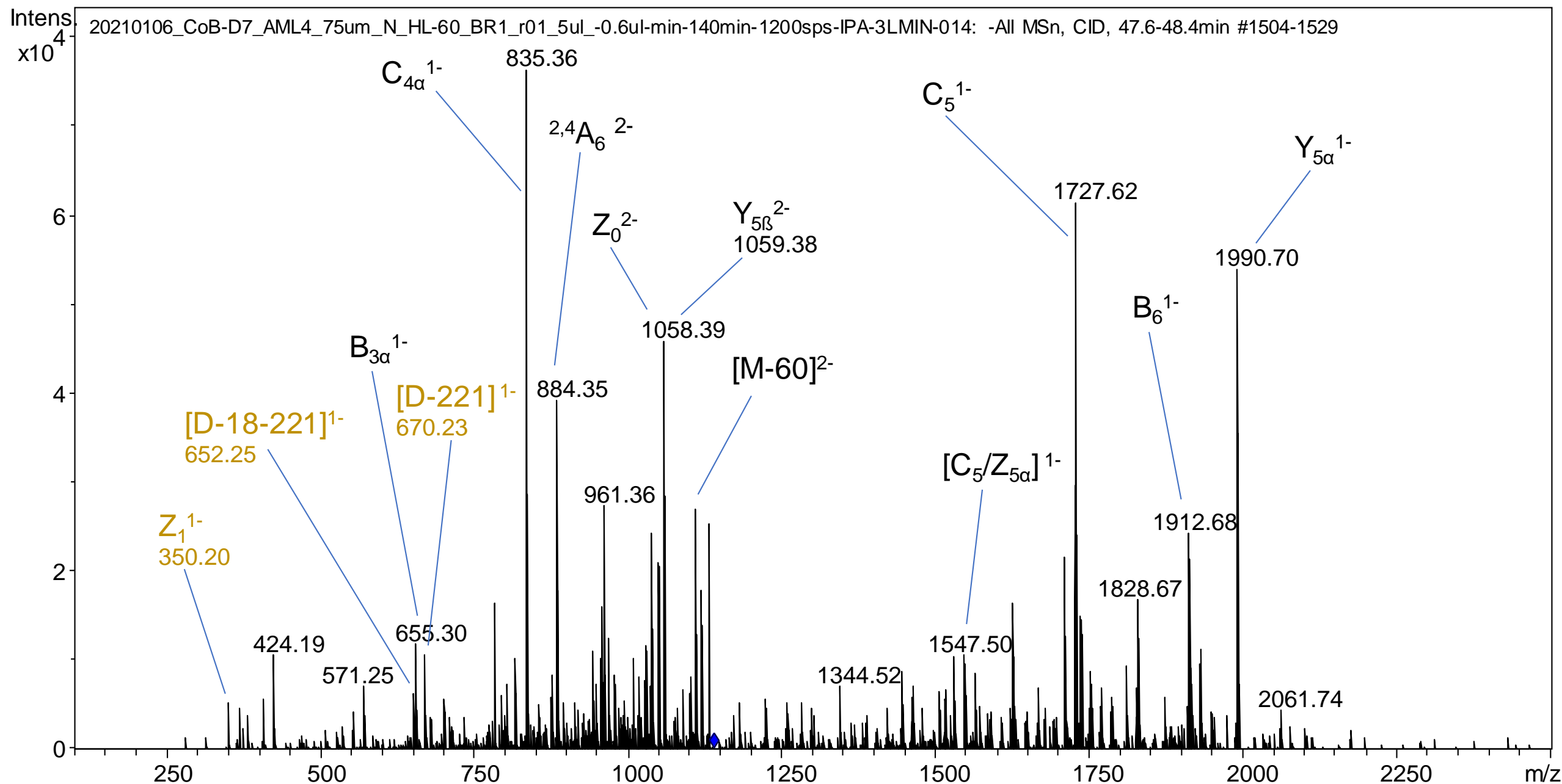
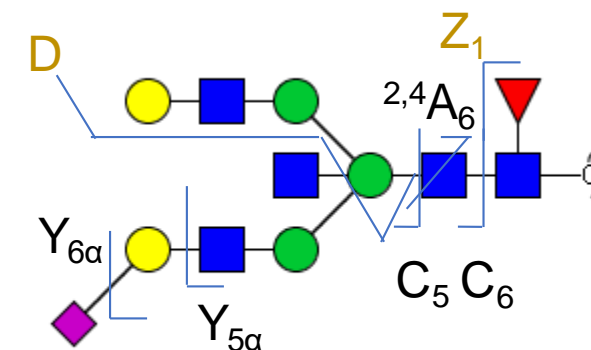
# Glycan 34b

H5N5F1S1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: HL-60

Monoisotopic mass: 2282.85 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1140.41  
Observed ion: *m/z* 1140.40  
Mass deviation: *m/z* 0.01  
Retention time: 48.1 min  
Note:  $\alpha$ -2,3 sialic acid linkage confirmed by  
neuraminidase S and A treatment

UniCarb-DB: #2395

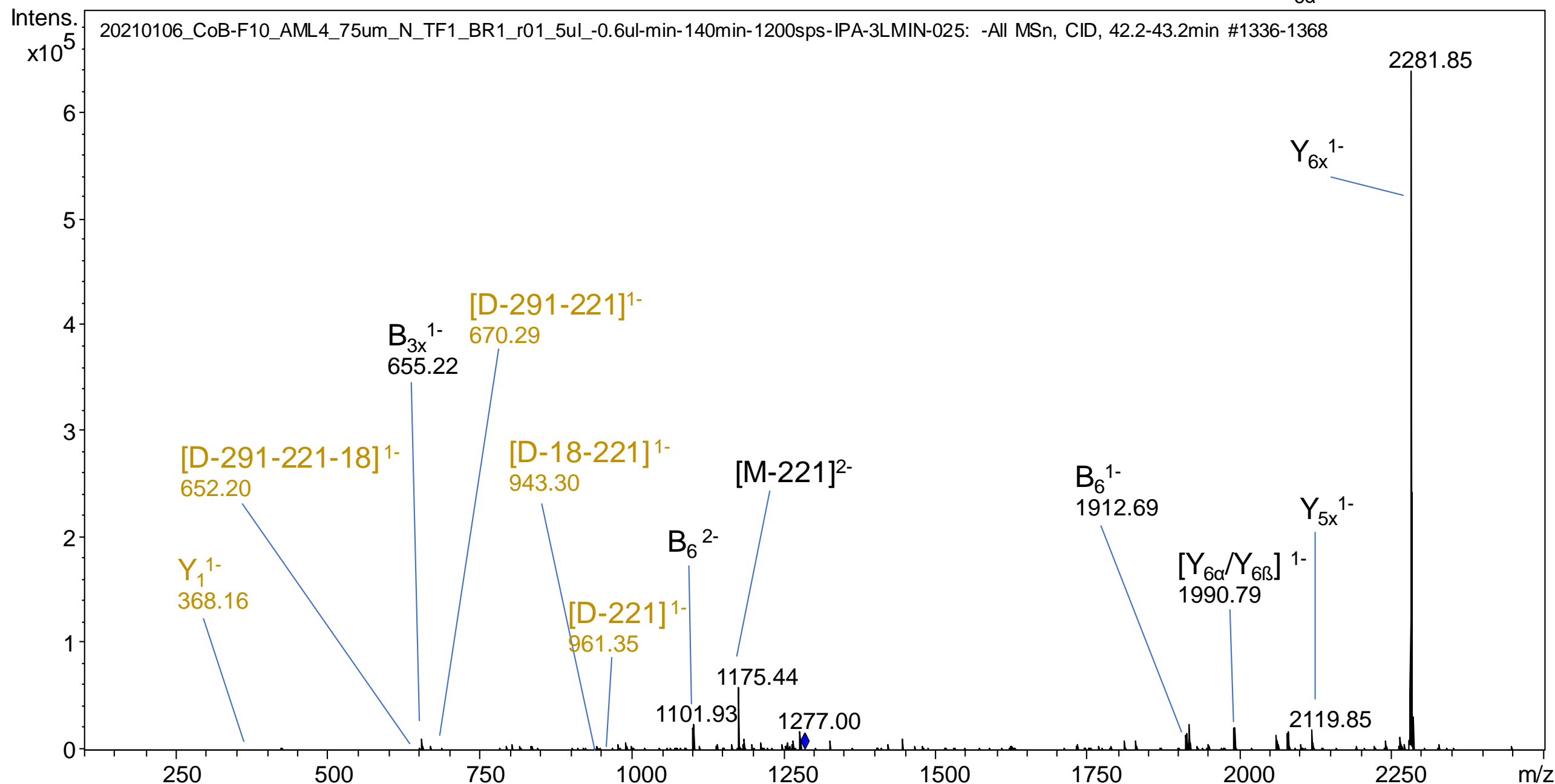
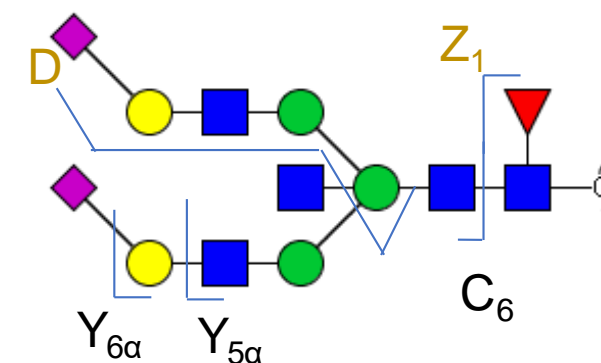


# Glycan 35a

H5N5F1S2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: TF-1

Monoisotopic mass: 2573.94 Da  
Charge observed: 2-  
Theoretical ion:  $m/z$  1285.96  
Observed ion:  $m/z$  1285.96  
Mass deviation:  $m/z$  0.00  
Retention time: 42.4 min  
Note:  $\alpha$ -2,6 sialic acid linkage confirmed by  
neuraminidase S and A treatment

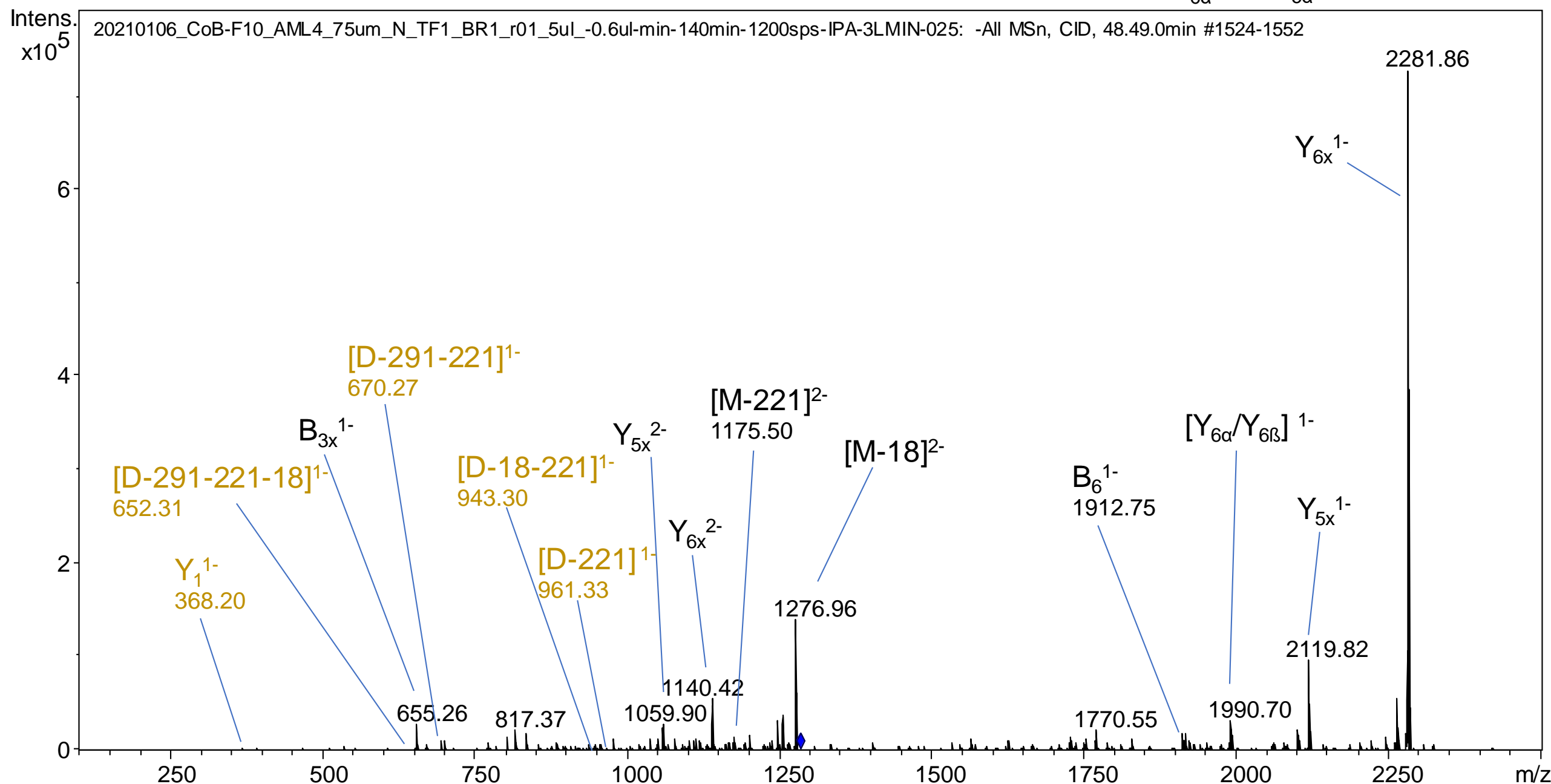
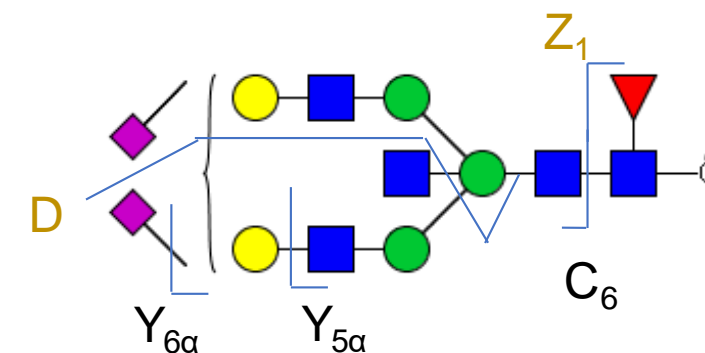


# Glycan 35b

H5N5F1S2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: TF-1

Monoisotopic mass: 2573.94 Da  
Charge observed: 2-  
Theoretical ion:  $m/z$  1285.96  
Observed ion:  $m/z$  1285.95  
Mass deviation:  $m/z$  0.01  
Retention time: 48.4 min  
Note: Sialic acid linkages confirmed by  
neuraminidase S and A treatment

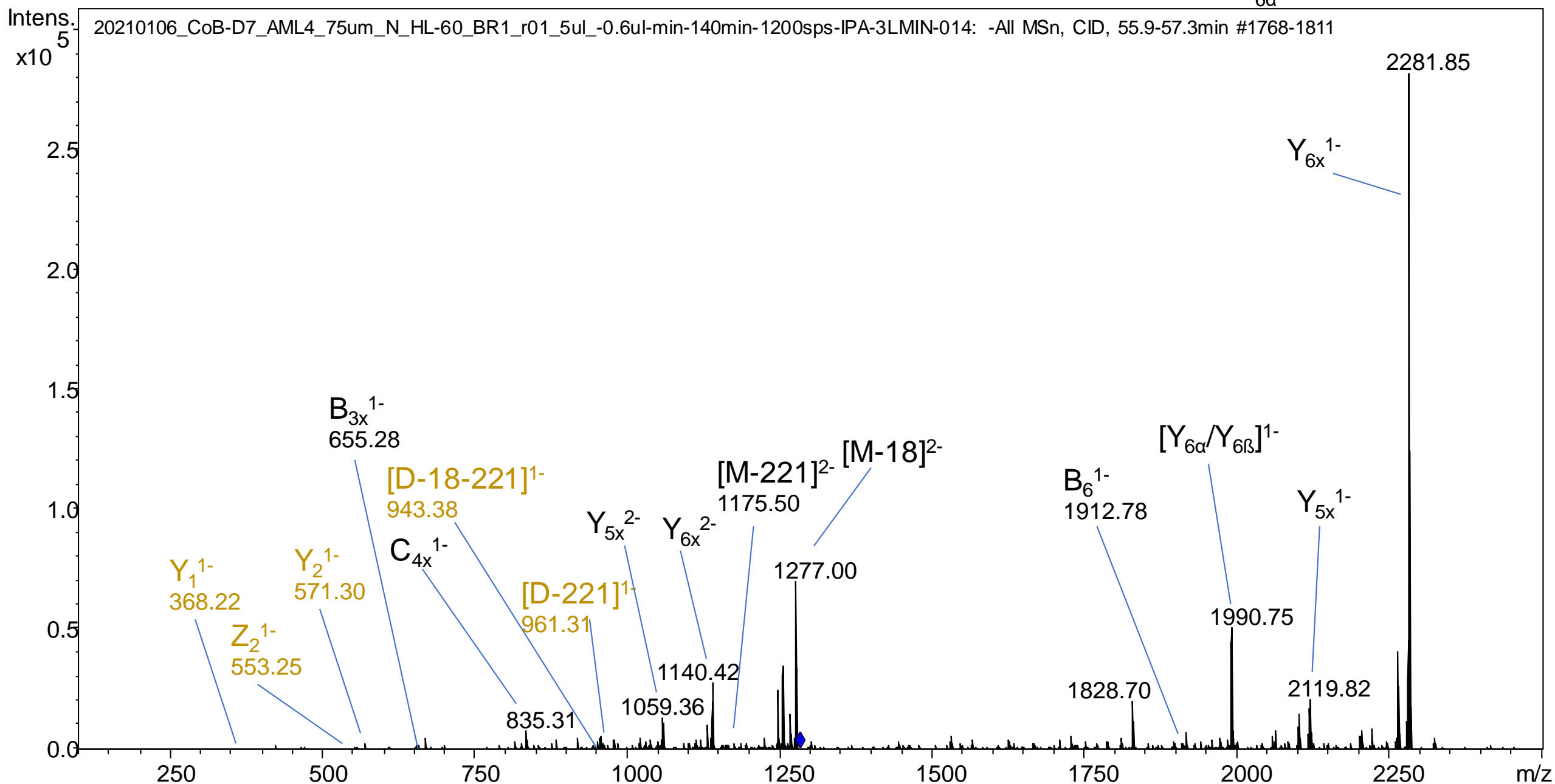
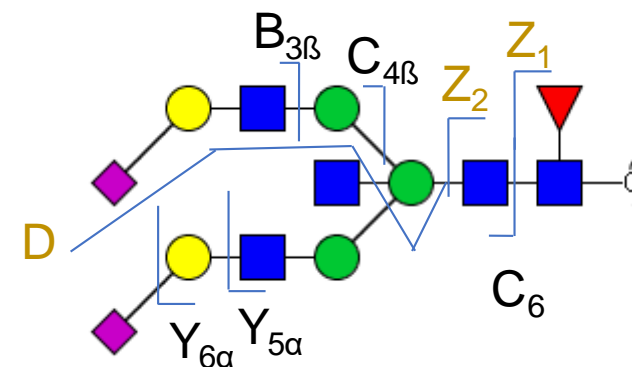


# Glycan 35c

H5N5F1S2

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: HL-60

Monoisotopic mass: 2573.94 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 1285.96  
Observed ion: *m/z* 1285.96  
Mass deviation: *m/z* 0.00  
Retention time: 56.1 min  
Note: Sialic acid linkages confirmed by  
neuraminidase S and A treatment



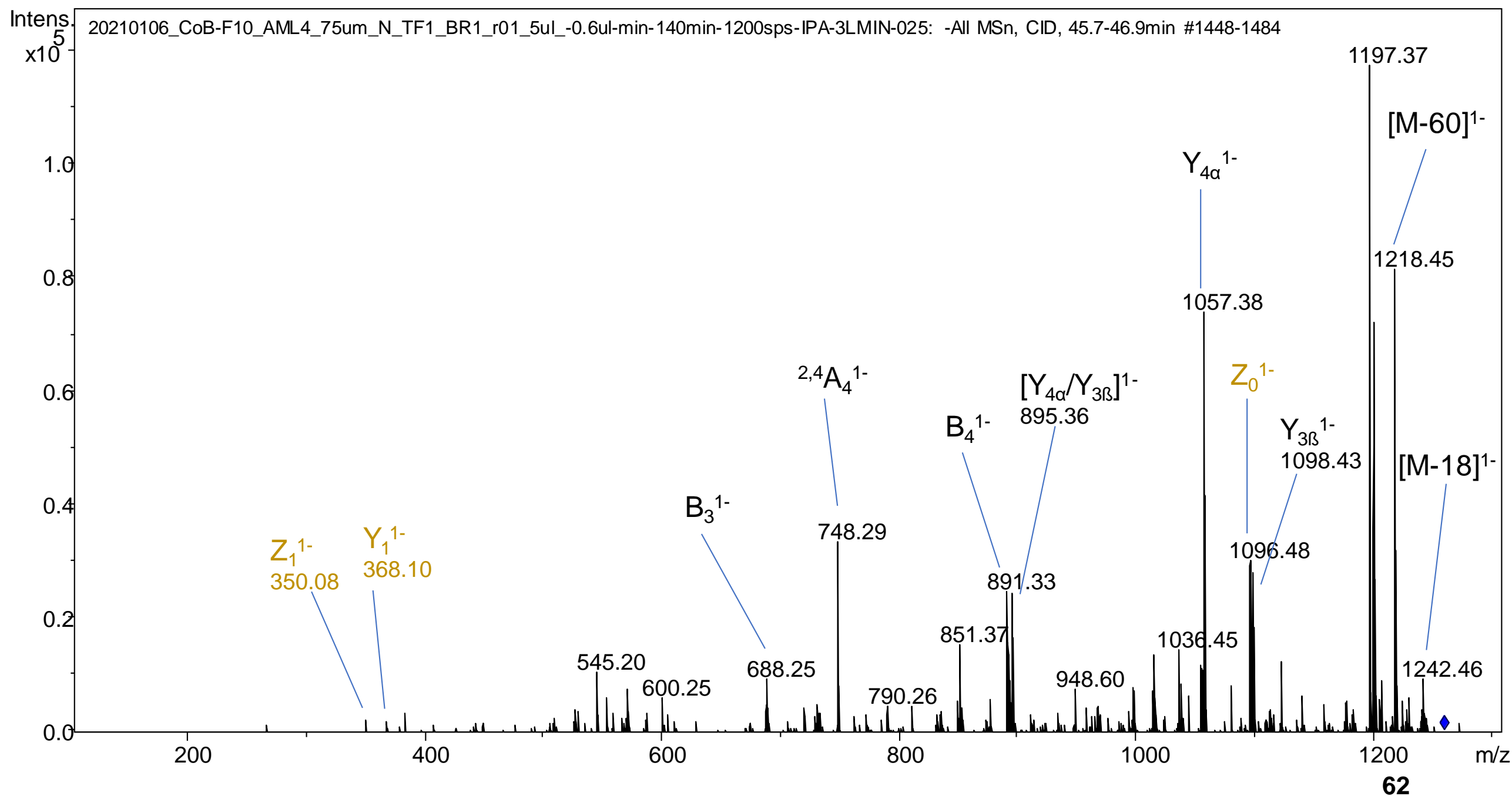
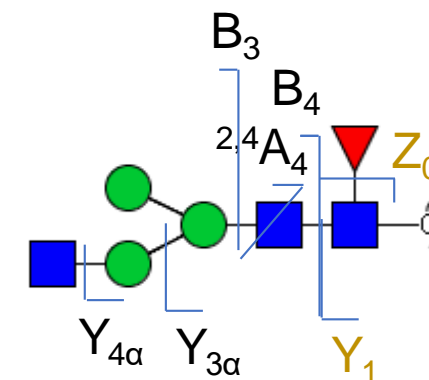
# Glycan 36a

## H3N3F1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: TF-1

Monoisotopic mass: 1261.48 Da  
Charge observed: 1-  
Theoretical ion: *m/z* 1260.47  
Observed ion: *m/z* 1260.48  
Mass deviation: *m/z* 0.01  
Retention time: 46.2 min  
Note: No D-ion at *m/z* 526 which would  
indicate that the GlcNAc is on the 3-arm

UniCarb-DB: #396



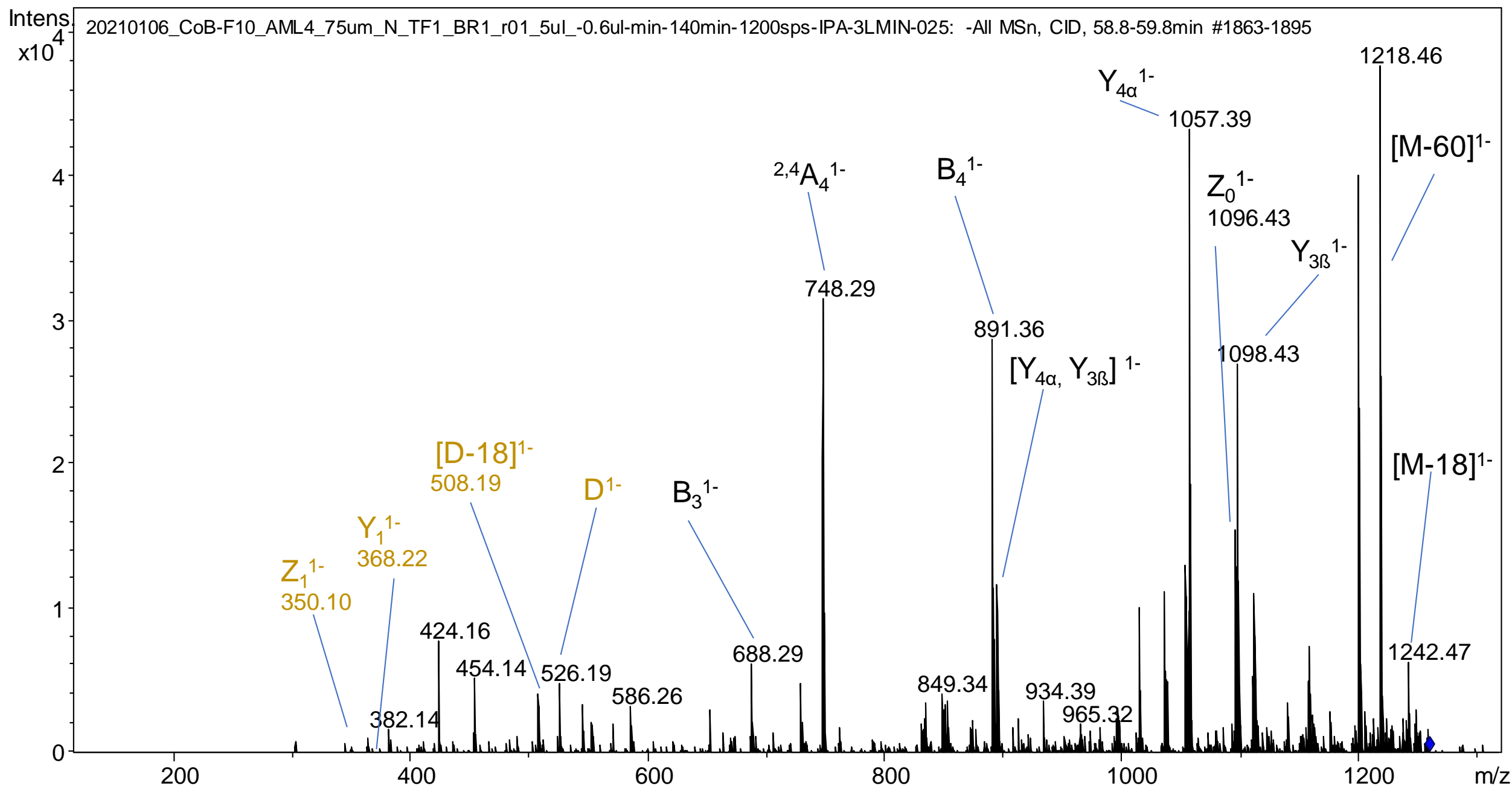
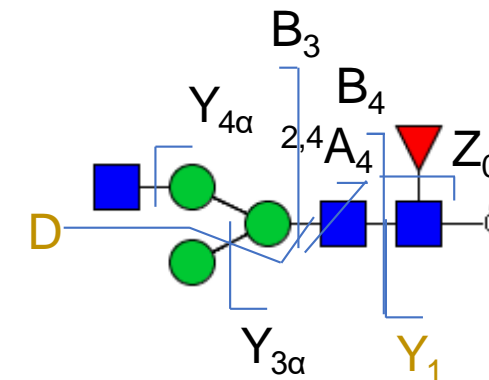
# Glycan 36b

H3N3F1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: TF-1

Monoisotopic mass: 1261.48 Da  
Charge observed: 1-  
Theoretical ion: *m/z* 1260.47  
Observed ion: *m/z* 1260.49  
Mass deviation: *m/z* 0.02  
Retention time: 59.1 min

UniCarb-DB: #2574



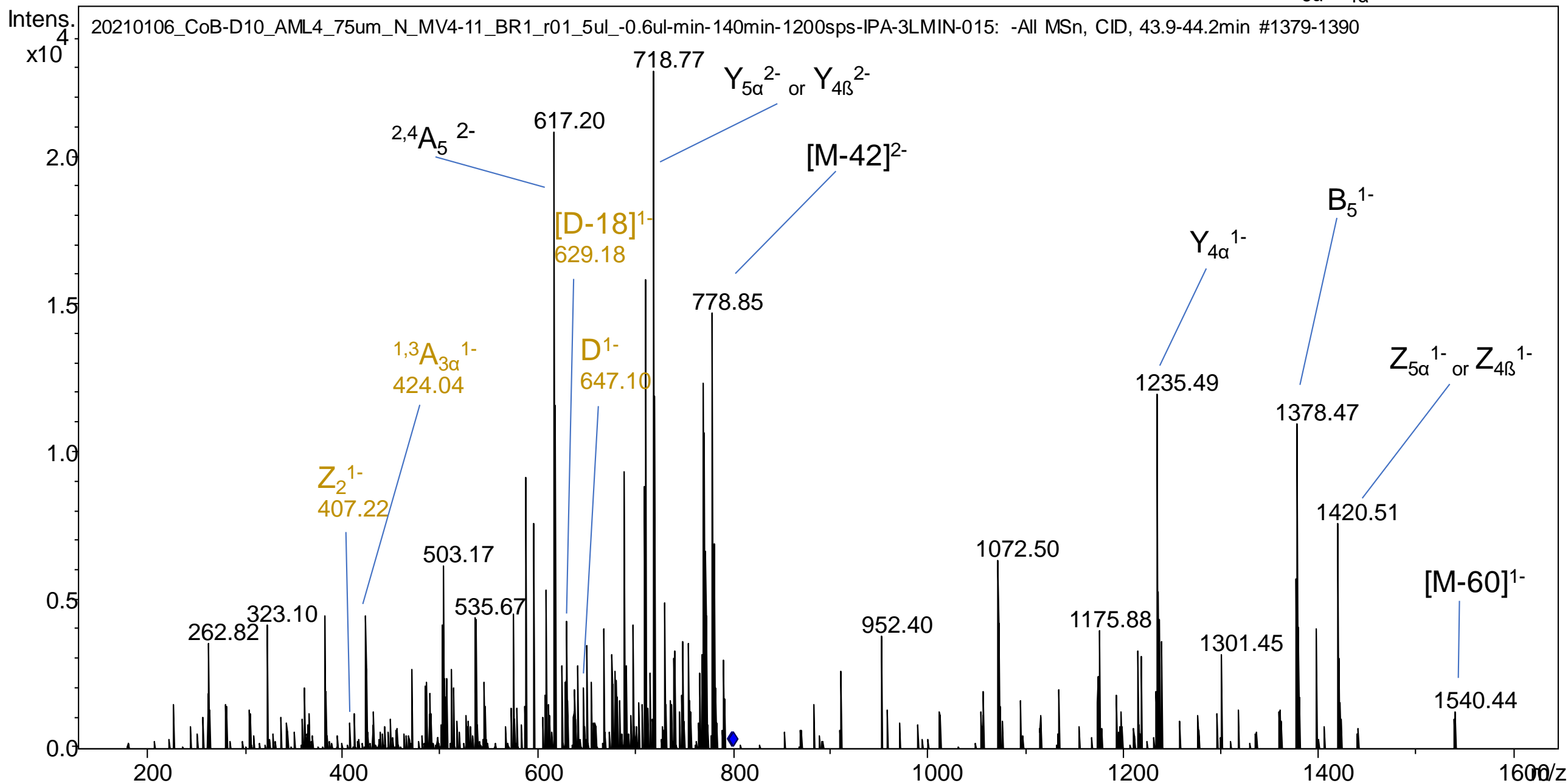
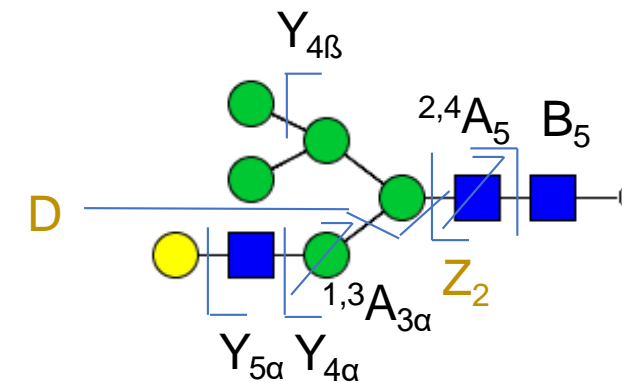
# Glycan 37

## H6N3

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MV4-11

Monoisotopic mass: 1601.59 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 799.78  
Observed ion: *m/z* 799.82  
Mass deviation: *m/z* 0.04  
Retention time: 34.9 min

UniCarb-DB: #2482



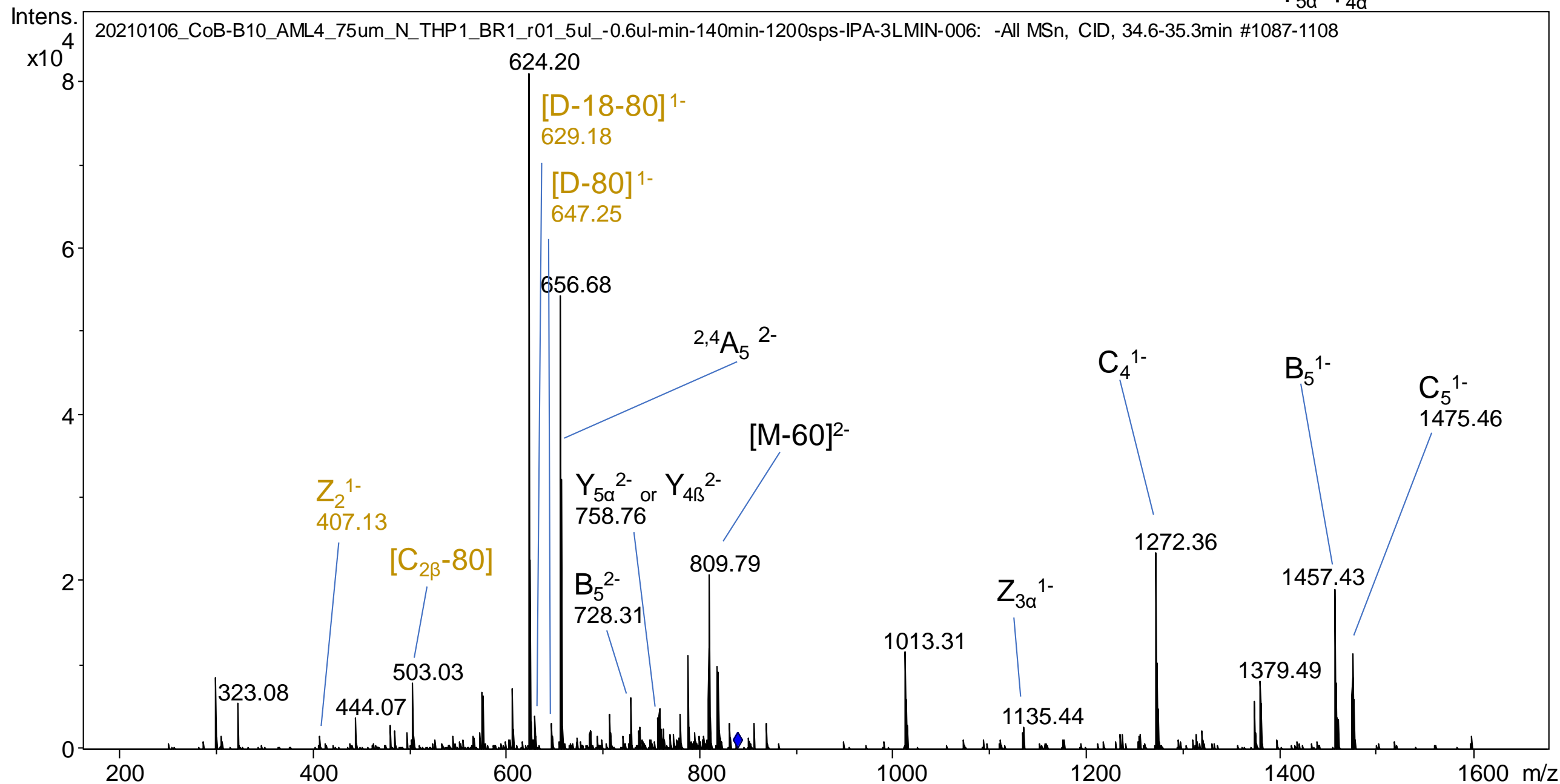
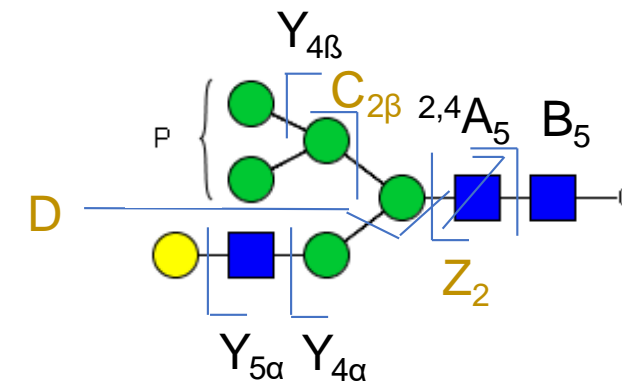


# Glycan 38

H6N3P1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: THP-1

Monoisotopic mass: 1681.55 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 839.77  
Observed ion: *m/z* 839.79  
Mass deviation: *m/z* 0.02  
Retention time: 34.8 min



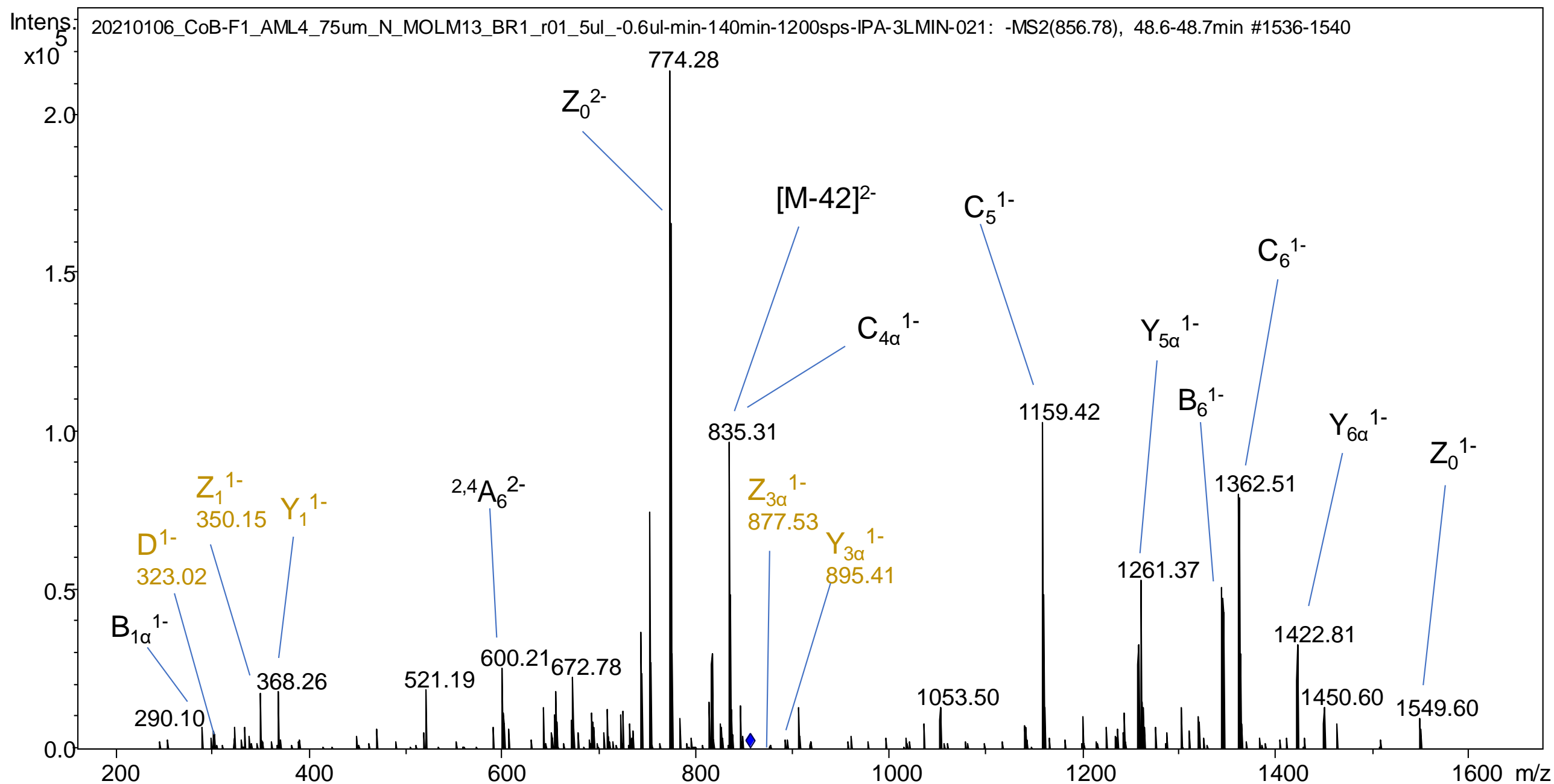
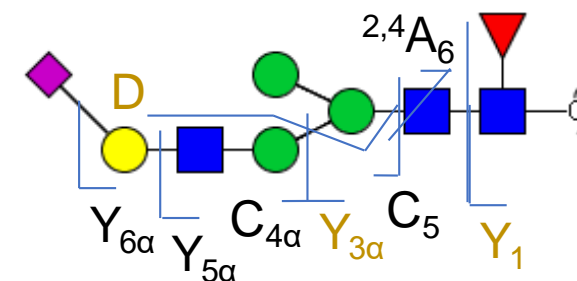
# Glycan 39a

H4N3F1S1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 1714.63 Da  
Charge observed: 2-  
Theoretical ion:  $m/z$  856.30  
Observed ion:  $m/z$  856.35  
Mass deviation:  $m/z$  0.05  
Retention time: 48.7 min  
Note:  $\alpha$ -2.6 sialic acid linkage confirmed by  
neuraminidase S and A treatment

UniCarb-DB: #416



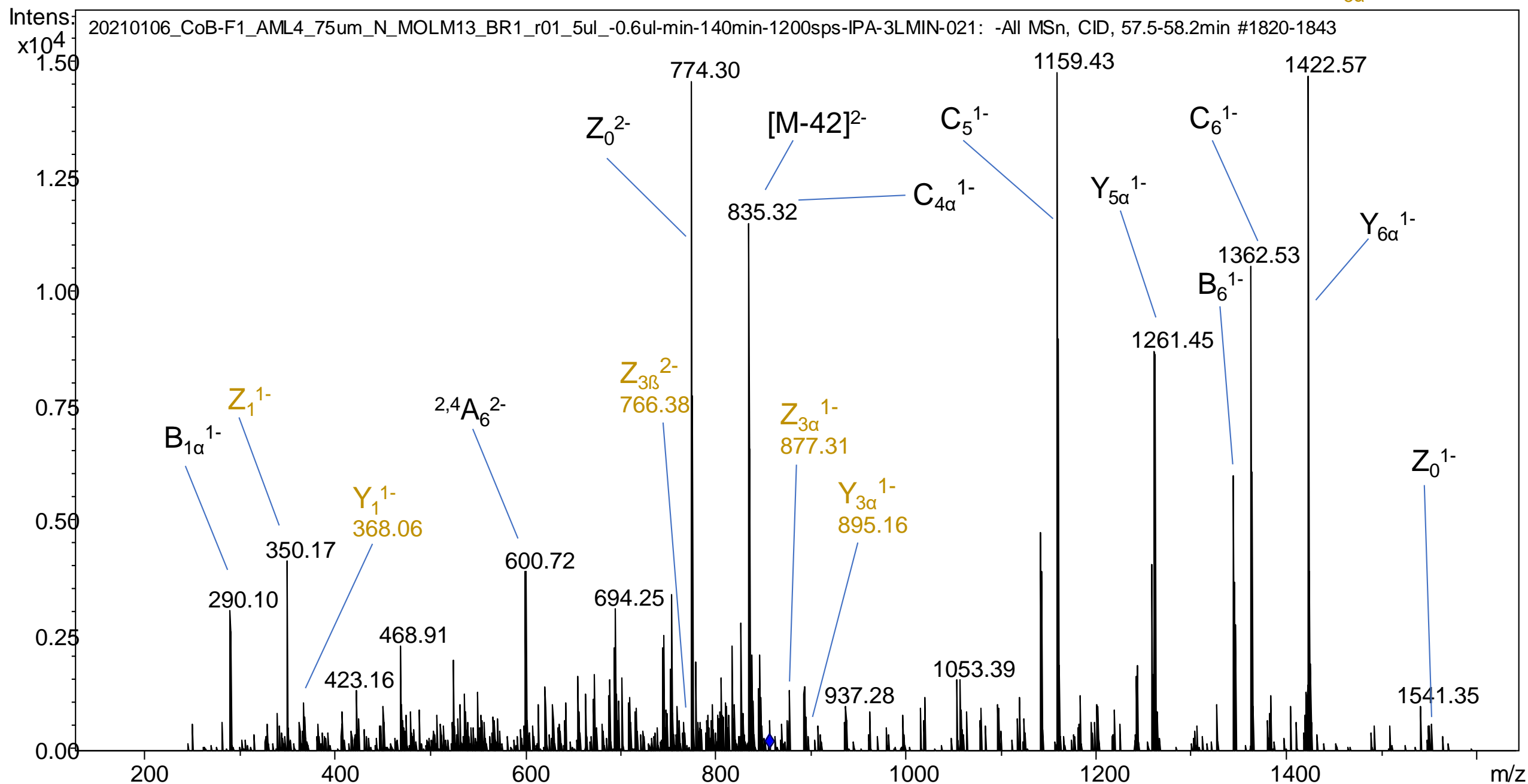
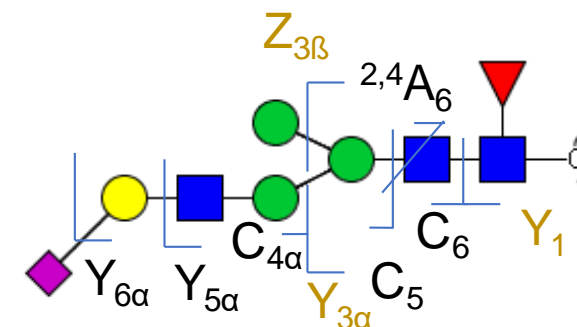
# Glycan 39b

H4N3F1S1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: MOLM-13

Monoisotopic mass: 1714.63 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 856.30  
Observed ion: *m/z* 856.36  
Mass deviation: *m/z* 0.06  
Retention time: 57.9 min  
Note:  $\alpha$ -2,3 sialic acid linkage confirmed by  
neuraminidase S and A treatment

UniCarb-DB: #2220

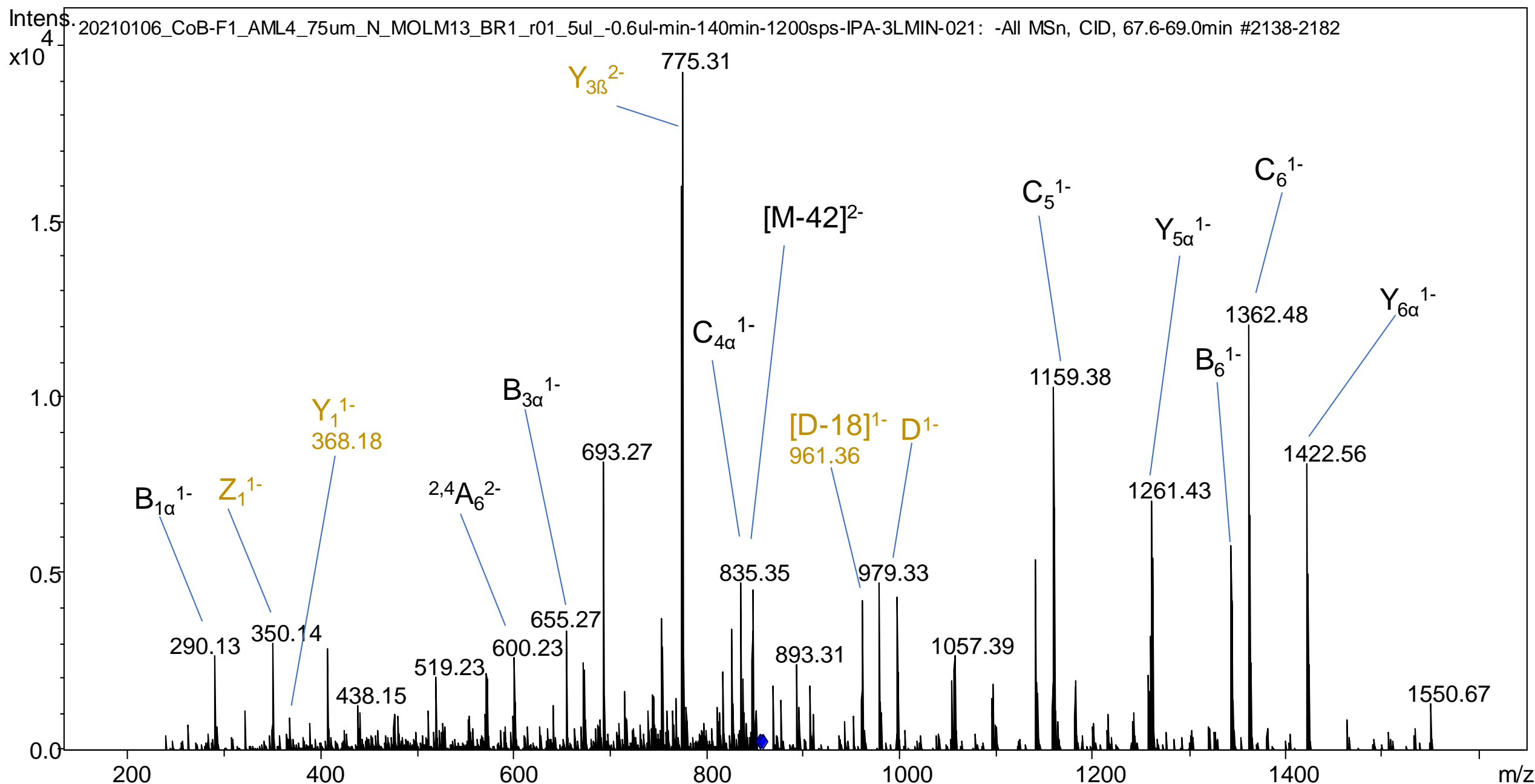
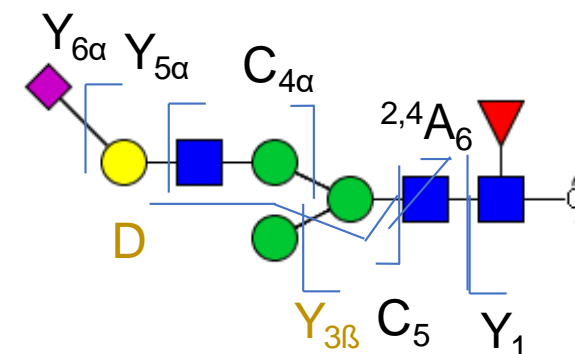


H4N3F1S1

**Depicted MS<sup>2</sup> was obtained from analysis of cell line: MOLM-13**

<b>Monoisotopic mass:</b>	<b>1714.63 Da</b>
<b>Charge observed:</b>	<b>2-</b>
<b>Theoretical ion:</b>	<b><i>m/z</i> 856.30</b>
<b>Observed ion:</b>	<b><i>m/z</i> 856.34</b>
<b>Mass deviation:</b>	<b><i>m/z</i> 0.04</b>
<b>Retention time:</b>	<b>67.7 min</b>
<b>Note: <math>\alpha</math>-2,6 sialic acid linkage confirmed by neuraminidase S and A treatment</b>	

**UniCarb-DB: #2488**



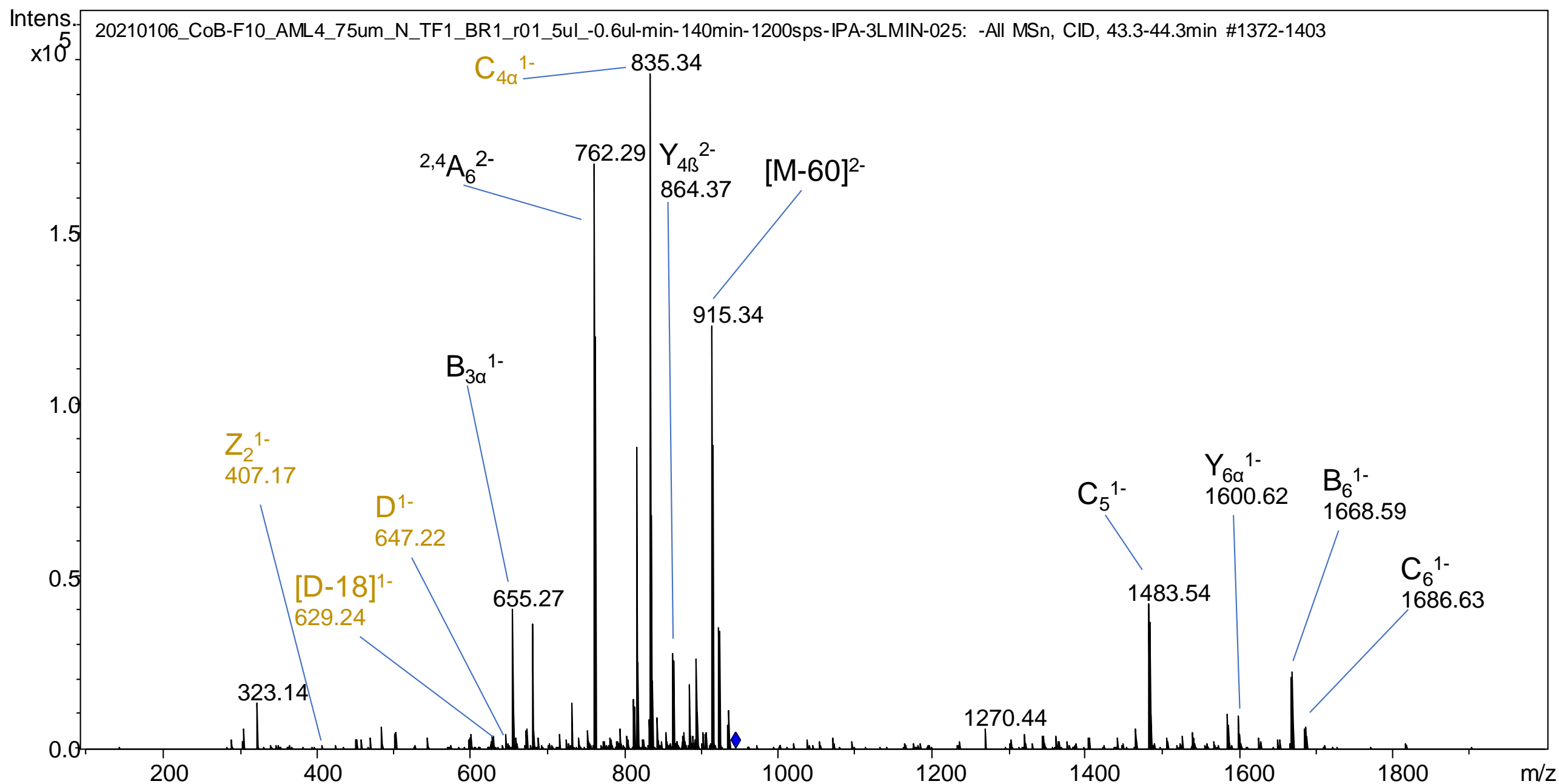
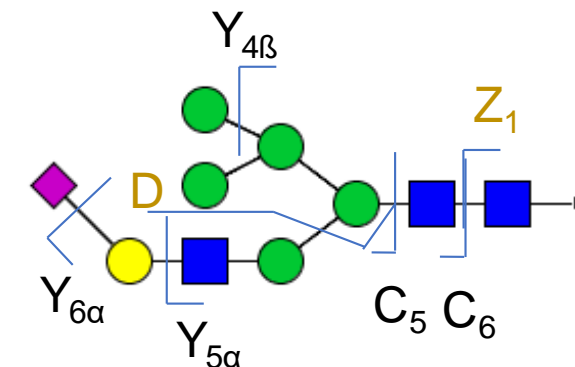
# Glycan 40a

H6N3S1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: TF-1

Monoisotopic mass: 1892.68 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 945.33  
Observed ion: *m/z* 945.36  
Mass deviation: *m/z* 0.03  
Retention time: 43.5 min  
Note:  $\alpha$ -2,6 sialic acid linkage confirmed by  
neuraminidase S and A treatment

UniCarb-DB: #430



# Glycan 40b

## H6N3S1

Depicted MS<sup>2</sup> was obtained from  
analysis of cell line: TF-1

Monoisotopic mass: 1892.68 Da  
Charge observed: 2-  
Theoretical ion: *m/z* 945.35  
Observed ion: *m/z* 945.36  
Mass deviation: *m/z* 0.01  
Retention time: 53.0 min  
Note:  $\alpha$ -2,3 sialic acid linkage confirmed by  
neuraminidase S and A treatment

UniCarb-DB: #2523

