

N-glycosylation of colorectal cancer tissues: a liquid chromatography and mass spectrometry-based investigation

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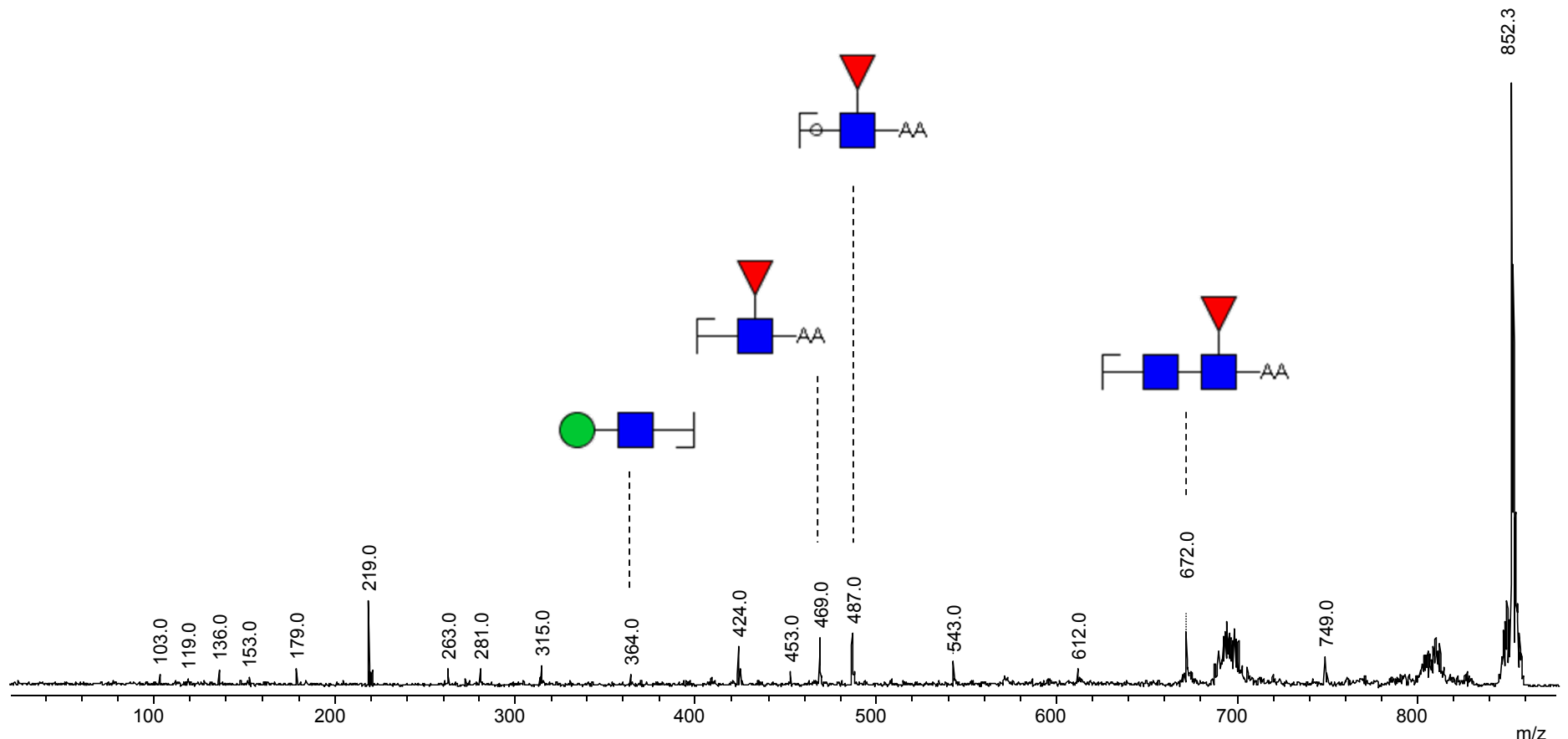
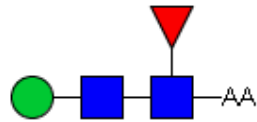
² Department of Surgery, Leiden University Medical Center, Leiden, The Netherlands

Supplementary Figure 1. MS/MS spectra of N-glycan structures detected in colorectal cancer tissues. The pooled AA-labeled glycans released from the colorectal cancer tissues were fractionated by HILIC-HPLC, and subsequently all fractions were analyzed by MALDI-ToF-MS. In addition, many HILIC-fractions were analyzed by ESI-ion trap-MS/MS (positive-ion mode) and MALDI-ToF-MS/MS (negative-ion mode). The obtained fragmentation spectra, in combination with general knowledge of human glycobiology, were used for structural assignments. Based on this interpretation, the presence of structural isomers can not be excluded. The MS/MS fragmentation spectra were interpreted manually and using ProteinScape software. Glycan compositions as well as proposed schematic structures are given where possible. The spectrum numbers refer to Supplementary Table 1. Glycan schemes were prepared using GlycoWorkbench (*Red triangle*, dHex, fucose; *yellow circle*, Hex, galactose; *green circle*, Hex, mannose; *blue square*, HexNAc, *N*-acetylglucosamine; *white square*, HexNAc, *N*-acetylhexosamine; *purple diamond*, Neu5Ac, sialic acid; *S*, sulfate; *Ac*, acetyl group). Lift, MALDI-ToF/ToF-MS experiment.

Spectrum 1

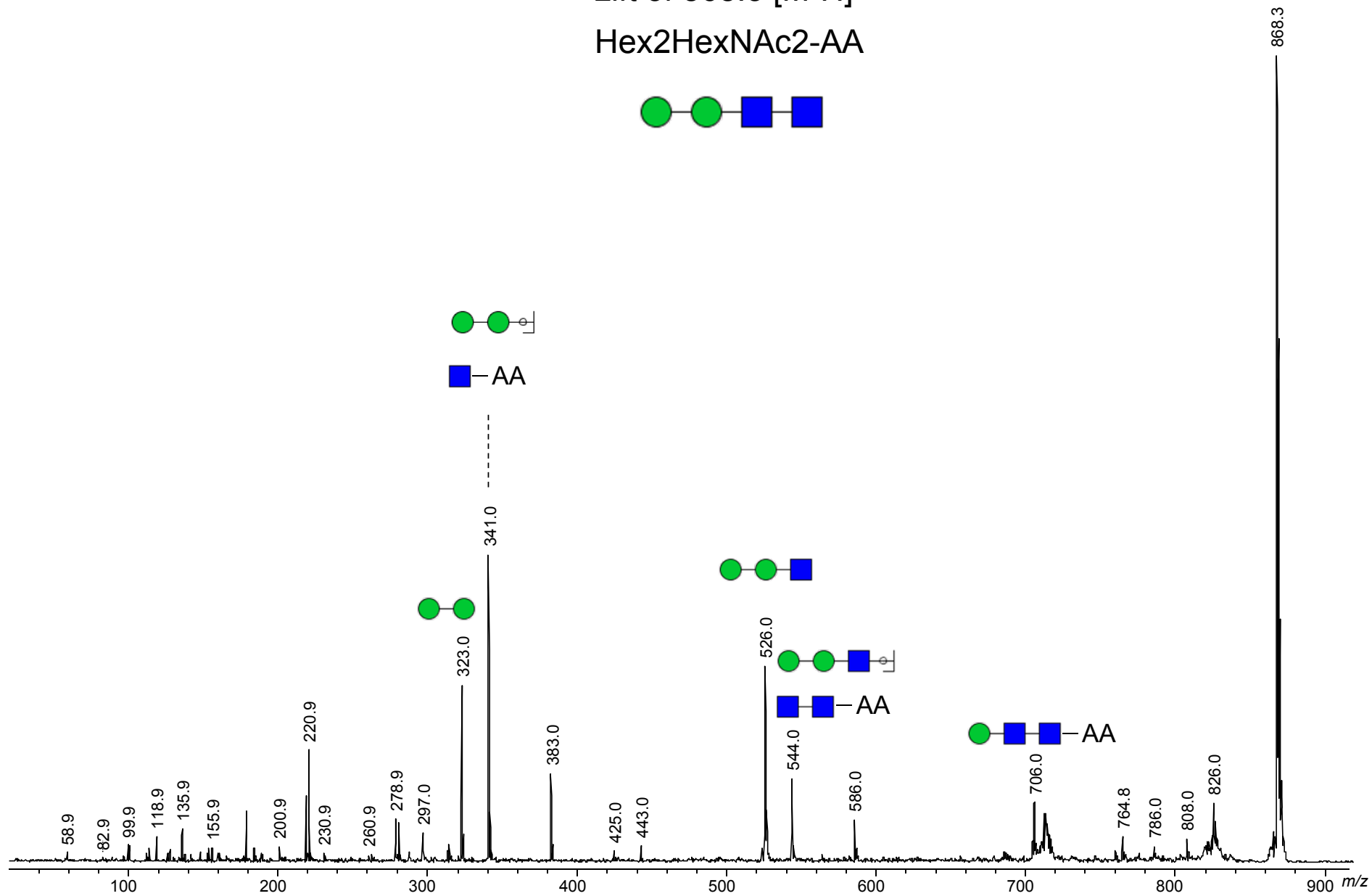
Lift of 852.3 [M-H]⁻

dHex1Hex1HexNAc2-AA



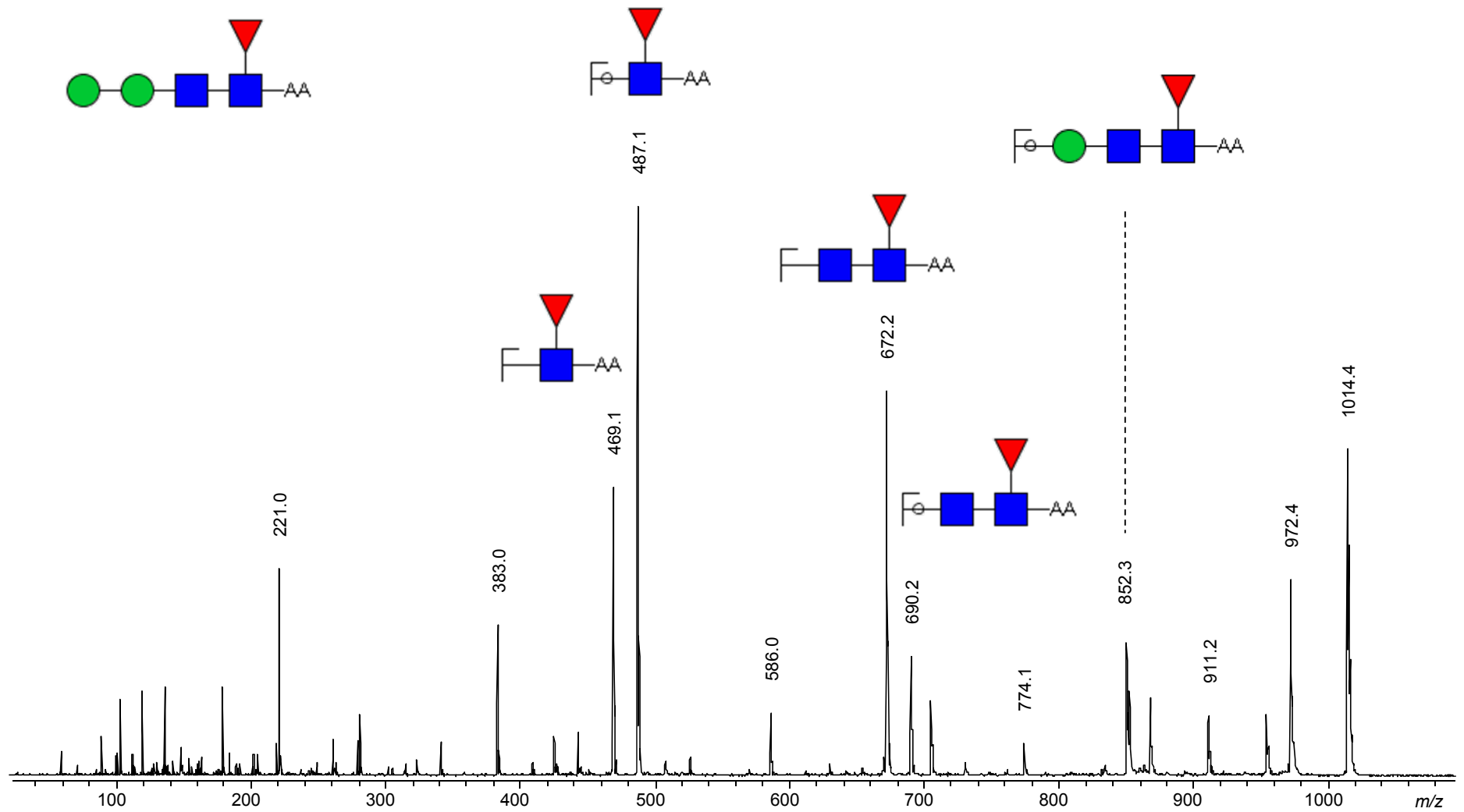
Spectrum 2

Lift of 868.3 [M-H]⁻
Hex2HexNAc2-AA



Spectrum 3

Lift of 1014.4 [M-H]⁻
dHex1Hex2HexNAc2-AA

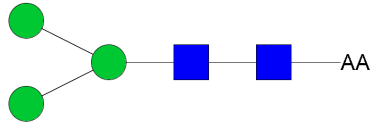


Spectrum 4



Glycan Search Report

Glycan: 1



Project path: /N-glycans cancer/Lift spectra 02/CombinedUNKNOWN

MS data: c:/documents and settings/ciabalog/desktop/lift/lift of 1030/0_a24/1/1030.4000.lift/1sref/pdata/1/1r

Parent m/z: 1030.3732 -1

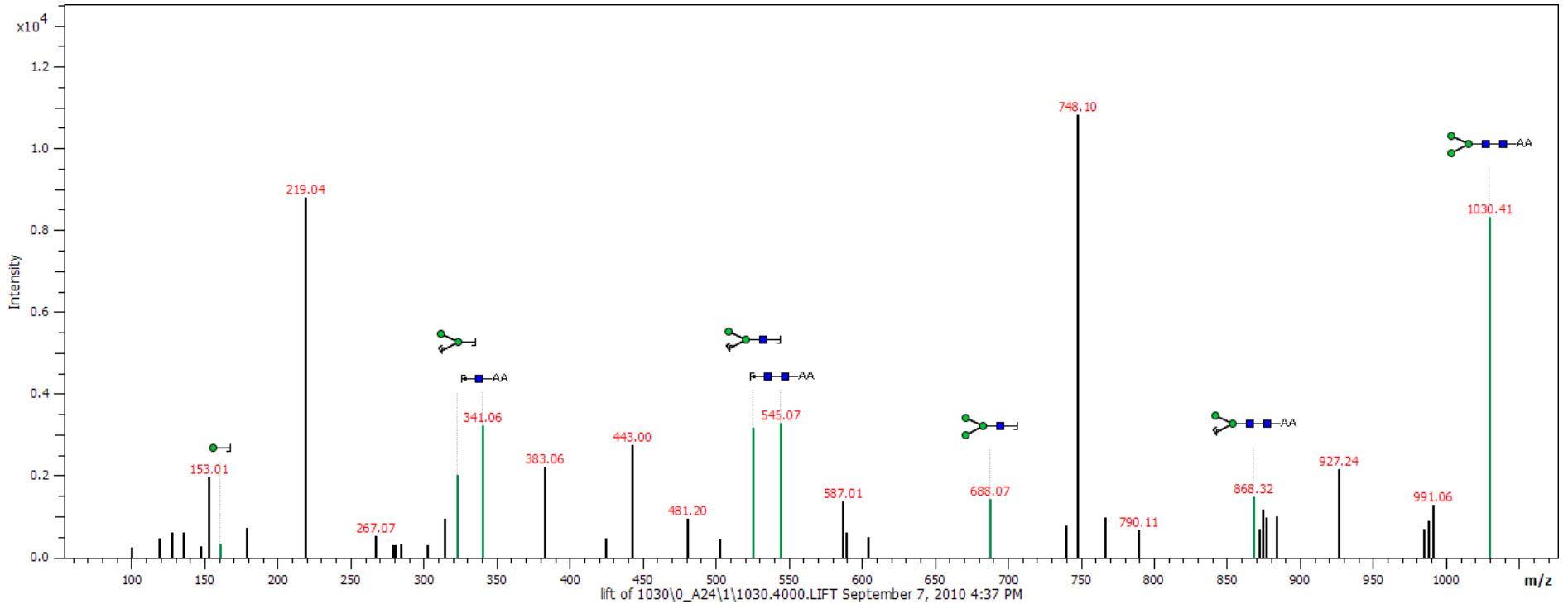
Score: 48.849

Composition: Hex3HexNAc2-AA

Intensity coverage [%]: 0.33

Accession: 36759

Fragment coverage [%]: 0.73

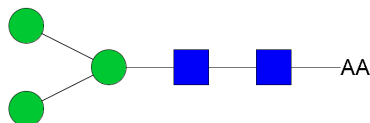


Spectrum 5



Glycan Search Report

Glycan: 1



Project path: /N-glycans cancer/25140/comp_25140.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25140_01.d/comp_25140.mgf

Parent m/z: 516.6975 2+

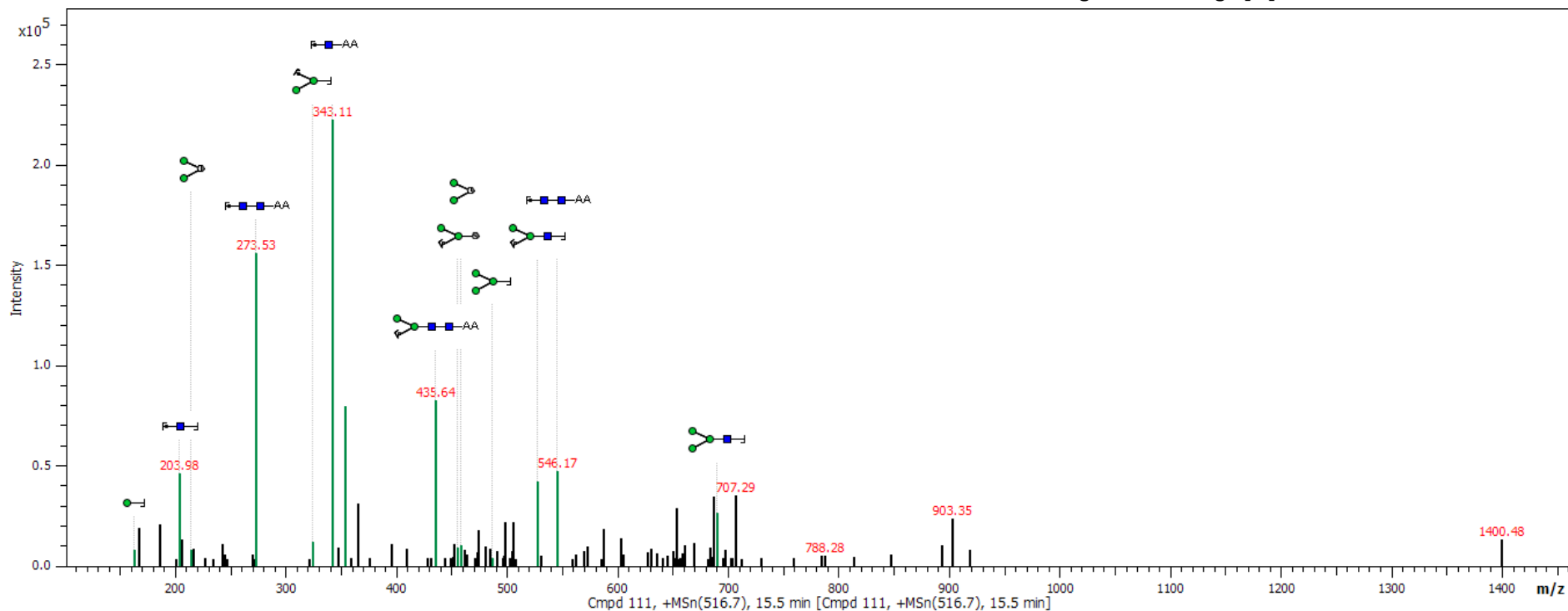
Score: 51.434

Composition: Hex3HexNAc2-AA

Intensity coverage [%]: 0.52

Accession: 954

Fragment coverage [%]: 0.51

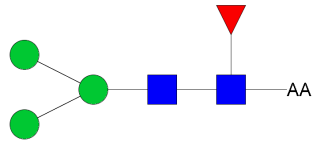


Spectrum 6



Glycan Search Report

Glycan: 2



Project path: /N-glycans cancer/Lift spectra 02/CombinedUNKNOWN

MS data: c:/documents and settings/ciabalog/desktop/lift/lift of 1176/0_b4/1/1176.4000.lift/1sref/pdata/1/1r

Parent m/z: 1176.4311 -1

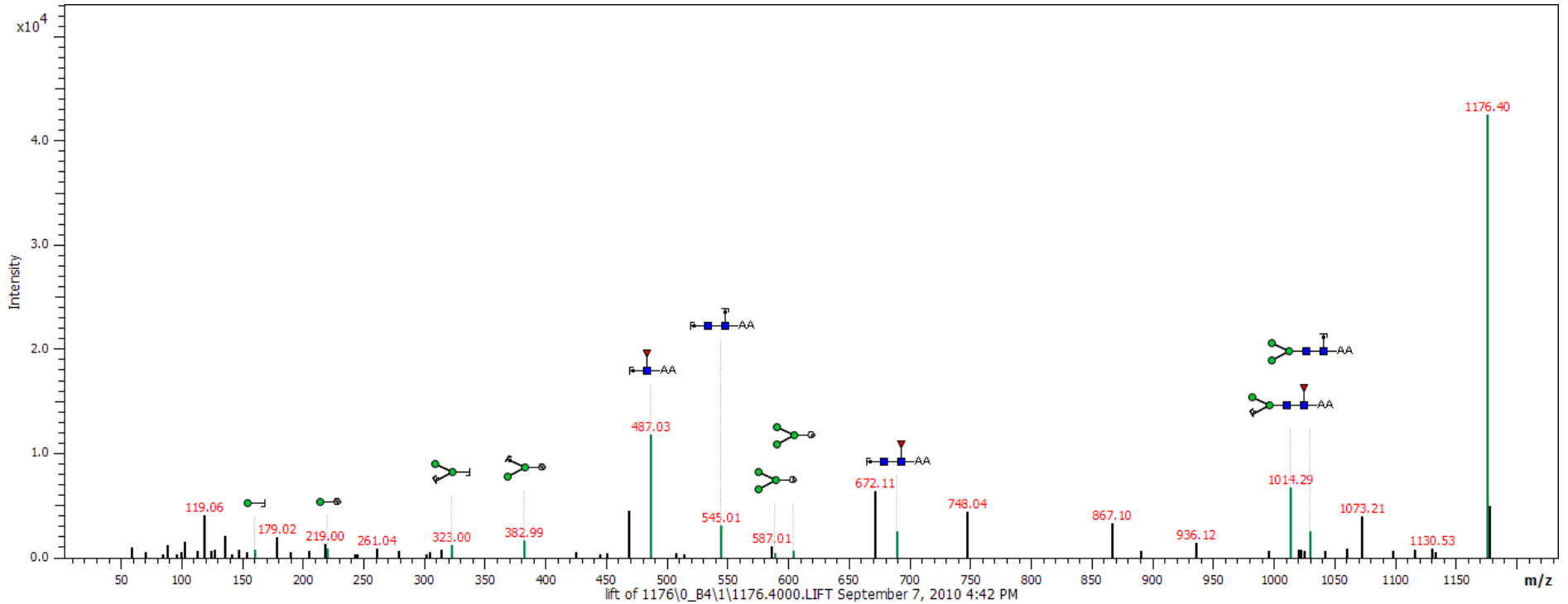
Score: 45.195

Composition: Hex3HexNAc2dHex1-AA

Intensity coverage [%]: 0.55

Accession: 1020

Fragment coverage [%]: 0.37

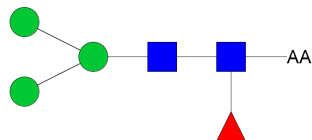


Spectrum 7



Glycan Search Report

Glycan: 1



Project path: /N-glycans cancer/25144/comp_25144.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25144_01.d/comp_25144.mgf

Parent m/z: 589.7265 2+

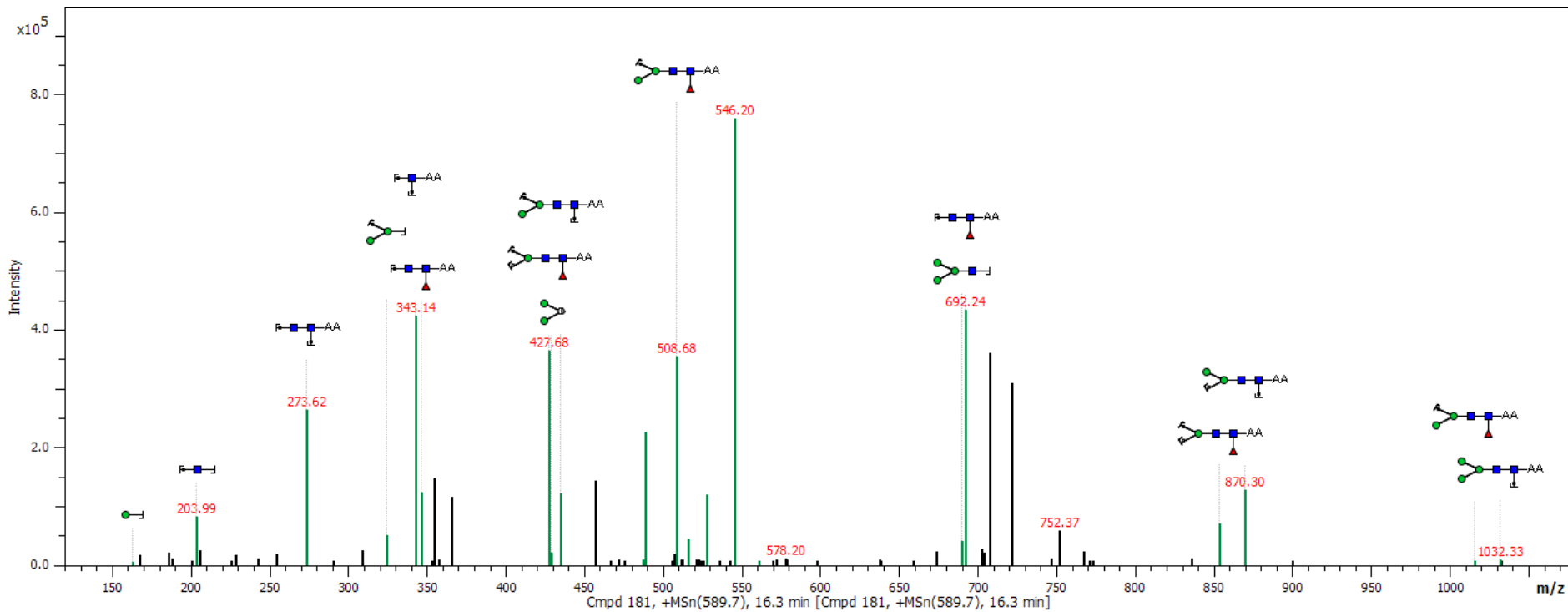
Score: 67.874

Composition: Hex3HexNAc2dHex1-AA

Intensity coverage [%]: 0.69

Accession: 9259

Fragment coverage [%]: 0.67

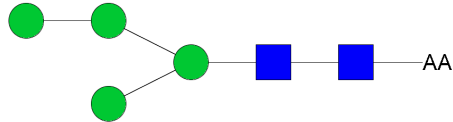


Spectrum 8



Glycan Search Report

Glycan: 6



Project path: /N-glycans cancer/Lift spectra/CombinedLIFT

MS data: c:/documents and settings/ciabalog/desktop/new folder/lift of 1192/0_b8/1/1192.4000.lift/
1sref/pdata/1/1r

Parent m/z: 1192.4260 -1

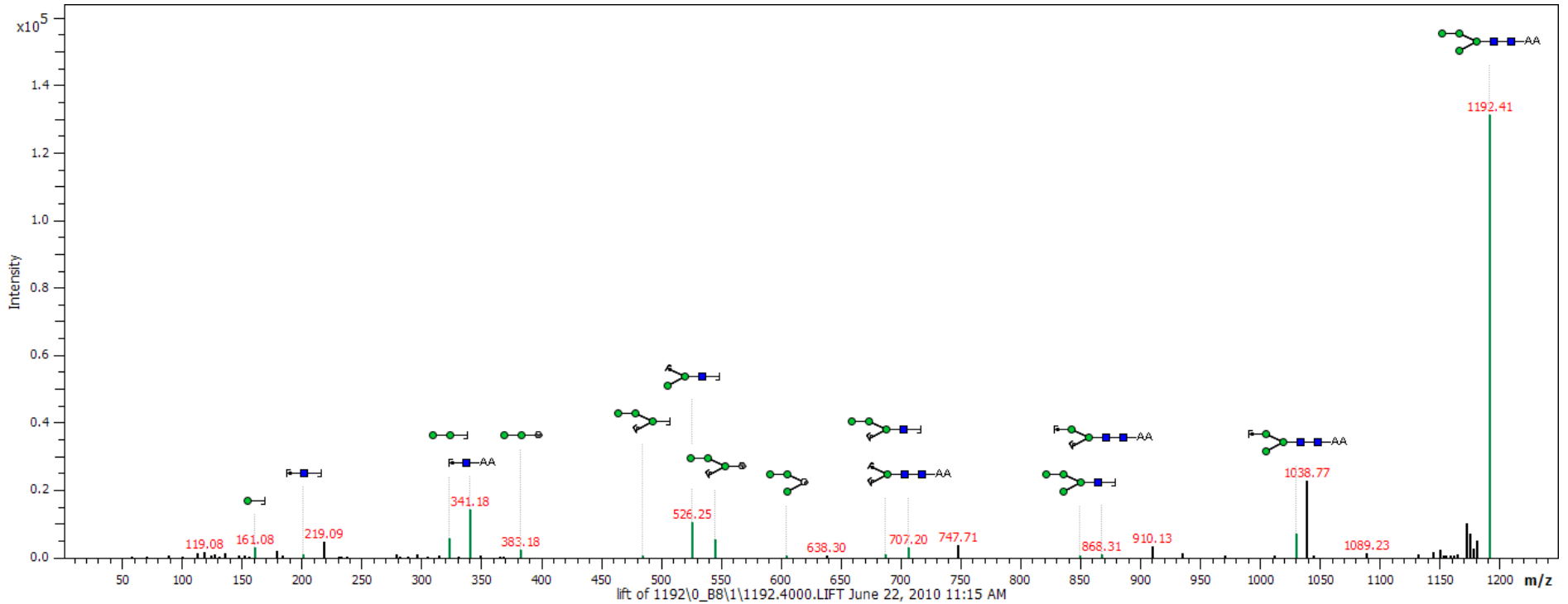
Score: 53.623

Composition: Hex4HexNAc2-AA

Intensity coverage [%]: 0.68

Accession: 951

Fragment coverage [%]: 0.42

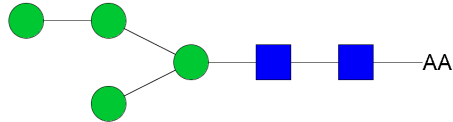


Spectrum 9



Glycan Search Report

Glycan: 3



Project path: /N-glycans cancer/25140/comp_25140.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25140_01.d/comp_25140.mgf

Parent m/z: 597.7239 2+

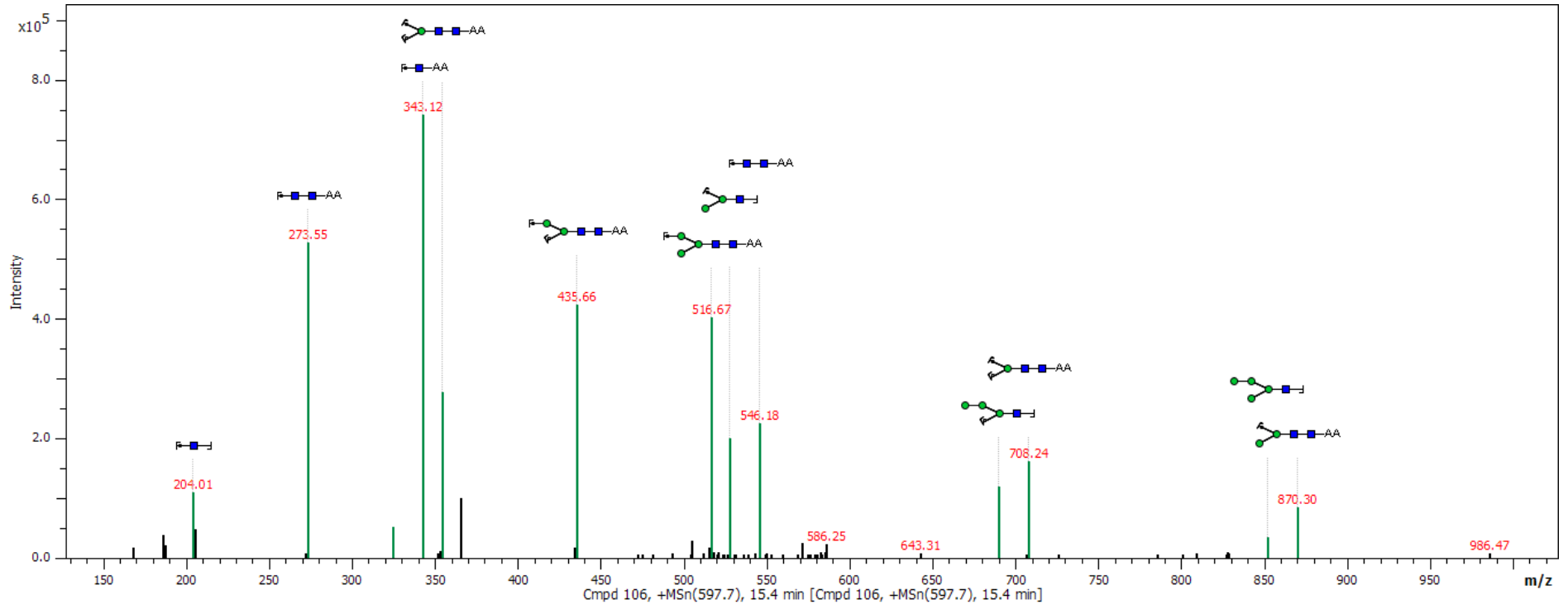
Score: 50.347

Composition: Hex4HexNAc2-AA

Intensity coverage [%]: 0.85

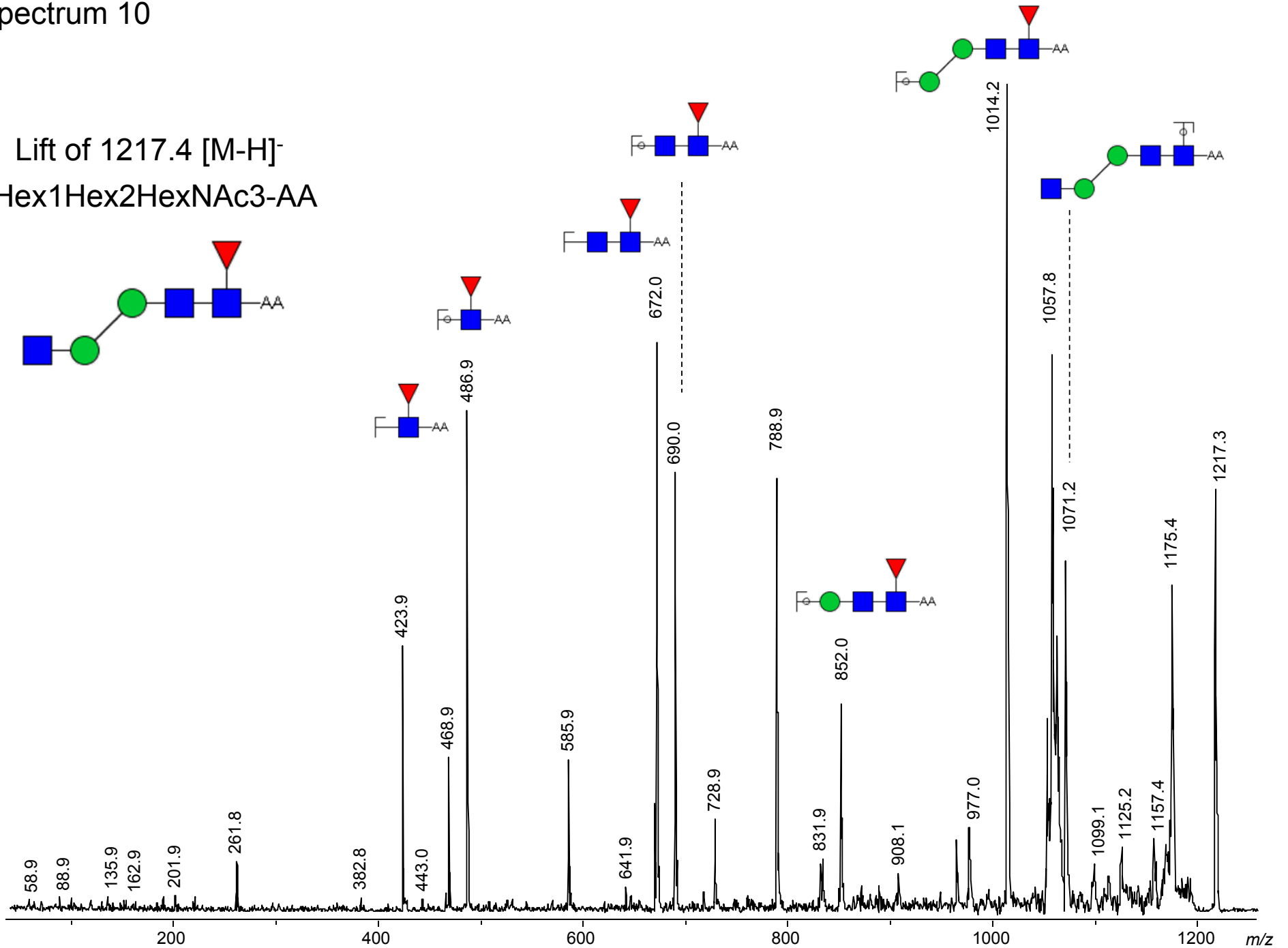
Accession: 951

Fragment coverage [%]: 0.30



Spectrum 10

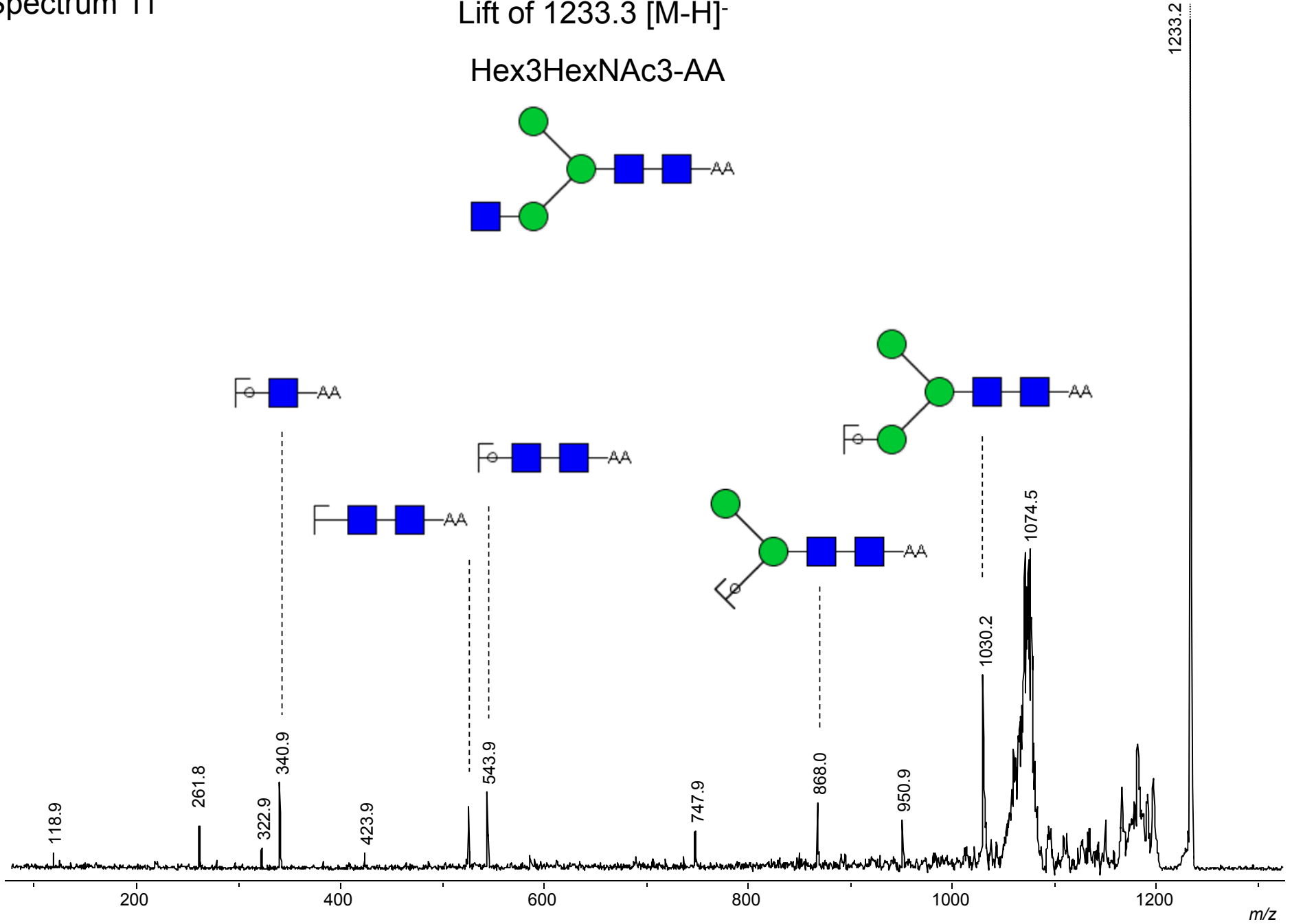
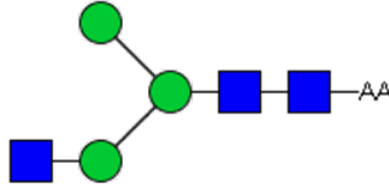
Lift of 1217.4 [M-H]⁻
dHex1Hex2HexNAc3-AA



Spectrum 11

Lift of 1233.3 [M-H]⁻

Hex3HexNAc3-AA

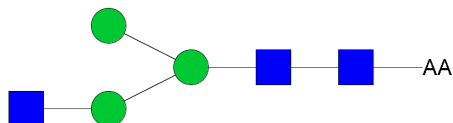


Spectrum 12



Glycan Search Report

Glycan: 2



Project path: /N-glycans cancer/25144/comp_25144.mgf

MS data: K:/Cancer-CCR/N-glycans raw_data_MS/LC-MS of the discriminators/25144_01.d/comp_25144.mgf

Parent m/z: 618.2372 2+

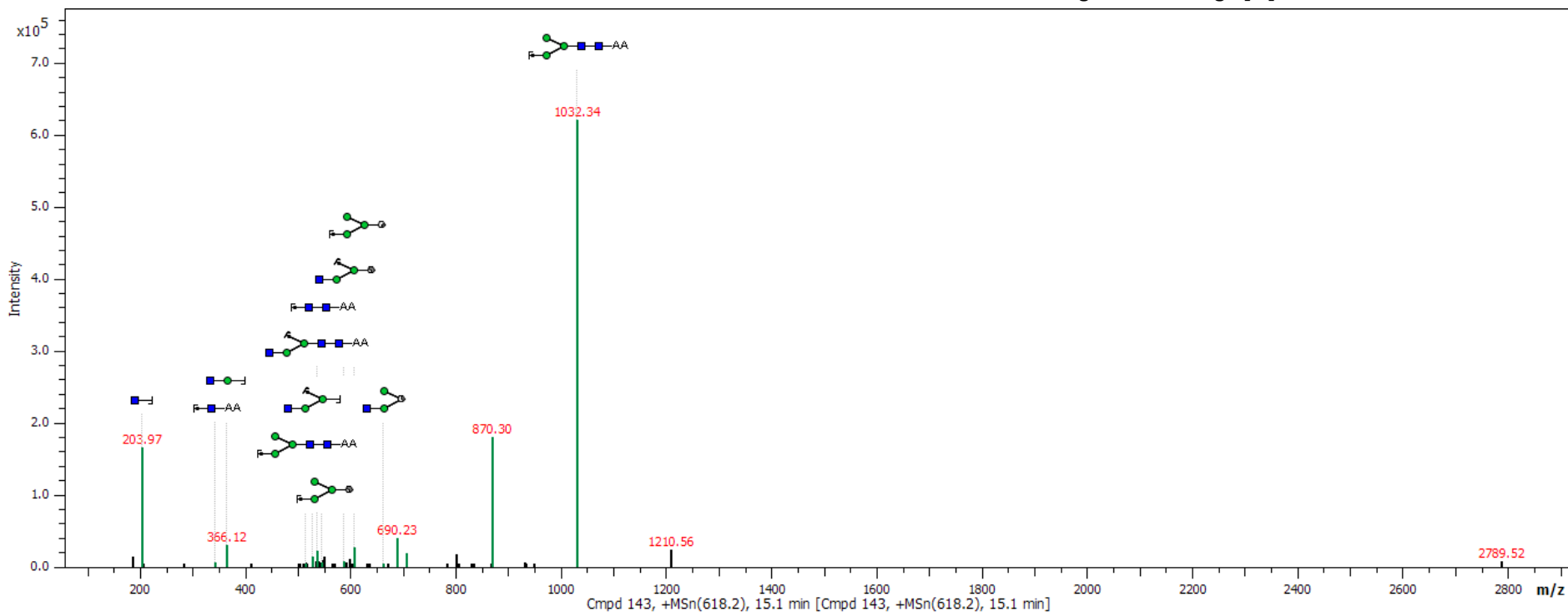
Score: 48.973

Composition: Hex3HexNAc3-AA

Intensity coverage [%]: 0.80

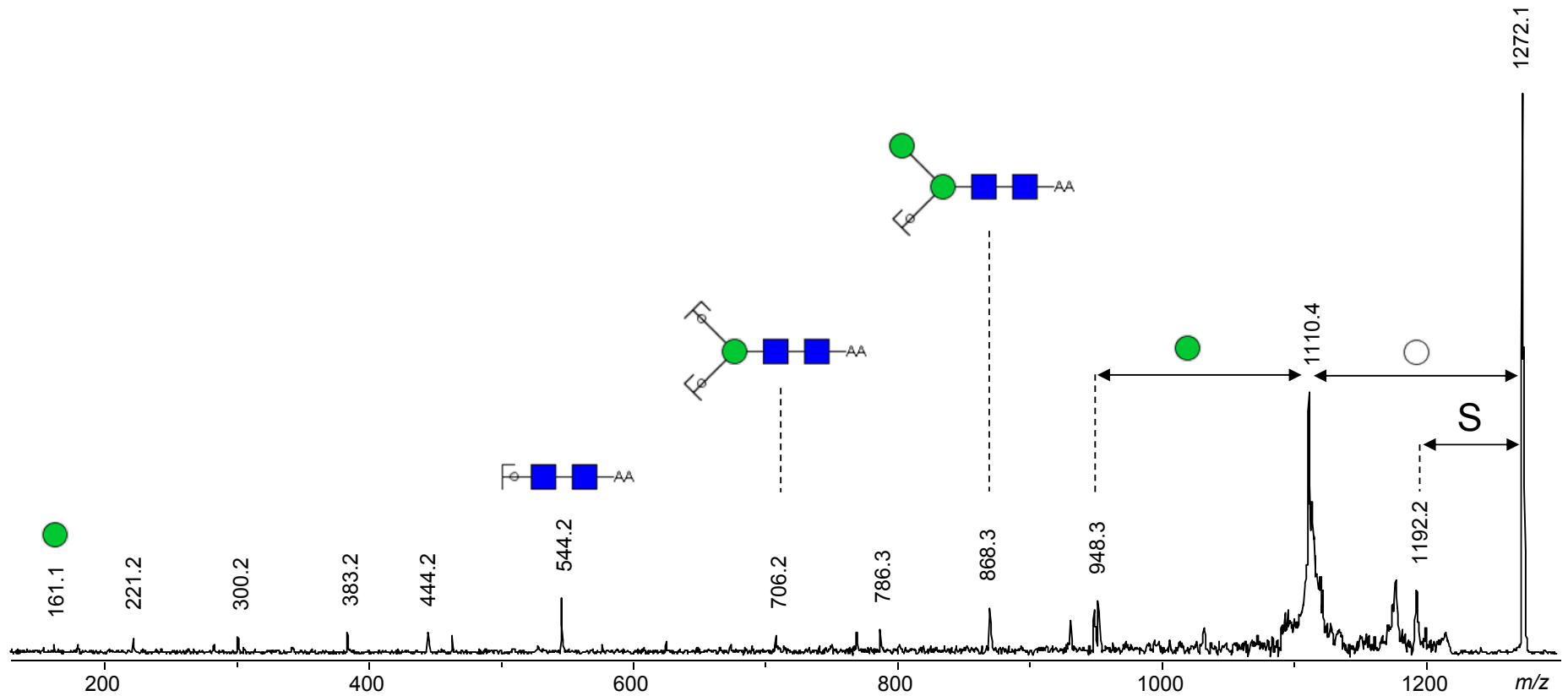
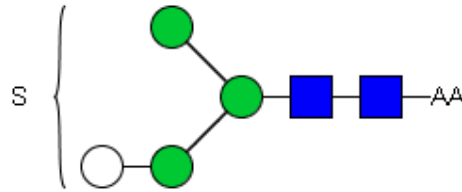
Accession: 1014

Fragment coverage [%]: 0.30



Spectrum 13

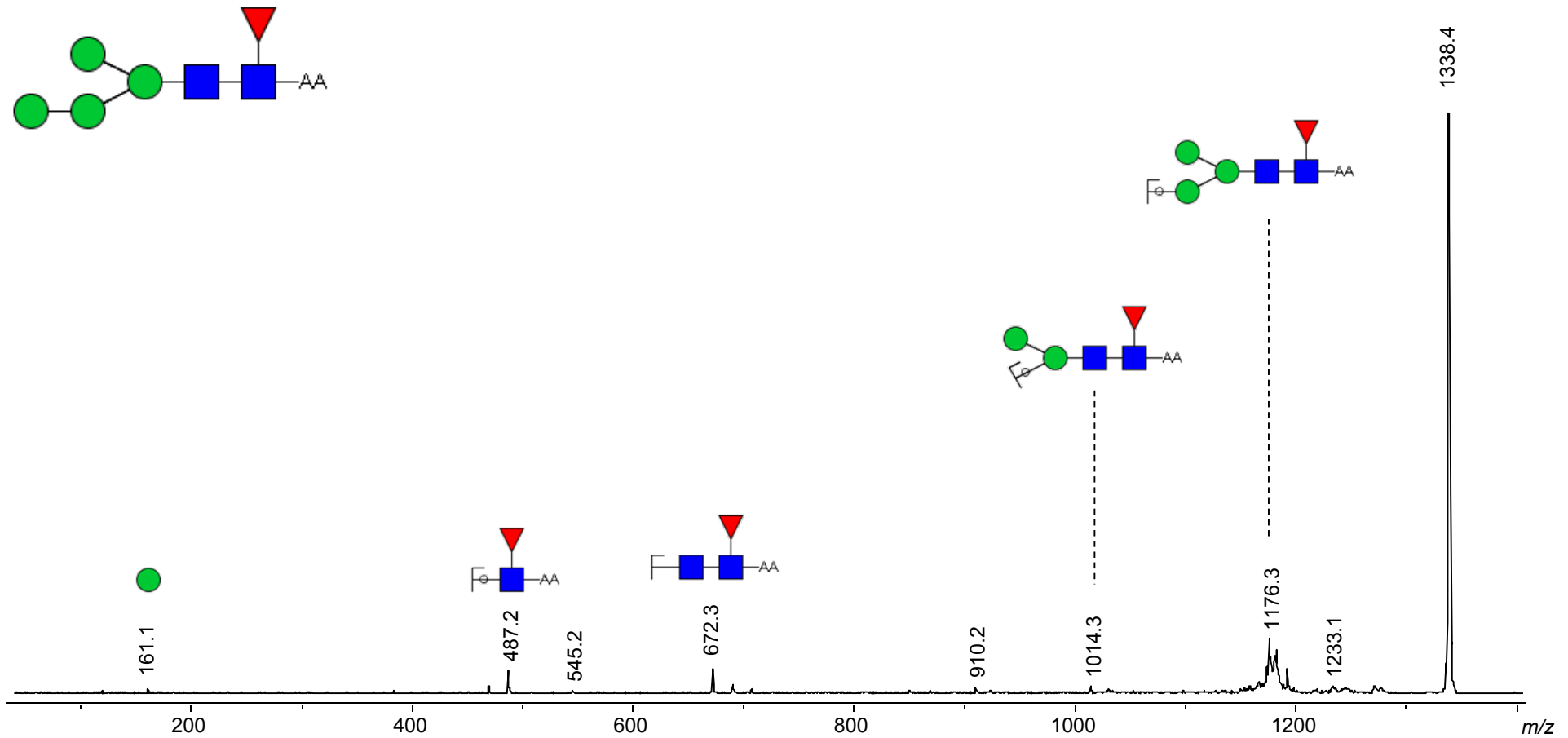
Lift of 1272.3 [M-H]⁻
S1Hex4HexNAc2-AA



Spectrum 14

Lift of 1238.4 [M-H]⁻

dHex1Hex4HexNAc2-AA

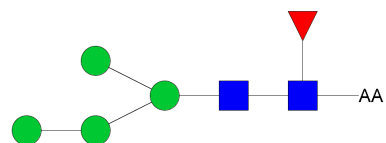




Spectrum 15

Glycan Search Report

Glycan: 5



Project path: /N-glycans cancer/25146/comp_25146.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25146_02.d/comp_25146.mgf

Parent m/z: 670.7529 2+

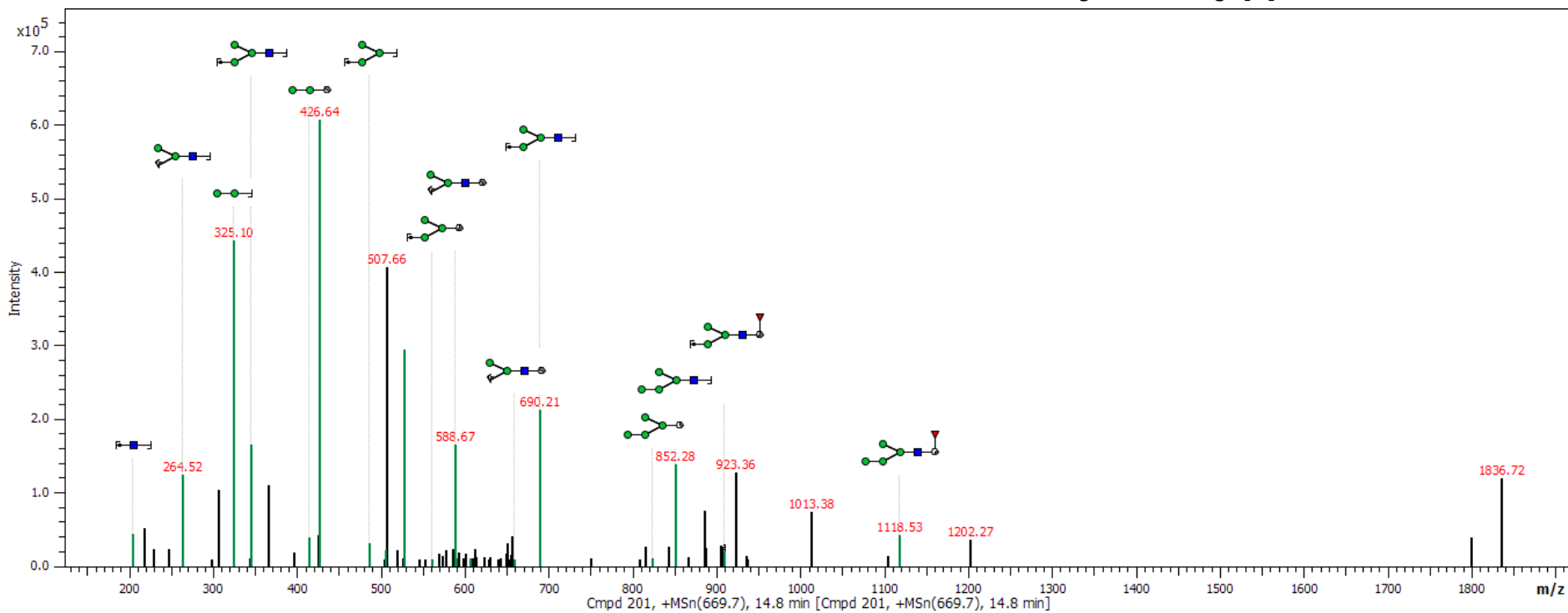
Score: 39.194

Composition: Hex4HexNAc2dHex1-AA

Intensity coverage [%]: 0.55

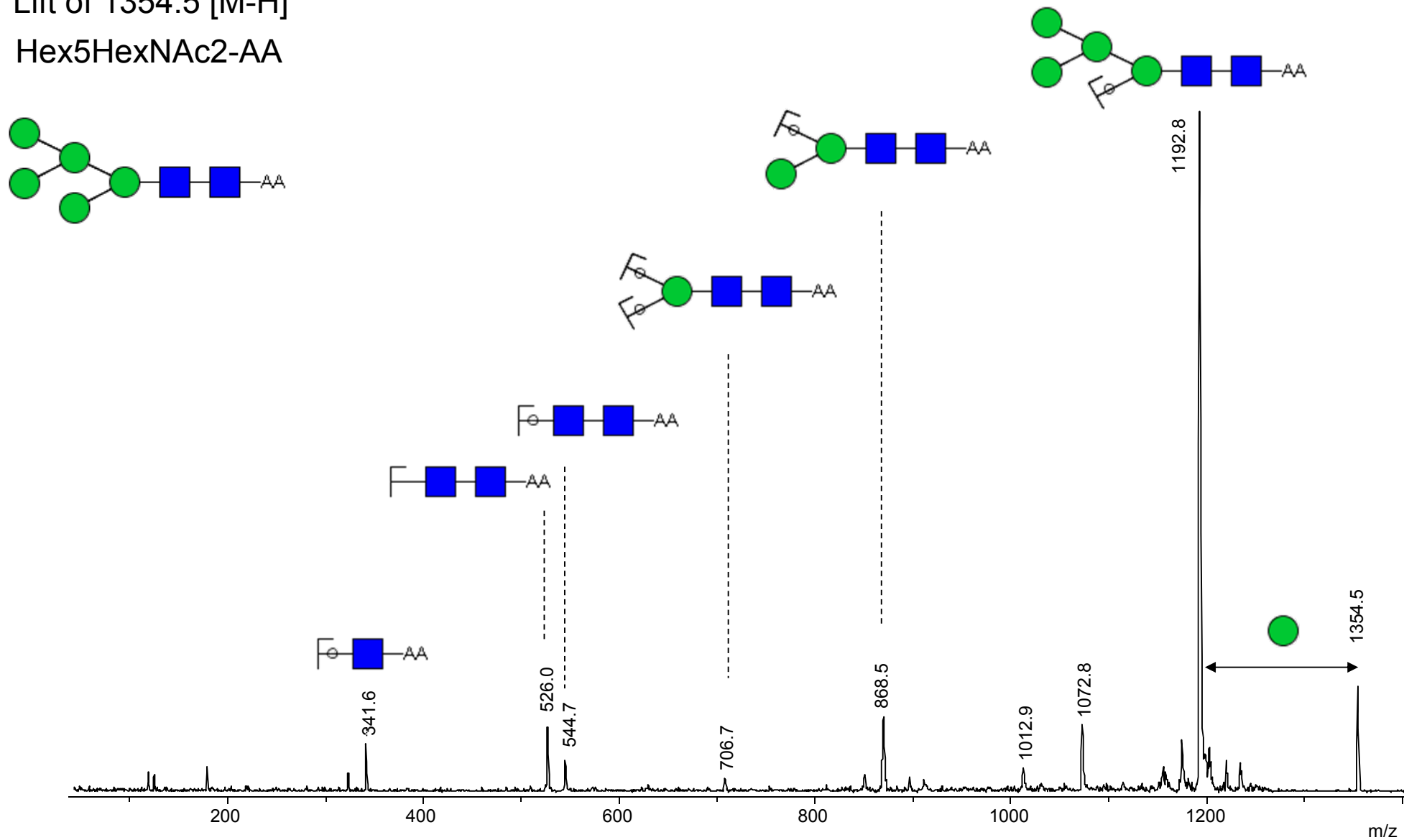
Accession: 24432

Fragment coverage [%]: 0.28



Spectrum 16

Lift of 1354.5 [M-H]⁻
Hex5HexNAc2-AA

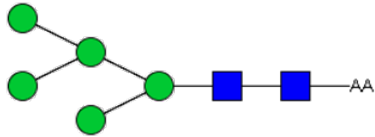


Spectrum 17



Glycan Search Report

Glycan: 1



Project path: /N-glycans cancer/25142/comp_25142_01.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25142_01.d/comp_25142_01.mgf

Parent m/z: 678.7503 2+

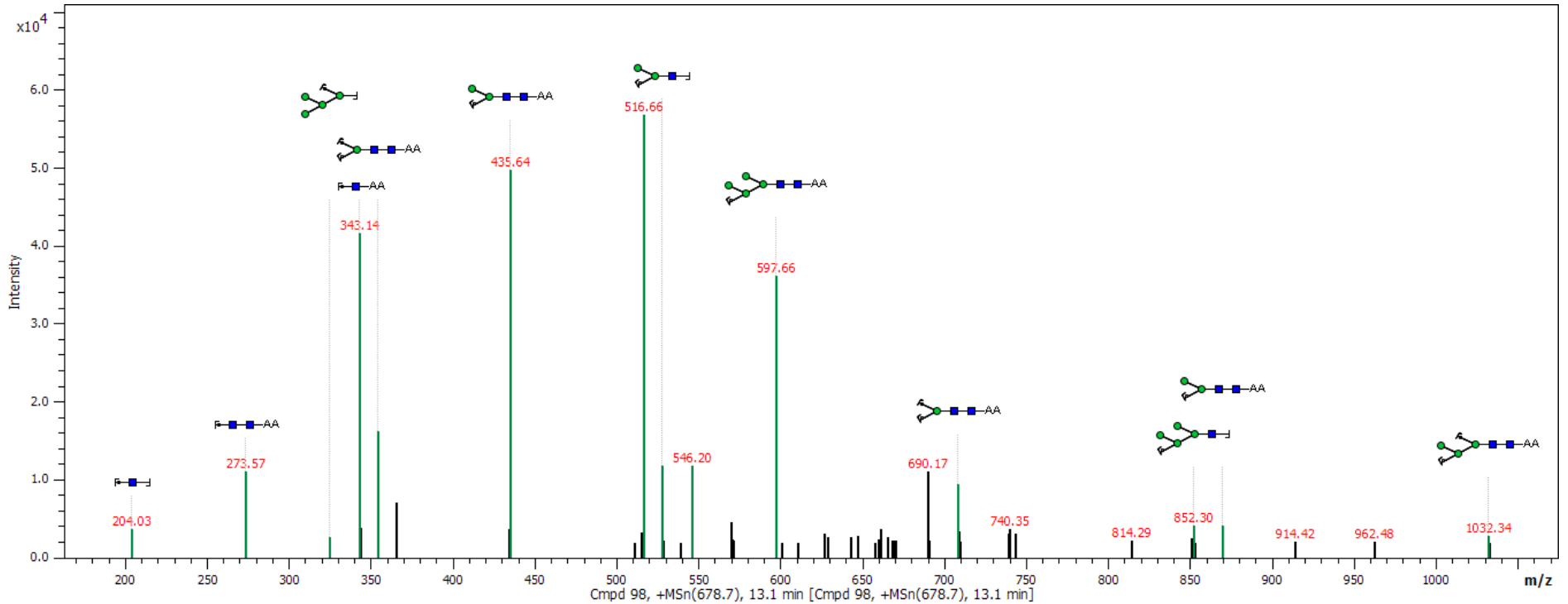
Score: 84.572

Composition: Hex5HexNAc2-AA

Intensity coverage [%]: 0.72

Accession: 36312

Fragment coverage [%]: 1.00

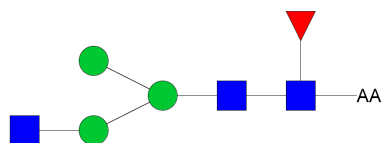




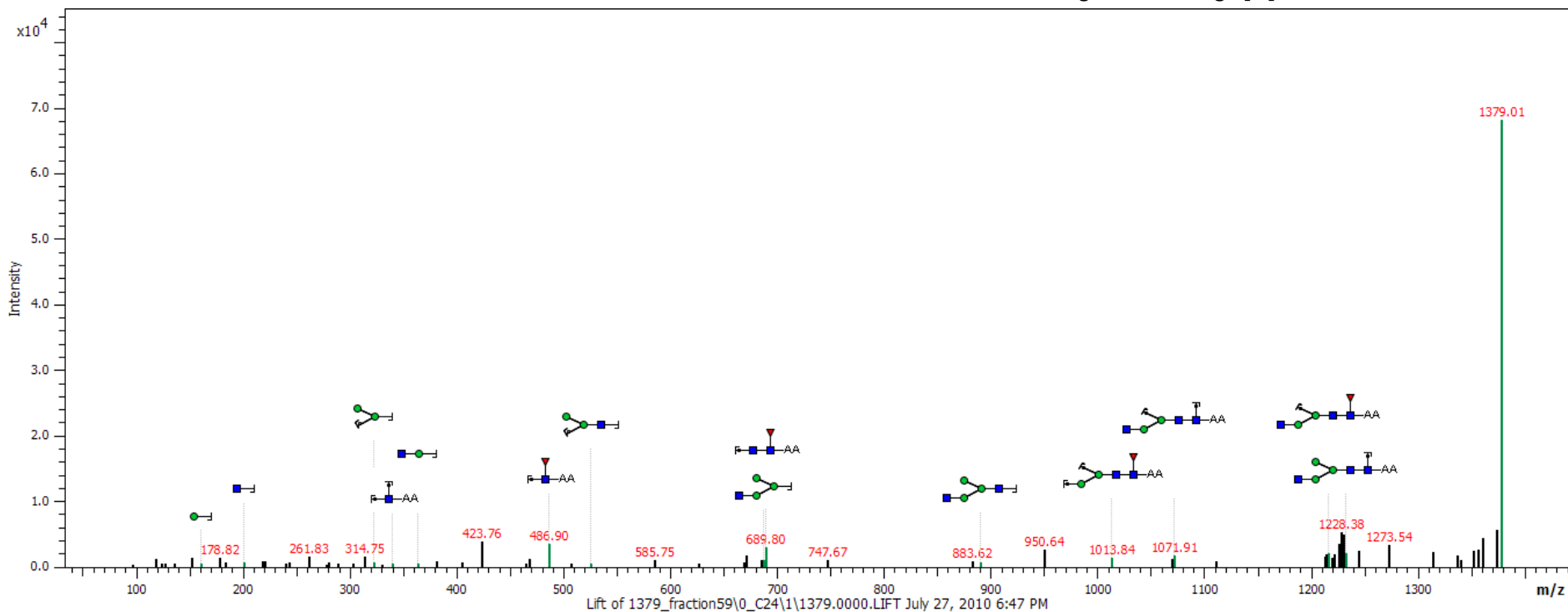
Spectrum 18

Glycan Search Report

Glycan: 4



Project path: /N-glycans cancer/Lift spectra/CombinedLIFT
MS data: c:/documents and settings/ciabalog/desktop/new folder/lift of 1379_fraction59/0_c24/1/1379.0000.lift/1sref/pdata/1/1r
Parent m/z: 1379.5105 -1 **Score:** 61.330
Composition: Hex3HexNAc3dHex1-AA **Intensity coverage [%]:** 0.53
Accession: 36110 **Fragment coverage [%]:** 0.71

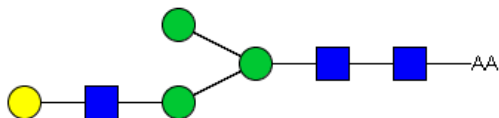




Spectrum 19

Glycan Search Report

Glycan: 2



Project path: /N-glycans cancer/25146/comp_25146.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25146_02.d/comp_25146.mgf

Parent m/z: 699.2636 2+

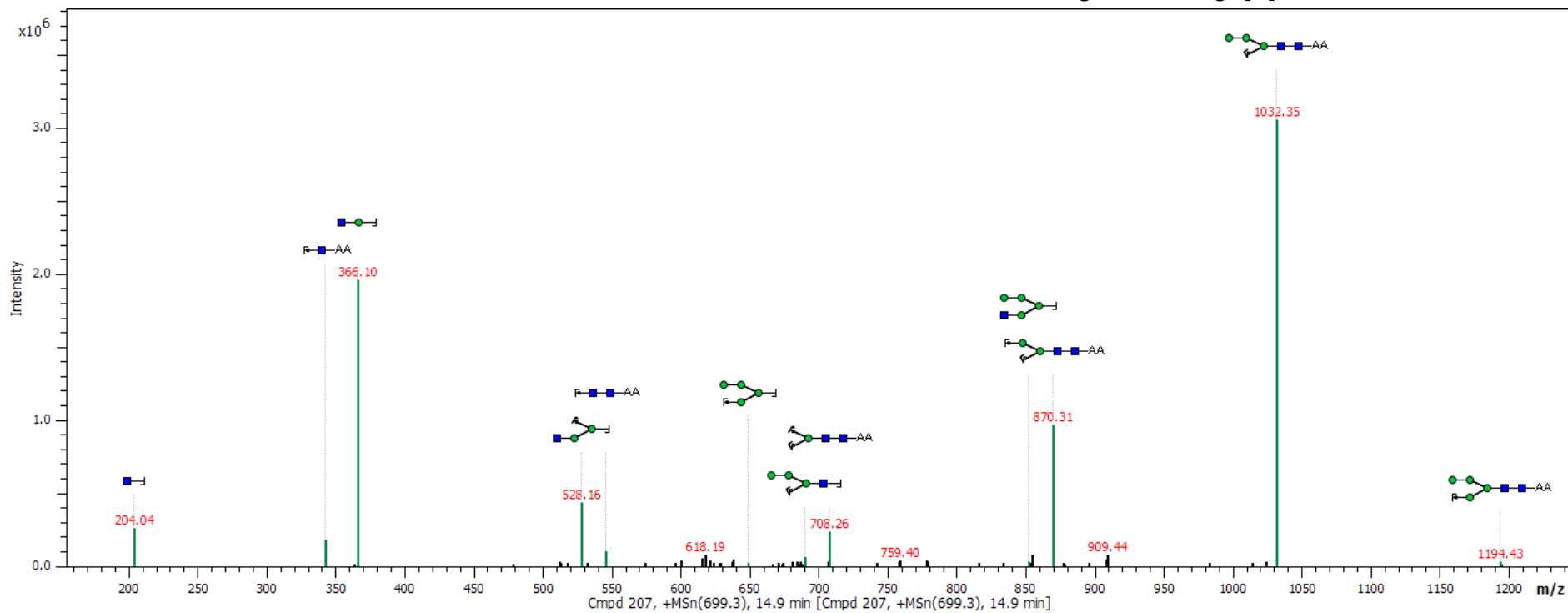
Score: 71.904

Composition: Hex4HexNAc3-AA

Intensity coverage [%]: 0.85

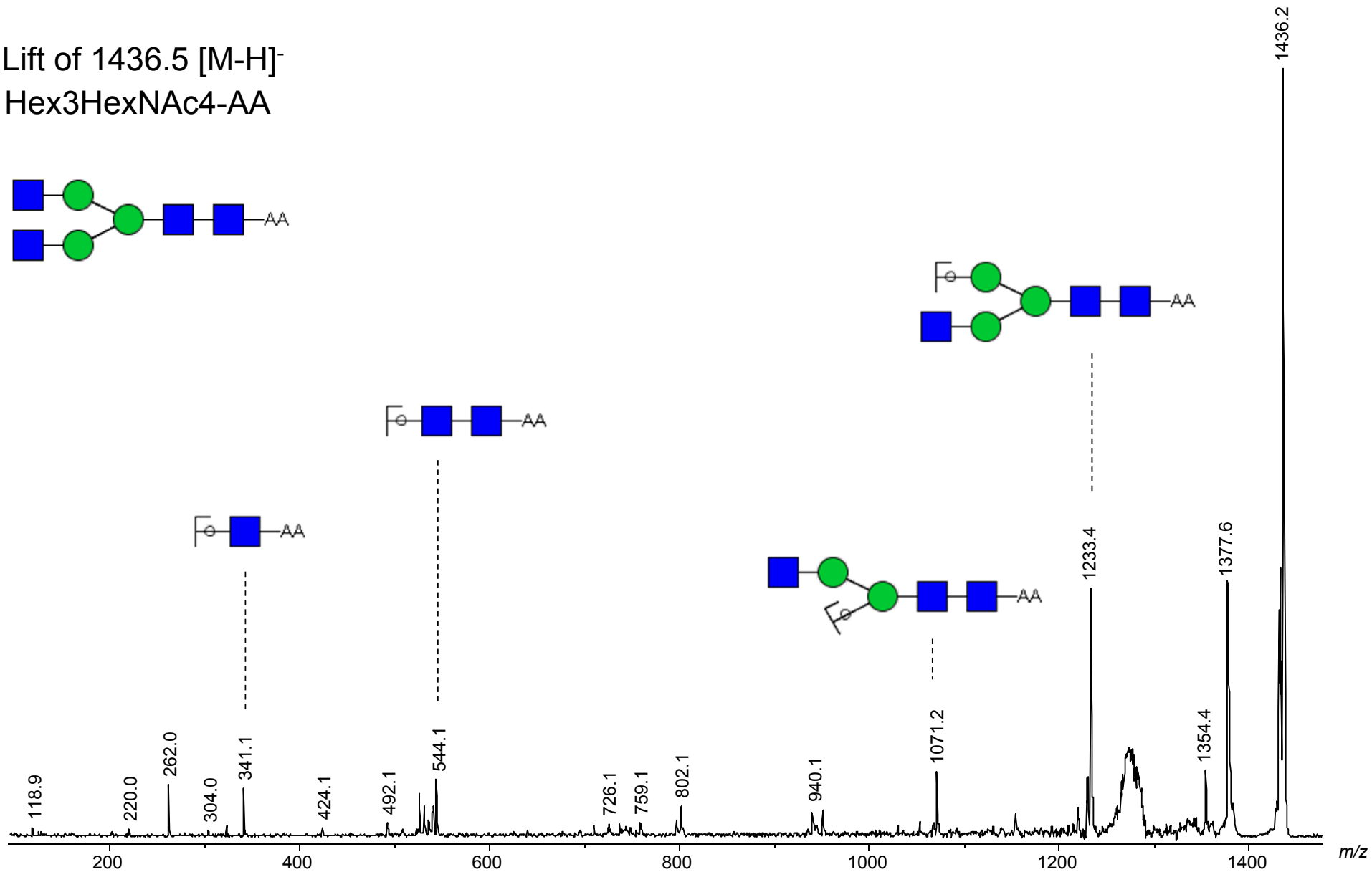
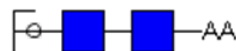
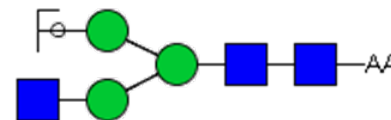
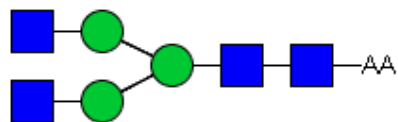
Accession: 36335

Fragment coverage [%]: 0.61



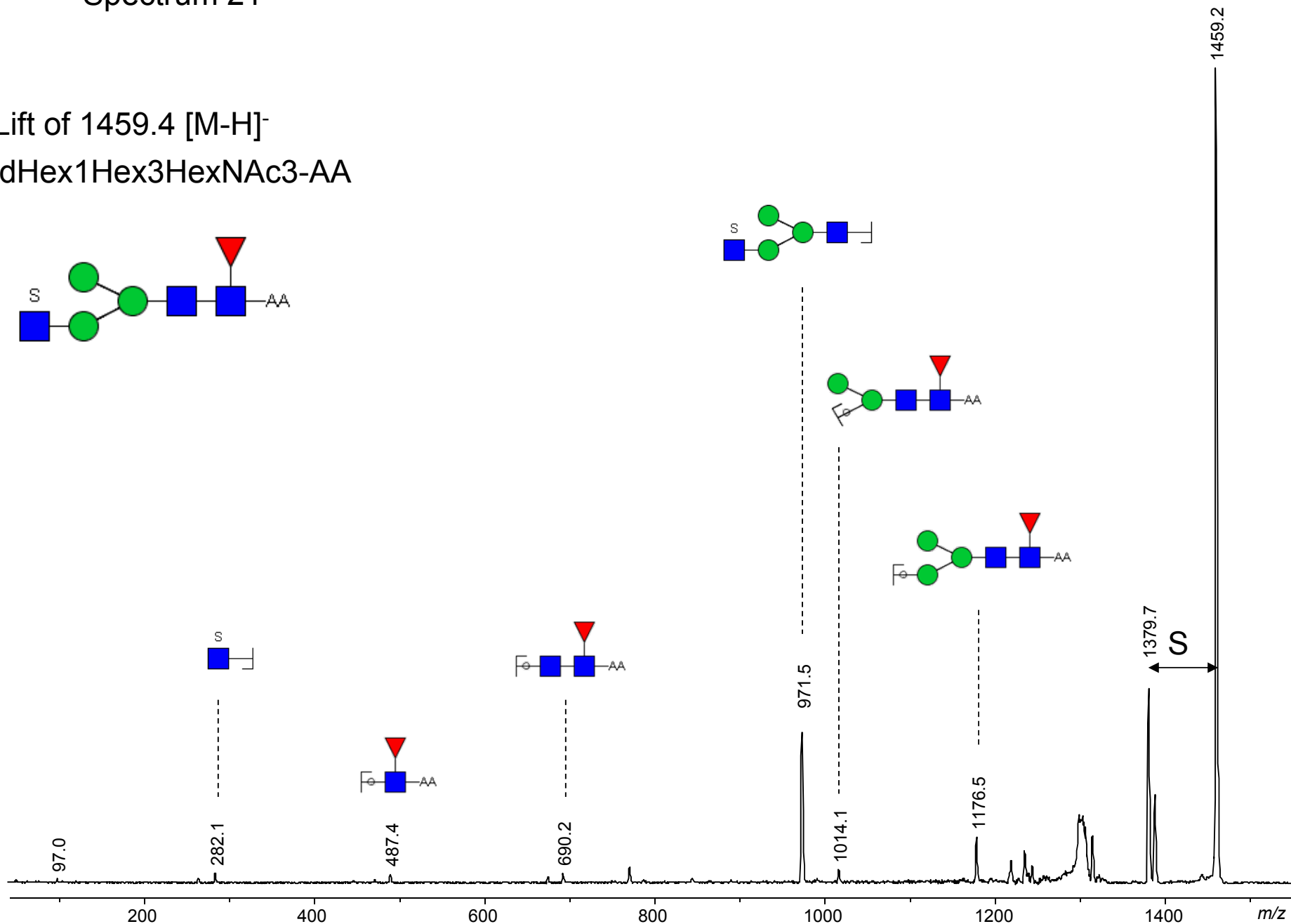
Spectrum 20

Lift of 1436.5 [M-H]⁻
Hex3HexNAc4-AA



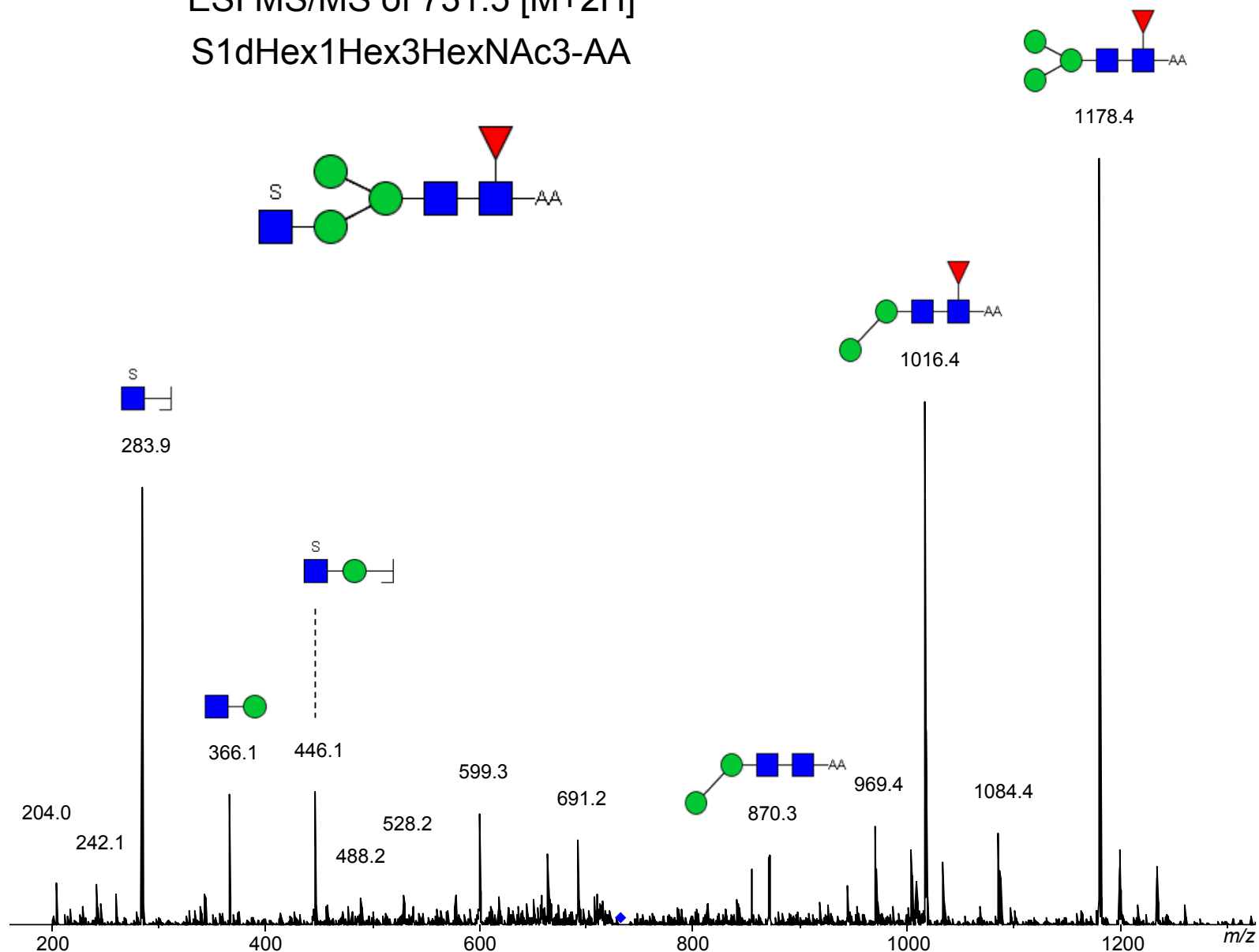
Spectrum 21

Lift of 1459.4 [M-H]⁻
S1dHex1Hex3HexNAc3-AA



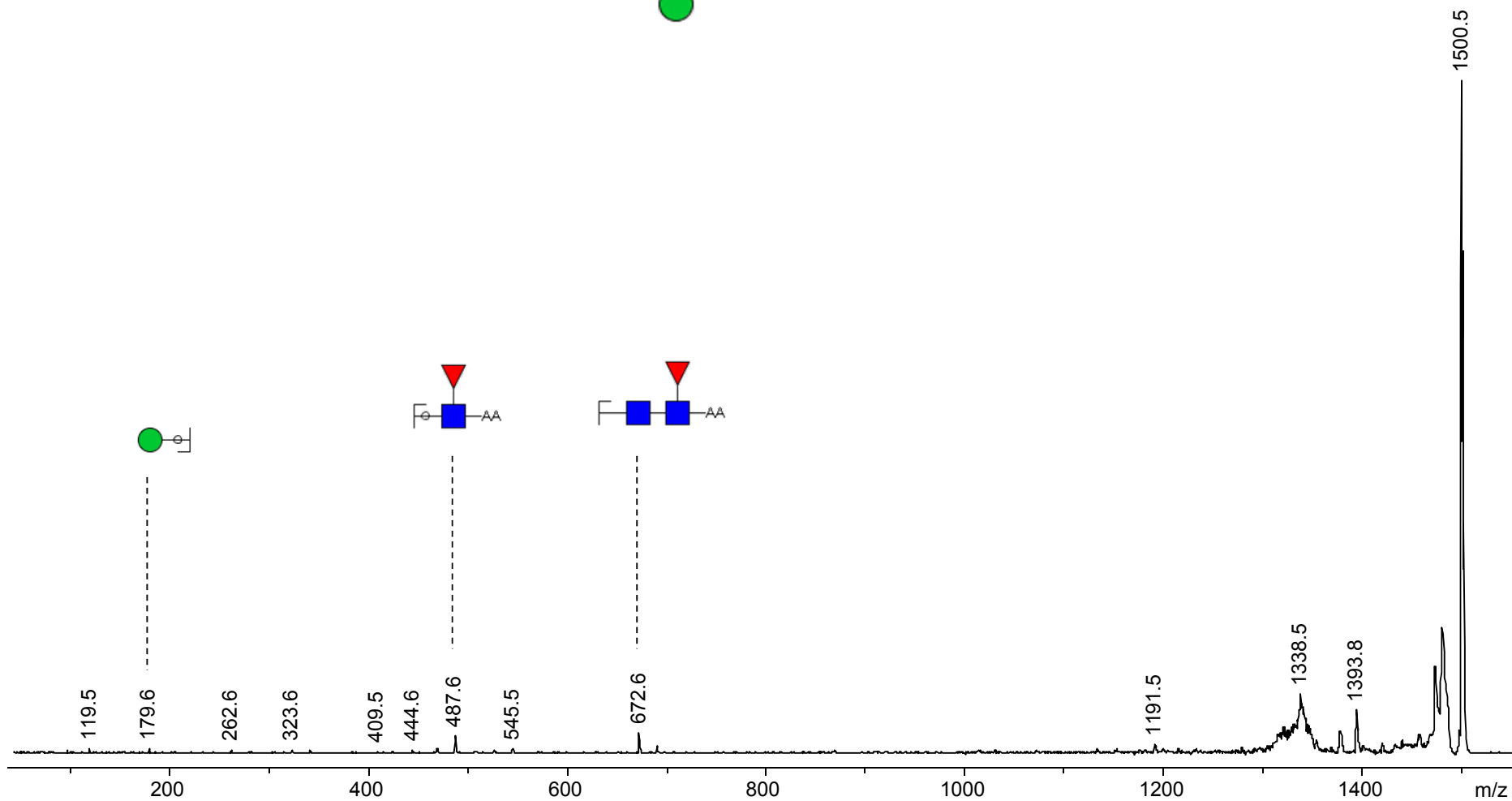
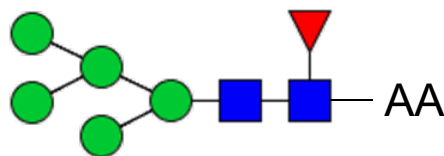
Spectrum 22

ESI MS/MS of 731.5 [M+2H]²⁺
S1dHex1Hex3HexNAc3-AA



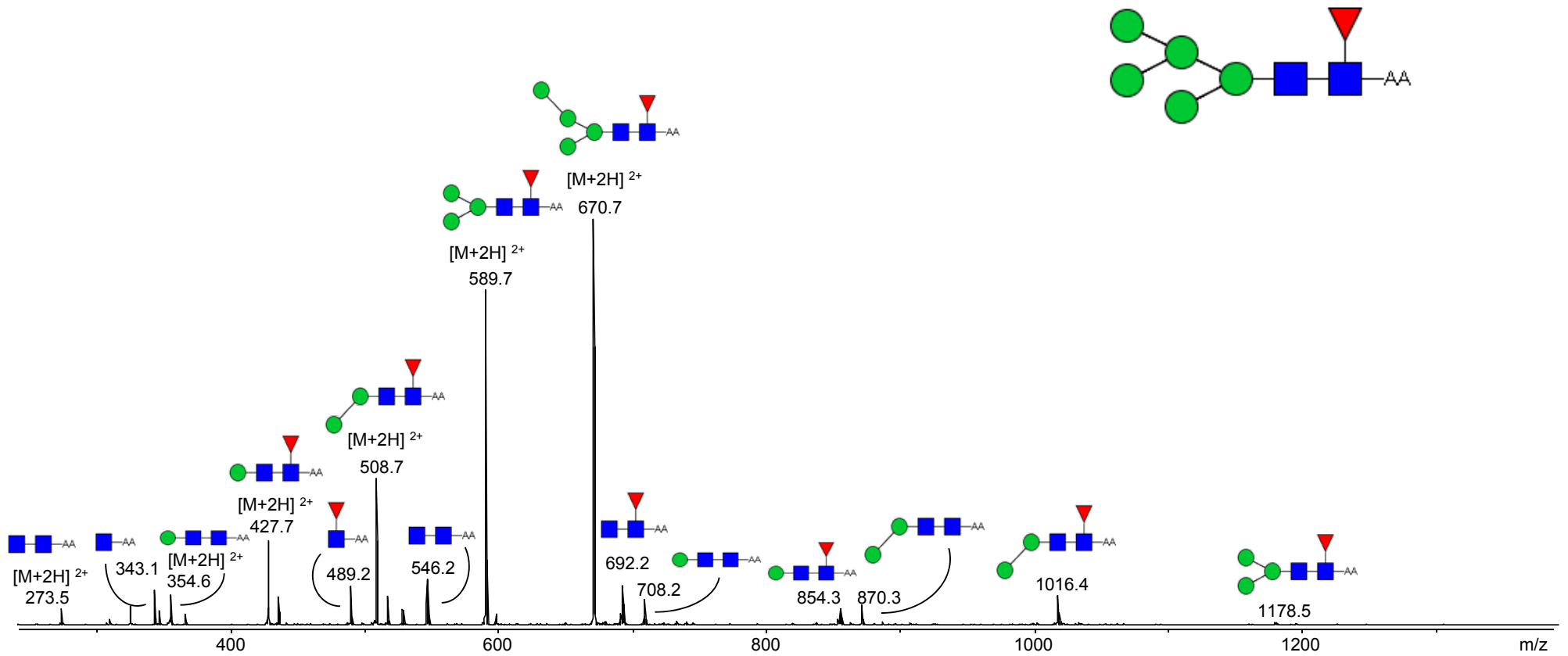
Spectrum 23

Lift of 1500.5 [M-H]⁻
dHex1Hex5HexNAc2-AA



Spectrum 24

ESI MS/MS of $[751.9 + 2H]^{2+}$
dHex1Hex5HexNAc2-AA

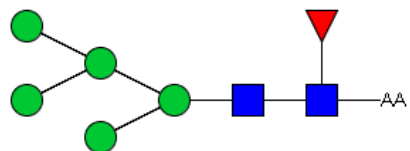




Spectrum 24

Glycan Search Report

Glycan: 5



Project path: /N-glycans cancer/25141/comp_25141.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25141_01.d/comp_25141.mgf

Parent m/z: 751.7793 2+

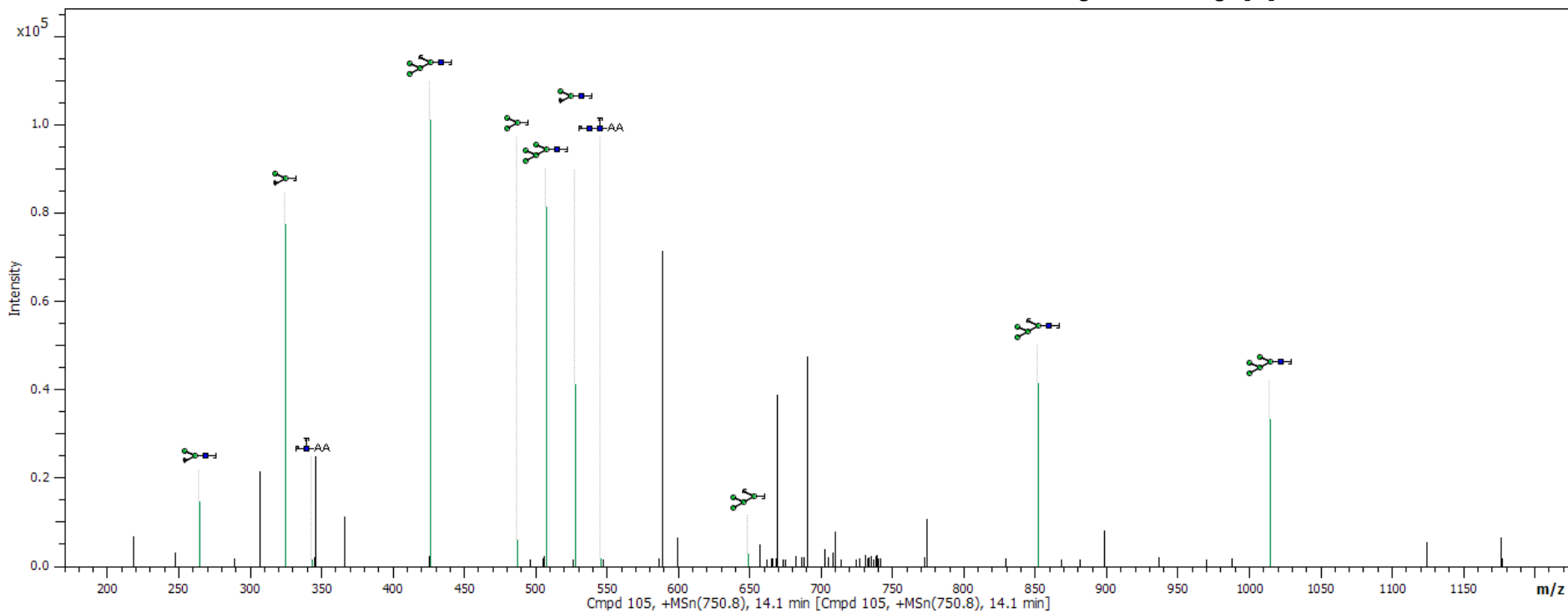
Score: 53.396

Composition: Hex5HexNAc2dHex1-AA

Intensity coverage [%]: 0.53

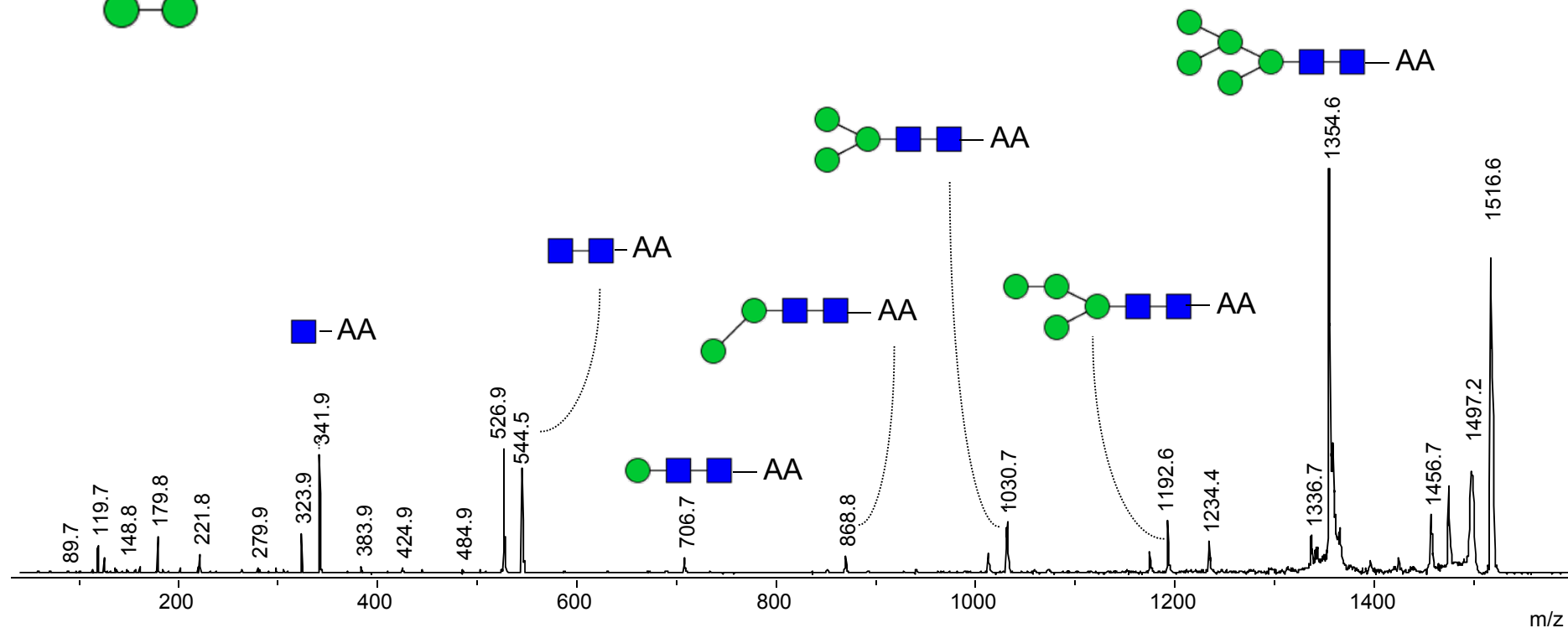
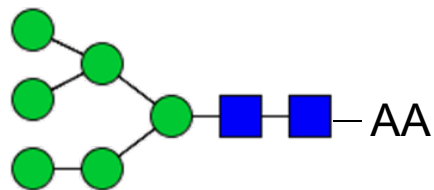
Accession: 36116

Fragment coverage [%]: 0.54



Spectrum 25

Lift of 1516.5 [M-H]⁻
Hex6HexNAc2-AA

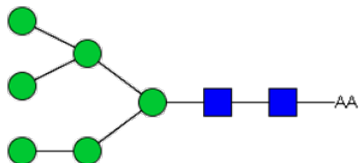




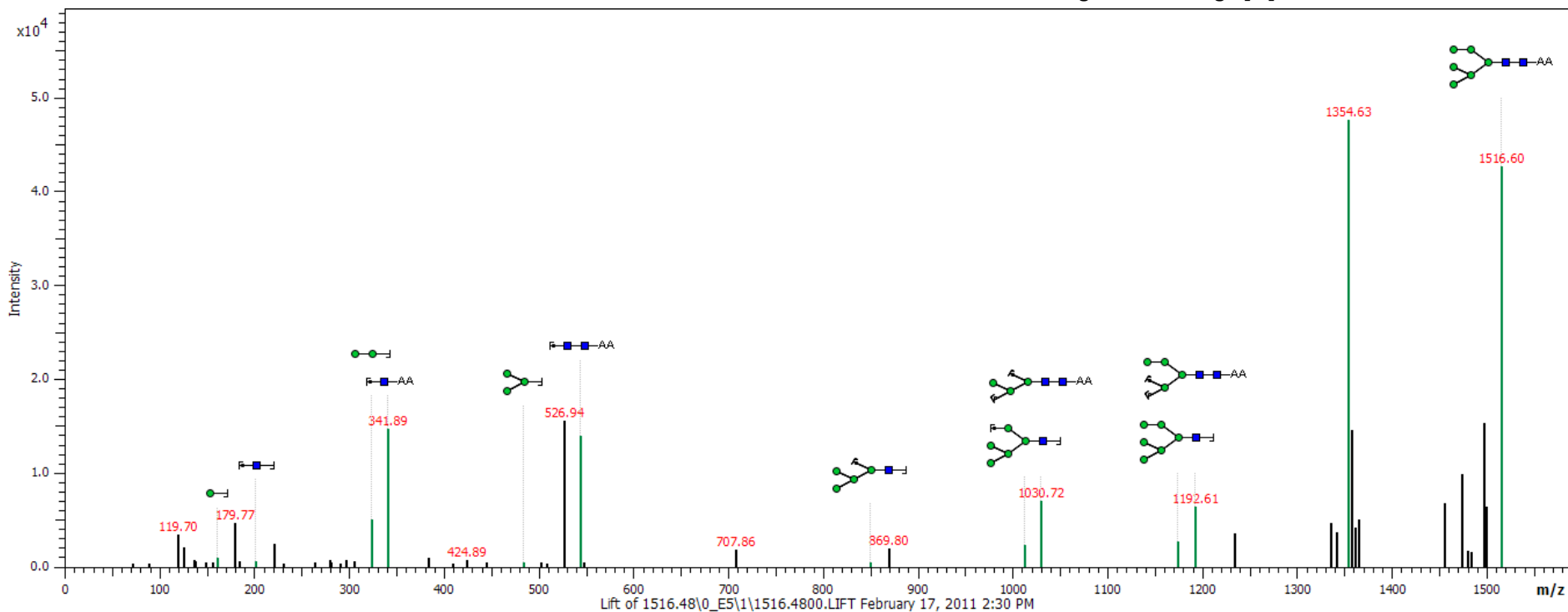
Spectrum 25

Glycan Search Report

Glycan: 1



Project path: /N-glycans cancer/Lift spectra 01/CombinedUNKNOWN
MS data: c:/documents and settings/ciabalog/desktop/17-02-11/lift of 1516.48/0_e5/1/1516.4800.lift/1sref/pdata/1/1r
Parent m/z: 1516.5316 -1 **Score:** 64.166
Composition: Hex6HexNAc2-AA **Intensity coverage [%]:** 0.55
Accession: 36315 **Fragment coverage [%]:** 0.75

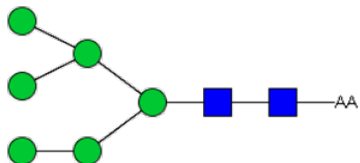




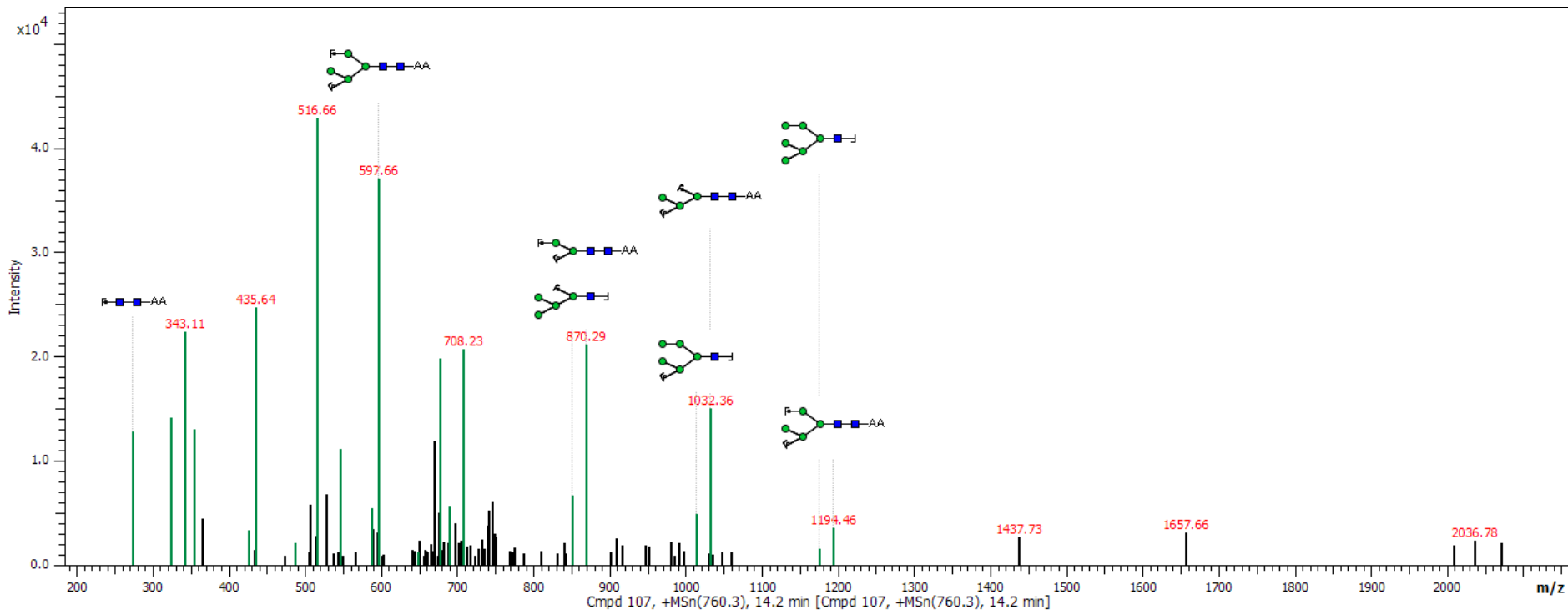
Spectrum 26

Glycan Search Report

Glycan: 2



Project path: /N-glycans cancer/25141/comp_25141.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25141_01.d/comp_25141.mgf
Parent m/z: 759.7767 2+ **Score:** 85.567
Composition: Hex6HexNAc2-AA **Intensity coverage [%]:** 0.64
Accession: 36315 **Fragment coverage [%]:** 1.14

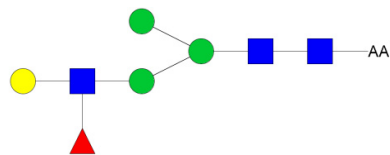




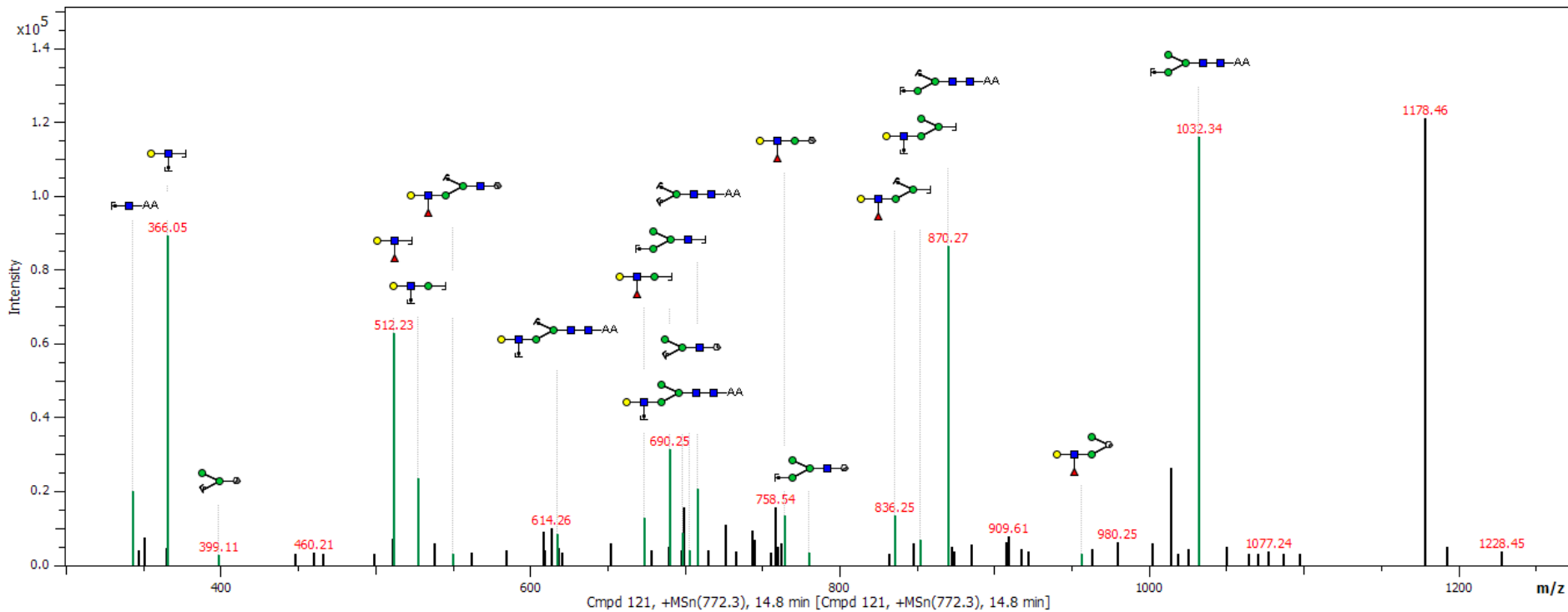
Spectrum 27

Glycan Search Report

Glycan: 9



Project path: /N-glycans cancer/25141/comp_25141.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25141_01.d/comp_25141.mgf
Parent m/z: 772.2926 2+ **Score:** 32.282
Composition: Hex4HexNAc3dHex1-AA **Intensity coverage [%]:** 0.56
Accession: 29050 **Fragment coverage [%]:** 0.19

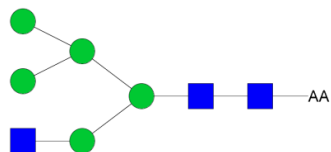




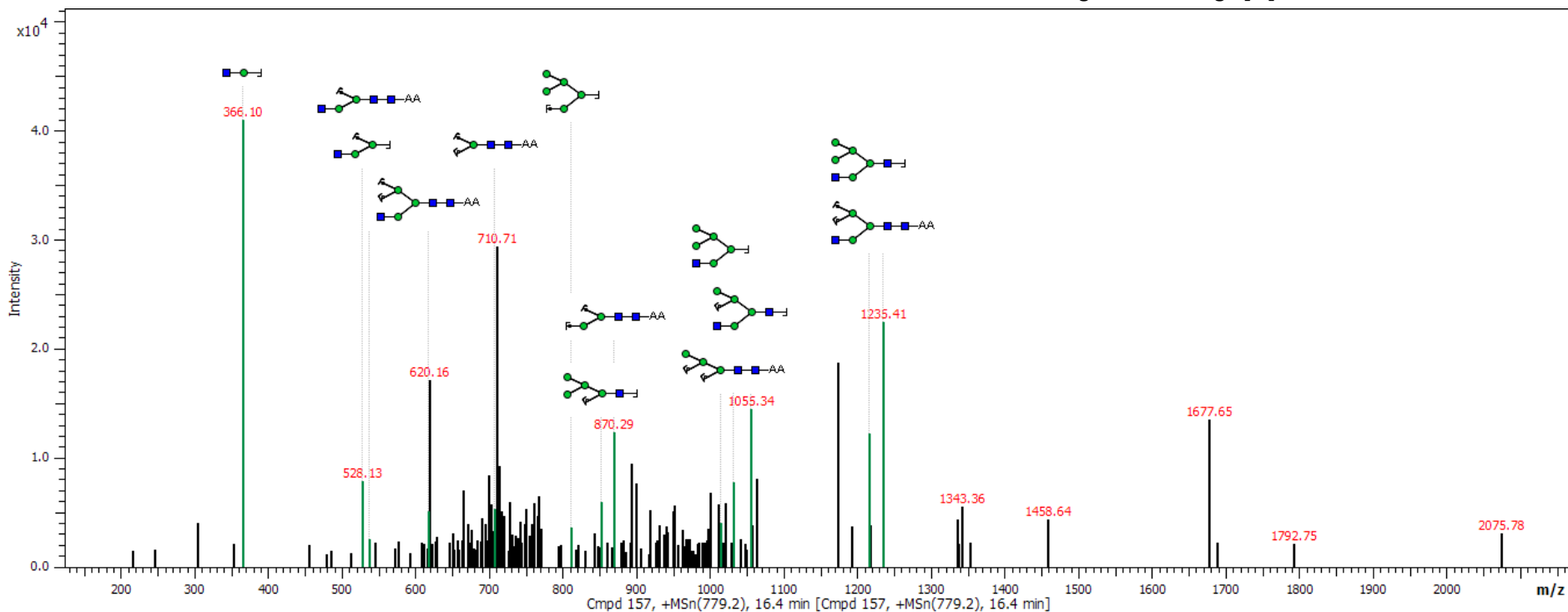
Spectrum 28

Glycan Search Report

Glycan: 9

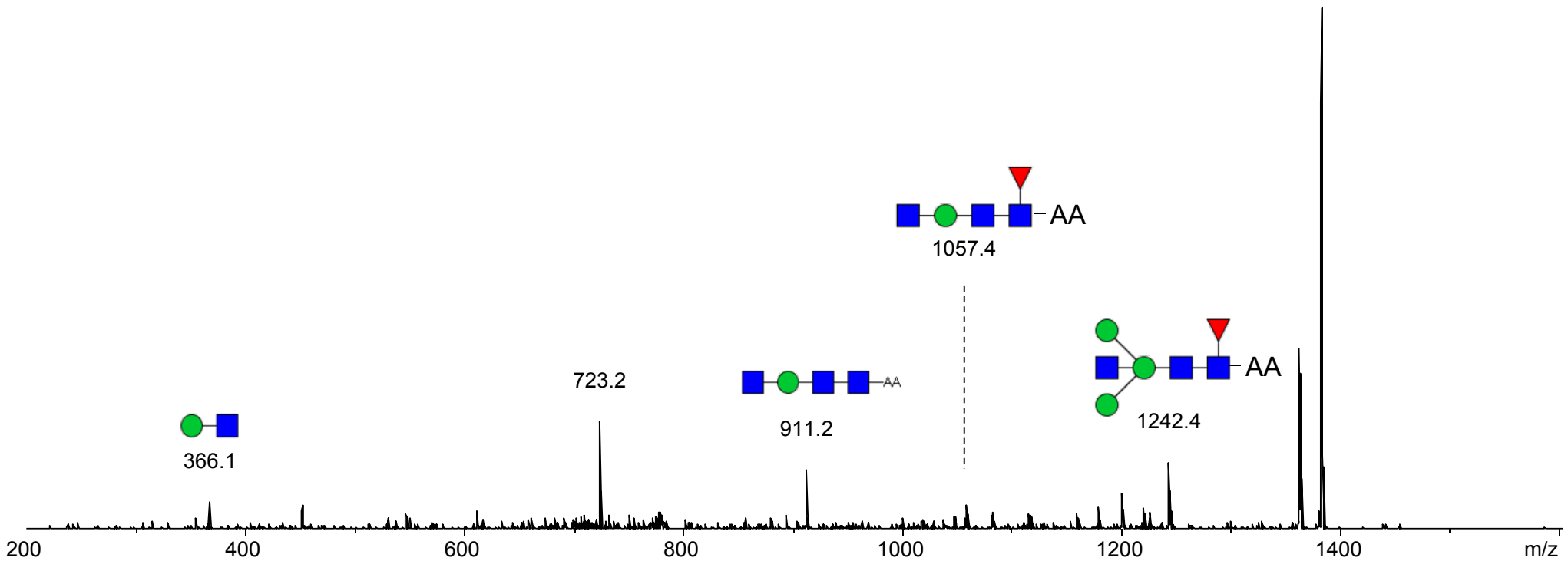
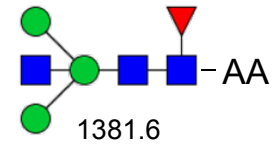
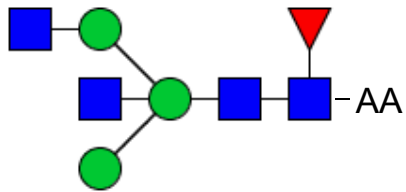


Project path: /N-glycans cancer/25141/comp_25141.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25141_01.d/comp_25141.mgf
Parent m/z: 780.2900 2+ **Score:** 34.511
Composition: Hex5HexNAc3-AA **Intensity coverage [%]:** 0.23
Accession: 36316 **Fragment coverage [%]:** 0.52



Spectrum 29

ESI MS/MS of 792.8 [M+2H]²⁺
dHex1Hex3HexNAc4-AA

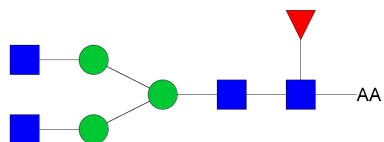




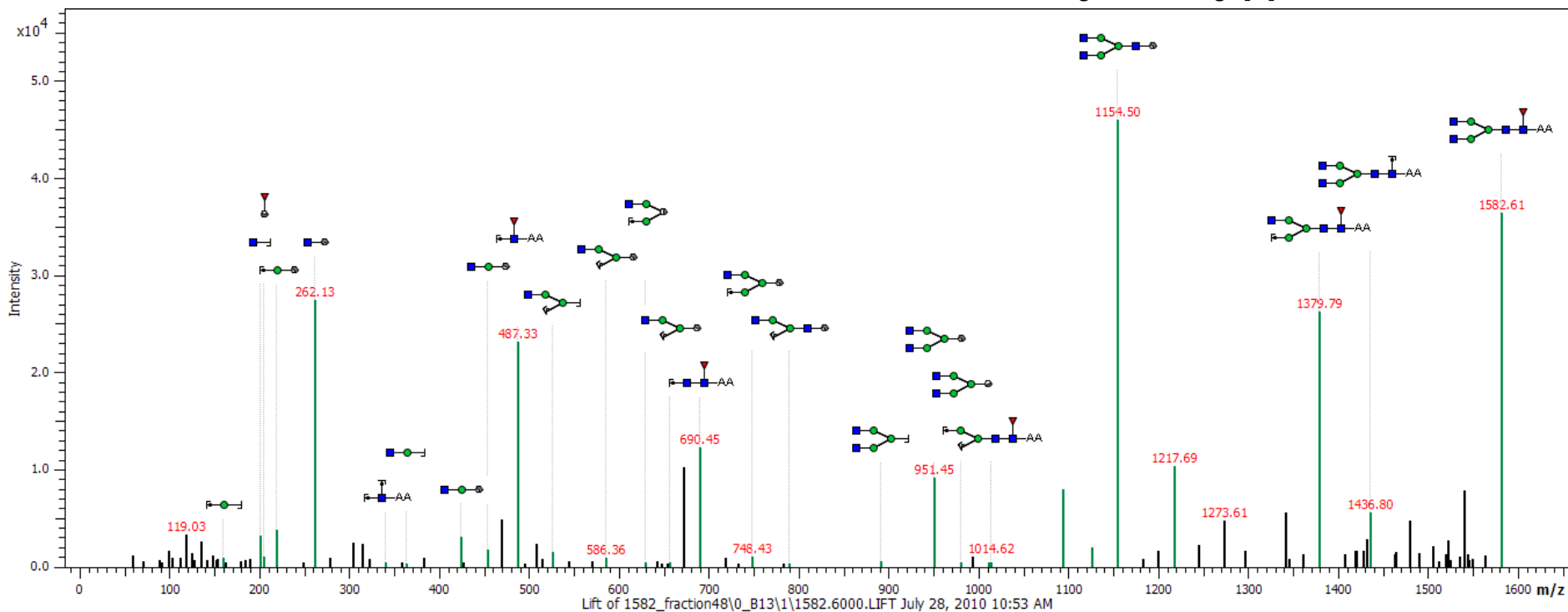
Spectrum 30

Glycan Search Report

Glycan: 7



Project path: /N-glycans cancer/Lift spectra/CombinedLIFT
MS data: c:/documents and settings/ciabalog/desktop/new folder/lift of 1582_fraction48/0_b13/1/1582.6000.lift/1sref/pdata/1/1r
Parent m/z: 1582.5899 -1 **Score:** 51.758
Composition: Hex3HexNAc4dHex1-AA **Intensity coverage [%]:** 0.68
Accession: 2620 **Fragment coverage [%]:** 0.39

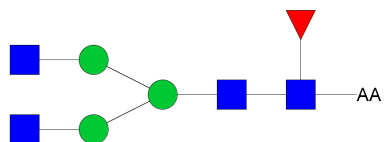




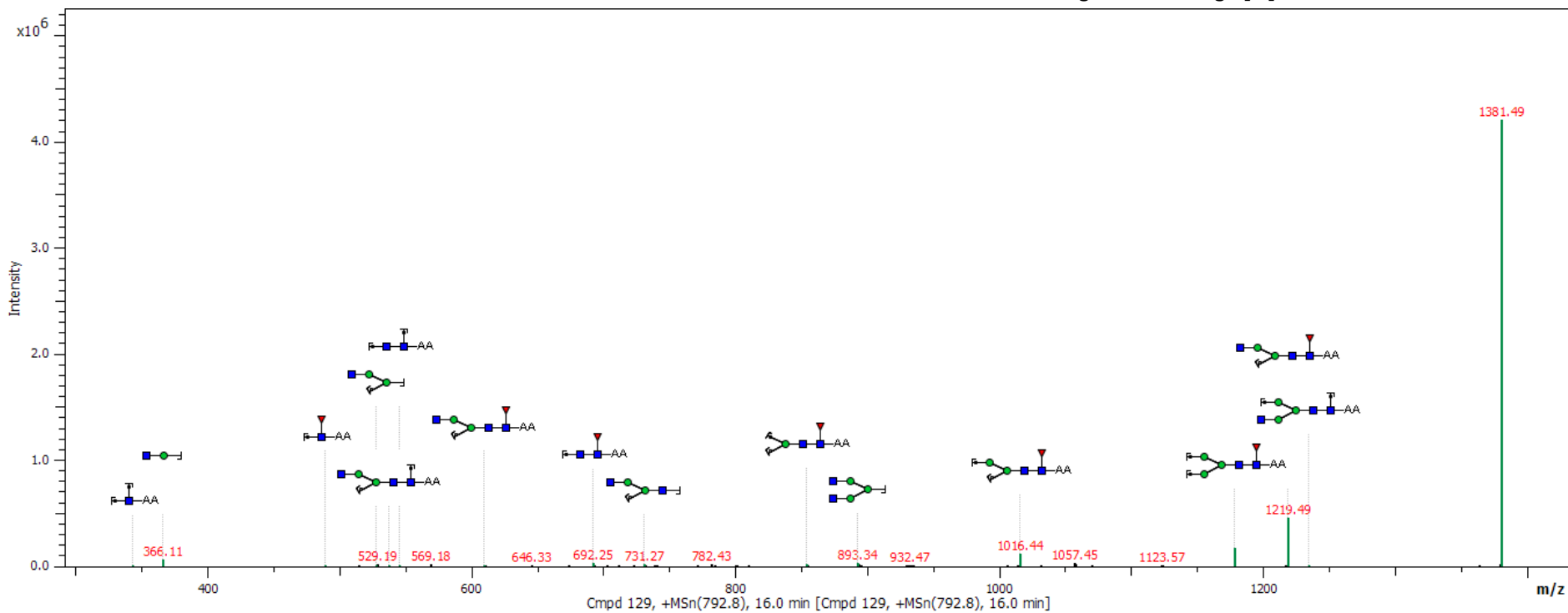
Spectrum 31

Glycan Search Report

Glycan: 1



Project path: /N-glycans cancer/25139/comp_25139.mgf
MS data: G:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25139_01.d/comp_25139.mgf
Parent m/z: 792.8059 2+ **Score:** 81.871
Composition: Hex3HexNAc4dHex1-AA **Intensity coverage [%]:** 0.94
Accession: 36231 **Fragment coverage [%]:** 0.71

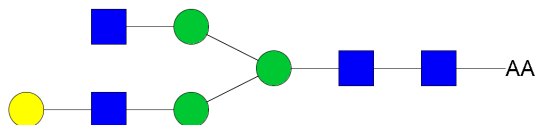




Spectrum 32

Glycan Search Report

Glycan: 2



Project path: /N-glycans cancer/25142/comp_25142_01.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25142_01.d/comp_25142_01.mgf

Parent m/z: 800.8033 2+

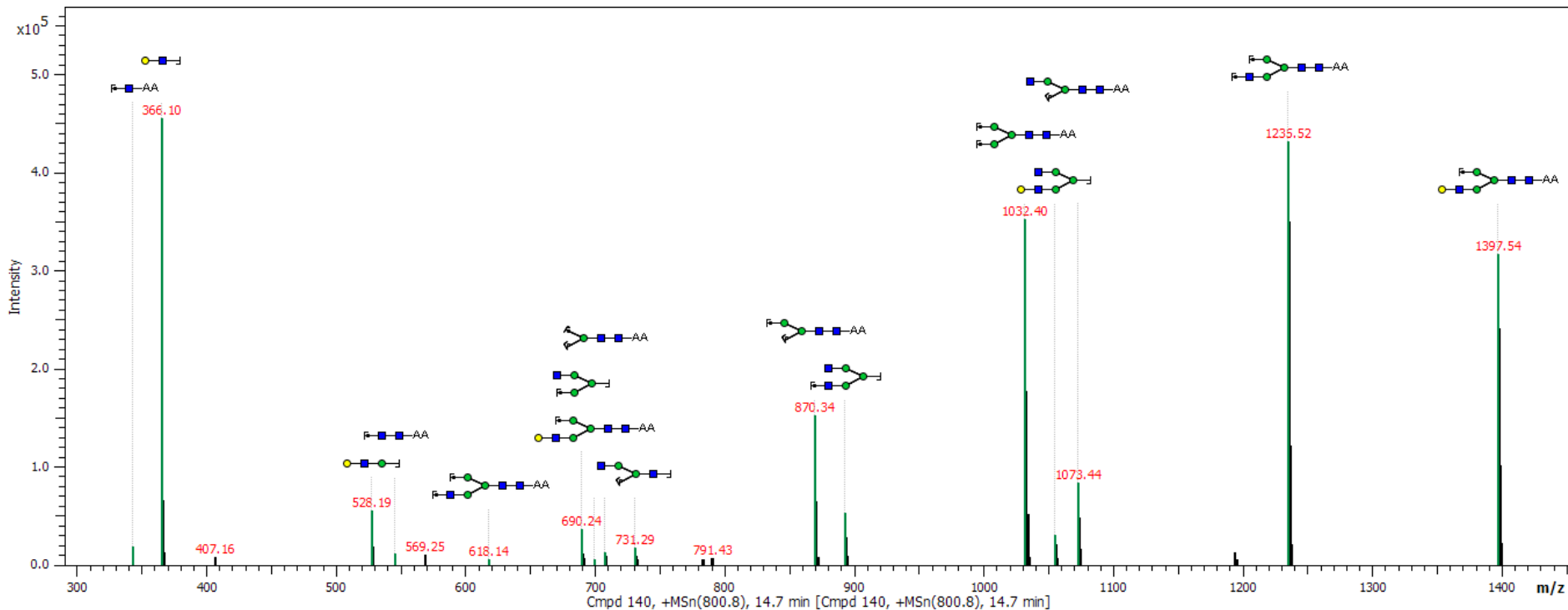
Score: 72.508

Composition: Hex4HexNAc4-AA

Intensity coverage [%]: 0.58

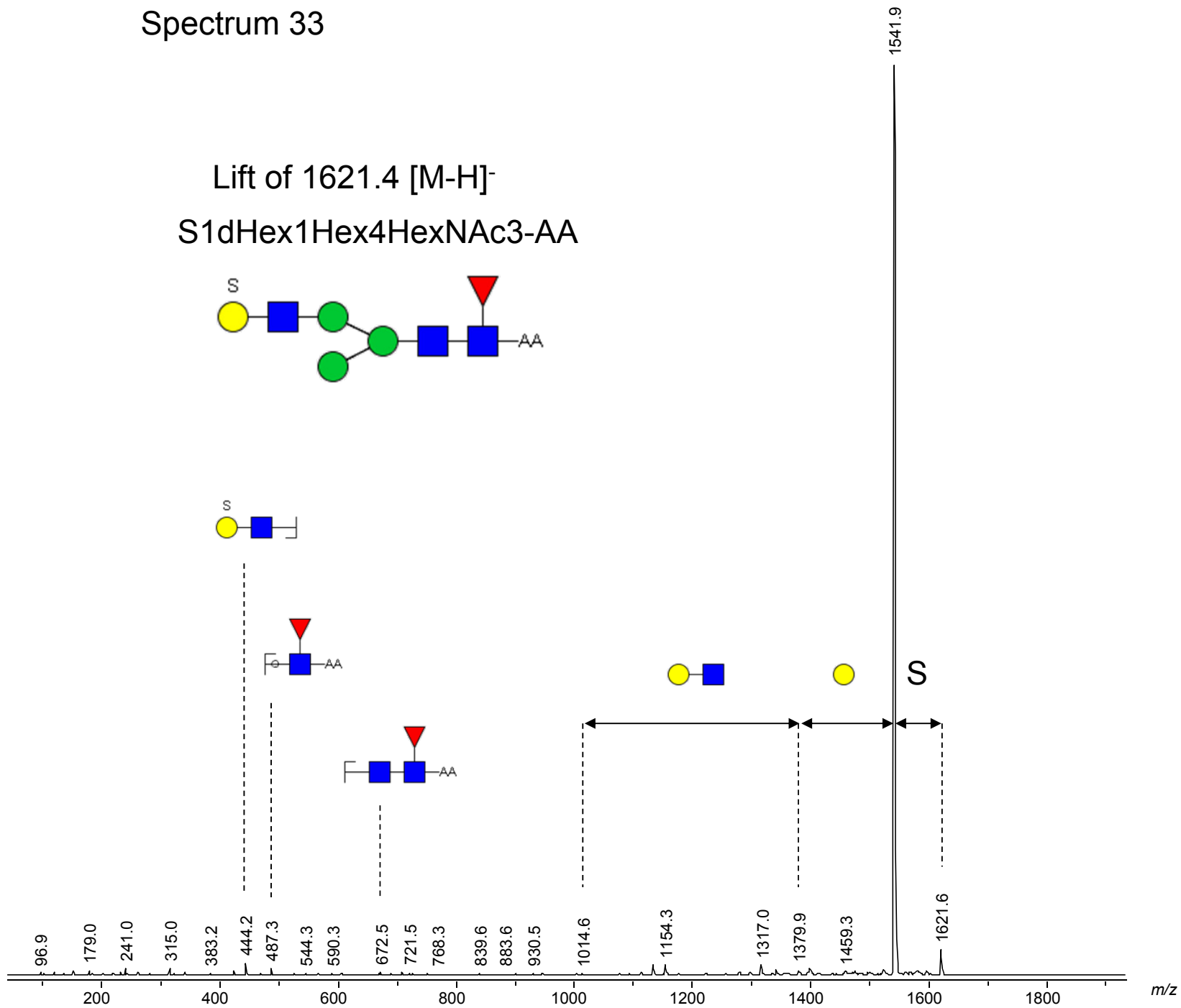
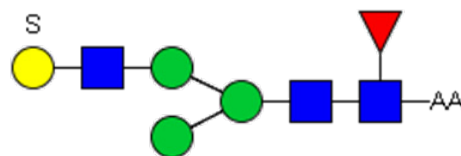
Accession: 36343

Fragment coverage [%]: 0.91



Spectrum 33

Lift of 1621.4 [M-H]⁻
S1dHex1Hex4HexNAc3-AA

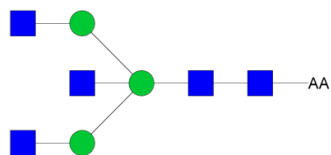




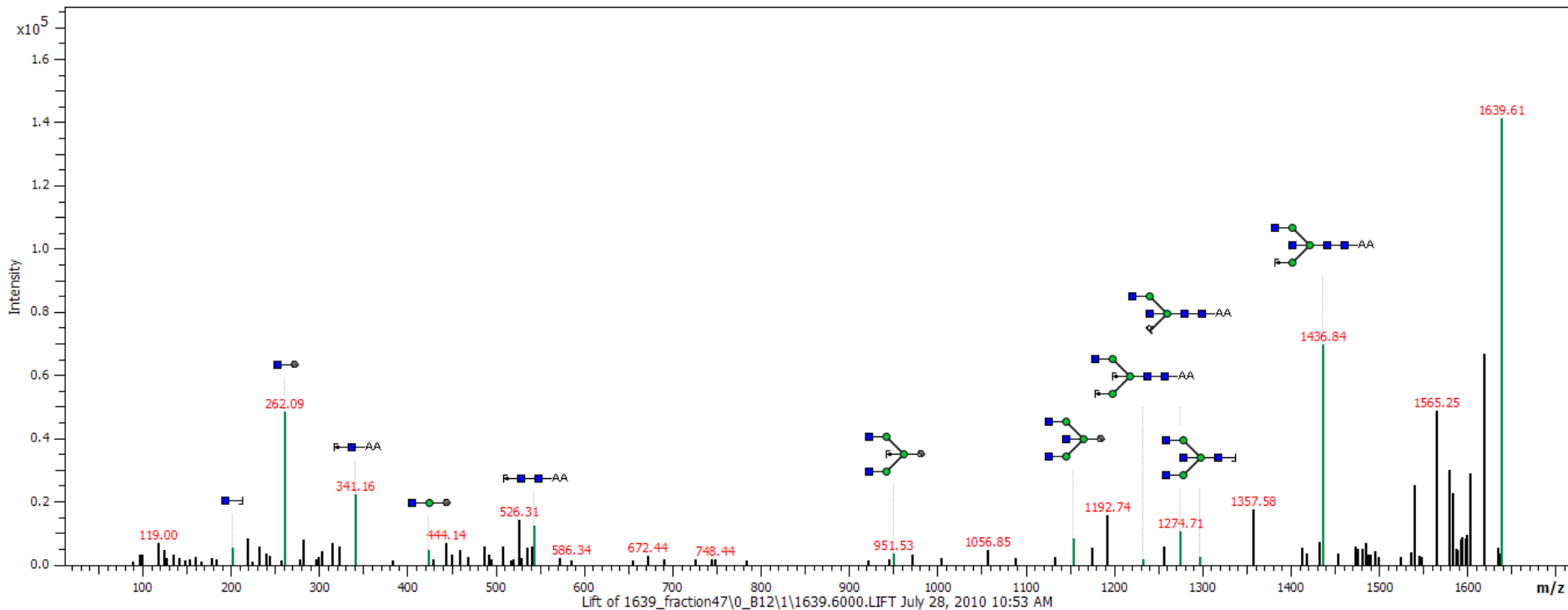
Spectrum 34

Glycan Search Report

Glycan: 13



Project path: /N-glycans cancer/Lift spectra/CombinedLIFT
MS data: c:/documents and settings/ciabalog/desktop/new folder/lift of 1639_fraction47/0_b12/1/1639.6000.lift/ 1sref/pdata/1/1r
Parent m/z: 1639.6114 -1 **Score:** 28.883
Composition: Hex3HexNAc5-AA **Intensity coverage [%]:** 0.37
Accession: 1032 **Fragment coverage [%]:** 0.23

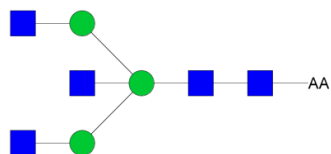




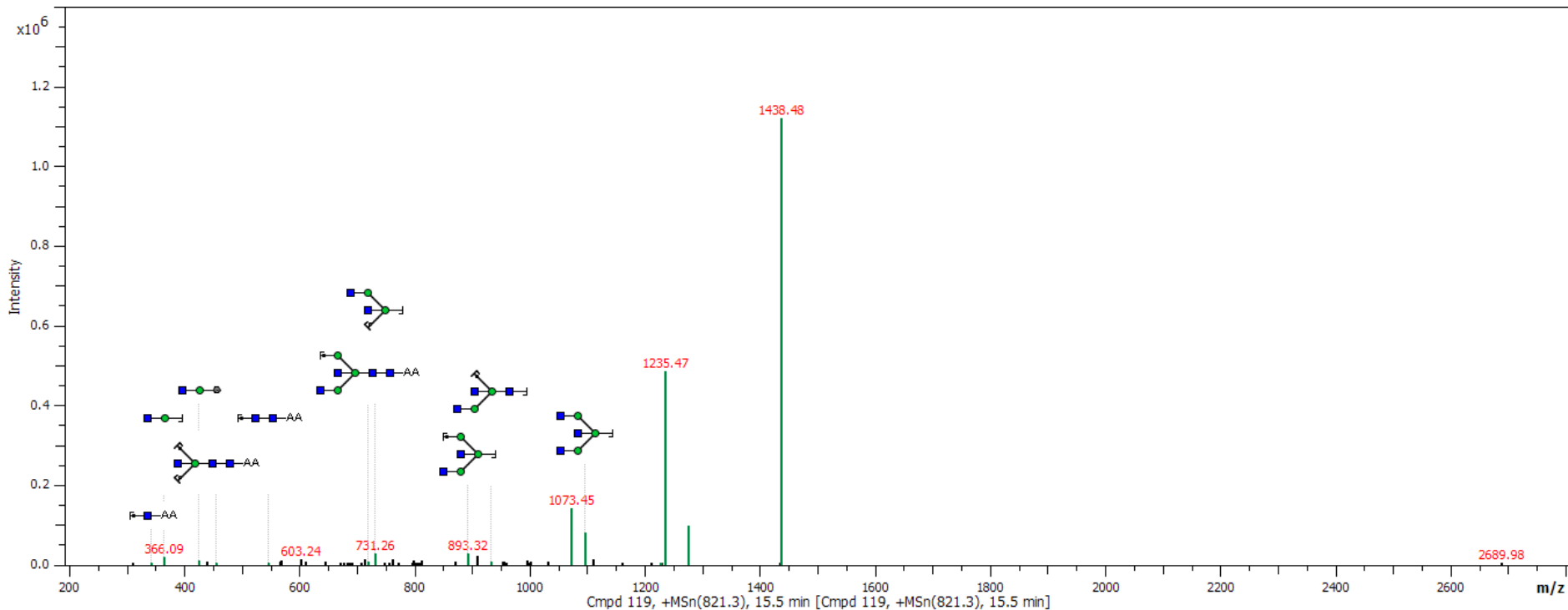
Spectrum 35

Glycan Search Report

Glycan: 3

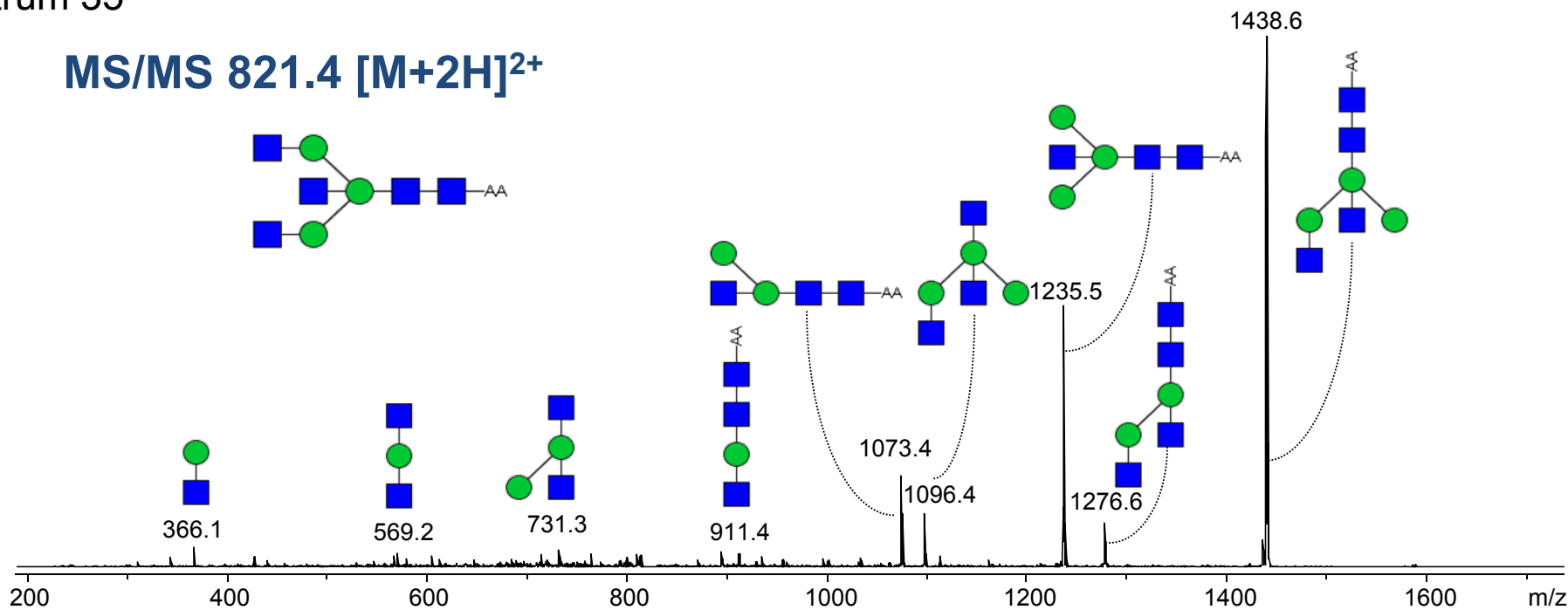


Project path: /N-glycans cancer/25139/comp_25139.mgf
MS data: G:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25139_01.d/comp_25139.mgf
Parent m/z: 821.3166 2+ **Score:** 61.071
Composition: Hex3HexNAc5-AA **Intensity coverage [%]:** 0.88
Accession: 1032 **Fragment coverage [%]:** 0.43



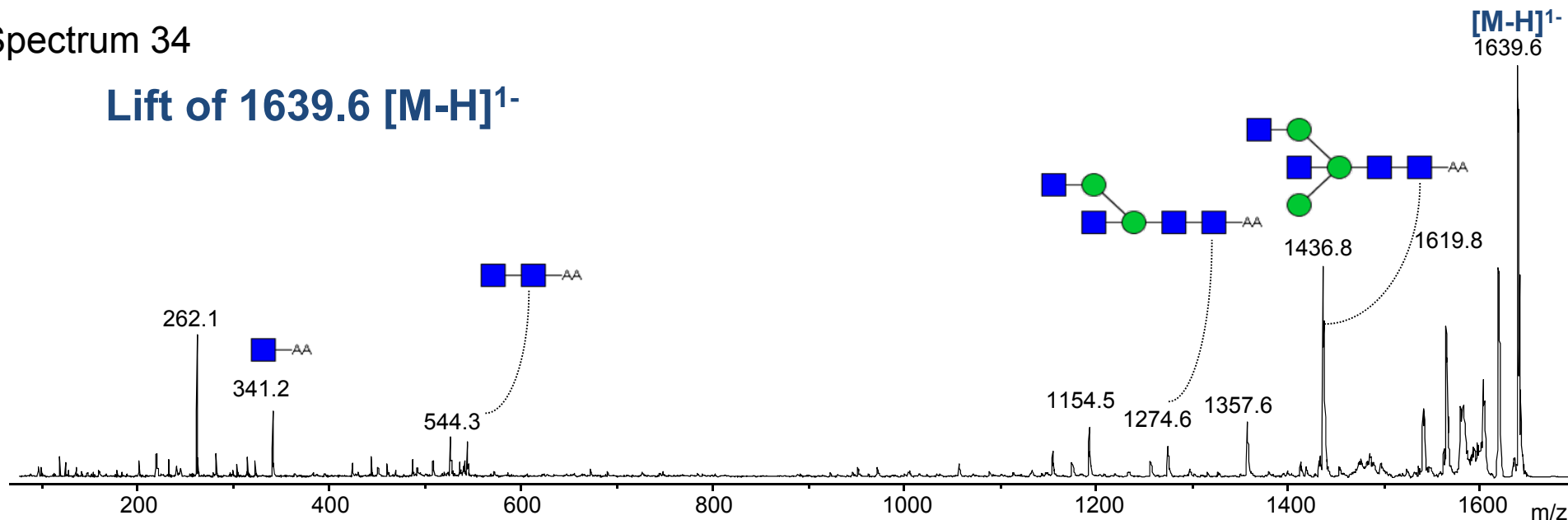
Spectrum 35

MS/MS 821.4 [M+2H]²⁺



Spectrum 34

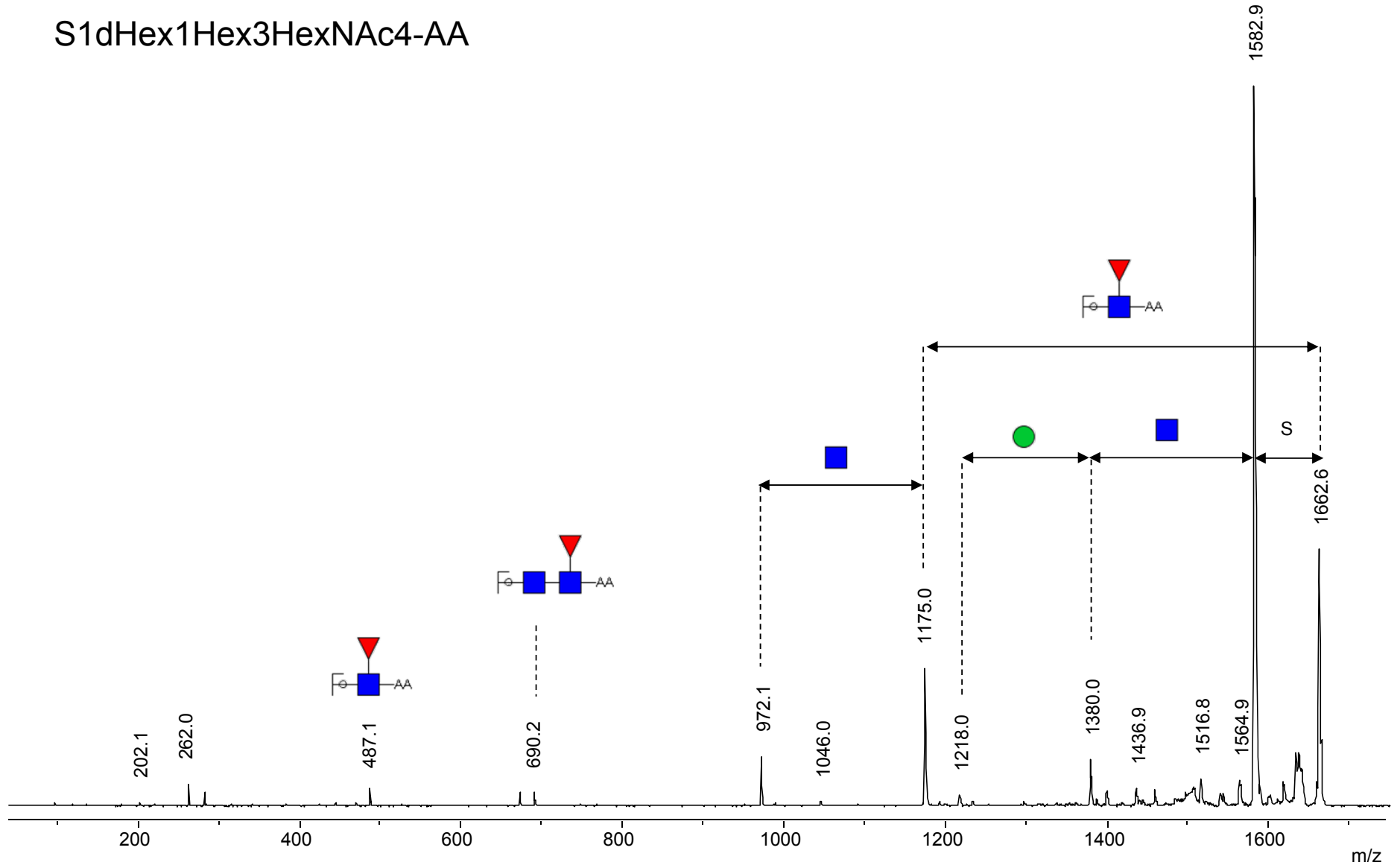
Lift of 1639.6 [M-H]¹⁻



Spectrum 36

Lift of 1662.5 [M-H]⁻

S1dHex1Hex3HexNAc4-AA

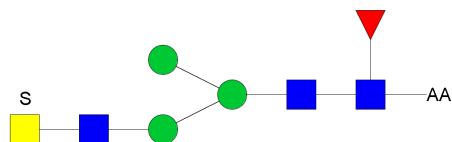




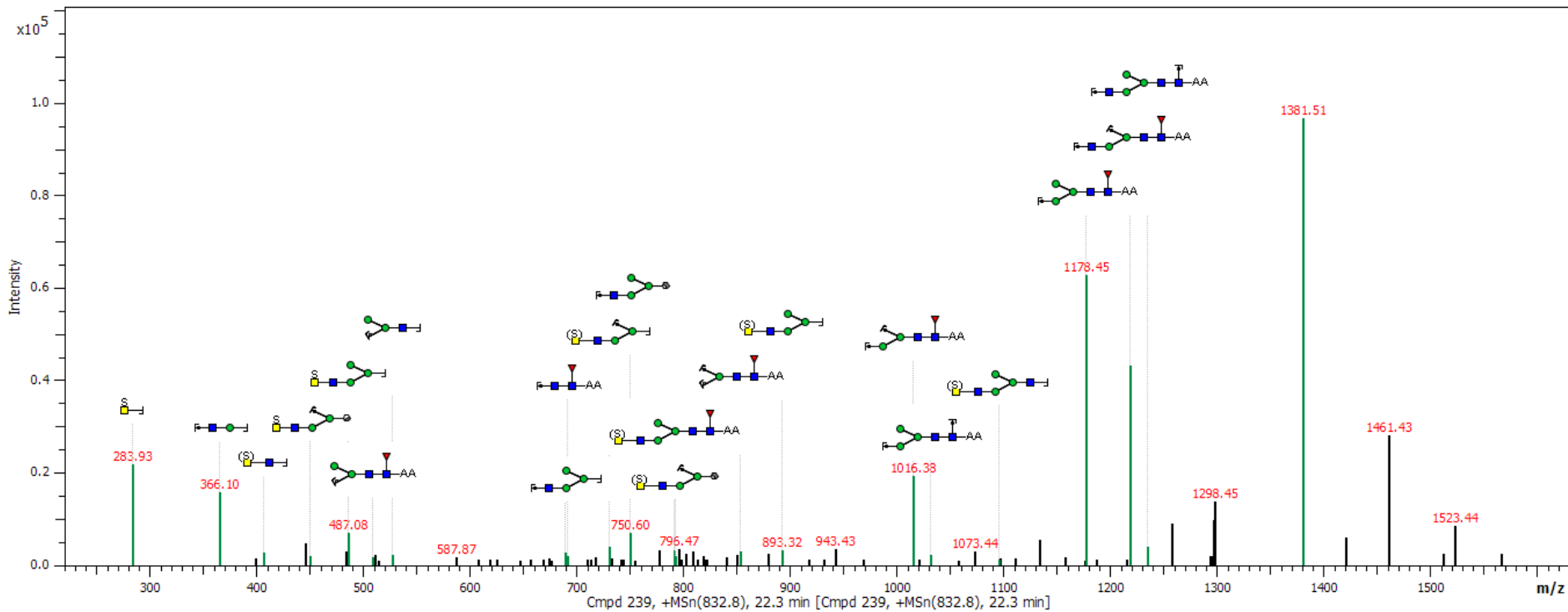
Spectrum 37

Glycan Search Report

Glycan: 5



Project path: /N-glycans cancer/25139/comp_25139.mgf
MS data: G:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25139_01.d/comp_25139.mgf
Parent m/z: 832.7843 2+ **Score:** 35.356
Composition: Hex3HexNAc4S1dHex1-AA **Intensity coverage [%]:** 0.65
Accession: 17280 **Fragment coverage [%]:** 0.19

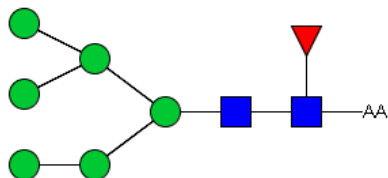




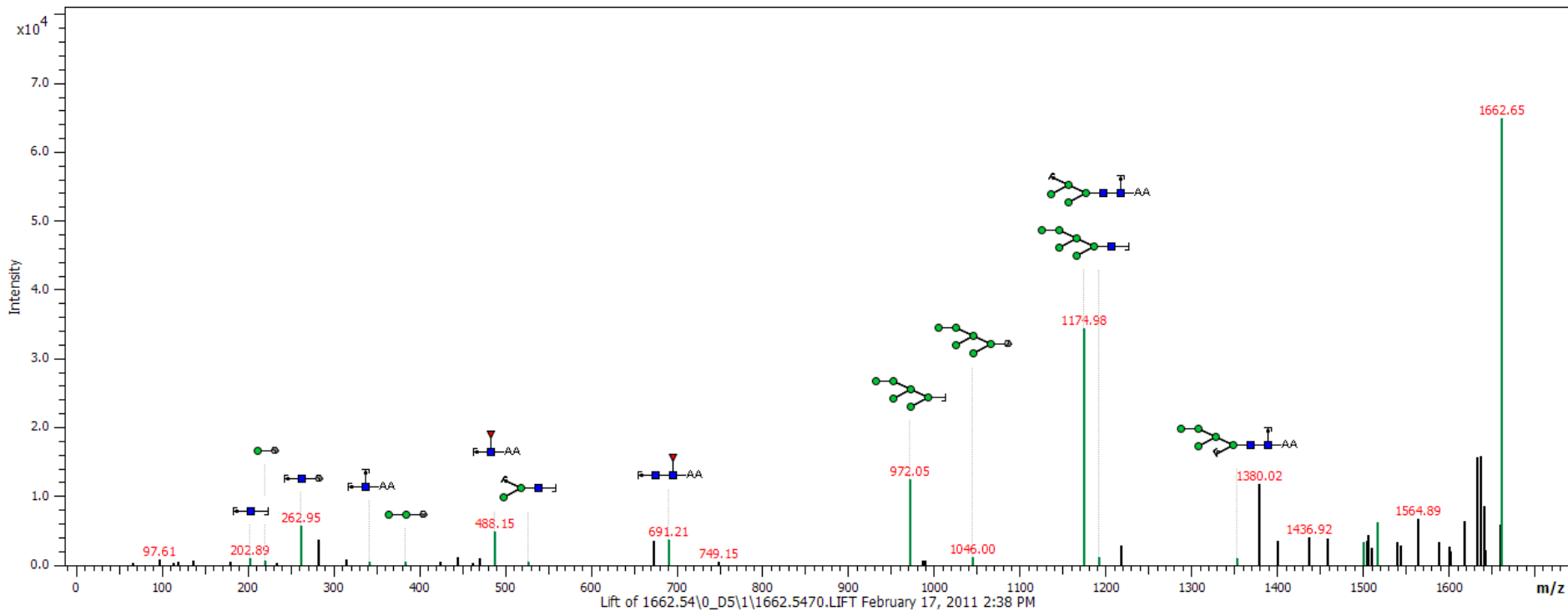
Spectrum 38

Glycan Search Report

Glycan: 4



Project path: /N-glycans cancer/Lift spectra 01/CombinedUNKNOWN
MS data: c:/documents and settings/ciabalog/desktop/17-02-11/17-02-11/lift of 1662.54/0_d5/1/1662.5470.lif/1sref/pdata/1/1r
Parent m/z: 1662.5895 -1 **Score:** 27.982
Composition: Hex6HexNAc2dHex1-AA **Intensity coverage [%]:** 0.53
Accession: 29018 **Fragment coverage [%]:** 0.15

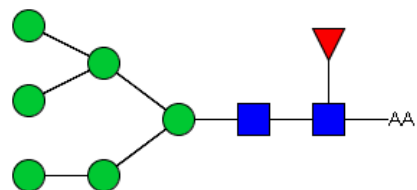




Spectrum 39

Glycan Search Report

Glycan: 25



Project path: /N-glycans cancer/25143/comp_25143_01.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25143_01.d/comp_25143_01.mgf

Parent m/z: 832.8057 2+

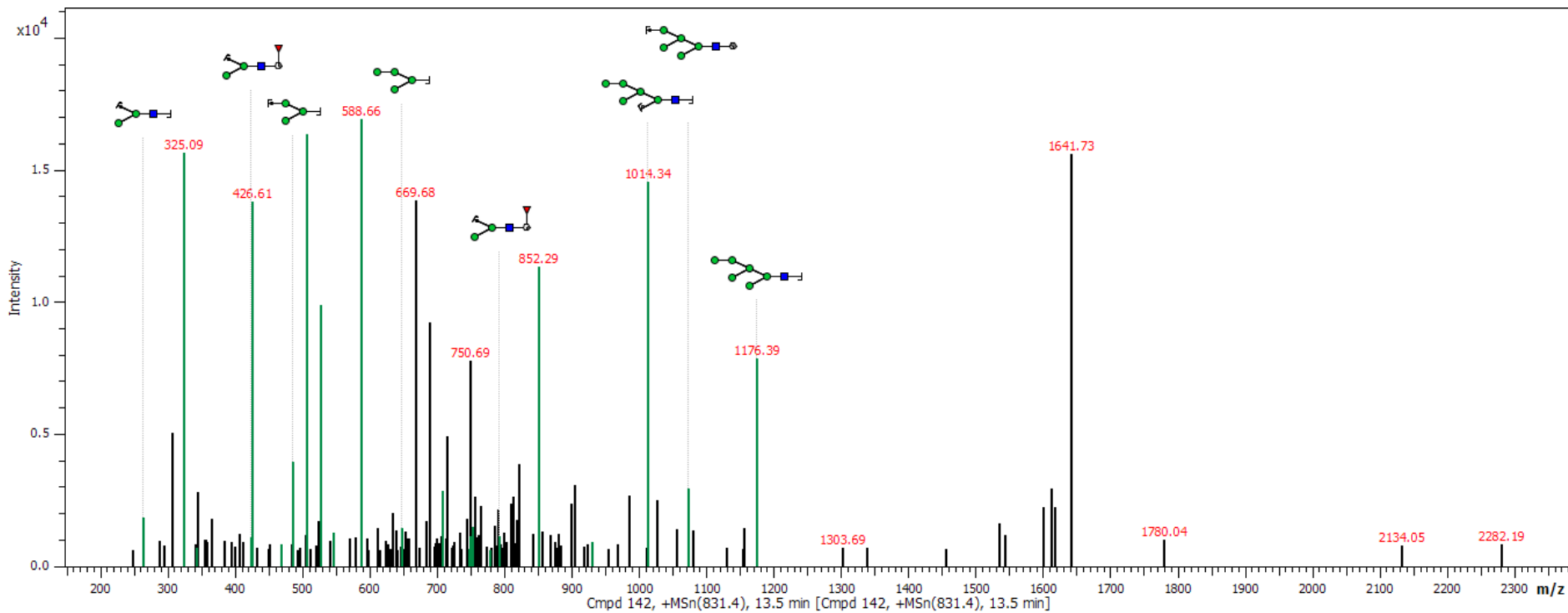
Score: 30.433

Composition: Hex6HexNAc2dHex1-AA

Intensity coverage [%]: 0.40

Accession: 29018

Fragment coverage [%]: 0.23

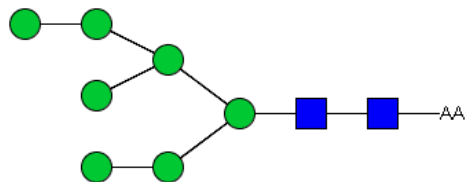




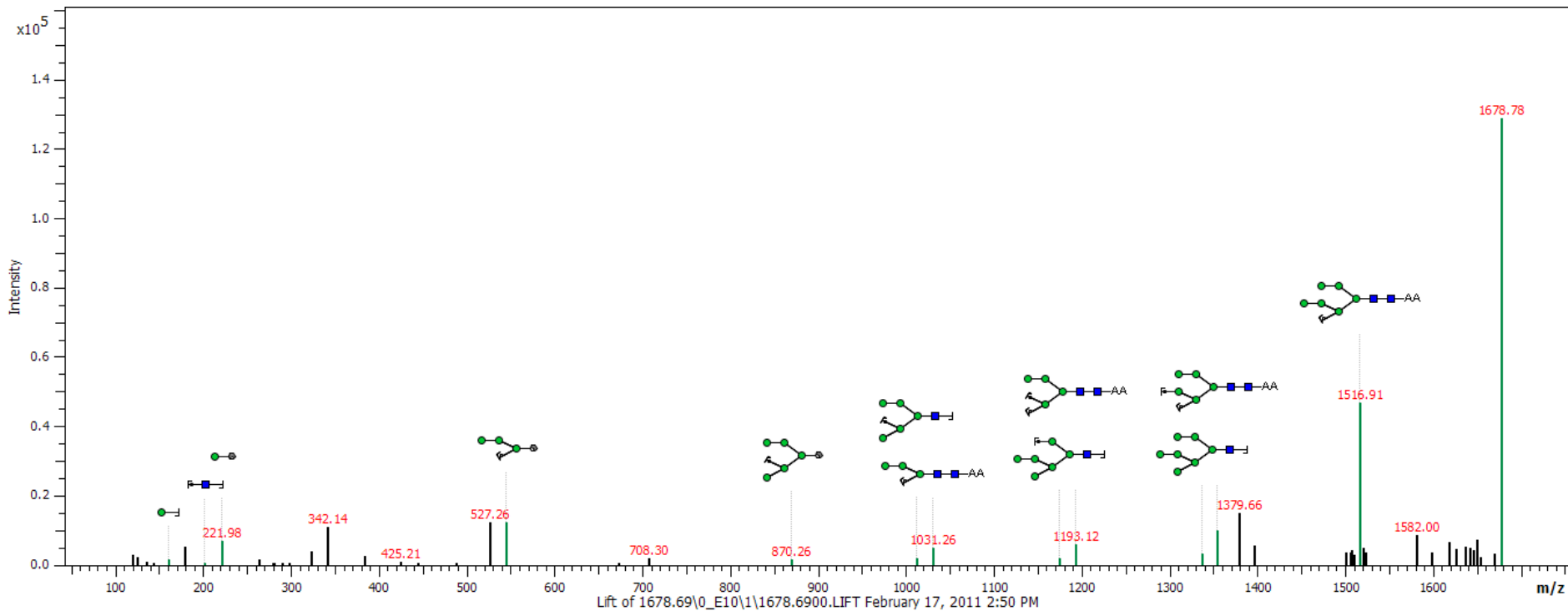
Spectrum 40

Glycan Search Report

Glycan: 2



Project path:	/N-glycans cancer/Lift spectra 01/CombinedUNKNOWN		
MS data:	c:/documents and settings/ciabalog/desktop/17-02-11/lift of 1678.69/0_e10/1/1678.6900.lift/1sref/pdata/1/1r		
Parent m/z:	1678.5844 -1	Score:	42.308
Composition:	Hex7HexNAc2-AA	Intensity coverage [%]:	0.61
Accession:	2255	Fragment coverage [%]:	0.29

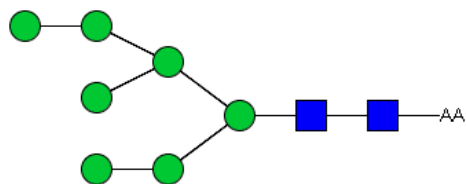




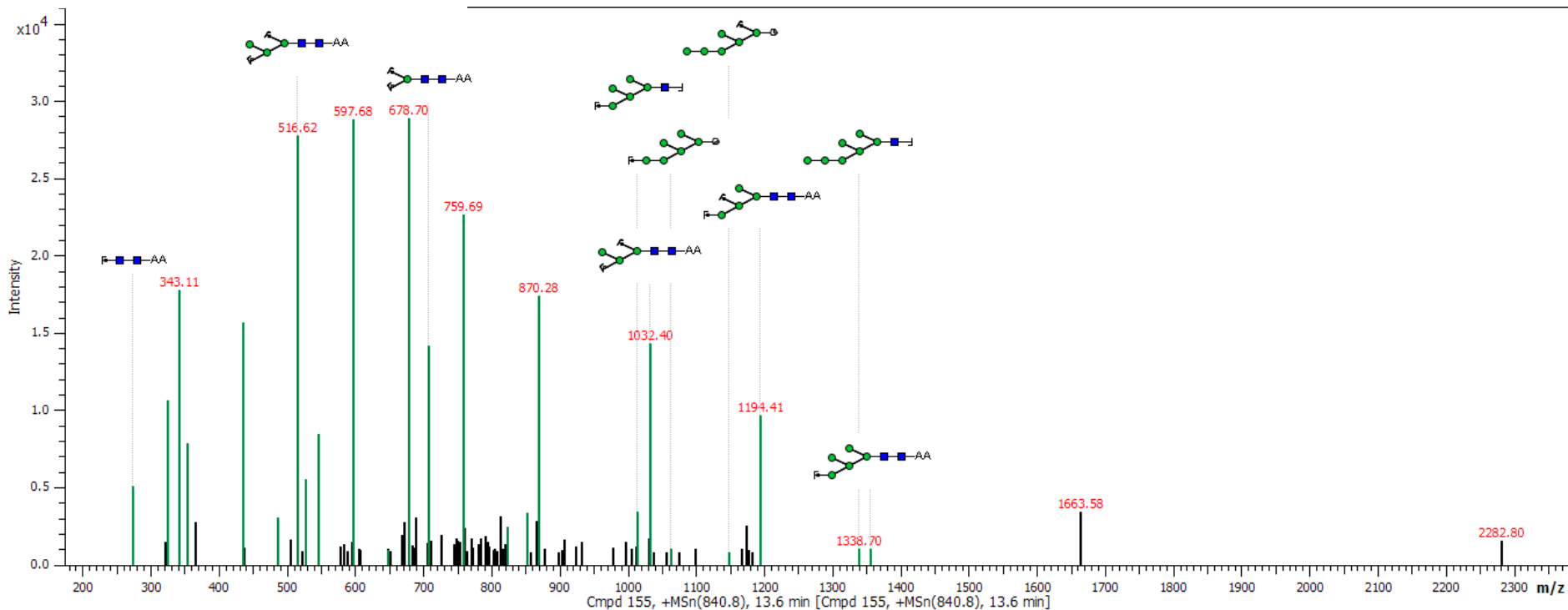
Spectrum 41

Glycan Search Report

Glycan: 6



Project path: /N-glycans cancer/25147/comp_25147.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25147_02.d/comp_25147.mgf
Parent m/z: 840.8031 2+ **Score:** 53.720
Composition: Hex7HexNAc2-AA **Intensity coverage [%]:** 0.72
Accession: 9035 **Fragment coverage [%]:** 0.40

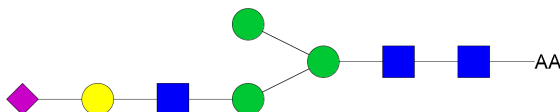




Spectrum 42

Glycan Search Report

Glycan: 4



Project path: /N-glycans cancer/25141/comp_25141.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25141_01.d/comp_25141.mgf

Parent m/z: 844.8113 2+

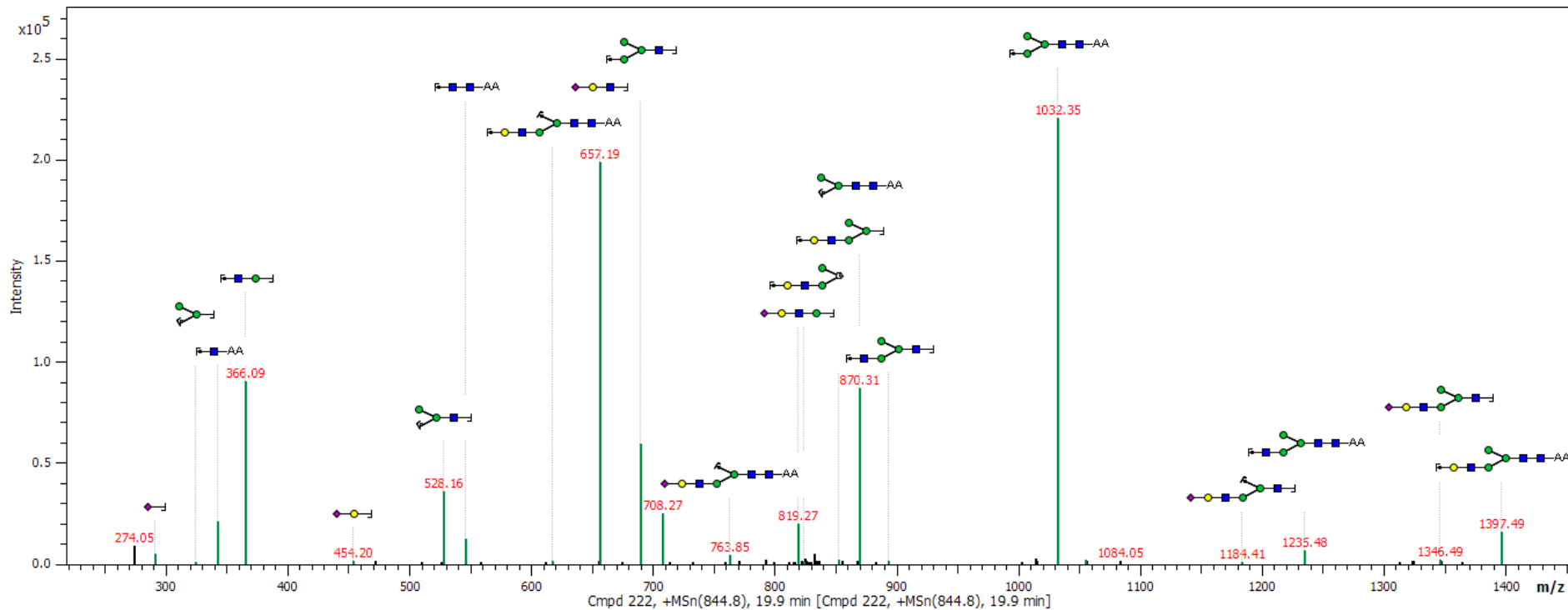
Score: 57.766

Composition: Hex4HexNAc3NeuAc1-AA

Intensity coverage [%]: 0.93

Accession: 13311

Fragment coverage [%]: 0.36

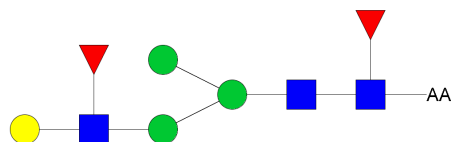




Spectrum 43

Glycan Search Report

Glycan: 10



Project path: /N-glycans cancer/25145/comp_25145.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25145_02.d/comp_25145.mgf

Parent m/z: 845.3215 2+

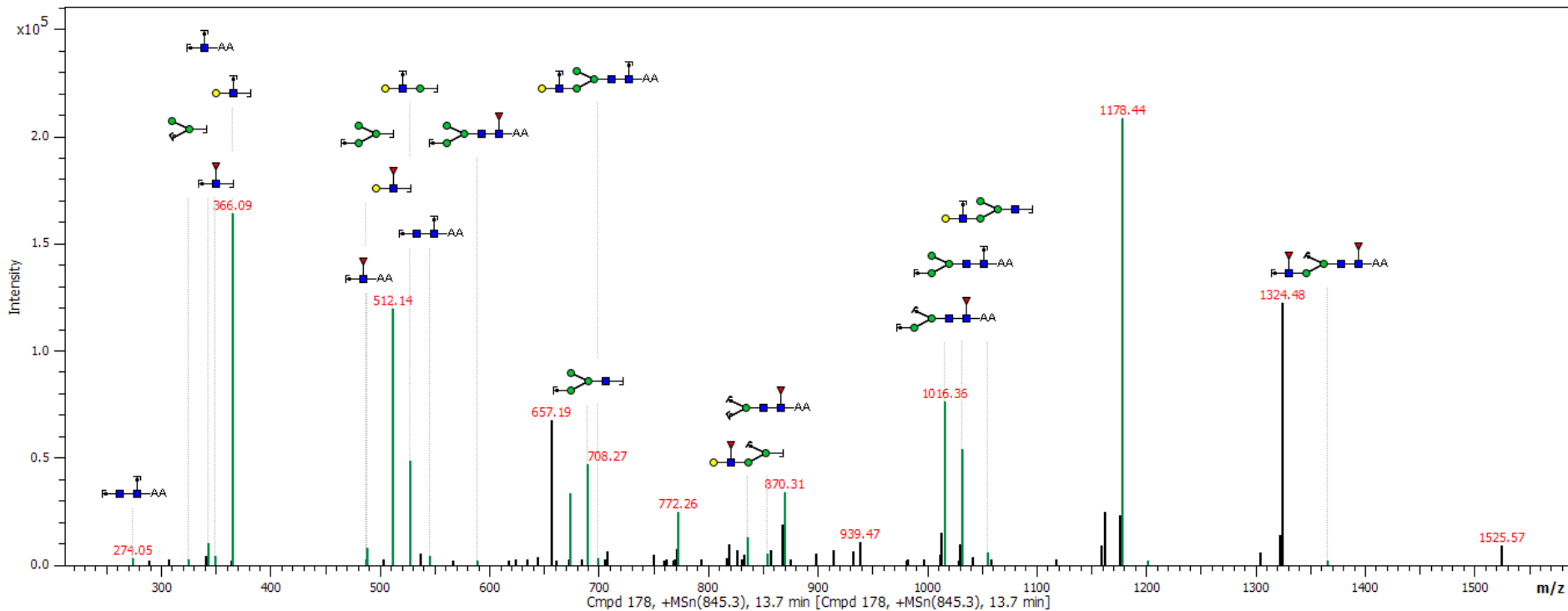
Score: 64.962

Composition: Hex4HexNAc3dHex2-AA

Intensity coverage [%]: 0.64

Accession: 36367

Fragment coverage [%]: 0.66

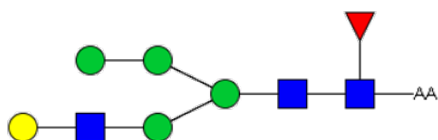




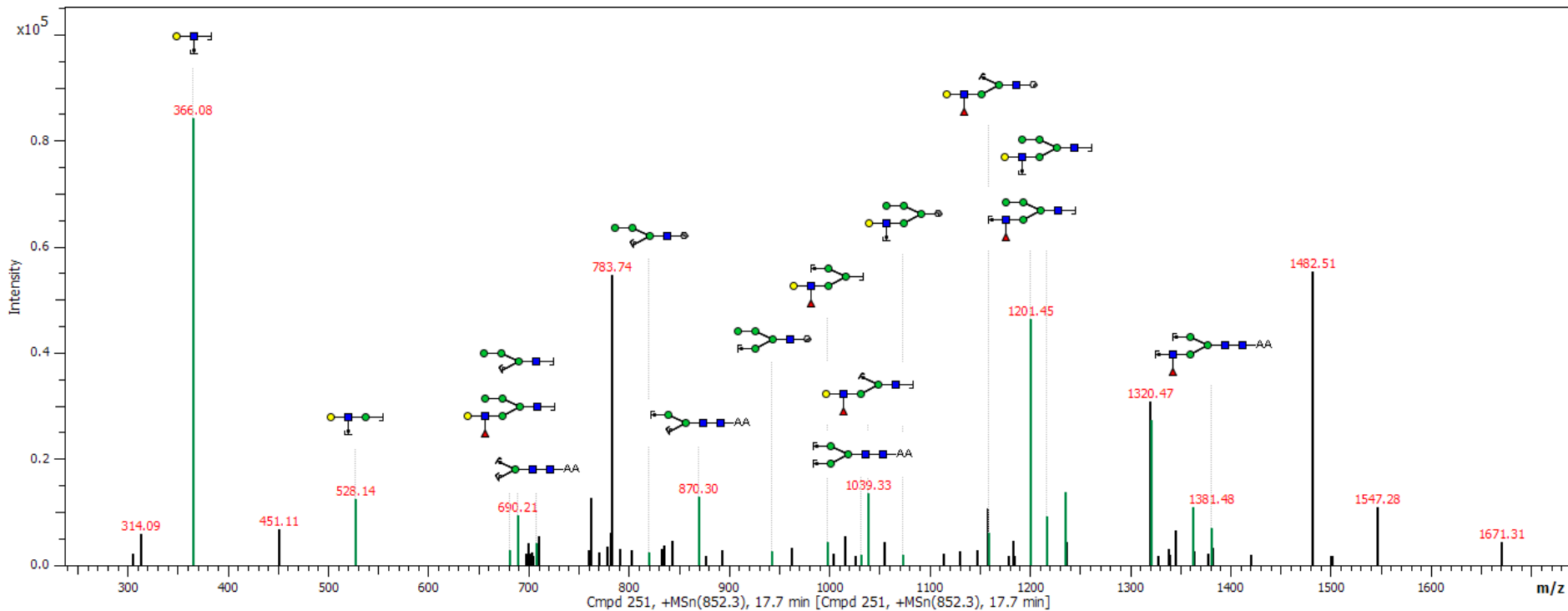
Spectrum 44

Glycan Search Report

Glycan: 24



Project path: /N-glycans cancer/25147/comp_25147.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25147_02.d/comp_25147.mgf
Parent m/z: 853.3190 2+ **Score:** 24.121
Composition: Hex5HexNAc3dHex1-AA **Intensity coverage [%]:** 0.46
Accession: 29095 **Fragment coverage [%]:** 0.13

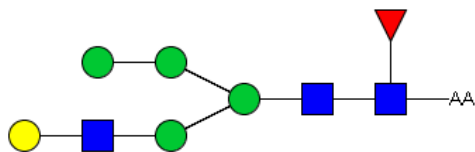




Spectrum 45

Glycan Search Report

Glycan: 17



Project path: /N-glycans cancer/25145/comp_25145.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25145_02.d/comp_25145.mgf

Parent m/z: 853.3190 2+

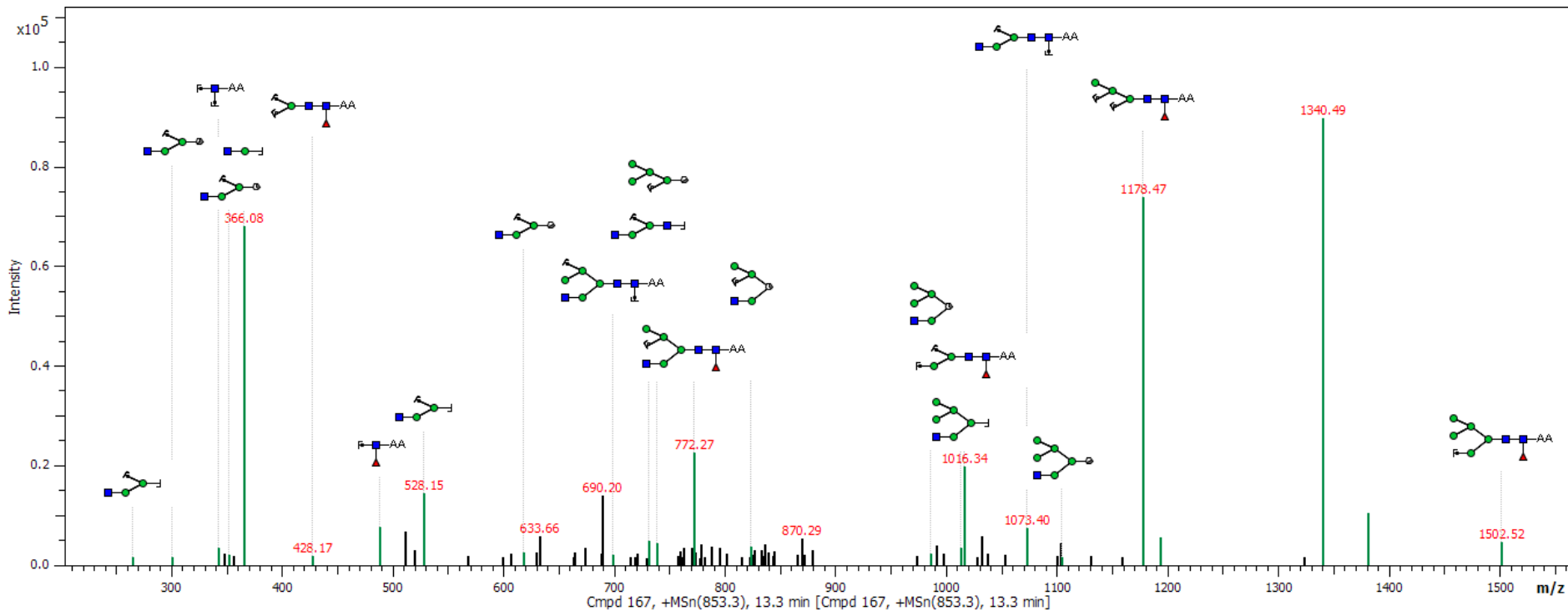
Score: 42.735

Composition: Hex5HexNAc3dHex1-AA

Intensity coverage [%]: 0.70

Accession: 8033

Fragment coverage [%]: 0.26

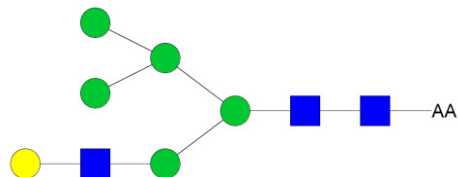




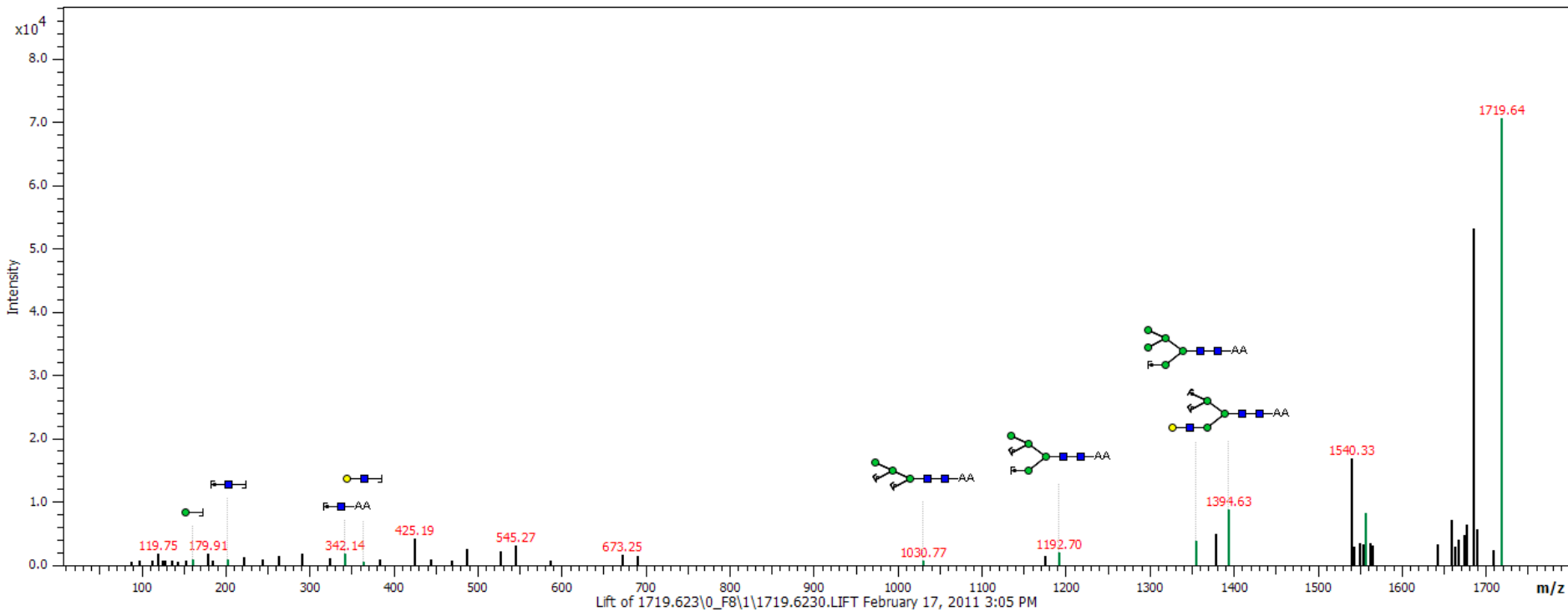
Spectrum 46

Glycan Search Report

Glycan: 3



Project path: /N-glycans cancer/Lift spectra 01/CombinedUNKNOWN
MS data: c:/documents and settings/ciabalog/desktop/17-02-11/17-02-11/lift of 1719.623/0_f8/1/1719.6230.lift/1sref/pdata/1/1r
Parent m/z: 1719.6110 -1 **Score:** 41.687
Composition: Hex6HexNAc3-AA **Intensity coverage [%]:** 0.38
Accession: 36317 **Fragment coverage [%]:** 0.46

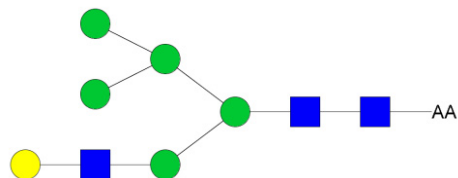




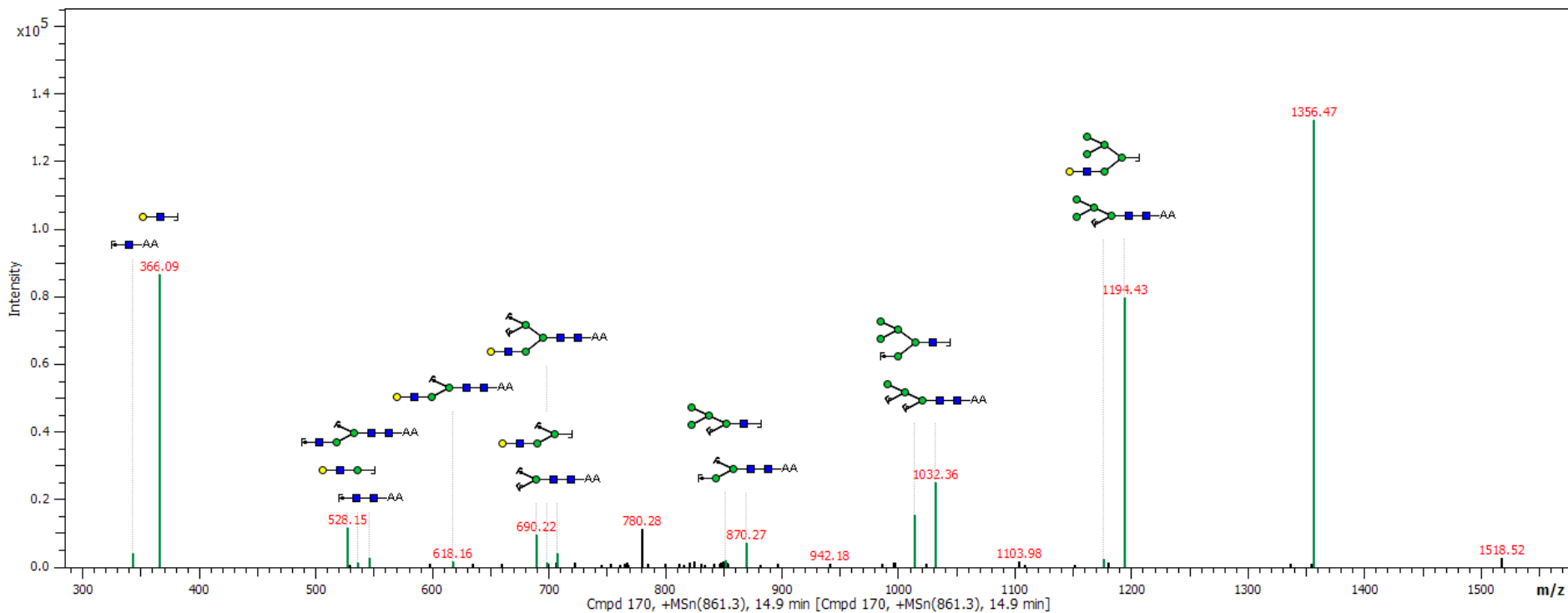
Spectrum 47

Glycan Search Report

Glycan: 5

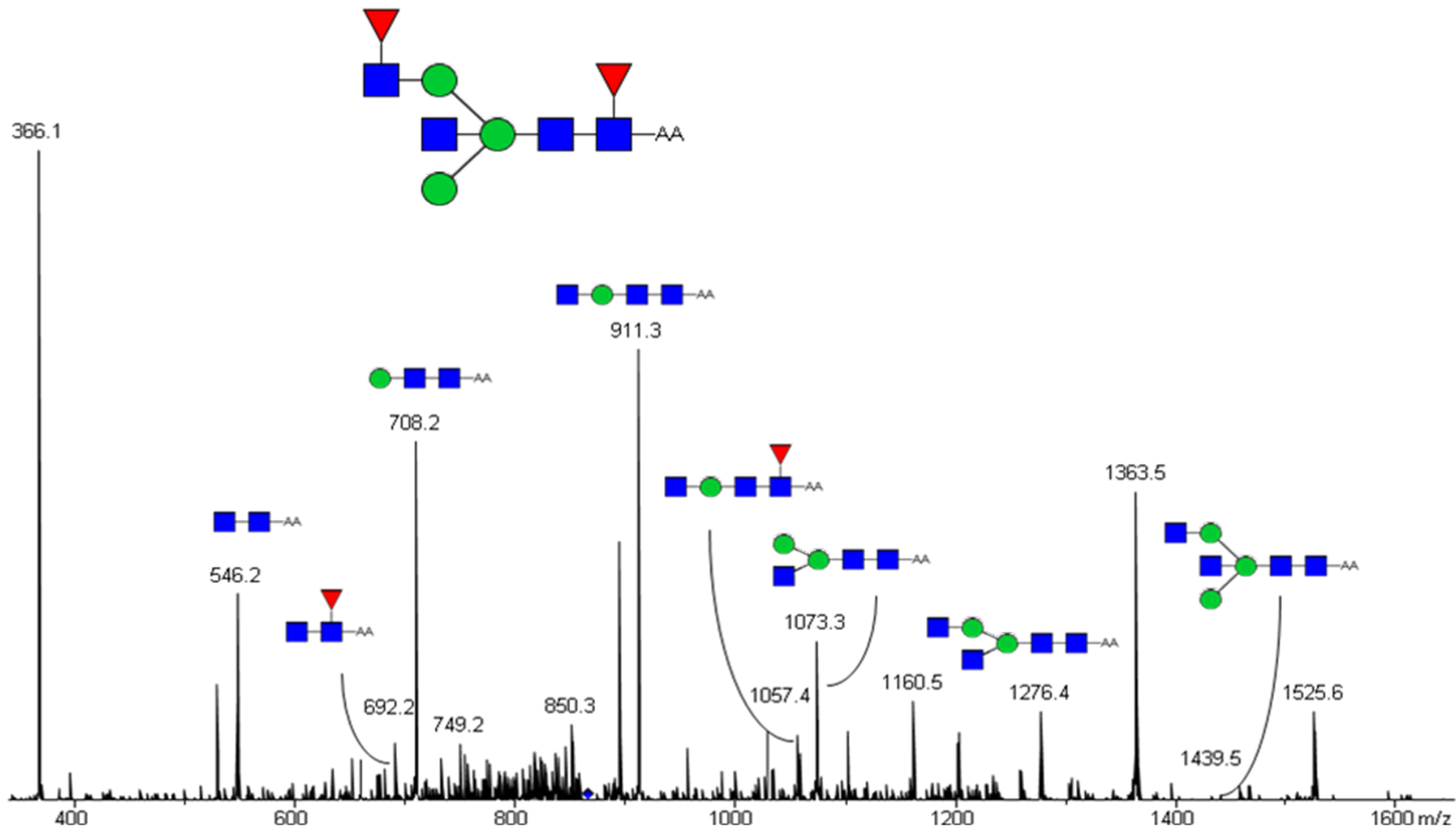


Project path: /N-glycans cancer/25143/comp_25143_01.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25143_01.d/comp_25143_01.mgf
Parent m/z: 861.3164 2+ **Score:** 70.455
Composition: Hex6HexNAc3-AA **Intensity coverage [%]:** 0.87
Accession: 36317 **Fragment coverage [%]:** 0.57



Spectrum 48

ESI MS/MS of 865.8 [M+2H]²⁺
dHex2Hex3HexNAc4-AA

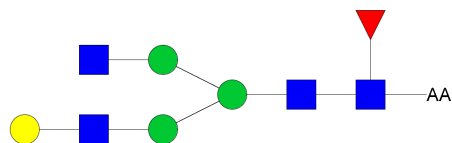




Spectrum 49

Glycan Search Report

Glycan: 9



Project path: /N-glycans cancer/Lift spectra/CombinedLIFT

MS data: c:/documents and settings/ciabalog/desktop/new folder/lift of 1744_fraction54/0_b19/1/1744.6000.lift/1sref/pdata/1/1r

Parent m/z: 1744.6427 -1

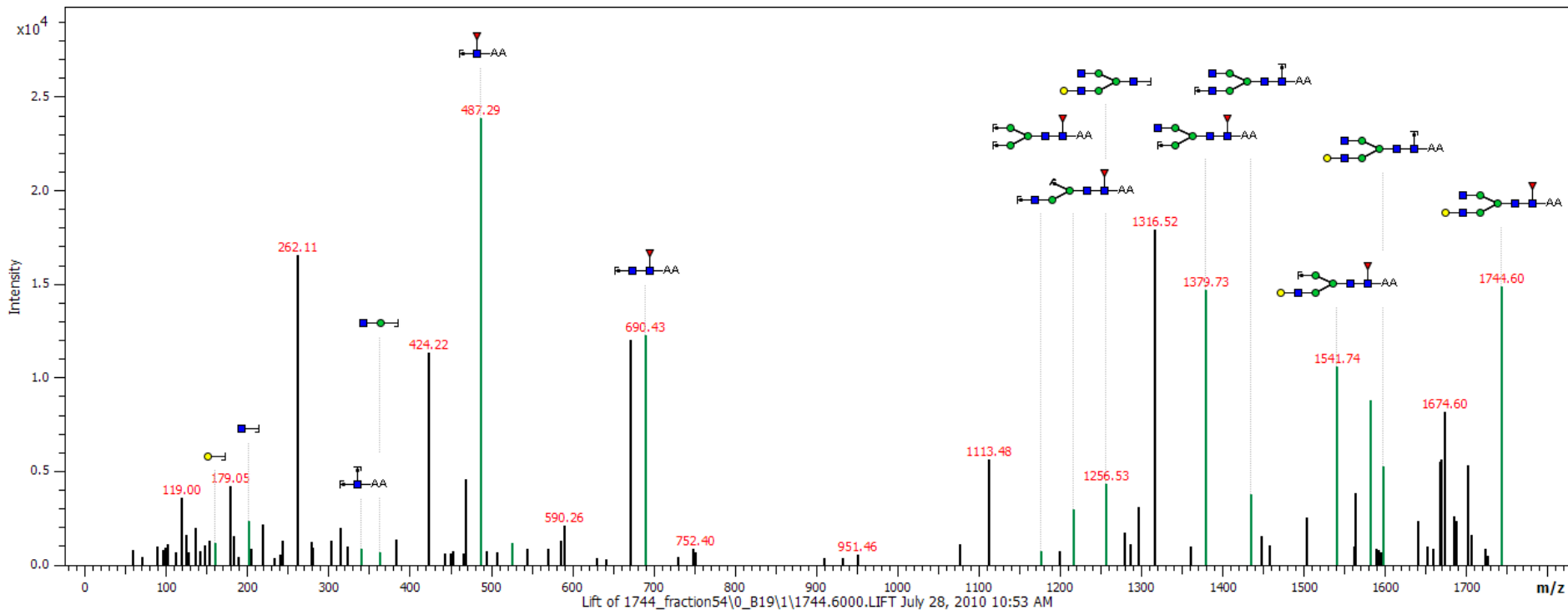
Score: 47.279

Composition: Hex4HexNAc4dHex1-AA

Intensity coverage [%]: 0.38

Accession: 36233

Fragment coverage [%]: 0.58

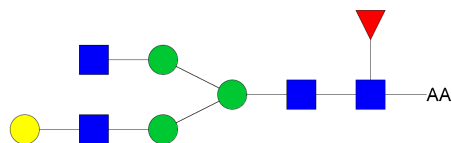




Spectrum 50

Glycan Search Report

Glycan: 1



Project path: /N-glycans cancer/25141/comp_25141.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25141_01.d/comp_25141.mgf

Parent m/z: 873.8323 2+

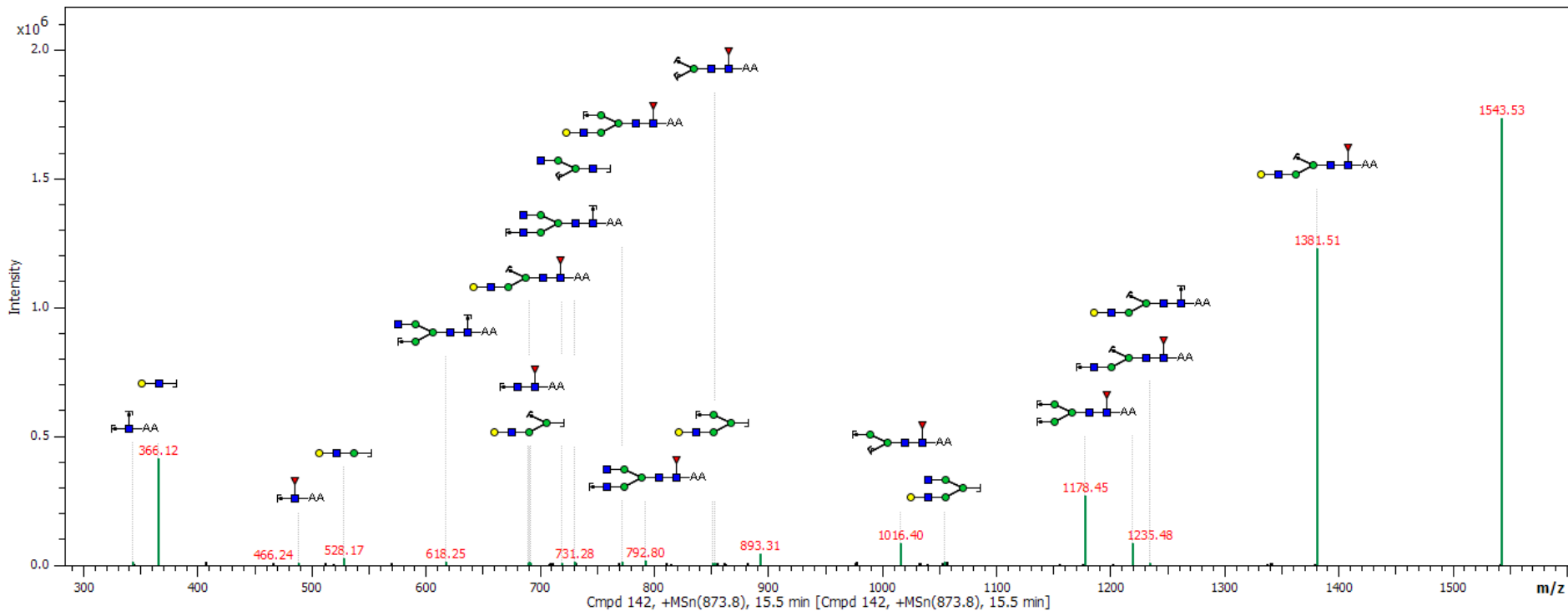
Score: 89.230

Composition: Hex4HexNAc4dHex1-AA

Intensity coverage [%]: 0.95

Accession: 36233

Fragment coverage [%]: 0.84

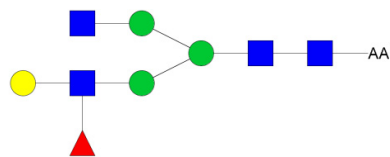




Spectrum 51

Glycan Search Report

Glycan: 19



Project path: /N-glycans cancer/25145/comp_25145.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25145_02.d/comp_25145.mgf

Parent m/z: 873.8323 2+

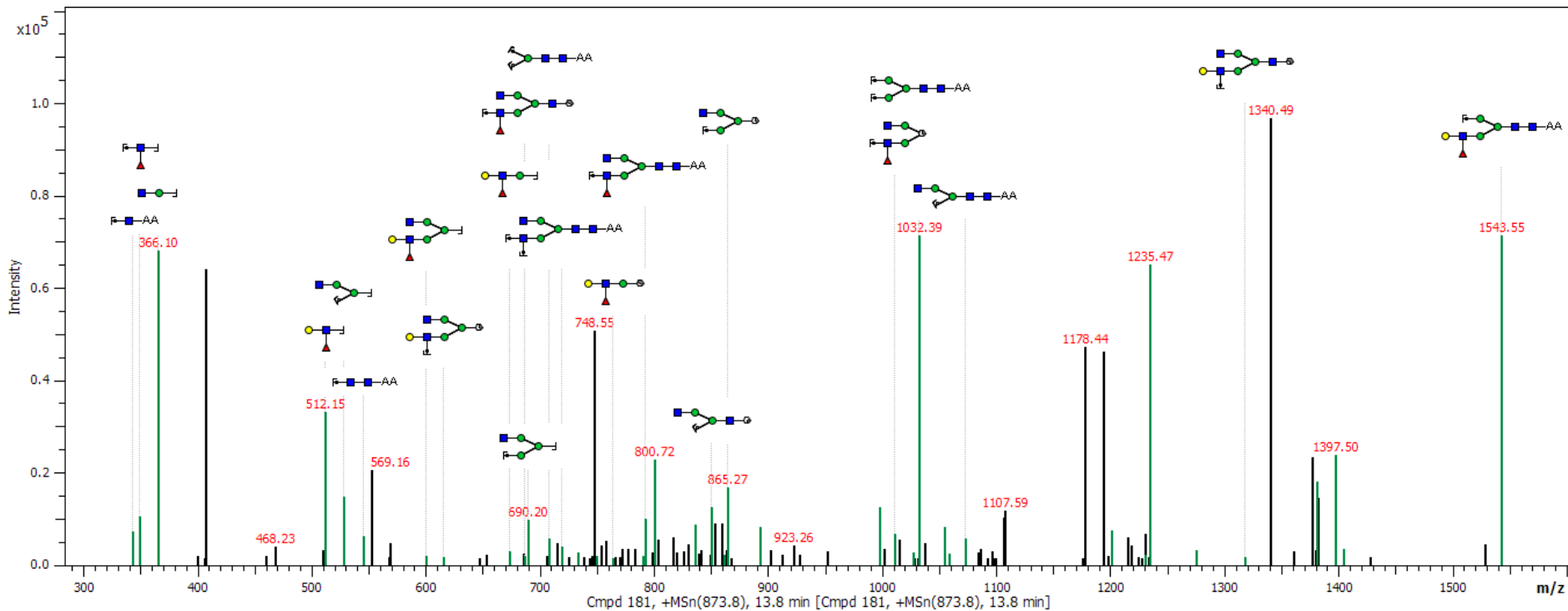
Score: 35.090

Composition: Hex4HexNAc4dHex1-AA

Intensity coverage [%]: 0.49

Accession: 29189

Fragment coverage [%]: 0.25

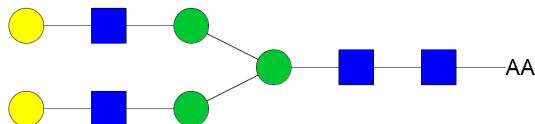




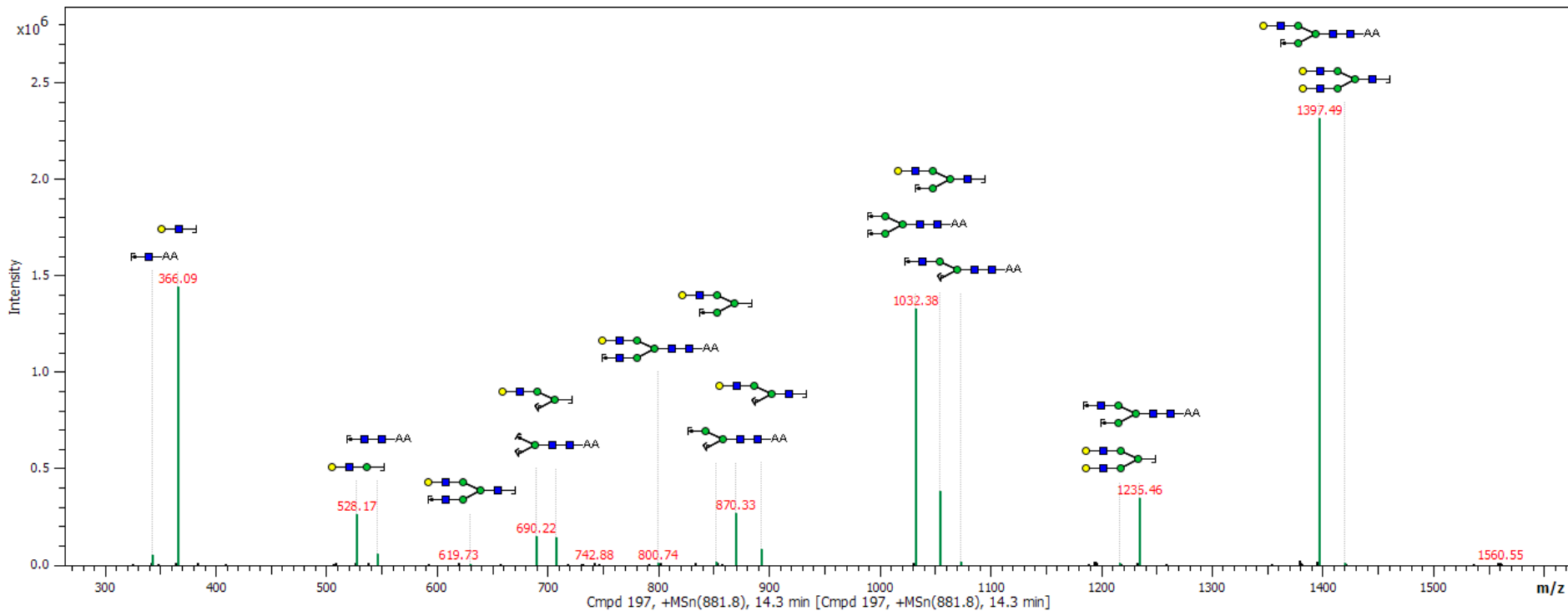
Spectrum 52

Glycan Search Report

Glycan: 2

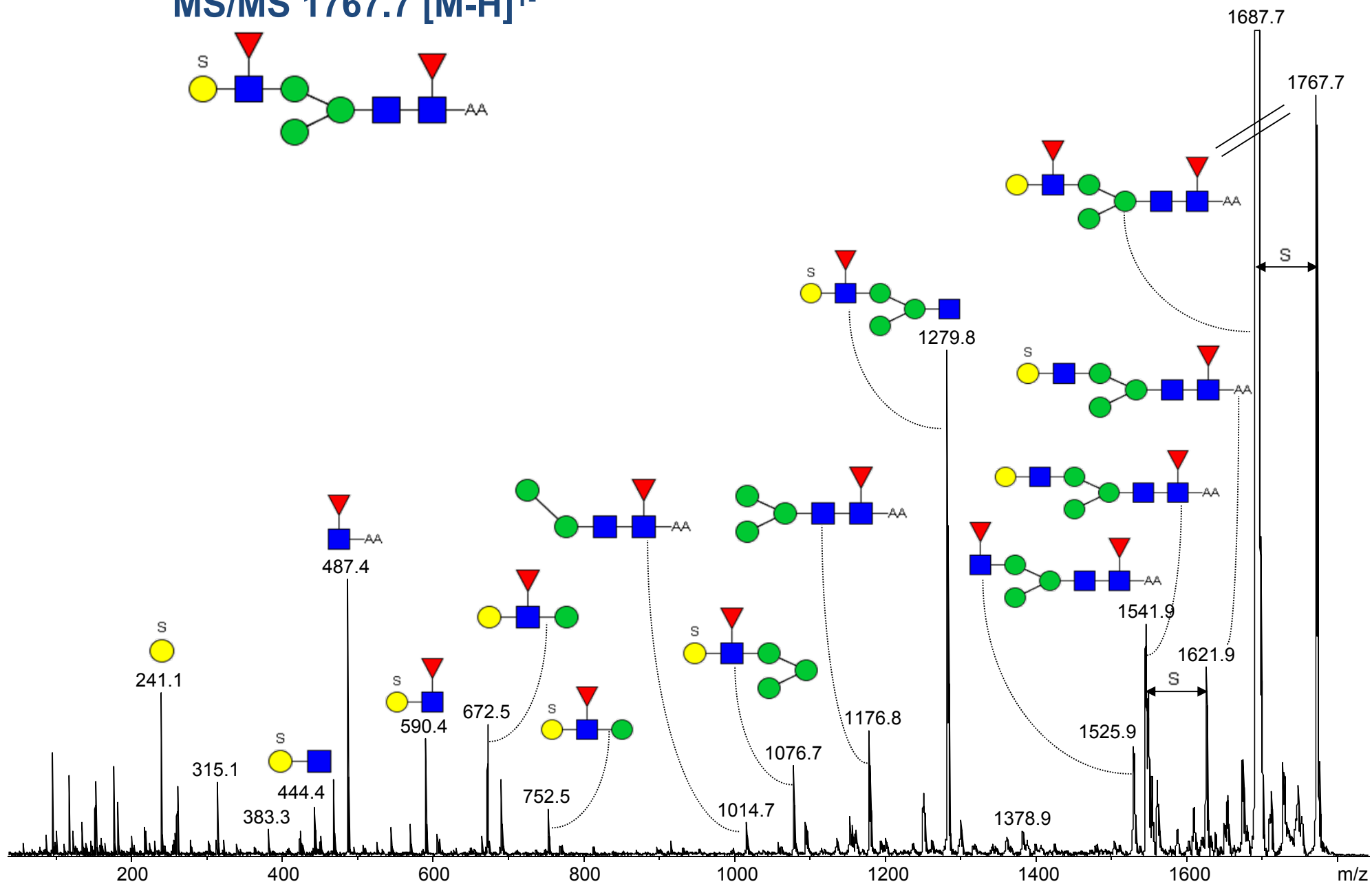


Project path: /N-glycans cancer/25145/comp_25145.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25145_02.d/comp_25145.mgf
Parent m/z: 881.8297 2+ **Score:** 86.713
Composition: Hex5HexNAc4-AA **Intensity coverage [%]:** 0.96
Accession: 32132 **Fragment coverage [%]:** 0.79



Spectrum 53

MS/MS 1767.7 [M-H]¹⁻

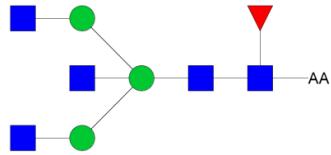


Spectrum 54

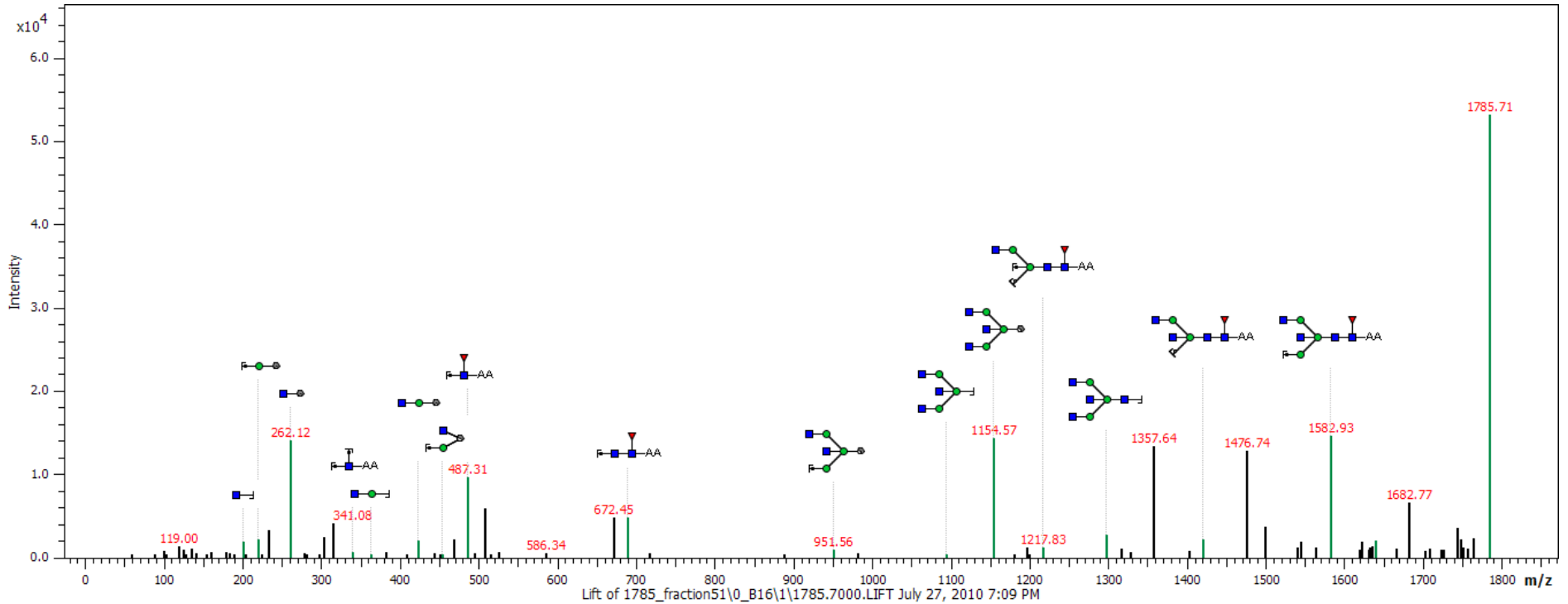


Glycan Search Report

Glycan: 11



Project path: /N-glycans cancer/Lift spectra/CombinedLIFT
MS data: c:/documents and settings/ciabalog/desktop/new folder/lift of 1785_fraction51/0_b16/1/1785.7000.lift/ 1sref/pdata/1/1r
Parent m/z: 1785.6693 -1 **Score:** 42.446
Composition: Hex3HexNAc5dHex1-AA **Intensity coverage [%]:** 0.55
Accession: 1040 **Fragment coverage [%]:** 0.33

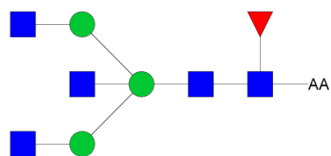


Spectrum 55

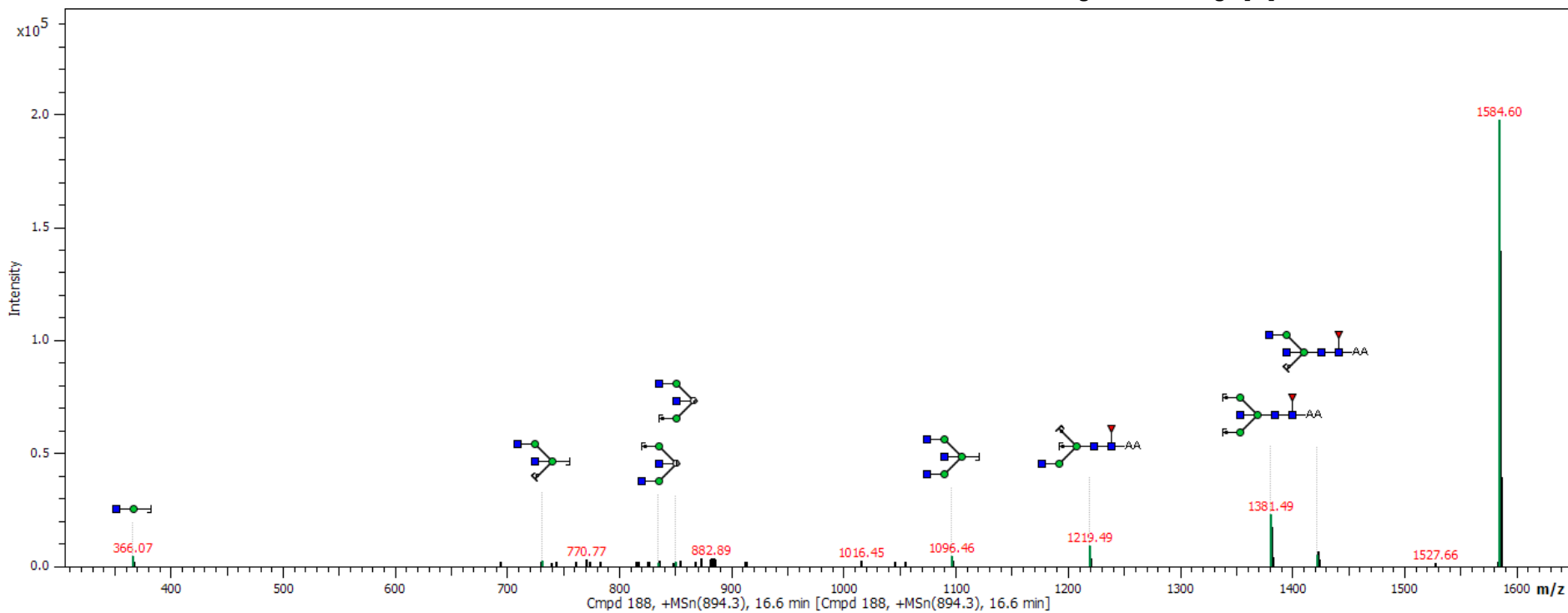


Glycan Search Report

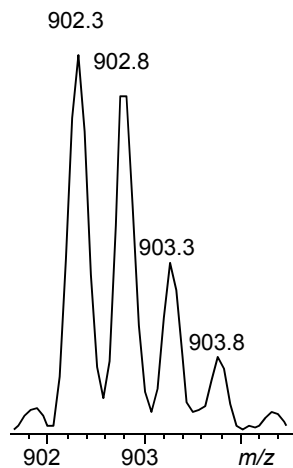
Glycan: 7



Project path: /N-glycans cancer/25142/comp_25142_01.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25142_01.d/comp_25142_01.mgf
Parent m/z: 894.3456 2+ **Score:** 35.761
Composition: Hex3HexNAc5dHex1-AA **Intensity coverage [%]:** 0.47
Accession: 1040 **Fragment coverage [%]:** 0.27

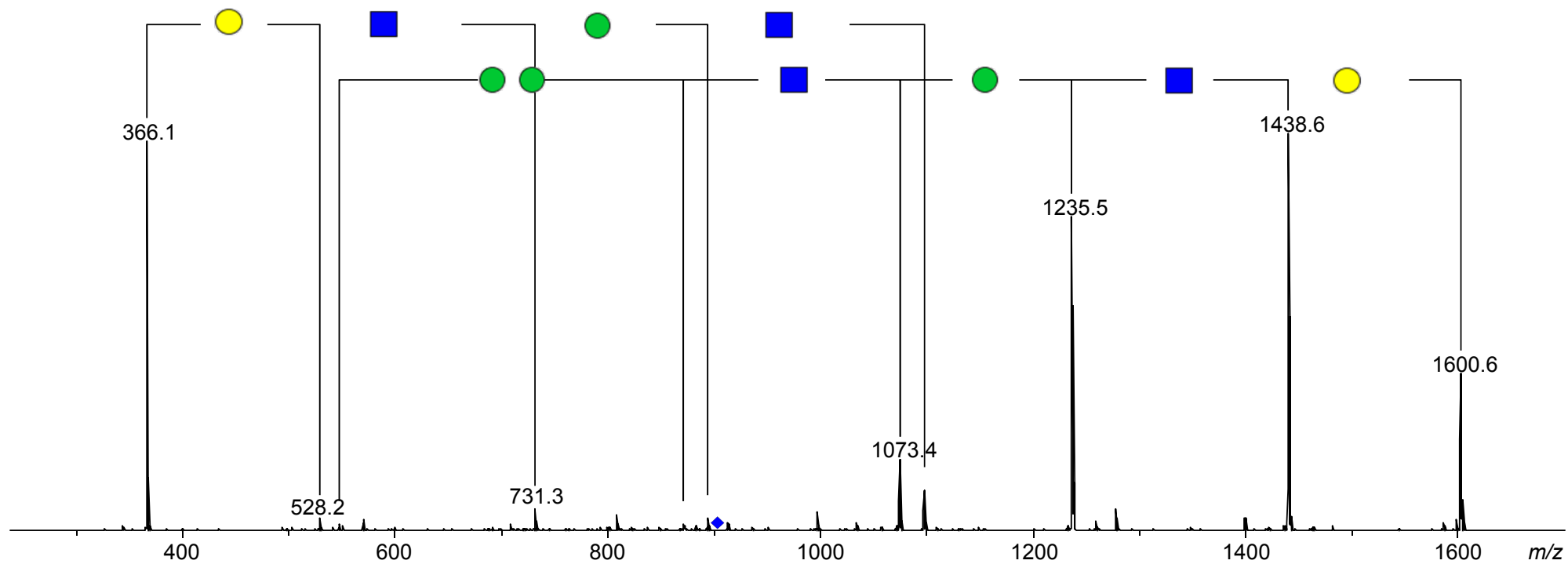
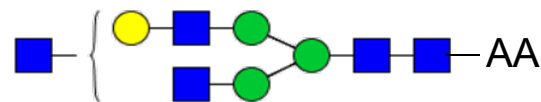


Spectrum 56



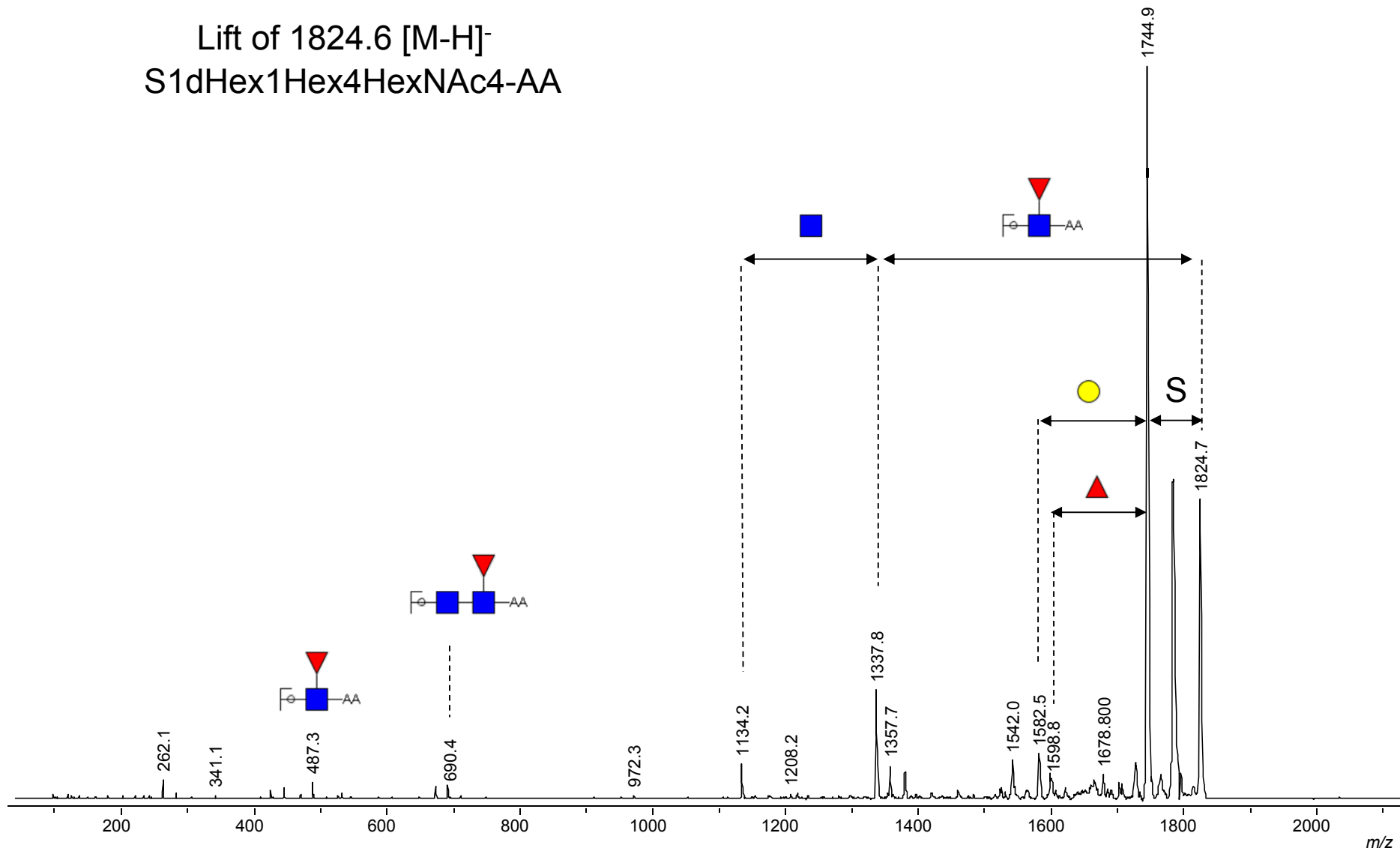
ESI MS/MS of $[902.2+2H]^{2+}$

Hex4HexNAc5-AA



Spectrum 57

Lift of 1824.6 [M-H]⁻
S1dHex1Hex4HexNAc4-AA

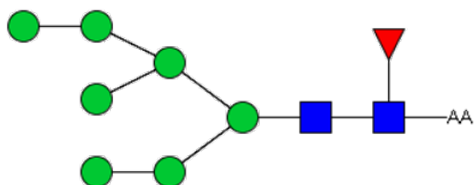


Spectrum 58

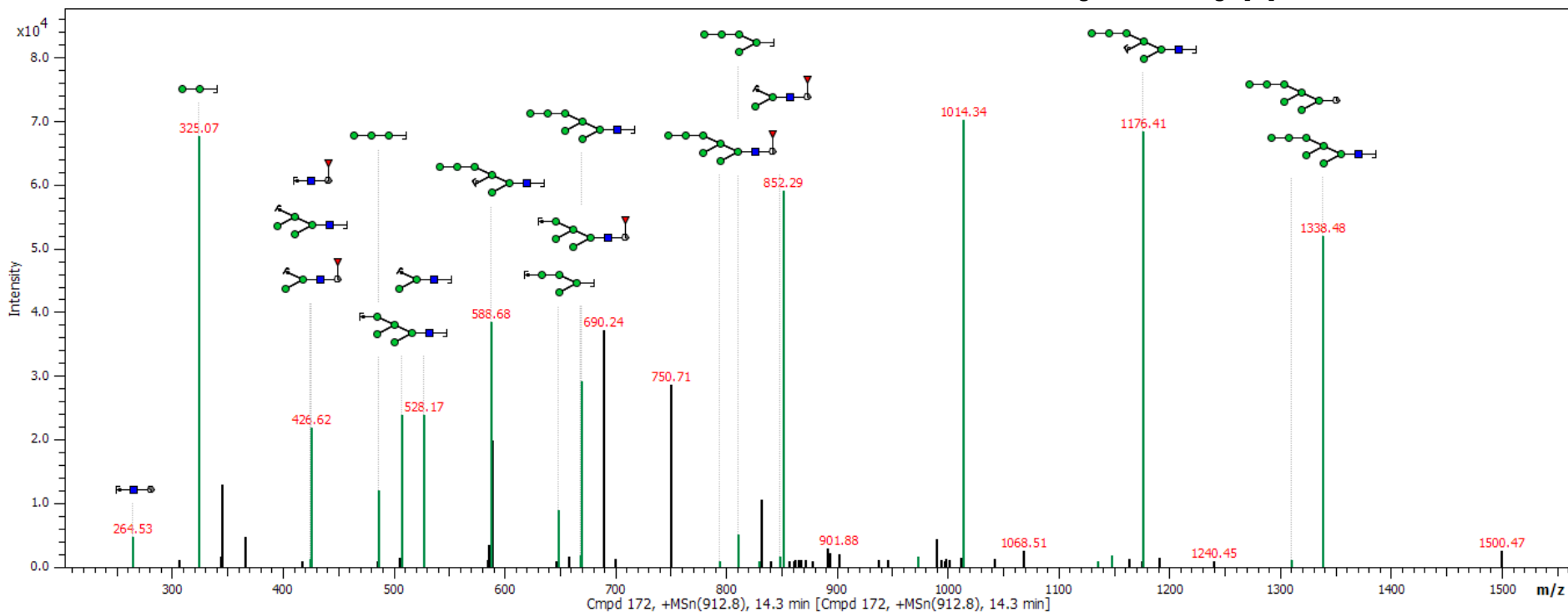


Glycan Search Report

Glycan: 18



Project path: /N-glycans cancer/25147/comp_25147.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25147_02.d/comp_25147.mgf
Parent m/z: 913.8321 2+ **Score:** 36.347
Composition: Hex7HexNAc2dHex1-AA **Intensity coverage [%]:** 0.74
Accession: 29019 **Fragment coverage [%]:** 0.18

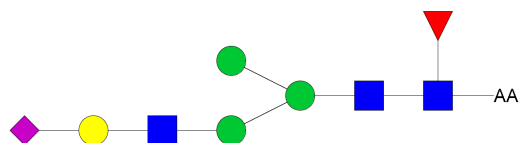




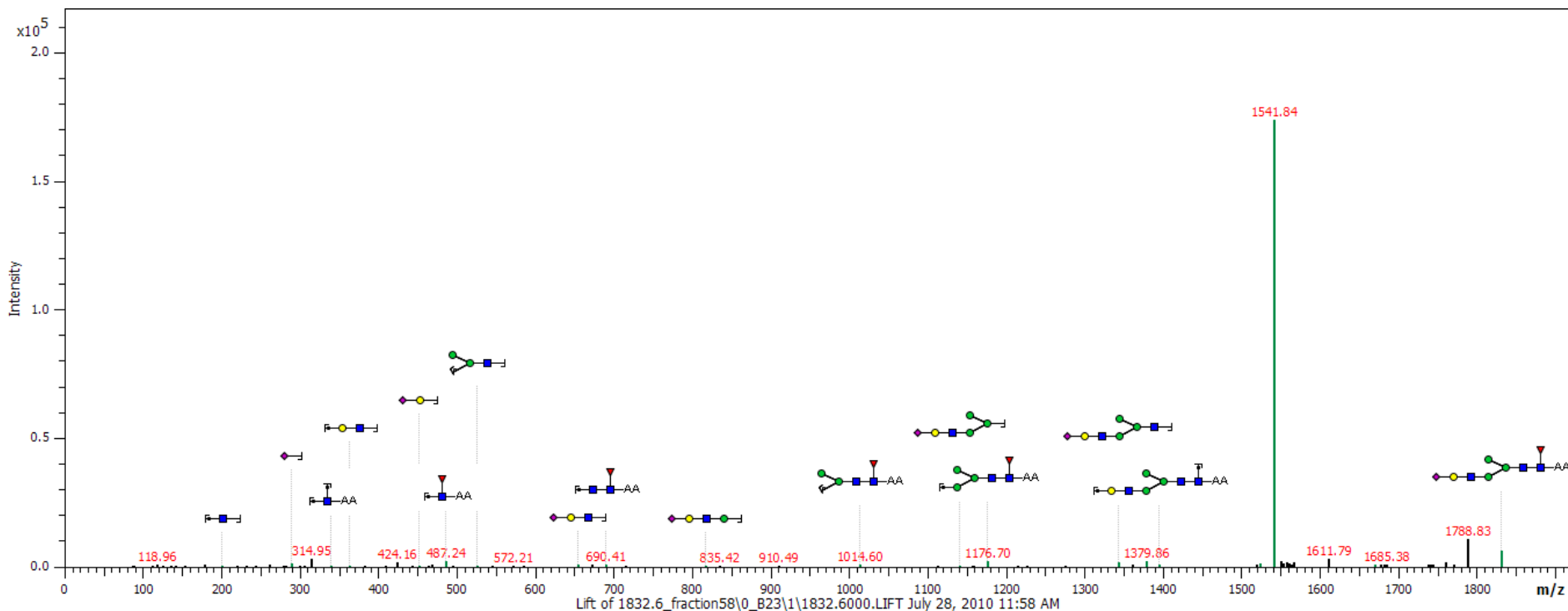
Spectrum 59

Glycan Search Report

Glycan: 2



Project path: /N-glycans cancer/Lift spectra/CombinedLIFT
MS data: c:/documents and settings/ciabalog/desktop/new folder/lift of 1832.6_fraction58/0_b23/1/1832.6000.lift/ 1sref/pdata/1/1r
Parent m/z: 1832.6587 -1 **Score:** 67.269
Composition: Hex4HexNAc3NeuAc1dHex1-AA **Intensity coverage [%]:** 0.81
Accession: 36111 **Fragment coverage [%]:** 0.56

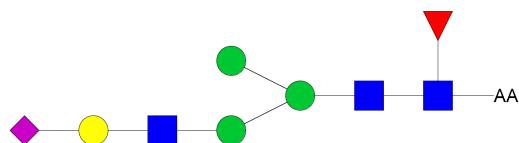




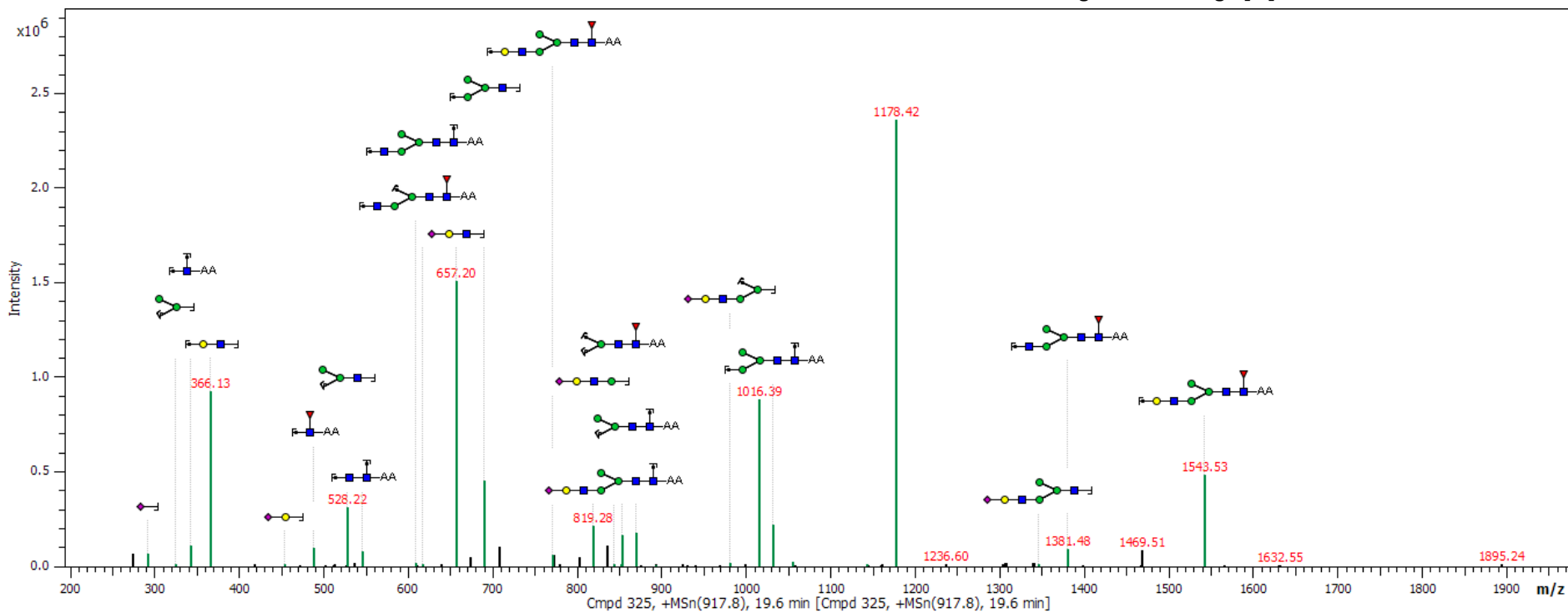
Spectrum 60

Glycan Search Report

Glycan: 4



Project path: /N-glycans cancer/25145/comp_25145.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25145_02.d/comp_25145.mgf
Parent m/z: 917.8403 2+ **Score:** 81.672
Composition: Hex4HexNAc3NeuAc1dHex1-AA **Intensity coverage [%]:** 0.91
Accession: 36111 **Fragment coverage [%]:** 0.73

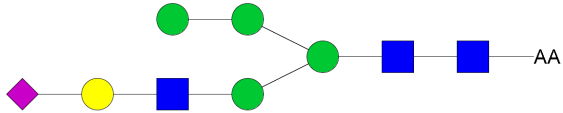


Spectrum 61



Glycan Search Report

Glycan: 1



Project path: /N-glycans cancer/25143/comp_25143_01.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25143_01.d/comp_25143_01.mgf

Parent m/z: 925.8377 2+

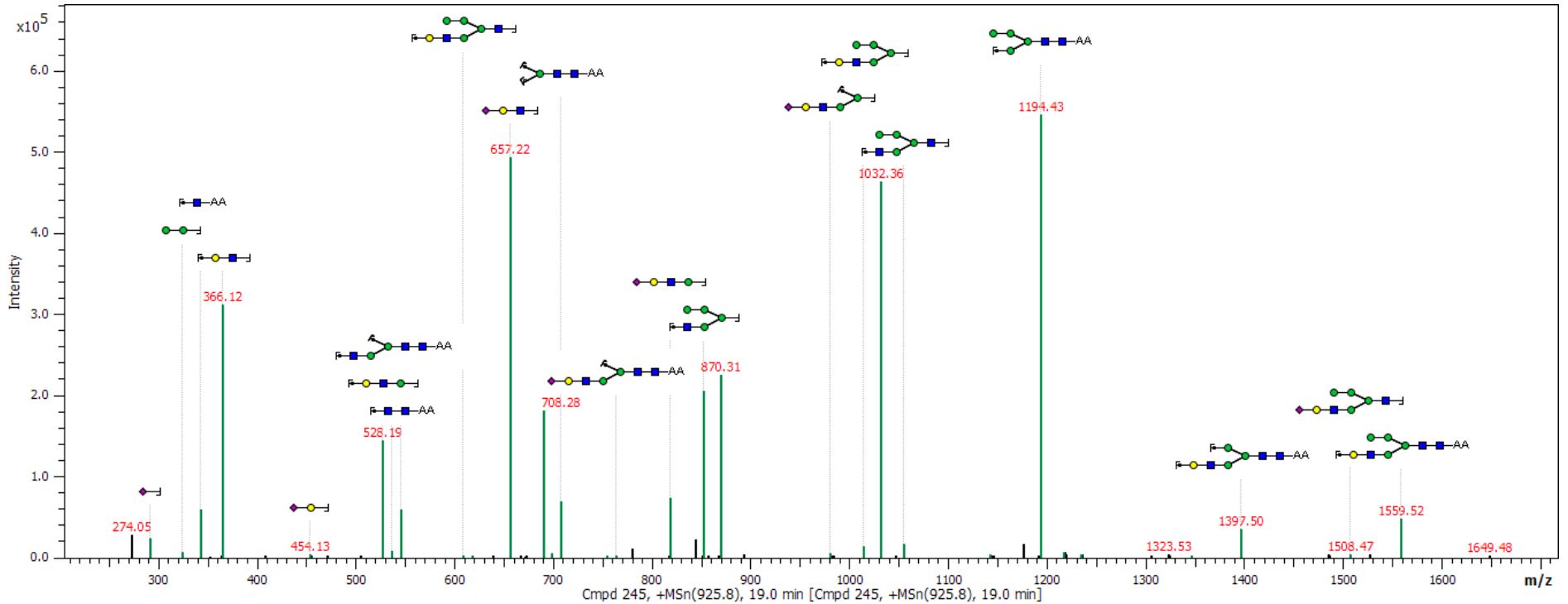
Score: 91.782

Composition: Hex5HexNAc3NeuAc1-AA

Intensity coverage [%]: 0.95

Accession: 36337

Fragment coverage [%]: 0.89

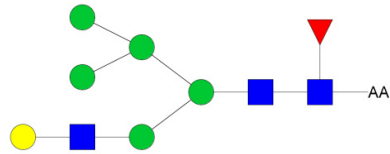


Spectrum 62



Glycan Search Report

Glycan: 8



Project path: /N-glycans cancer/25147/comp_25147.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25147_02.d/comp_25147.mgf

Parent m/z: 934.3454 2+

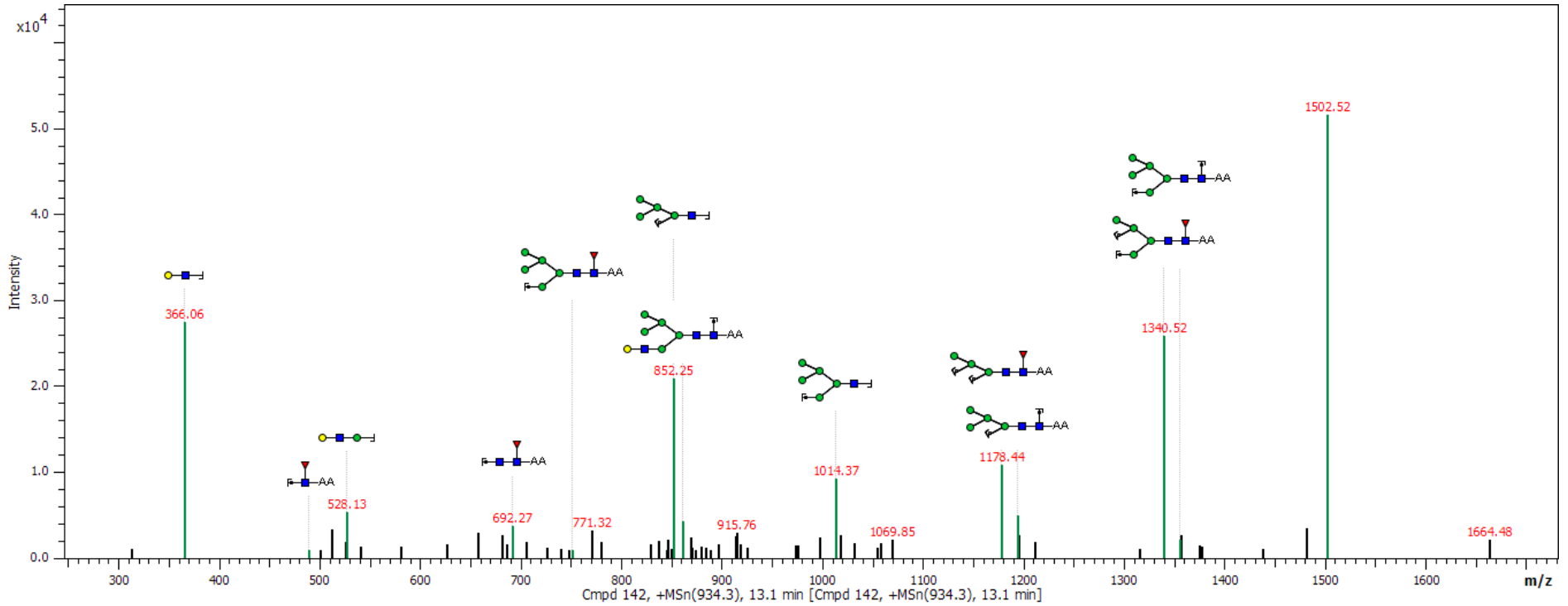
Score: 49.528

Composition: Hex6HexNAc3dHex1-AA

Intensity coverage [%]: 0.66

Accession: 36119

Fragment coverage [%]: 0.37

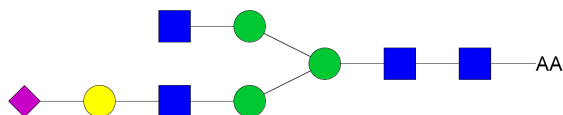


Spectrum 63

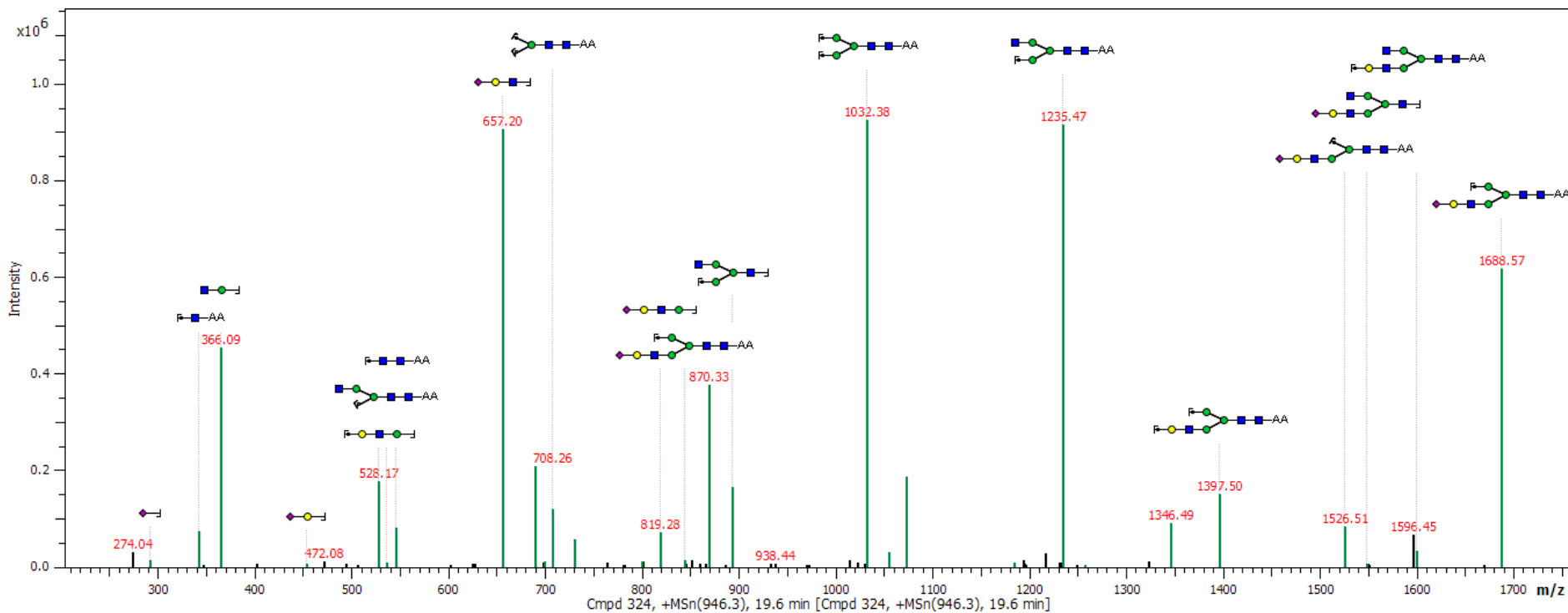


Glycan Search Report

Glycan: 1



Project path: /N-glycans cancer/25145/comp_25145.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25145_02.d/comp_25145.mgf
Parent m/z: 946.3510 2+ **Score:** 90.886
Composition: Hex4HexNAc4NeuAc1-AA **Intensity coverage [%]:** 0.93
Accession: 36345 **Fragment coverage [%]:** 0.88

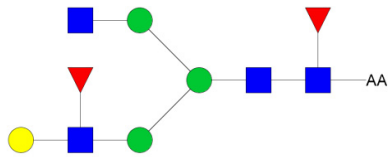


Spectrum 64



Glycan Search Report

Glycan: 4



Project path: /N-glycans cancer/25143/comp_25143_01.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25143_01.d/comp_25143_01.mgf

Parent m/z: 946.8612 2+

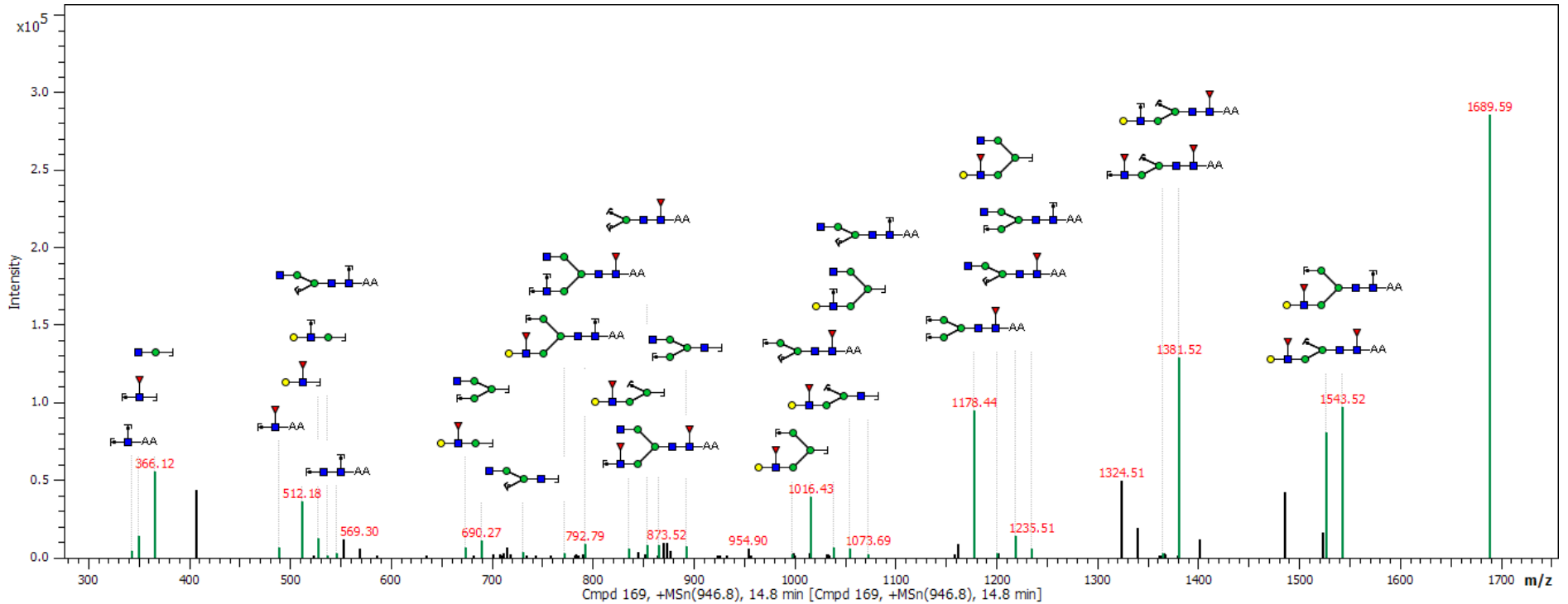
Score: 78.128

Composition: Hex4HexNAc4dHex2-AA

Intensity coverage [%]: 0.76

Accession: 36232

Fragment coverage [%]: 0.81

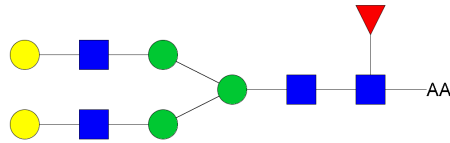


Spectrum 65

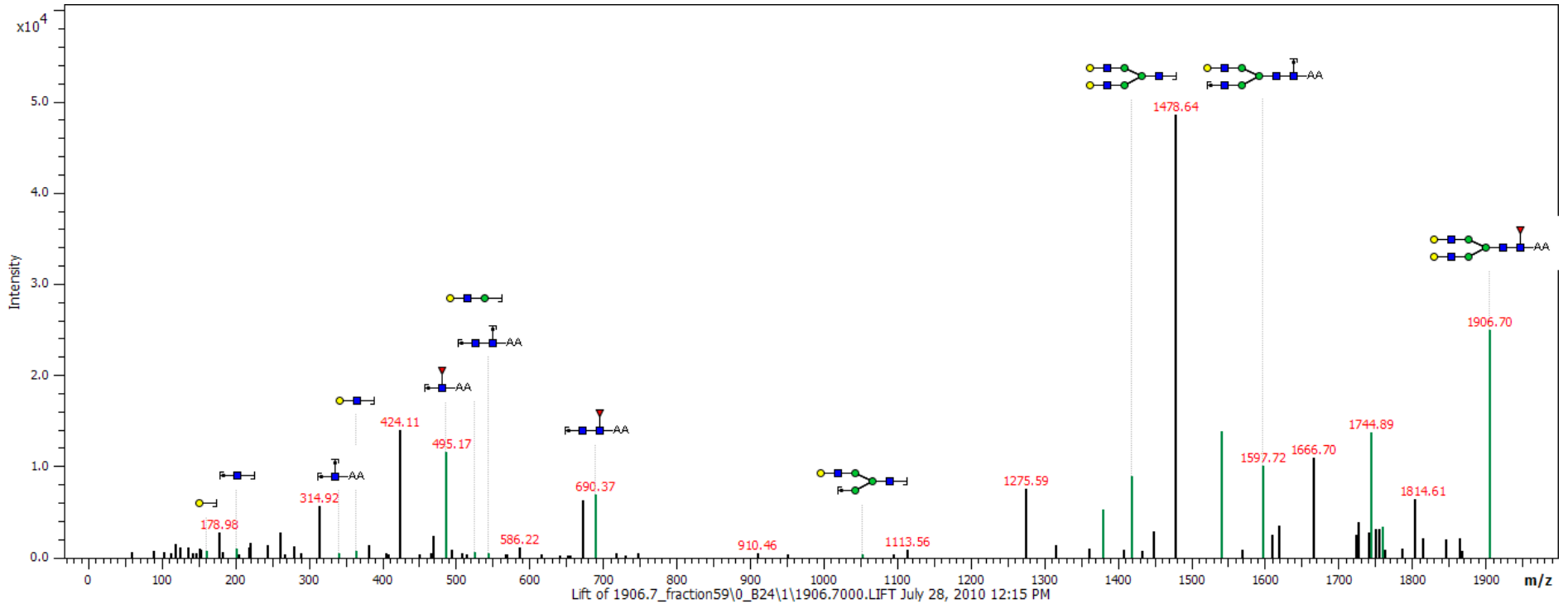


Glycan Search Report

Glycan: 8



Project path: /N-glycans cancer/Lift spectra/CombinedLIFT
MS data: c:/documents and settings/ciabalog/desktop/new folder/lift of 1906.7_fraction59/0_b24/1/1906.7000.lift/ 1sref/pdata/1/1r
Parent m/z: 1906.6955 -1 **Score:** 48.617
Composition: Hex5HexNAc4dHex1-AA **Intensity coverage [%]:** 0.38
Accession: 36269 **Fragment coverage [%]:** 0.63

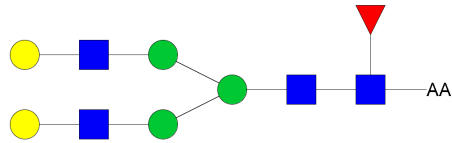


Spectrum 66



Glycan Search Report

Glycan: 2



Project path: /N-glycans cancer/25143/comp_25143_01.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25143_01.d/comp_25143_01.mgf

Parent m/z: 954.8587 2+

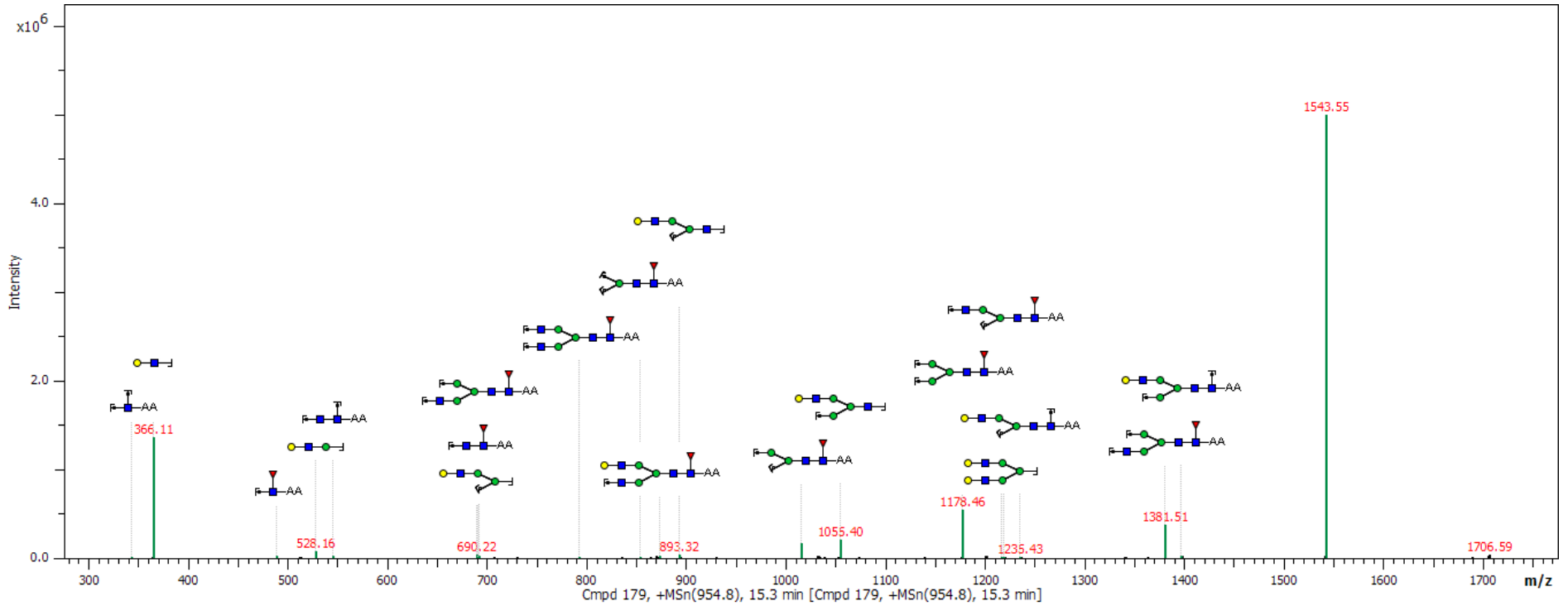
Score: 86.071

Composition: Hex5HexNAc4dHex1-AA

Intensity coverage [%]: 0.96

Accession: 36269

Fragment coverage [%]: 0.77

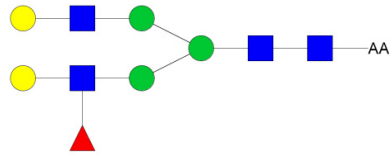


Spectrum 67



Glycan Search Report

Glycan: 13



Project path: /N-glycans cancer/25147/comp_25147.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25147_02.d/comp_25147.mgf

Parent m/z: 954.8587 2+

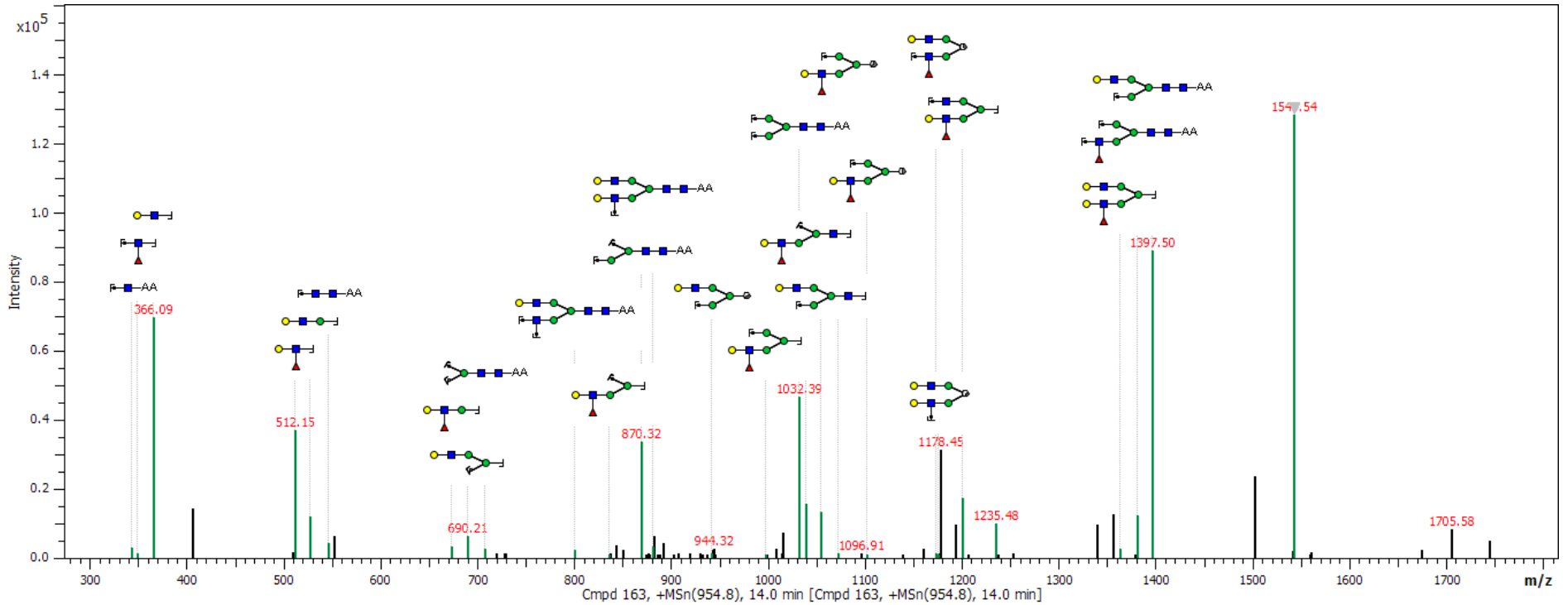
Score: 41.604

Composition: Hex5HexNAc4dHex1-AA

Intensity coverage [%]: 0.73

Accession: 10190

Fragment coverage [%]: 0.24



Spectrum 68



Glycan Search Report

Glycan: 18

Project path: /N-glycans cancer/25143/comp_25143_01.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25143_01.d/comp_25143_01.mgf

Parent m/z: 962.8561 2+

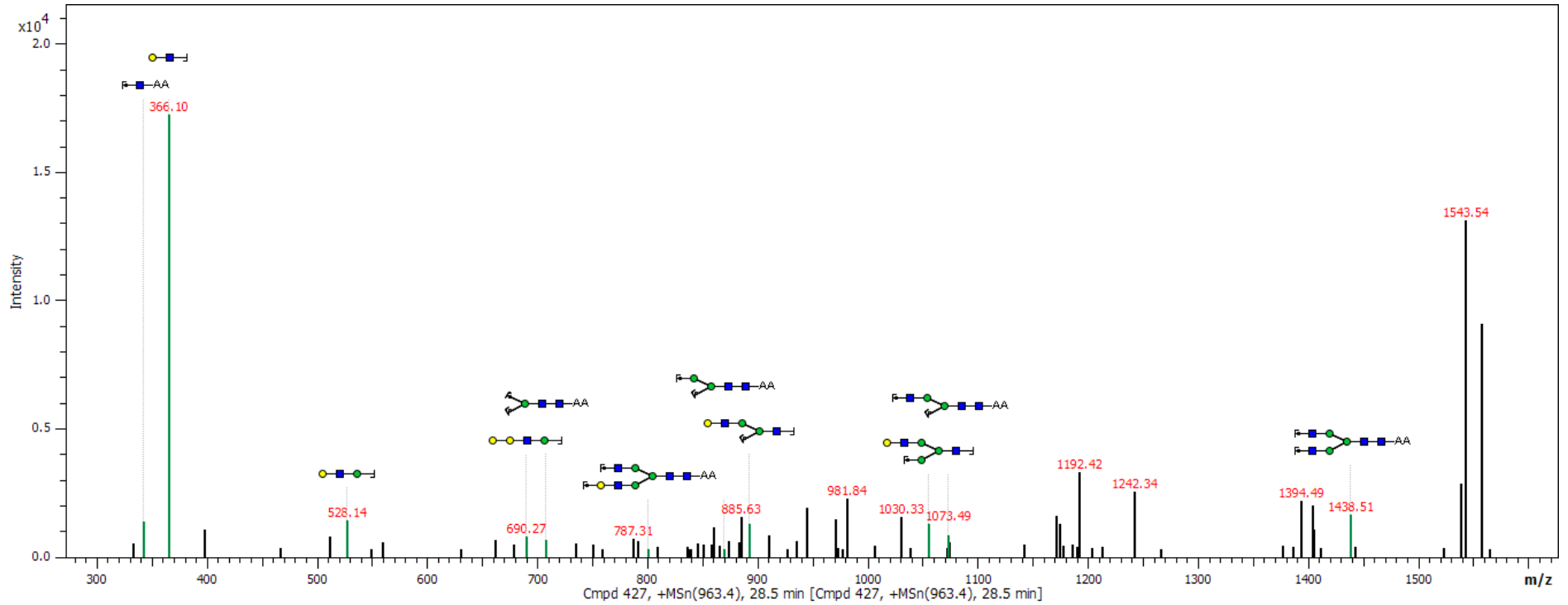
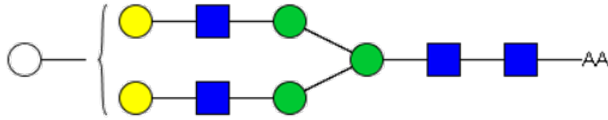
Score: 34.897

Composition: Hex6HexNAc4-AA

Intensity coverage [%]: 0.28

Accession: 36353

Fragment coverage [%]: 0.44

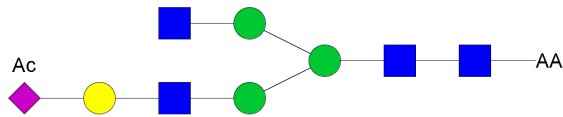


Spectrum 69



Glycan Search Report

Glycan: 8



Project path: /N-glycans cancer/25142/comp_25142_01.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25142_01.d/comp_25142_01.mgf

Parent m/z: 967.3563 2+

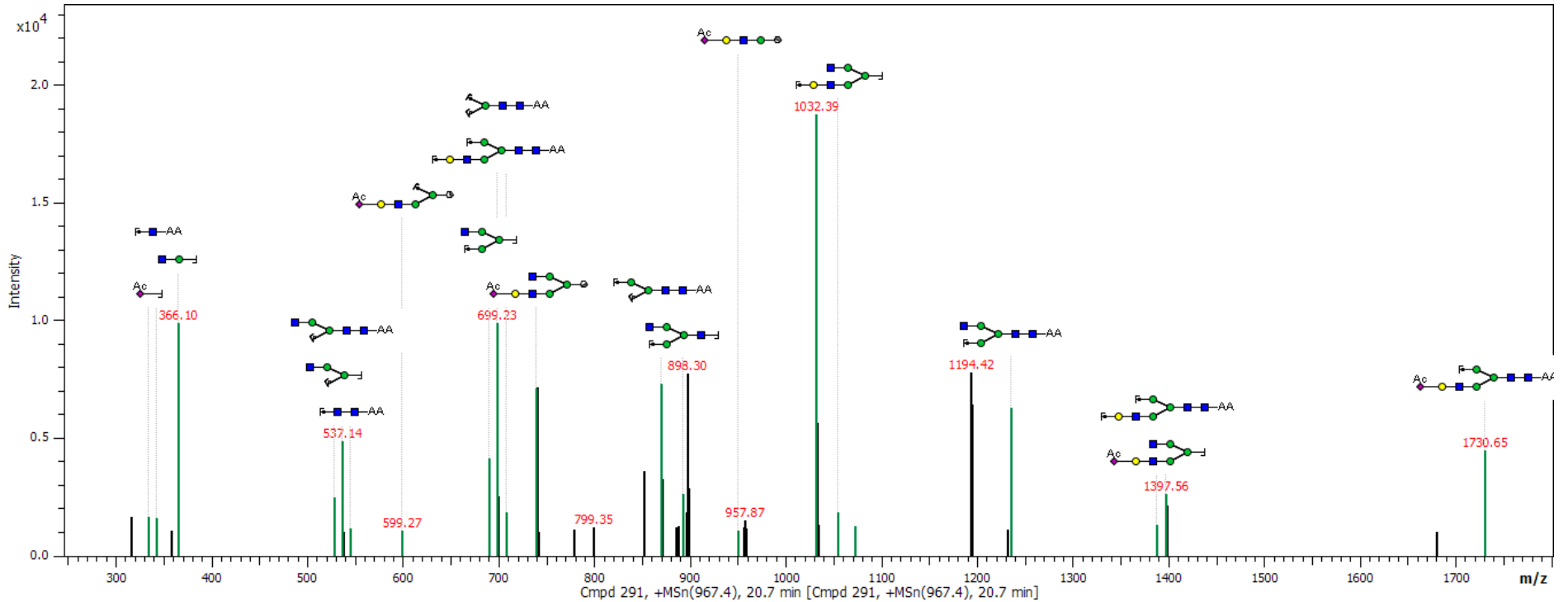
Score: 34.490

Composition: Ac1Hex4HexNAc4NeuAc1-AA

Intensity coverage [%]: 0.56

Accession: 7875

Fragment coverage [%]: 0.21

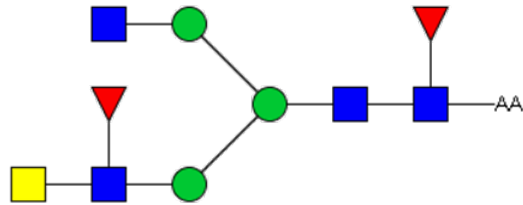


Spectrum 70



Glycan Search Report

Glycan: 12



Project path: /N-glycans cancer/25145/comp_25145.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25145_02.d/comp_25145.mgf

Parent m/z: 967.3745 2+

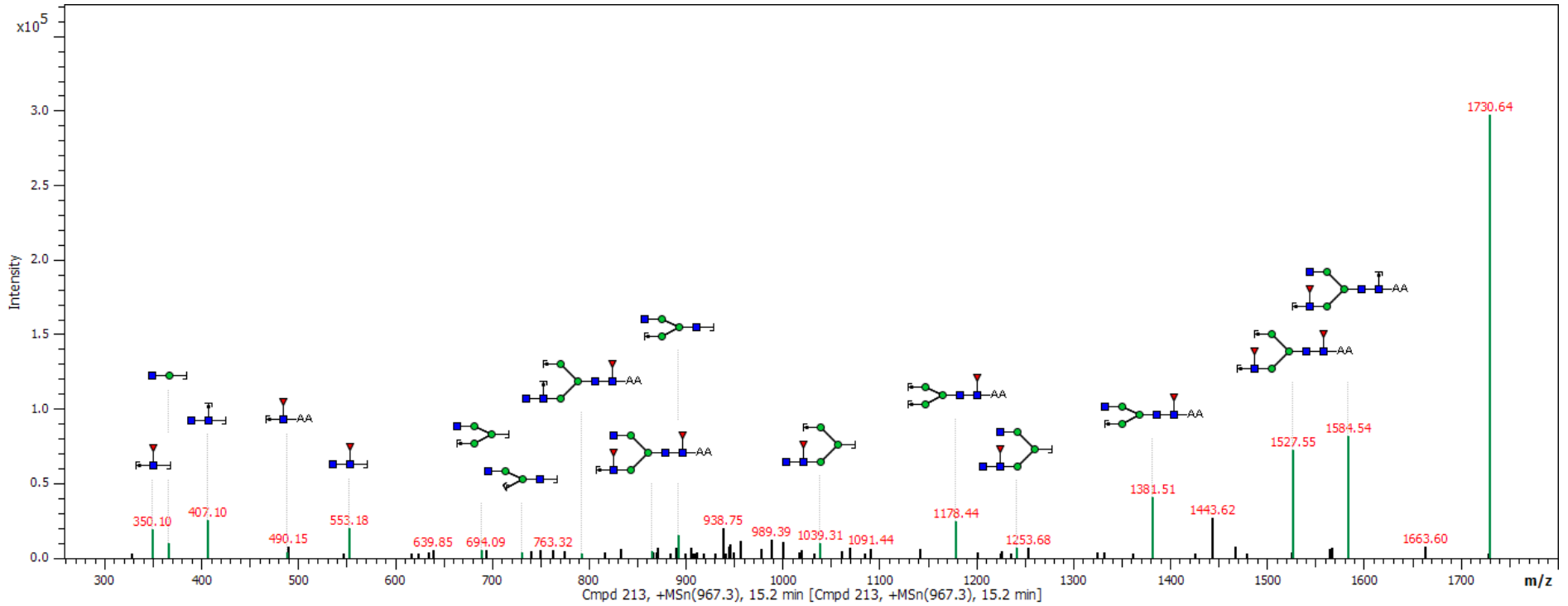
Score: 58.743

Composition: Hex3HexNAc5dHex2-AA

Intensity coverage [%]: 0.64

Accession: 36714

Fragment coverage [%]: 0.54

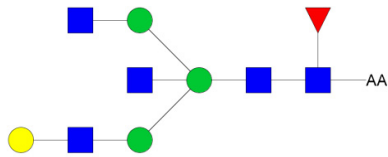


Spectrum 71

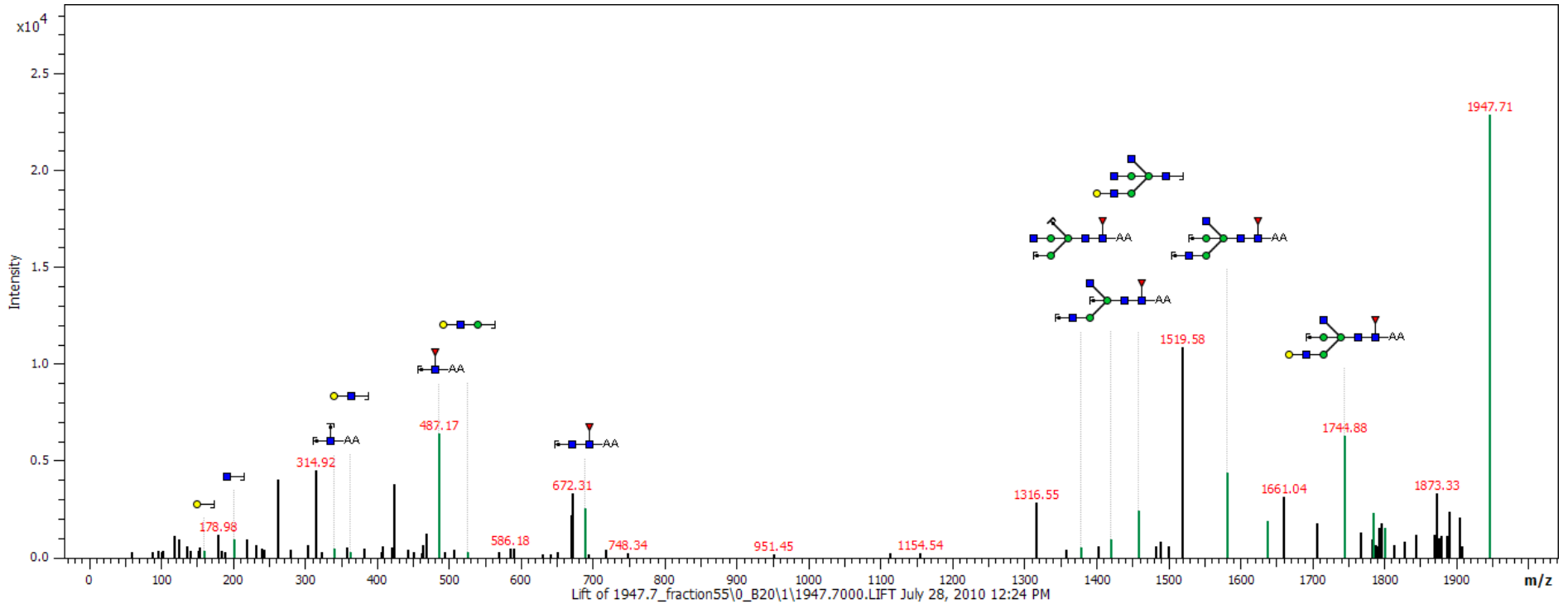


Glycan Search Report

Glycan: 10



Project path: /N-glycans cancer/Lift spectra/CombinedLIFT
MS data: c:/documents and settings/ciabalog/desktop/new folder/lift of 1947.7_fraction55/0_b20/1/1947.7000.lift/1sref/pdata/1/1r
Parent m/z: 1947.7221 -1 **Score:** 46.581
Composition: Hex4HexNAc5dHex1-AA **Intensity coverage [%]:** 0.40
Accession: 36228 **Fragment coverage [%]:** 0.54

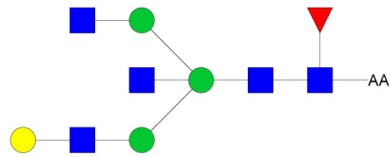


Spectrum 72

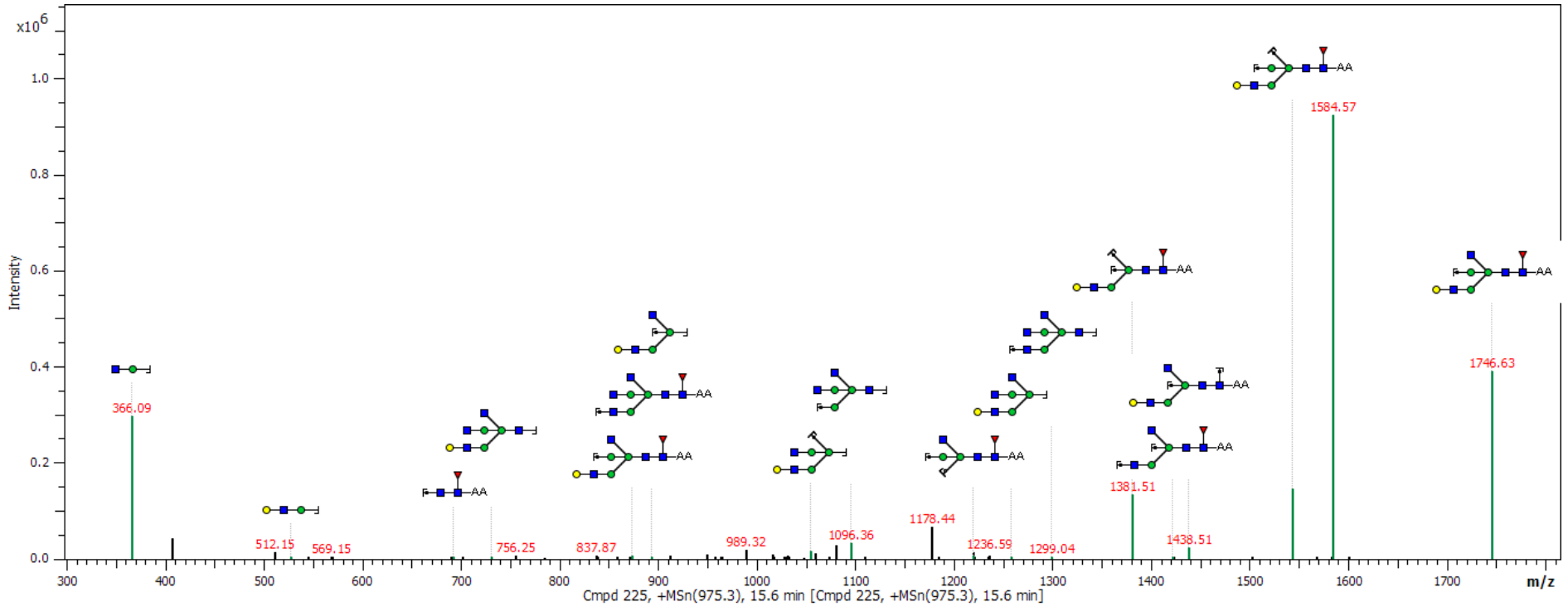


Glycan Search Report

Glycan: 5



Project path: /N-glycans cancer/25145/comp_25145.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25145_02.d/comp_25145.mgf
Parent m/z: 975.3720 2+ **Score:** 80.202
Composition: Hex4HexNAc5dHex1-AA **Intensity coverage [%]:** 0.86
Accession: 36228 **Fragment coverage [%]:** 0.75

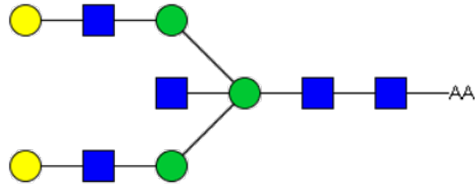


Spectrum 73



Glycan Search Report

Glycan: 8



Project path: /N-glycans cancer/25145/comp_25145.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25145_02.d/comp_25145.mgf

Parent m/z: 983.3694 2+

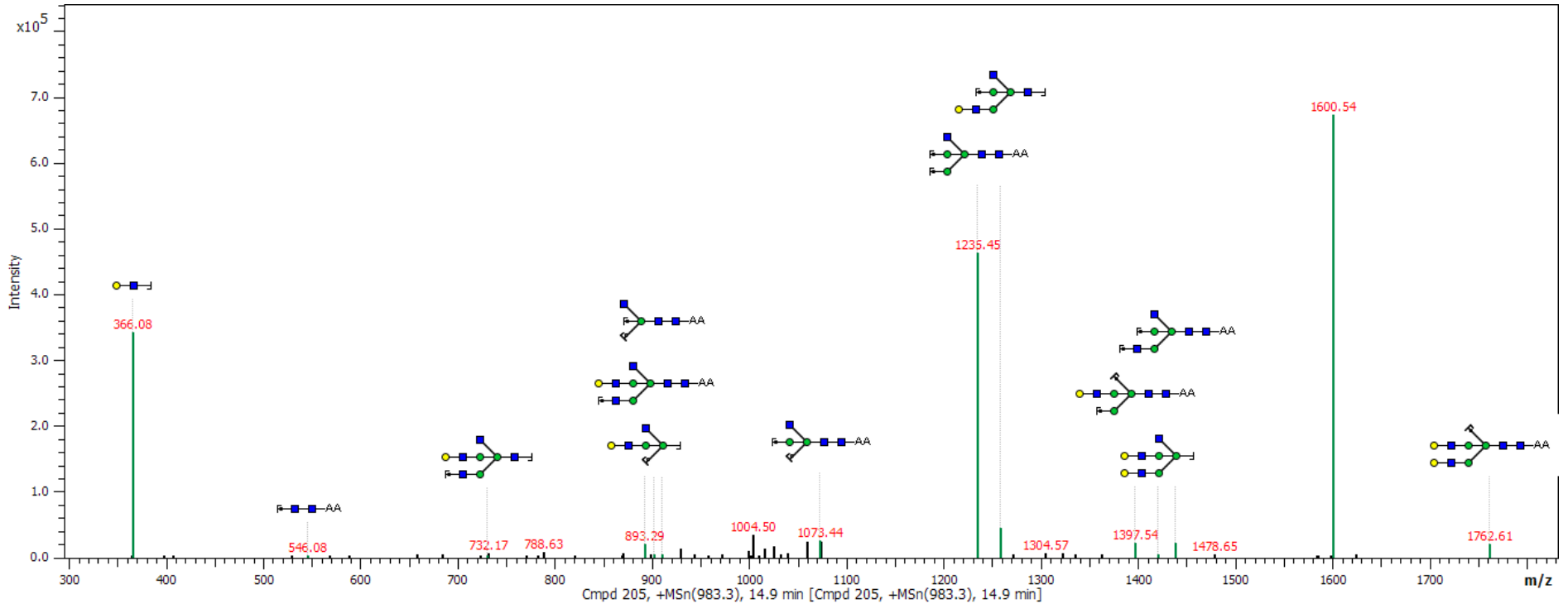
Score: 71.951

Composition: Hex5HexNAc5-AA

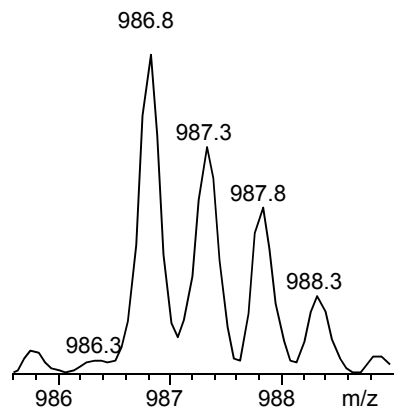
Intensity coverage [%]: 0.86

Accession: 36348

Fragment coverage [%]: 0.61

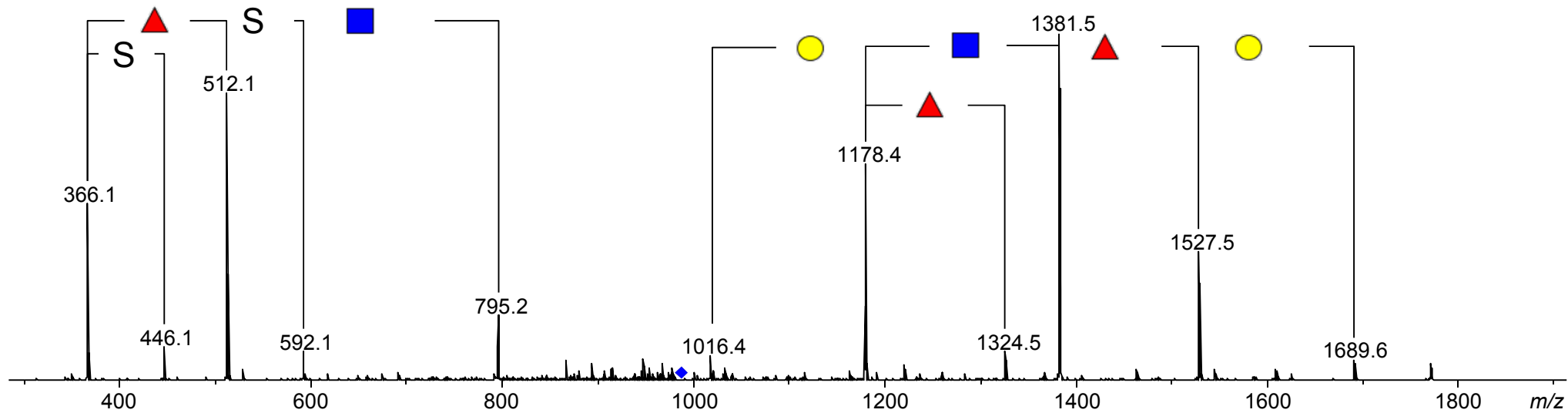
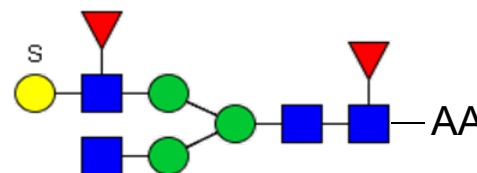


Spectrum 74



ESI MS/MS of $[986.8+2H]^{2+}$

S1dHex2Hex4HexNAc4-AA

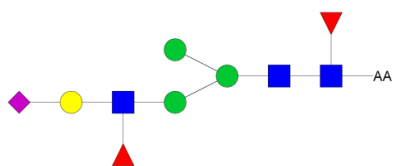


Spectrum 75



Glycan Search Report

Glycan: 19



Project path: /N-glycans cancer/25143/comp_25143_01.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25143_01.d/comp_25143_01.mgf

Parent m/z: 990.8692 2+

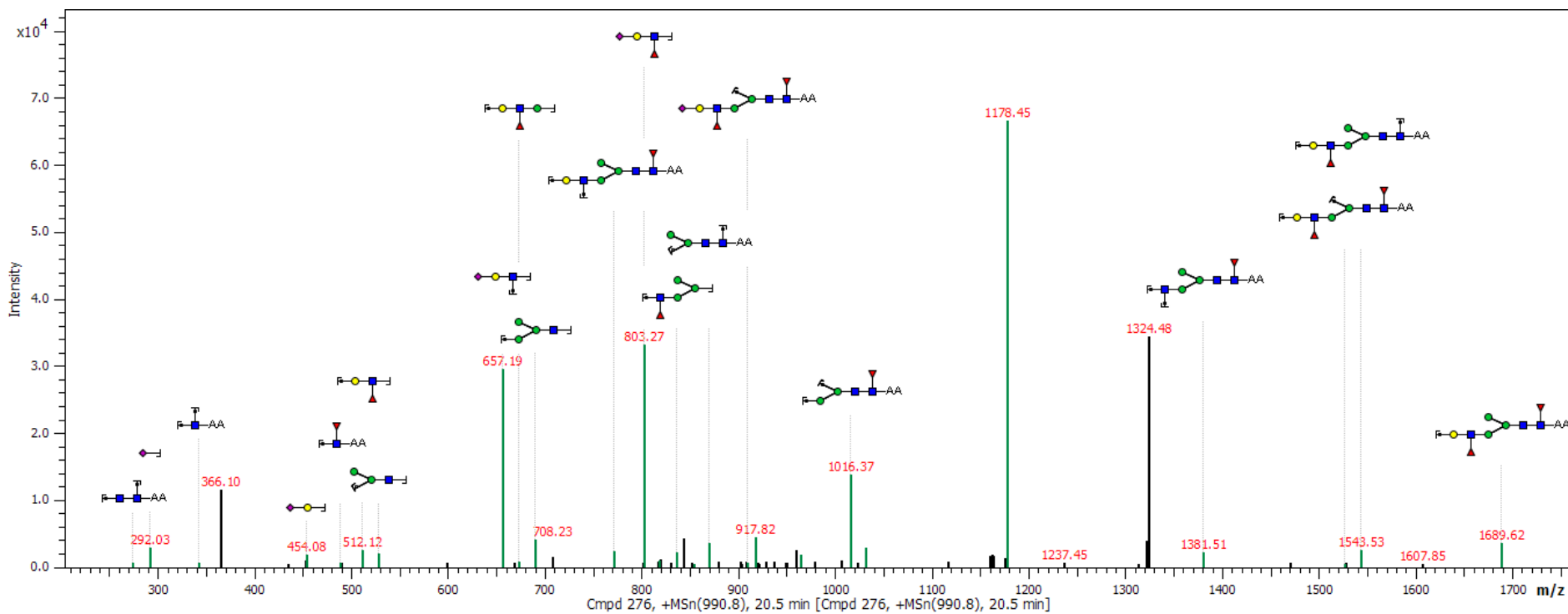
Score: 34.184

Composition: Hex4HexNAc3NeuAc1dHex2-AA

Intensity coverage [%]: 0.68

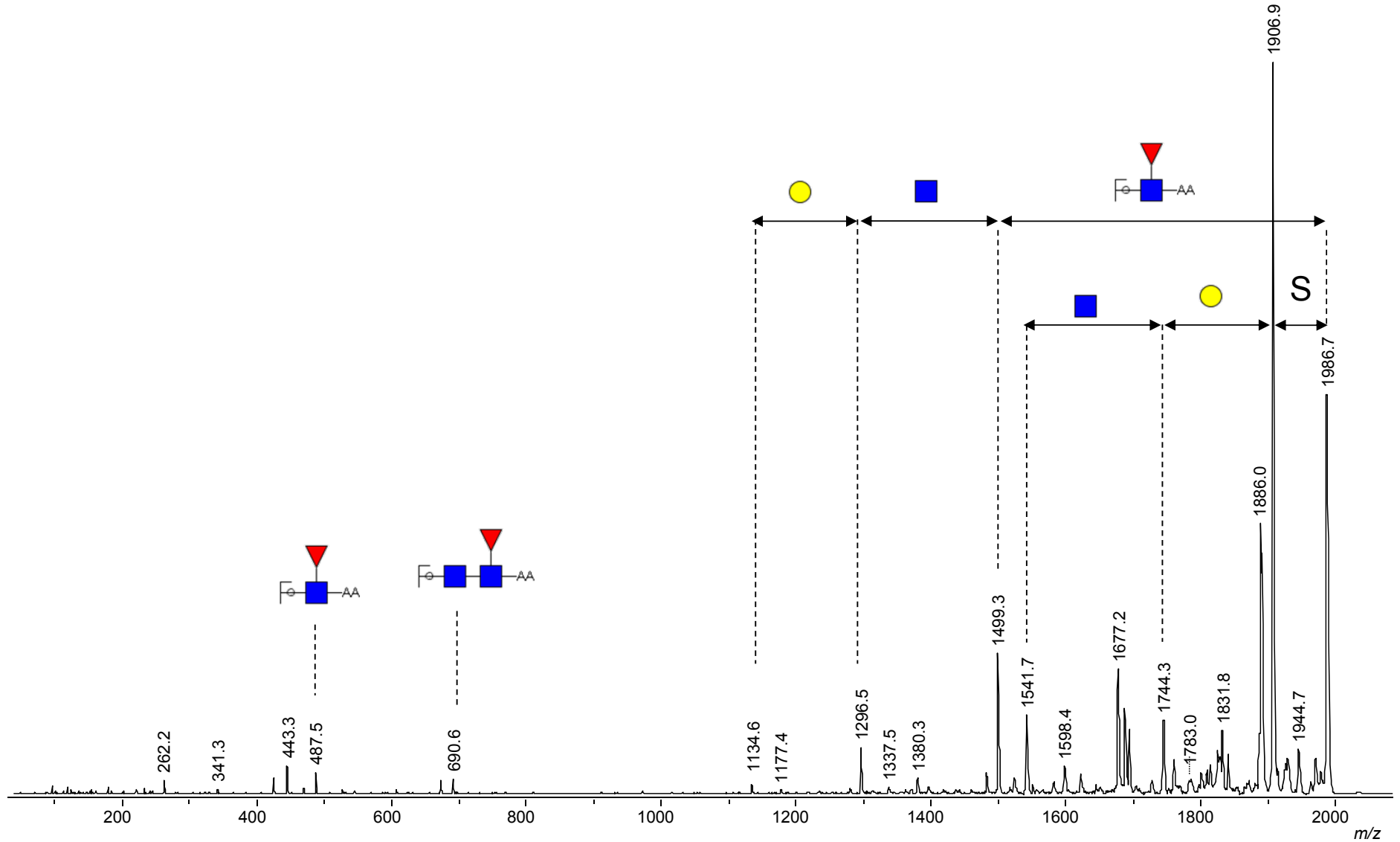
Accession: 29052

Fragment coverage [%]: 0.17



Spectrum 76

Lift of 1986.7 [M-H]⁻
S1dHex1Hex5HexNAc4-AA

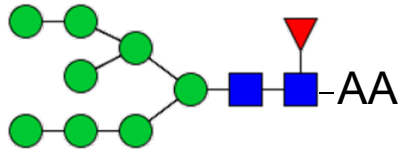


Spectrum 77



Glycan Search Report

Glycan: 34



Project path: /N-glycans cancer/25148/comp_25148.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf

Parent m/z: 994.8585 2+

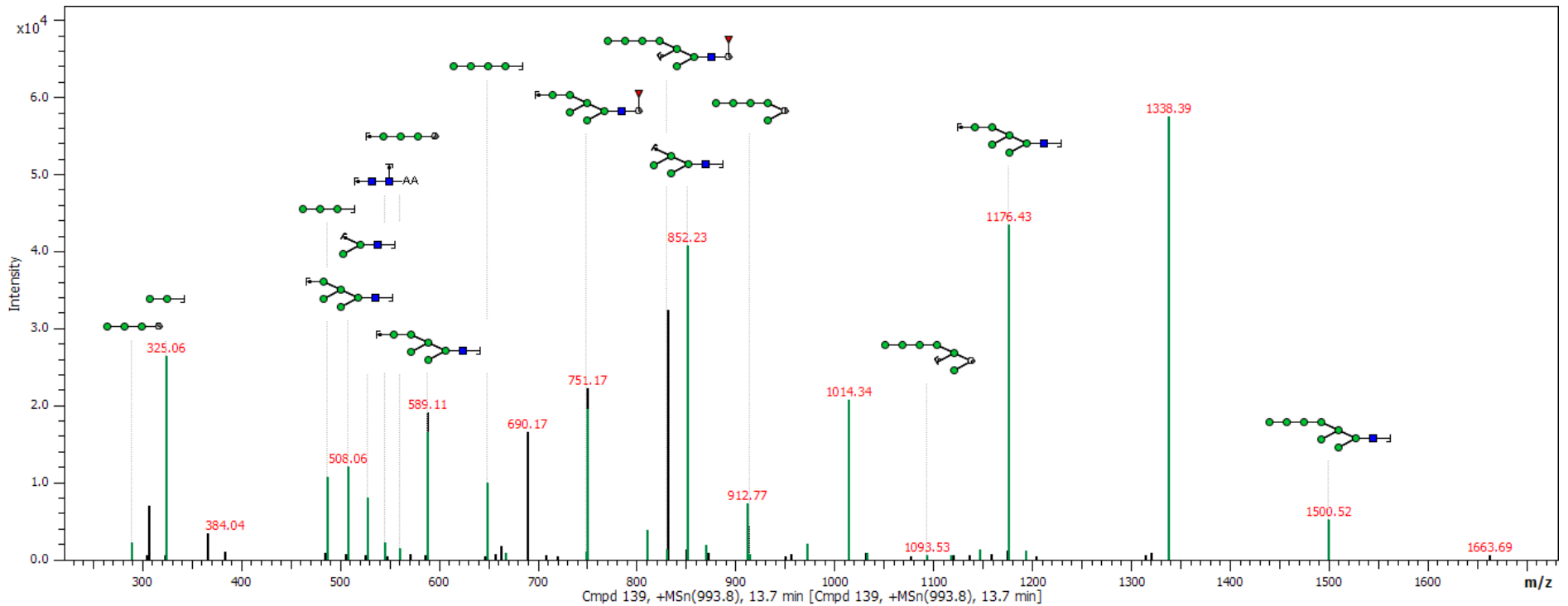
Score: 35.550

Composition: Hex8HexNAc2dHex1-AA

Intensity coverage [%]: 0.69

Accession: 29021

Fragment coverage [%]: 0.18

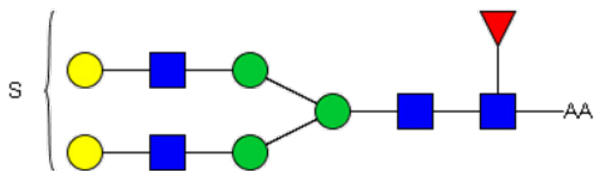


Spectrum 78



Glycan Search Report

Glycan: 22



Project path: /N-glycans cancer/25145/comp_25145.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25145_02.d/comp_25145.mgf

Parent m/z: 995.8853 2+

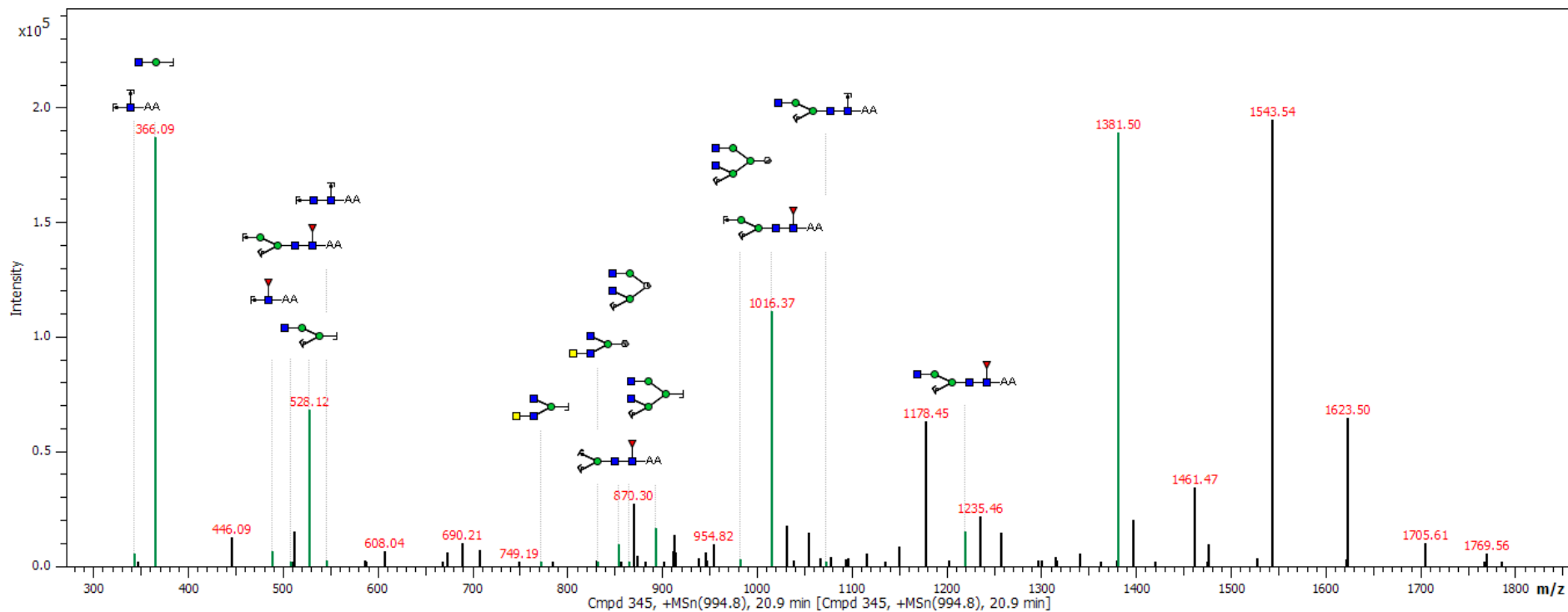
Score: 26.863

Composition: Hex3HexNAc6dHex1-AA

Intensity coverage [%]: 0.48

Accession: 1488

Fragment coverage [%]: 0.15

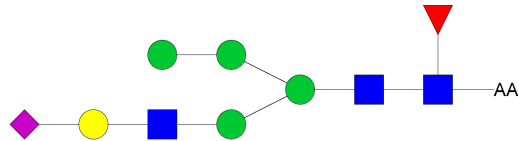


Spectrum 79



Glycan Search Report

Glycan: 10



Project path: /N-glycans cancer/25147/comp_25147.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25147_02.d/comp_25147.mgf

Parent m/z: 998.8667 2+

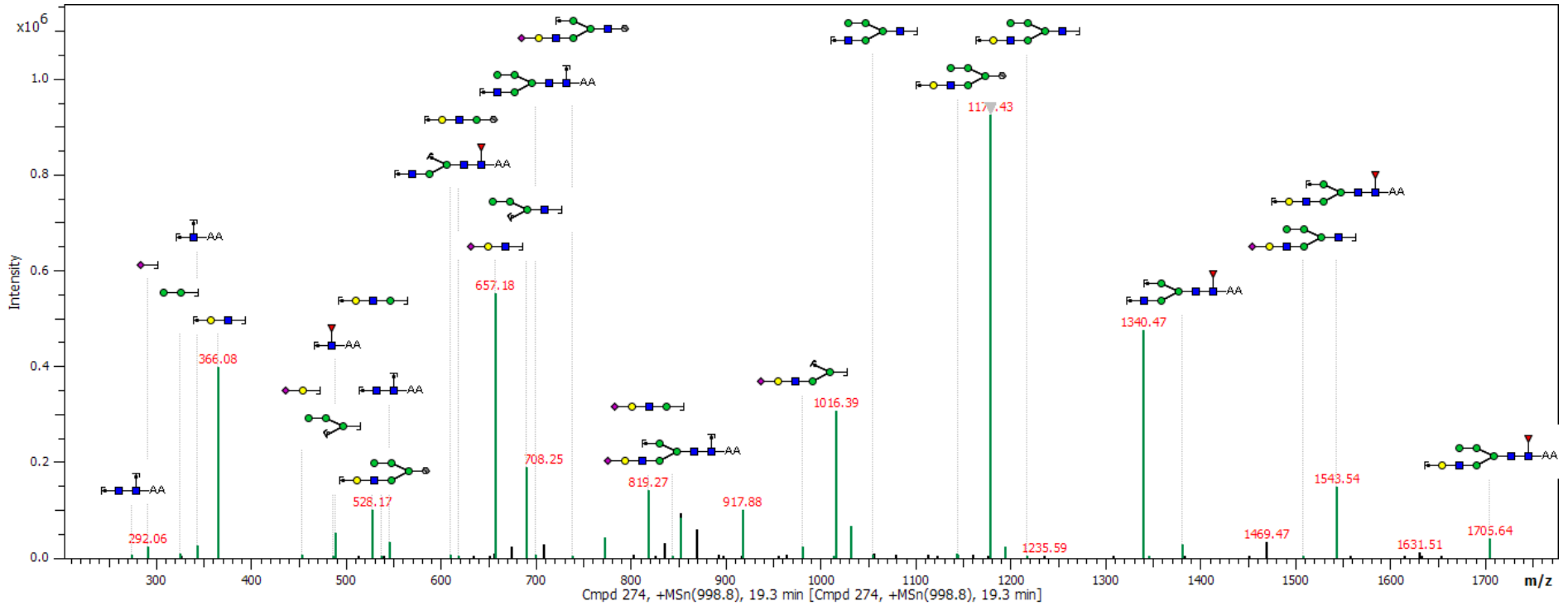
Score: 46.613

Composition: Hex5HexNAc3NeuAc1dHex1-AA

Intensity coverage [%]: 0.89

Accession: 36628

Fragment coverage [%]: 0.24

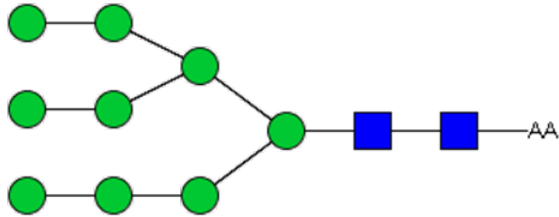


Spectrum 80

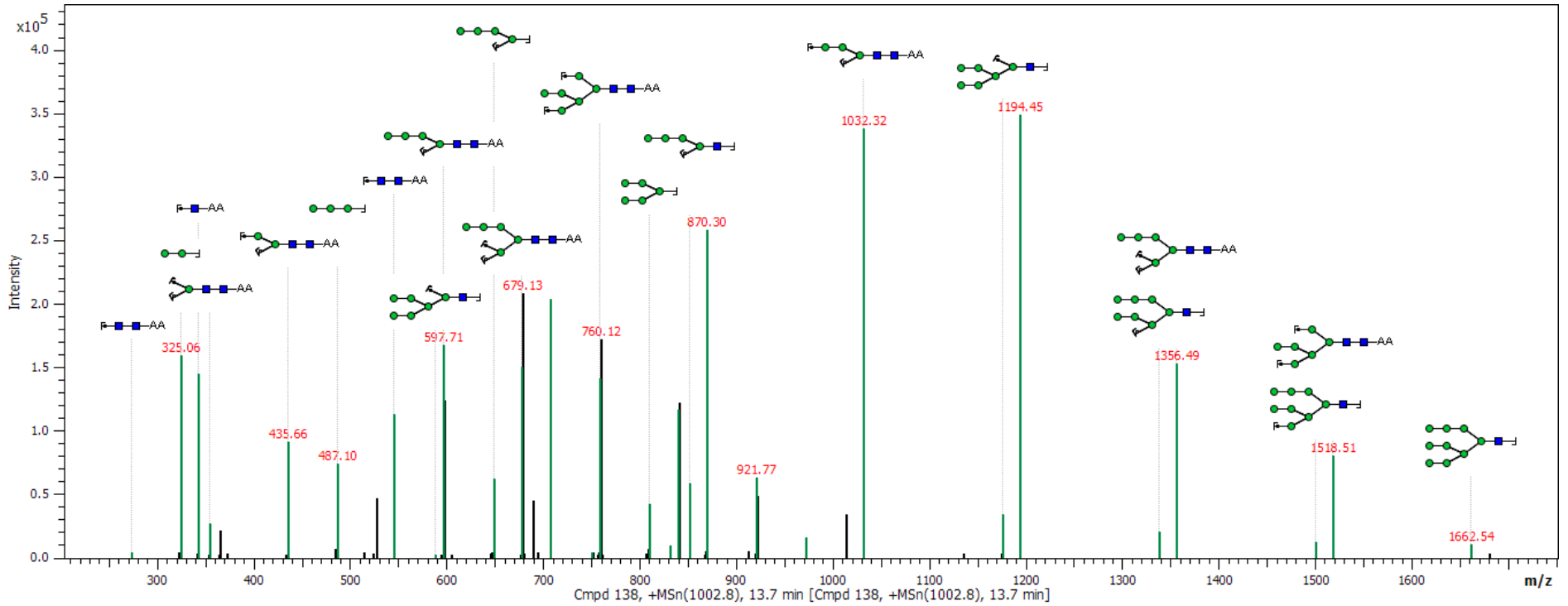


Glycan Search Report

Glycan: 1



Project path: /N-glycans cancer/25148/comp_25148.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf
Parent m/z: 1002.8559 2+ **Score:** 93.455
Composition: Hex9HexNAc2-AA **Intensity coverage [%]:** 0.75
Accession: 36321 **Fragment coverage [%]:** 1.16

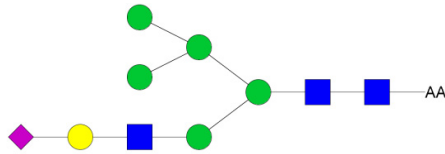


Spectrum 81

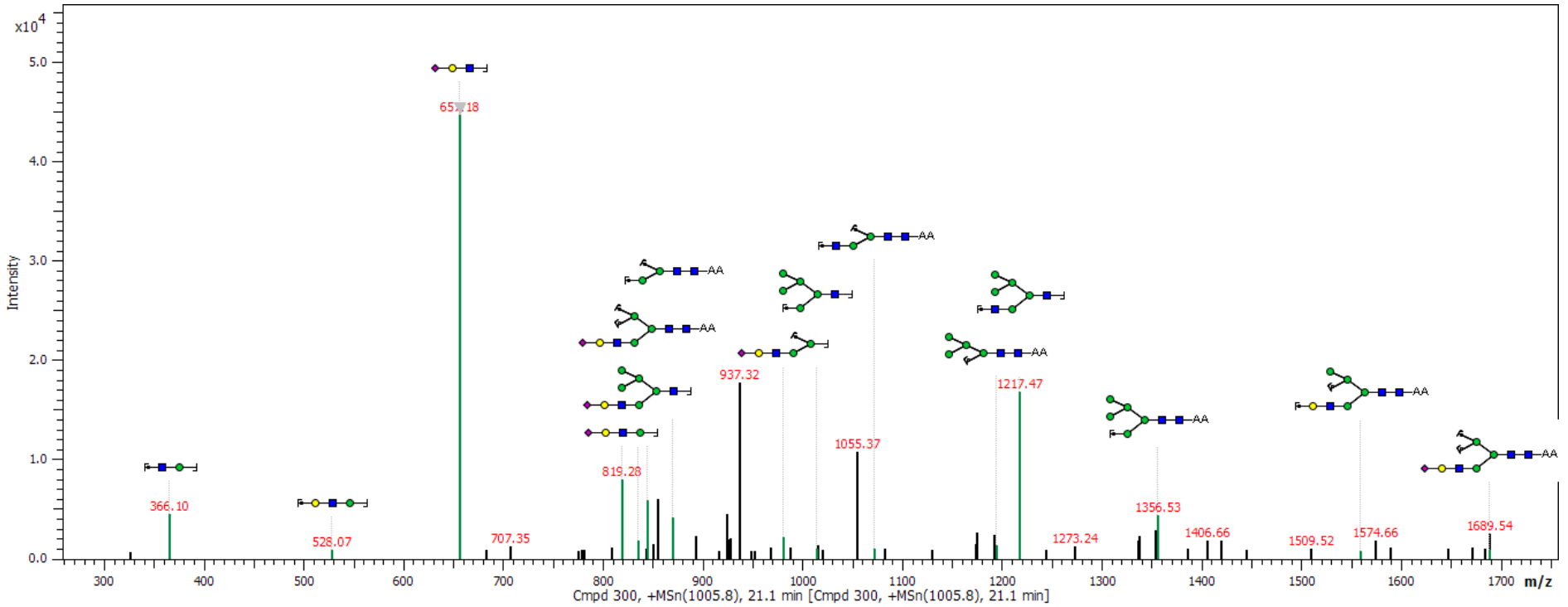


Glycan Search Report

Glycan: 11

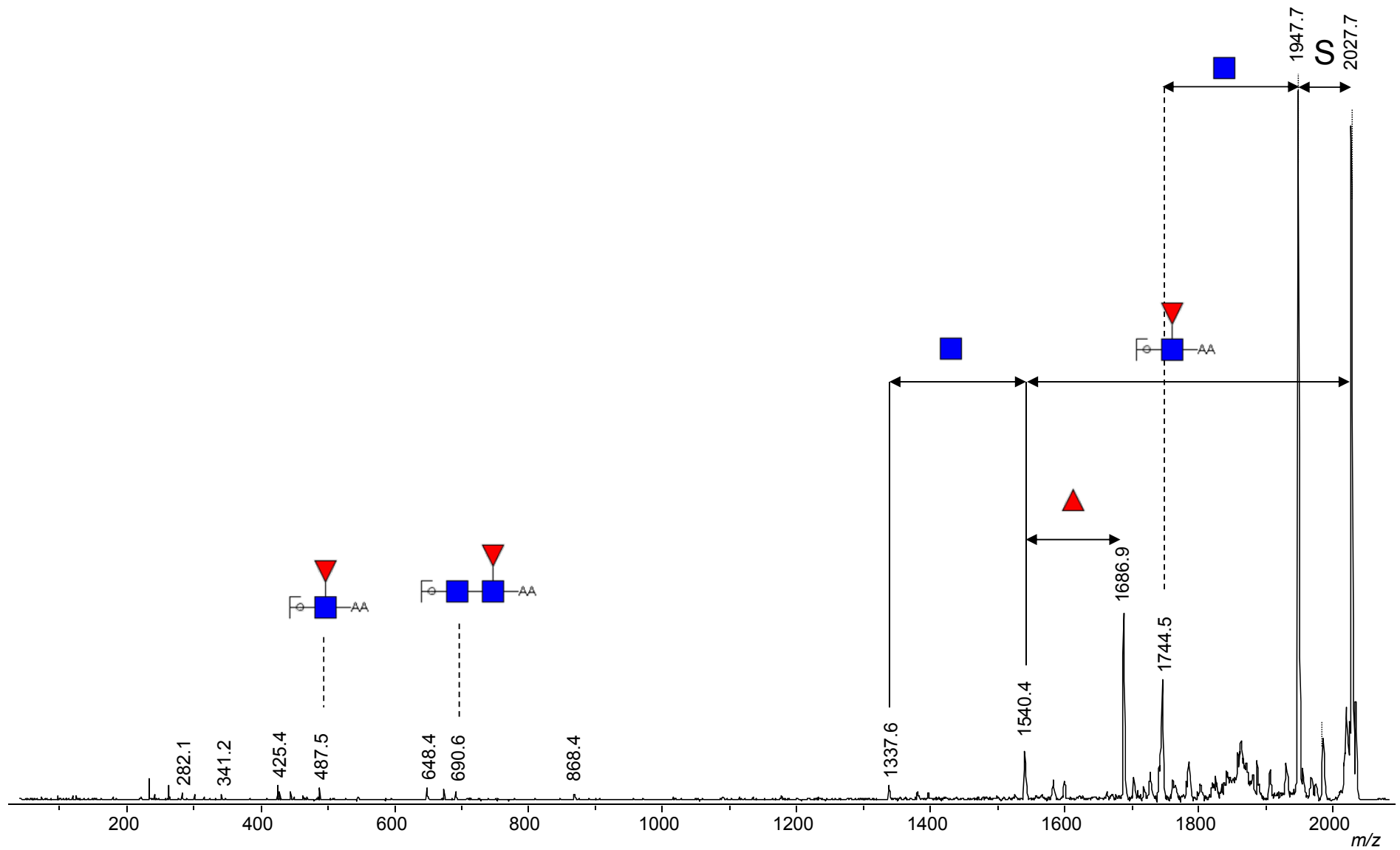


Project path: /N-glycans cancer/25147/comp_25147.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25147_02.d/comp_25147.mgf
Parent m/z: 1006.8641 2+ **Score:** 45.360
Composition: Hex6HexNAc3NeuAc1-AA **Intensity coverage [%]:** 0.50
Accession: 36319 **Fragment coverage [%]:** 0.41

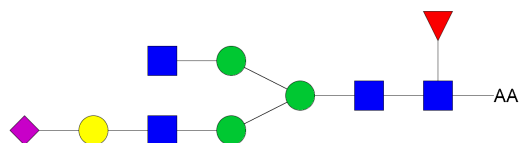


Spectrum 82

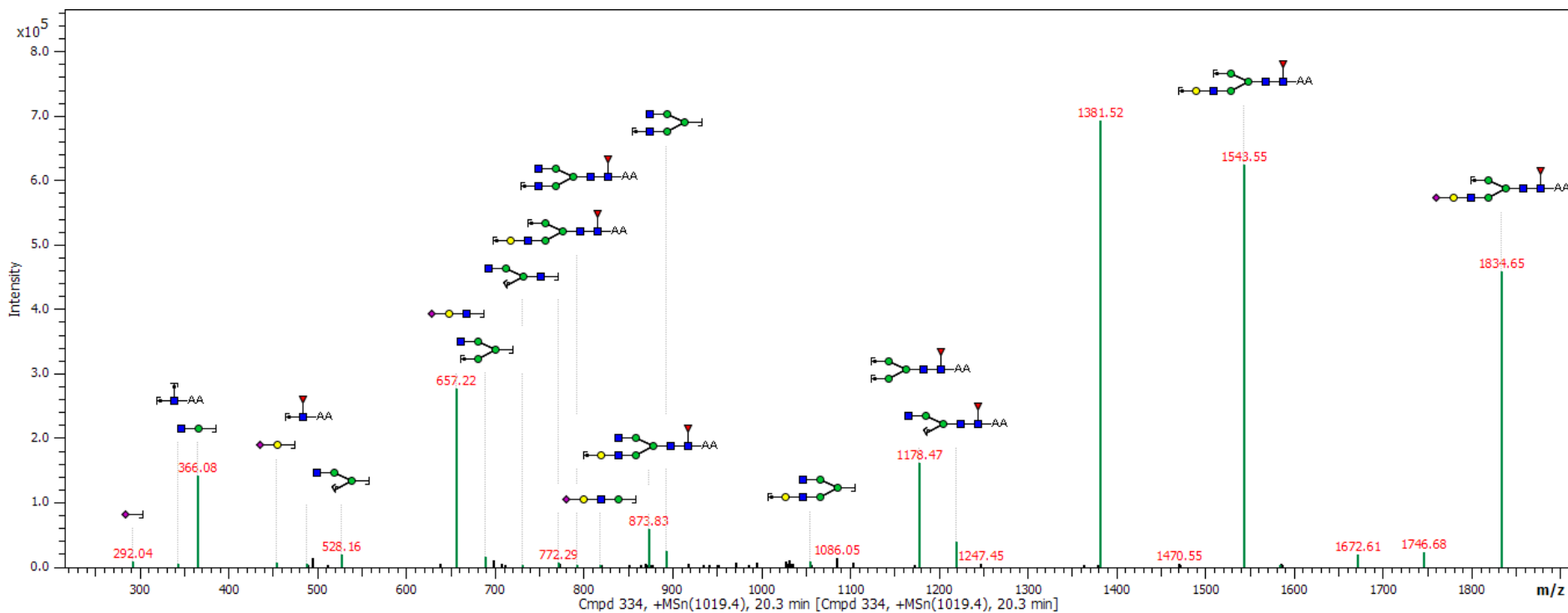
Lift of 2027.7 [M-H]⁻
S1dHex1Hex4HexNAc5-AA



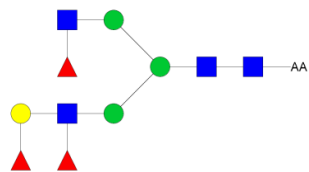
Glycan: 7



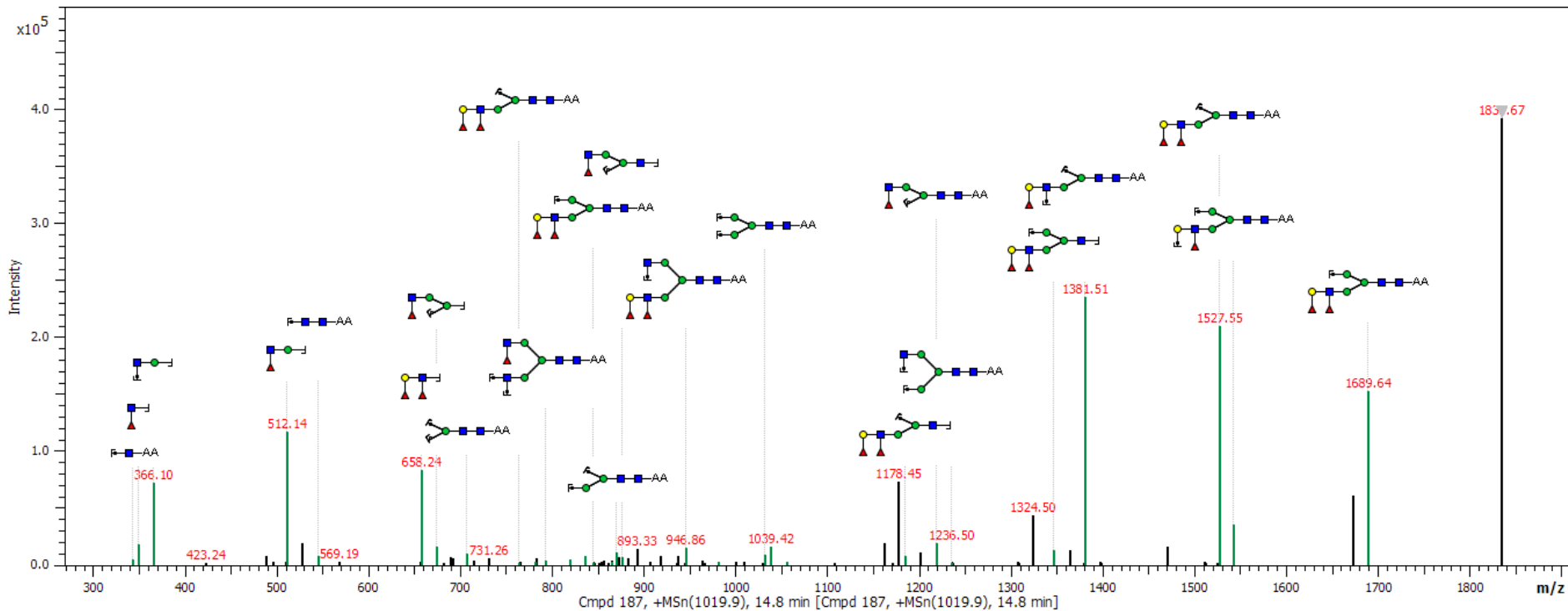
Project path: /N-glycans cancer/25145/comp_25145.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25145_02.d/comp_25145.mgf
Parent m/z: 1019.3800 2+ **Score:** 72.761
Composition: Hex4HexNAc4NeuAc1dHex1-AA **Intensity coverage [%]:** 0.94
Accession: 36235 **Fragment coverage [%]:** 0.57



Glycan: 23



Project path:	/N-glycans cancer/25147/comp_25147.mgf		
MS data:	K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25147_02.d/comp_25147.mgf		
Parent m/z:	1019.8902 2+	Score:	32.418
Composition:	Hex4HexNAc4dHex3-AA	Intensity coverage [%]:	0.57
Accession:	29221	Fragment coverage [%]:	0.18

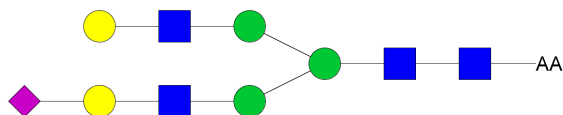




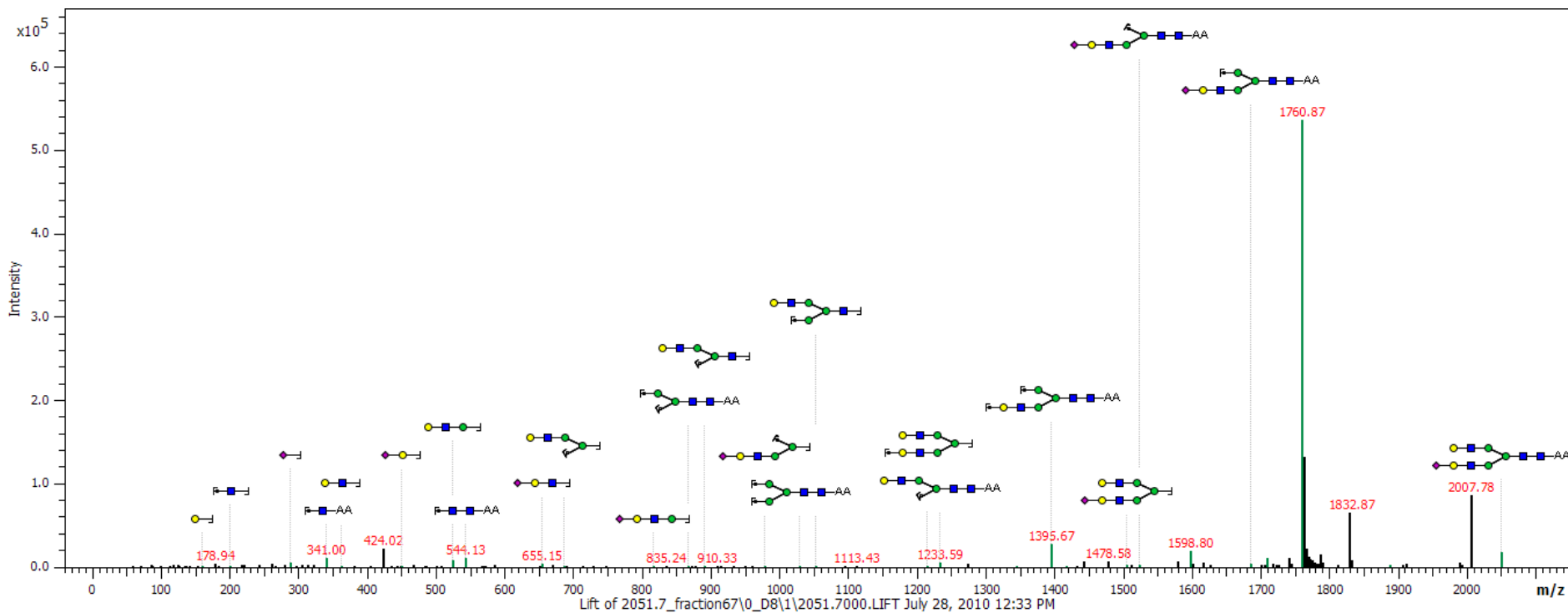
Spectrum 85

Glycan Search Report

Glycan: 1



Project path: /N-glycans cancer/Lift spectra/CombinedLIFT
MS data: c:/documents and settings/ciabalog/desktop/new folder/lift of 2051.7_fraction67/0_d8/1/2051.7000.lif/ 1sref/pdata/1/1r
Parent m/z: 2051.7330 -1 **Score:** 68.847
Composition: Hex5HexNAc4NeuAc1-AA **Intensity coverage [%]:** 0.56
Accession: 36355 **Fragment coverage [%]:** 0.84

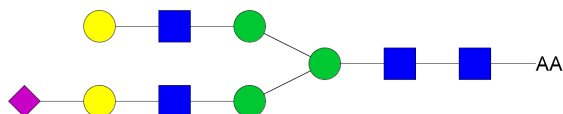




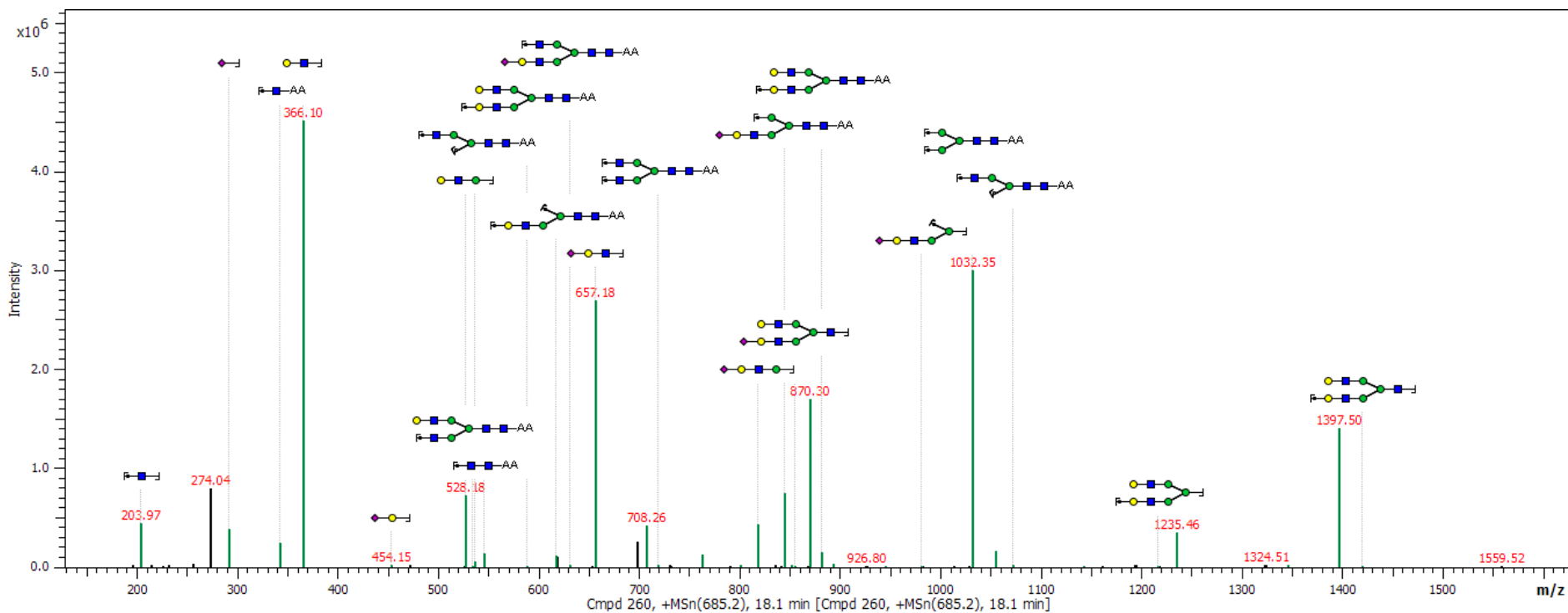
Spectrum 86

Glycan Search Report

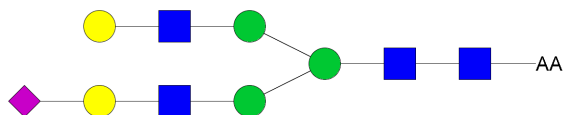
Glycan: 1



Project path: /N-glycans cancer/25147/comp_25147.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25147_02.d/comp_25147.mgf
Parent m/z: 685.2540 3+ **Score:** 96.069
Composition: Hex5HexNAc4NeuAc1-AA **Intensity coverage [%]:** 0.92
Accession: 36355 **Fragment coverage [%]:** 1.00



Glycan: 6



Project path: /N-glycans cancer/25143/comp_25143_01.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25143_01.d/comp_25143_01.mgf

Parent m/z: 1027.3774 2+

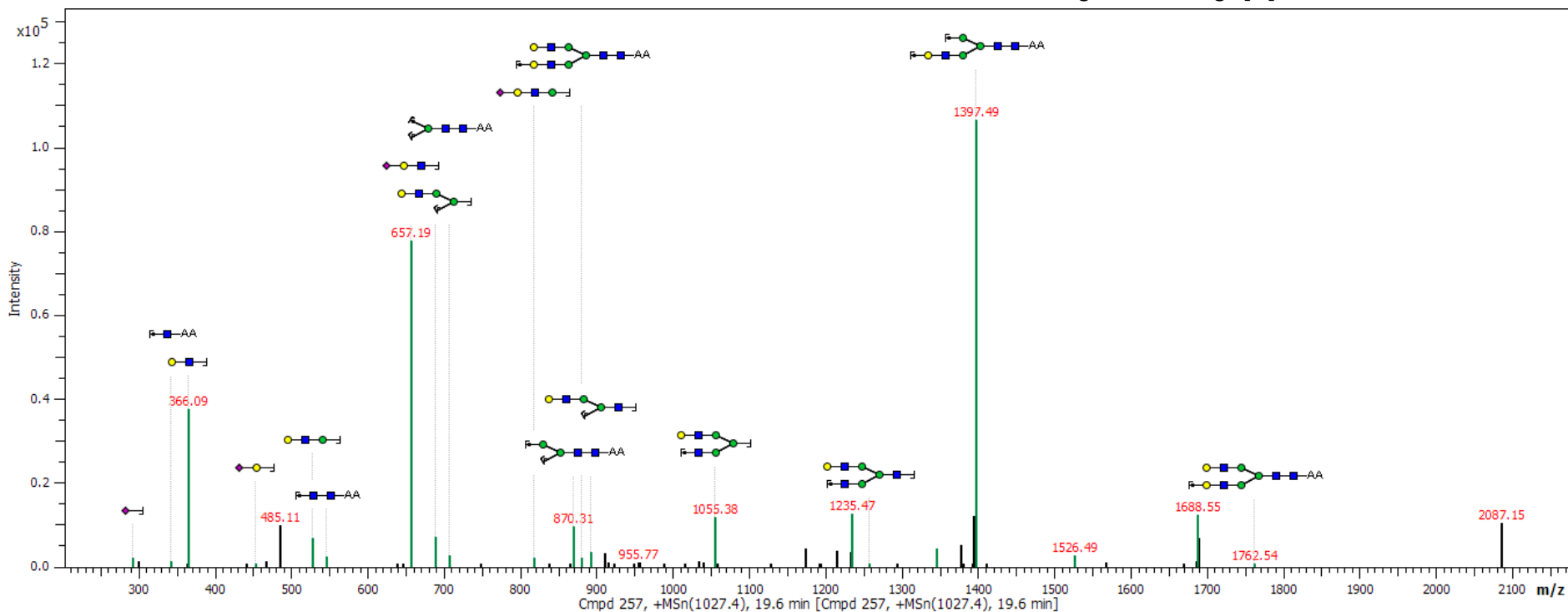
Score: 67.794

Composition: Hex5HexNAc4NeuAc1-AA

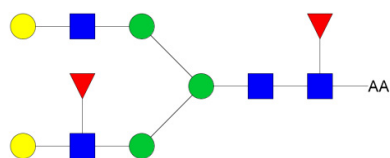
Intensity coverage [%]: 0.77

Accession: 36355

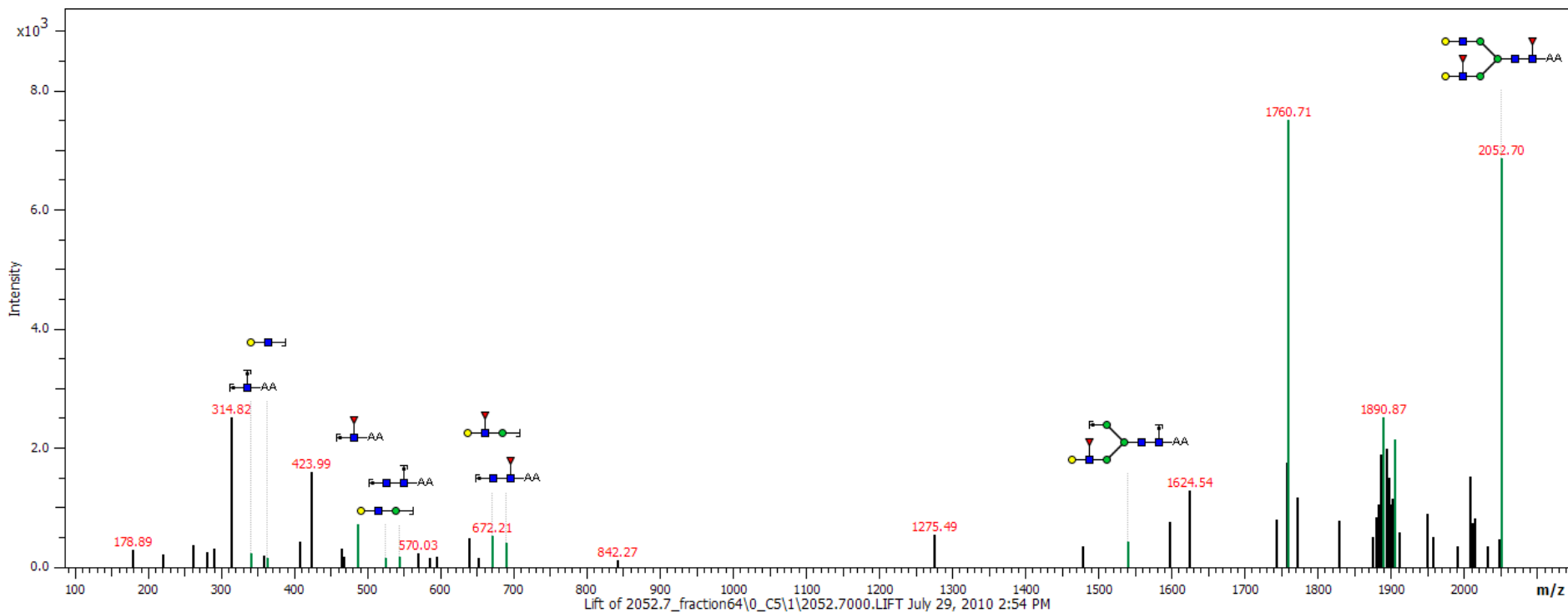
Fragment coverage [%]: 0.60



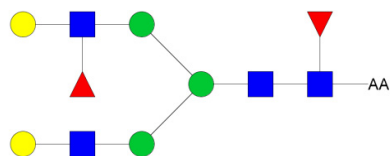
Glycan: 12



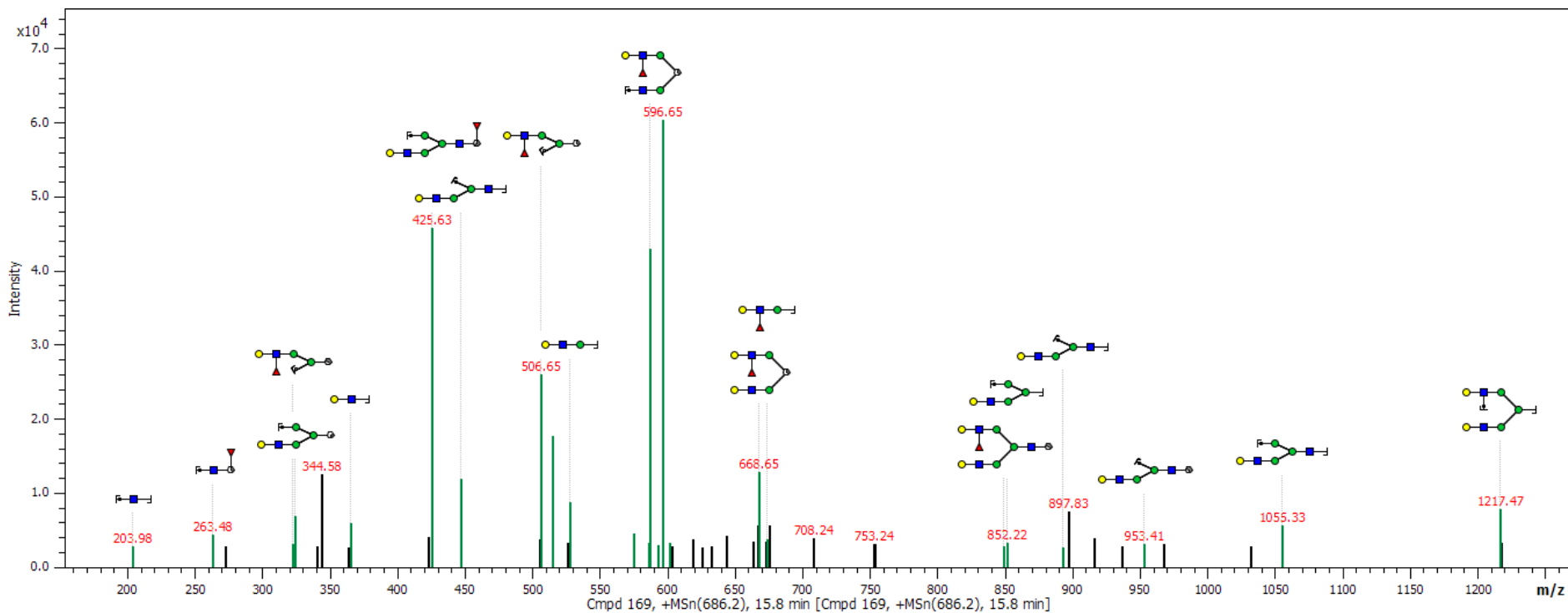
Project path:	/N-glycans cancer/Lift spectra/CombinedLIFT		
MS data:	c:/documents and settings/ciabalog/desktop/new folder/lift of 2052.7_fraction64/0_c5/1/2052.7000.lif/ 1sref/pdata/1/1r		
Parent m/z:	2052.7534 -1	Score:	35.486
Composition:	Hex5HexNAc4dHex2-AA	Intensity coverage [%]:	0.41
Accession:	36267	Fragment coverage [%]:	0.31



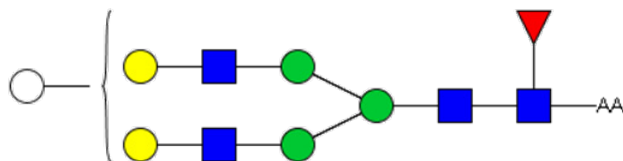
Glycan: 9



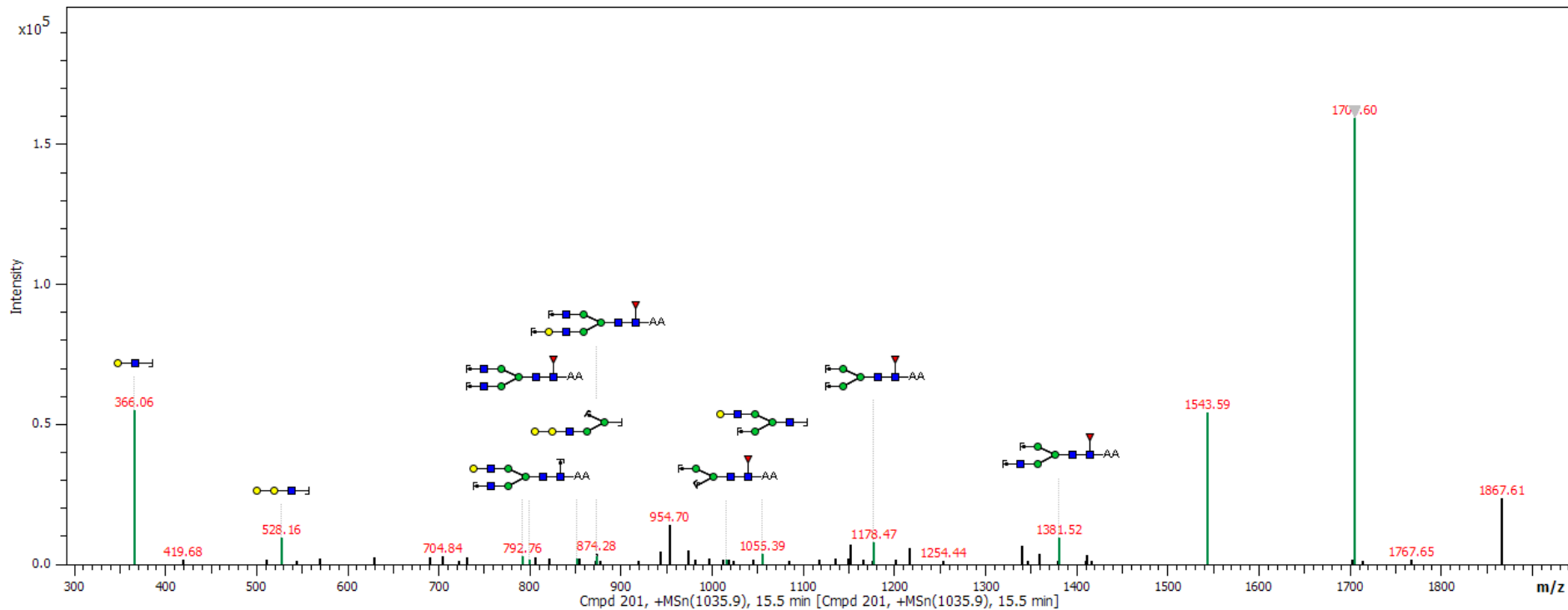
Project path:	/N-glycans cancer/25142/comp_25142_01.mgf		
MS data:	K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25142_01.d/comp_25142_01.mgf		
Parent m/z:	685.5942	3+	Score: 34.192
Composition:	Hex5HexNAc4dHex2-AA		Intensity coverage [%]: 0.74
Accession:	8659		Fragment coverage [%]: 0.16



Glycan: 5



Project path:	/N-glycans cancer/25147/comp_25147.mgf	Score:	56.983
MS data:	K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25147_02.d/comp_25147.mgf	Intensity coverage [%]:	0.71
Parent m/z:	1035.8851 2+	Fragment coverage [%]:	0.46
Composition:	Hex6HexNAc4dHex1-AA		
Accession:	36271		

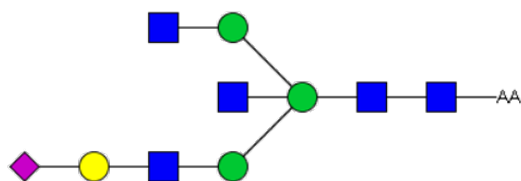




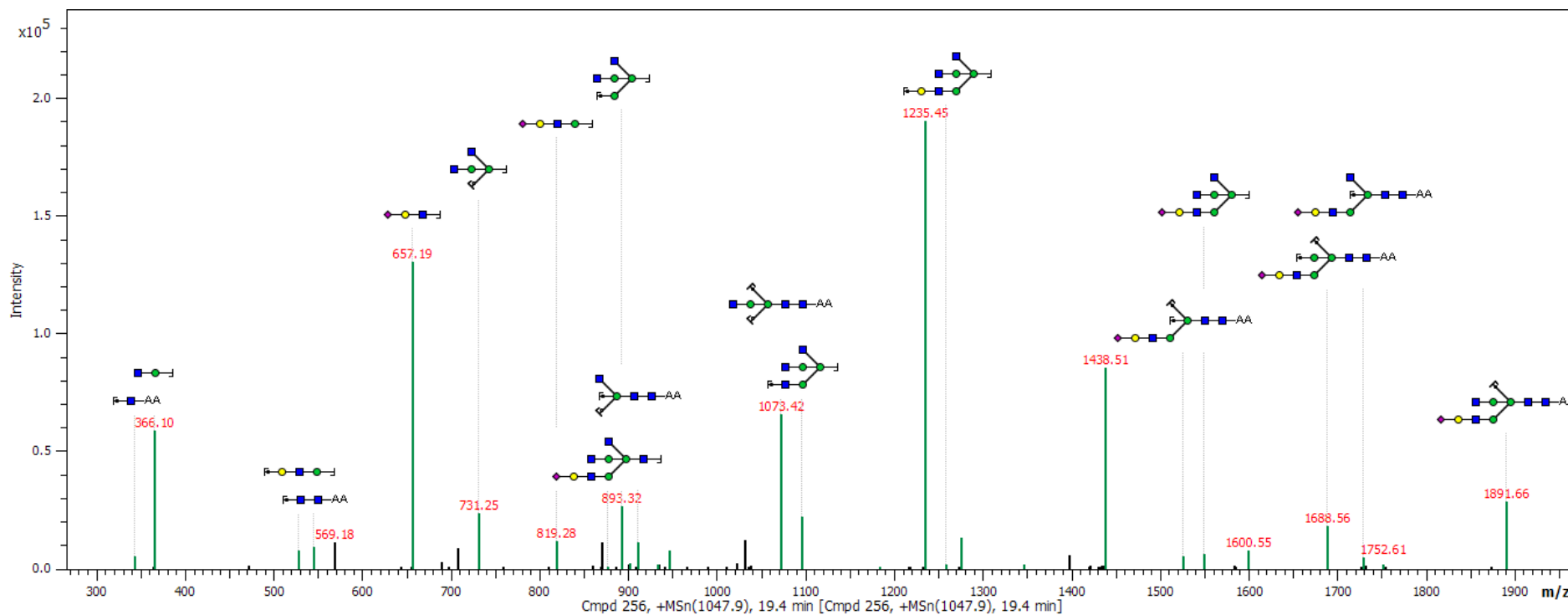
Spectrum 90

Glycan Search Report

Glycan: 3



Project path: /N-glycans cancer/25143/comp_25143_01.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25143_01.d/comp_25143_01.mgf
Parent m/z: 1047.8907 2+ **Score:** 86.017
Composition: Hex4HexNAc5NeuAc1-AA **Intensity coverage [%]:** 0.89
Accession: 36342 **Fragment coverage [%]:** 0.83

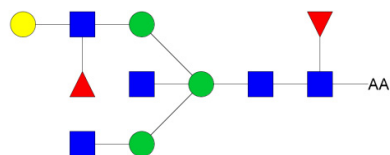




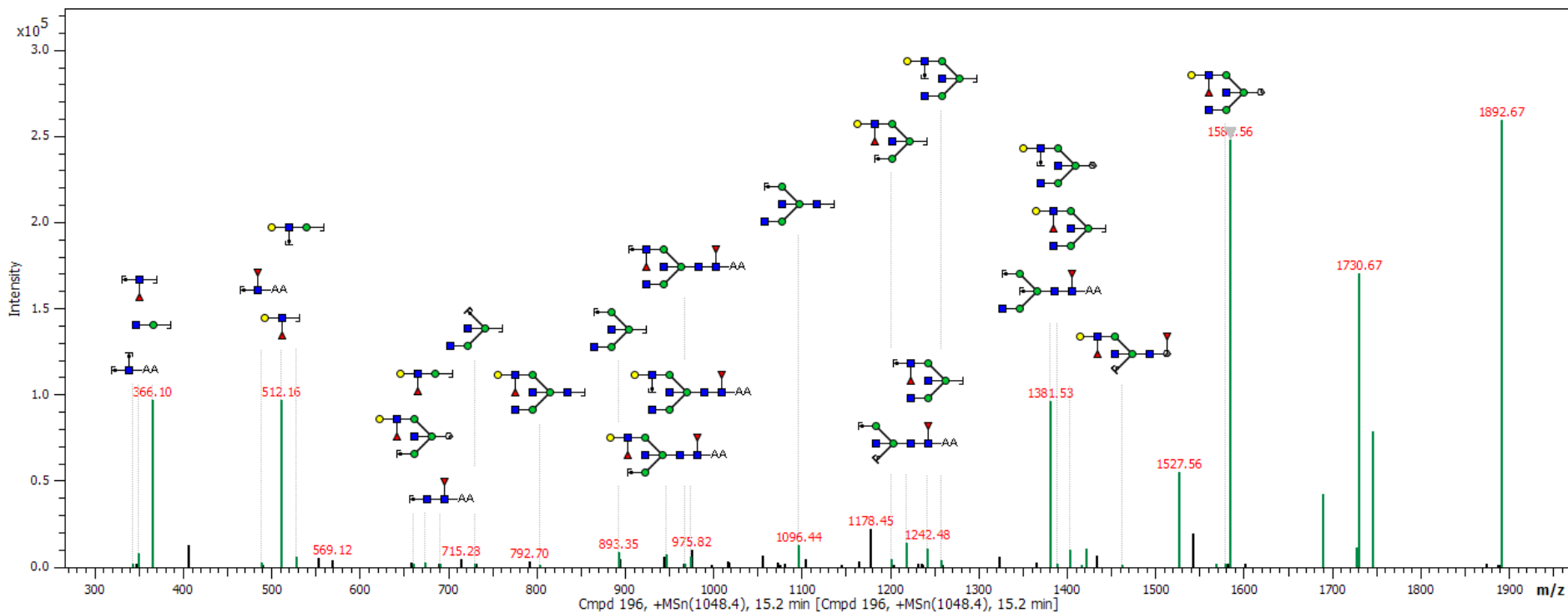
Spectrum 91

Glycan Search Report

Glycan: 9



Project path: /N-glycans cancer/25147/comp_25147.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25147_02.d/comp_25147.mgf
Parent m/z: 1048.4009 2+ **Score:** 48.304
Composition: Hex4HexNAc5dHex2-AA **Intensity coverage [%]:** 0.89
Accession: 5779 **Fragment coverage [%]:** 0.26

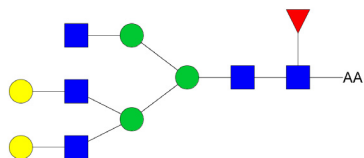




Spectrum 92

Glycan Search Report

Glycan: 10



Project path: /N-glycans cancer/25143/comp_25143_01.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25143_01.d/comp_25143_01.mgf

Parent m/z: 1056.3984 2+

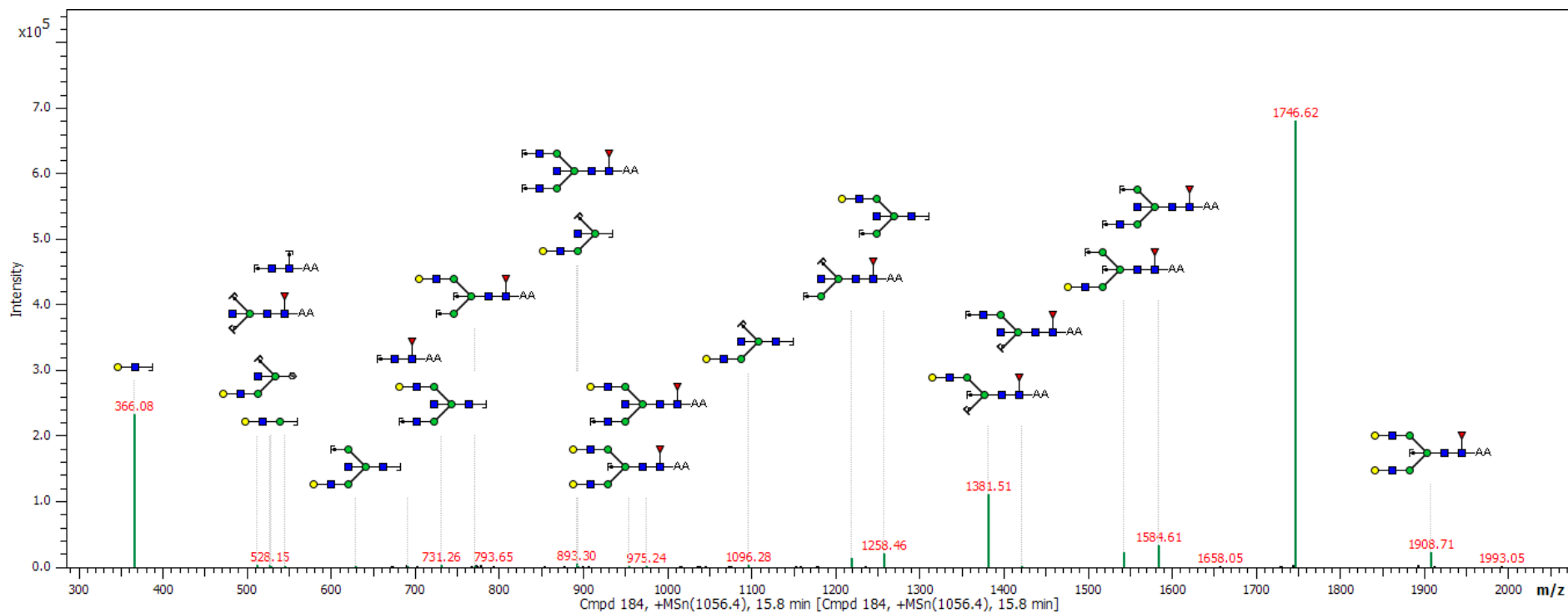
Score: 54.093

Composition: Hex5HexNAc5dHex1-AA

Intensity coverage [%]: 0.97

Accession: 1043

Fragment coverage [%]: 0.30

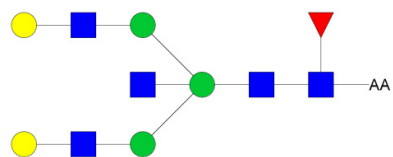




Spectrum 93

Glycan Search Report

Glycan: 4



Project path: /N-glycans cancer/25147/comp_25147.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25147_02.d/comp_25147.mgf

Parent m/z: 1056.3984 2+

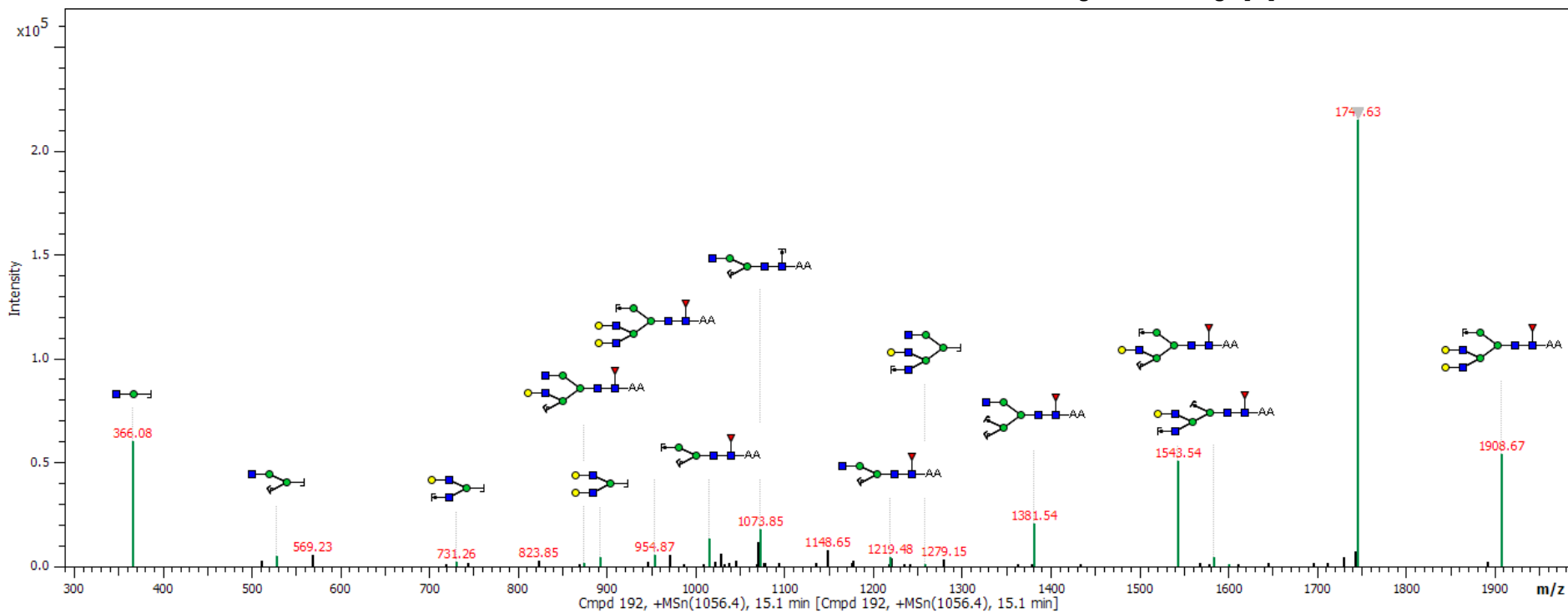
Score: 70.399

Composition: Hex5HexNAc5dHex1-AA

Intensity coverage [%]: 0.82

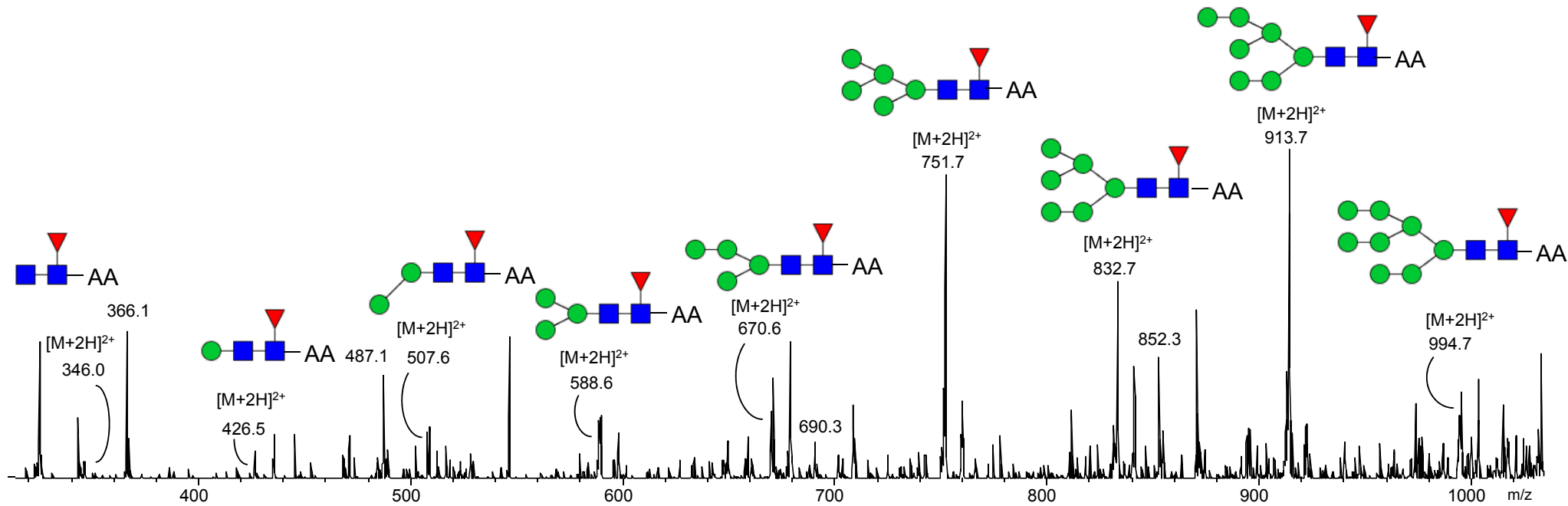
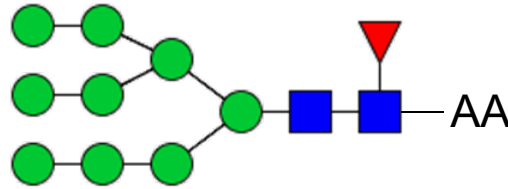
Accession: 36372

Fragment coverage [%]: 0.60



Spectrum 94

ESI MS/MS of $[1075.6 + 2H]^{2+}$

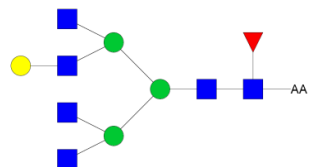




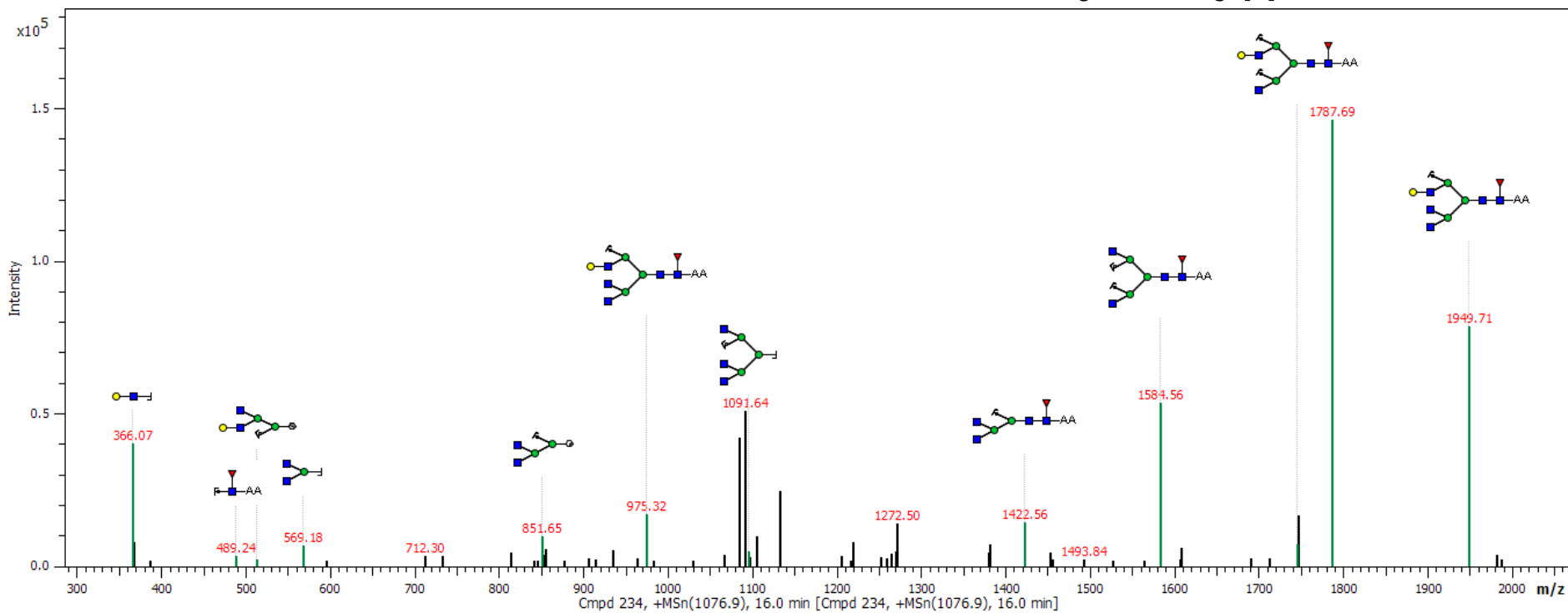
Spectrum 95

Glycan Search Report

Glycan: 20



Project path: /N-glycans cancer/25145/comp_25145.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25145_02.d/comp_25145.mgf
Parent m/z: 1076.9117 2+ **Score:** 31.327
Composition: Hex4HexNAc6dHex1-AA **Intensity coverage [%]:** 0.57
Accession: 566 **Fragment coverage [%]:** 0.17

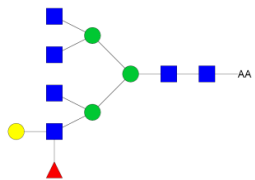


Spectrum 96

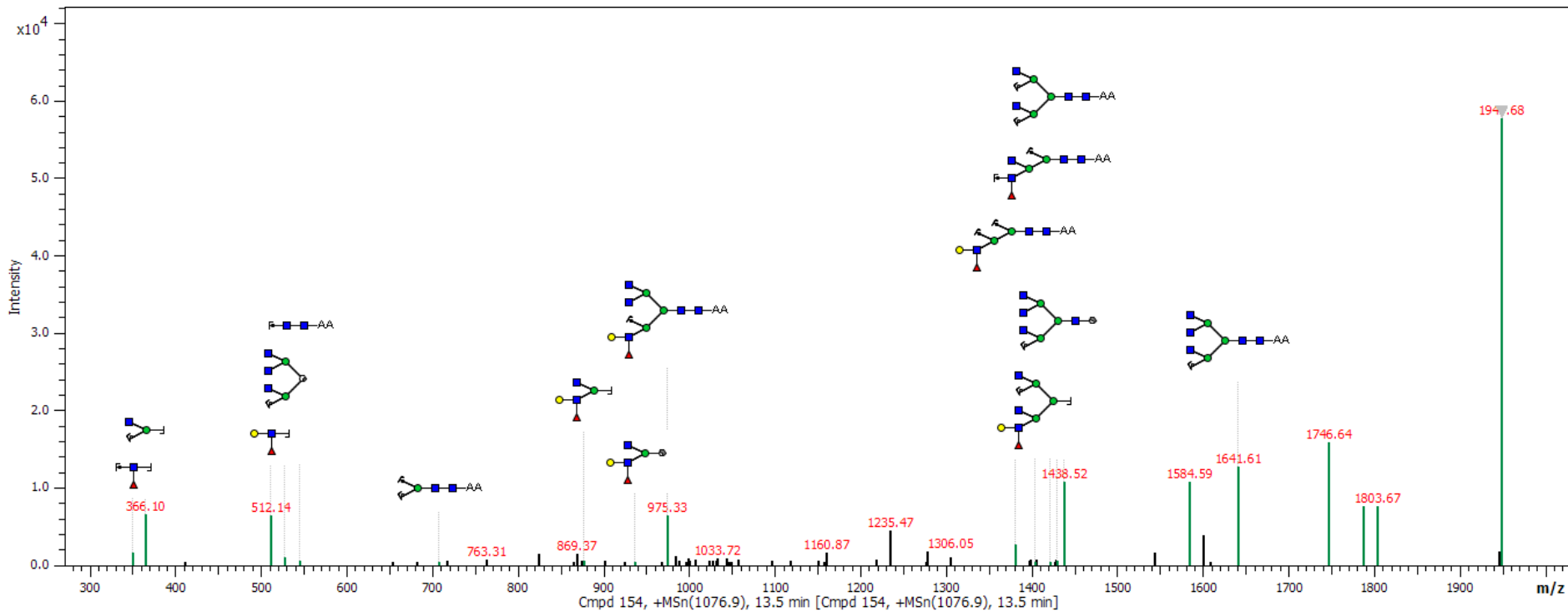


Glycan Search Report

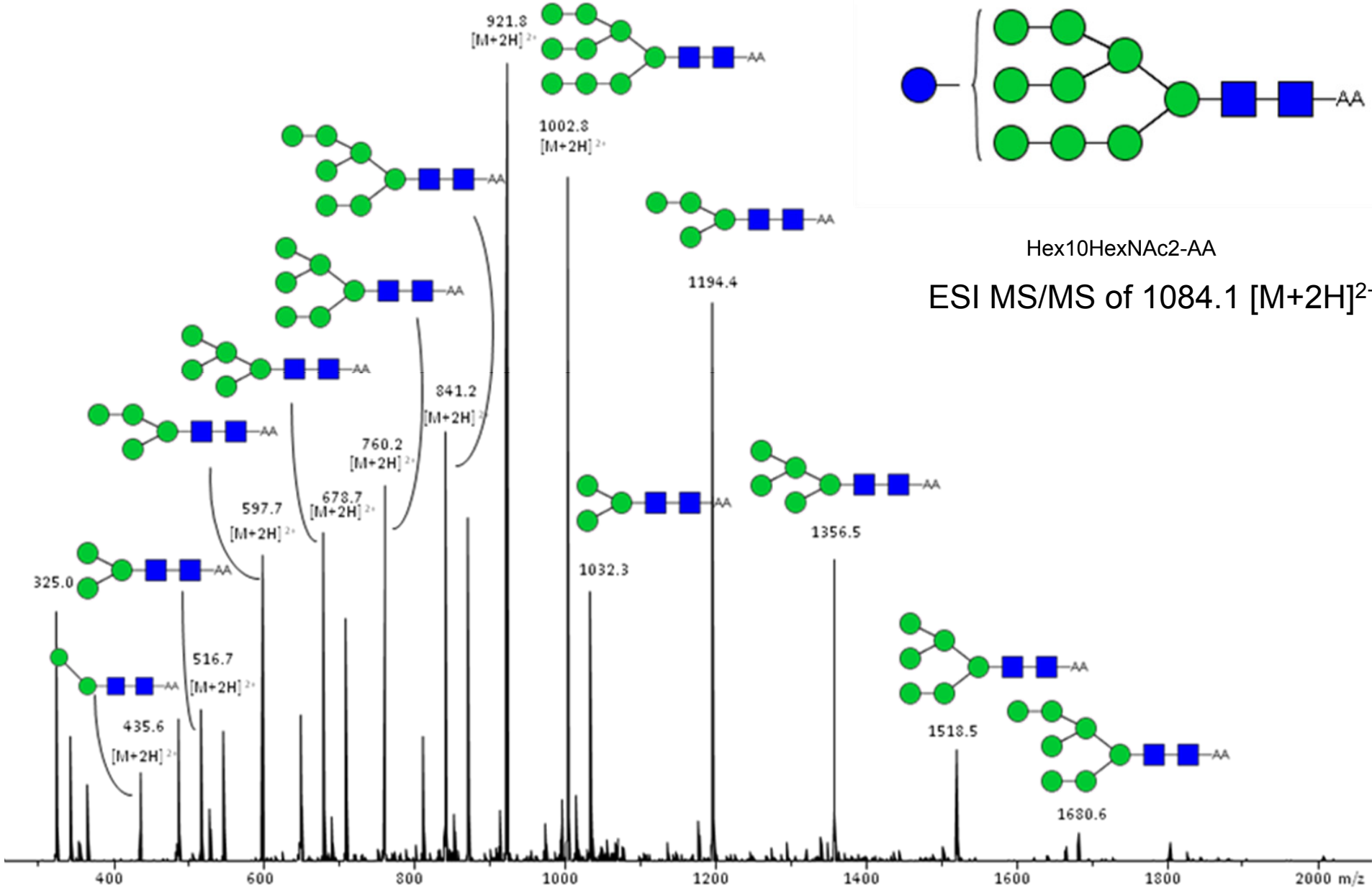
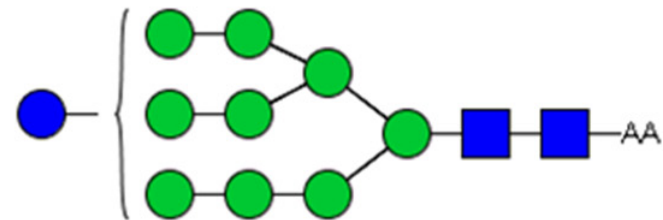
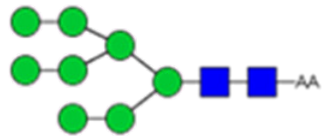
Glycan: 22



Project path: /N-glycans cancer/25147/comp_25147.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25147_02.d/comp_25147.mgf
Parent m/z: 1076.9117 2+ **Score:** 34.428
Composition: Hex4HexNAc6dHex1-AA **Intensity coverage [%]:** 0.79
Accession: 30044 **Fragment coverage [%]:** 0.15



Spectrum 97



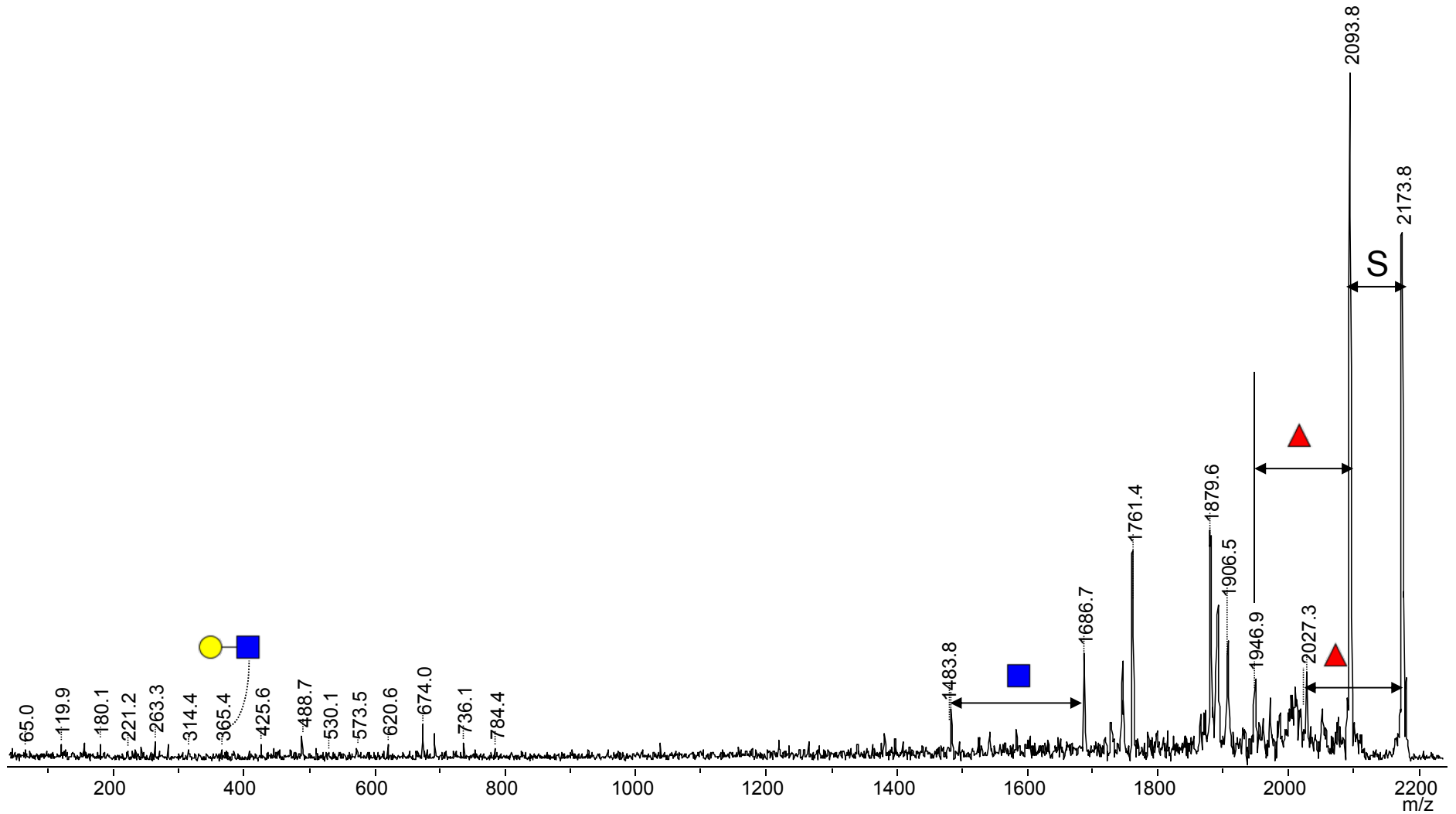
Hex10HexNAc2-AA

ESI MS/MS of 1084.1 $[M+2H]^{2+}$

Spectrum 98

Lift of 2173.8 [M-H]⁻

S1dHex2Hex4HexNAc5-AA

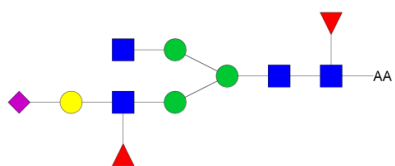


Spectrum 99



Glycan Search Report

Glycan: 22



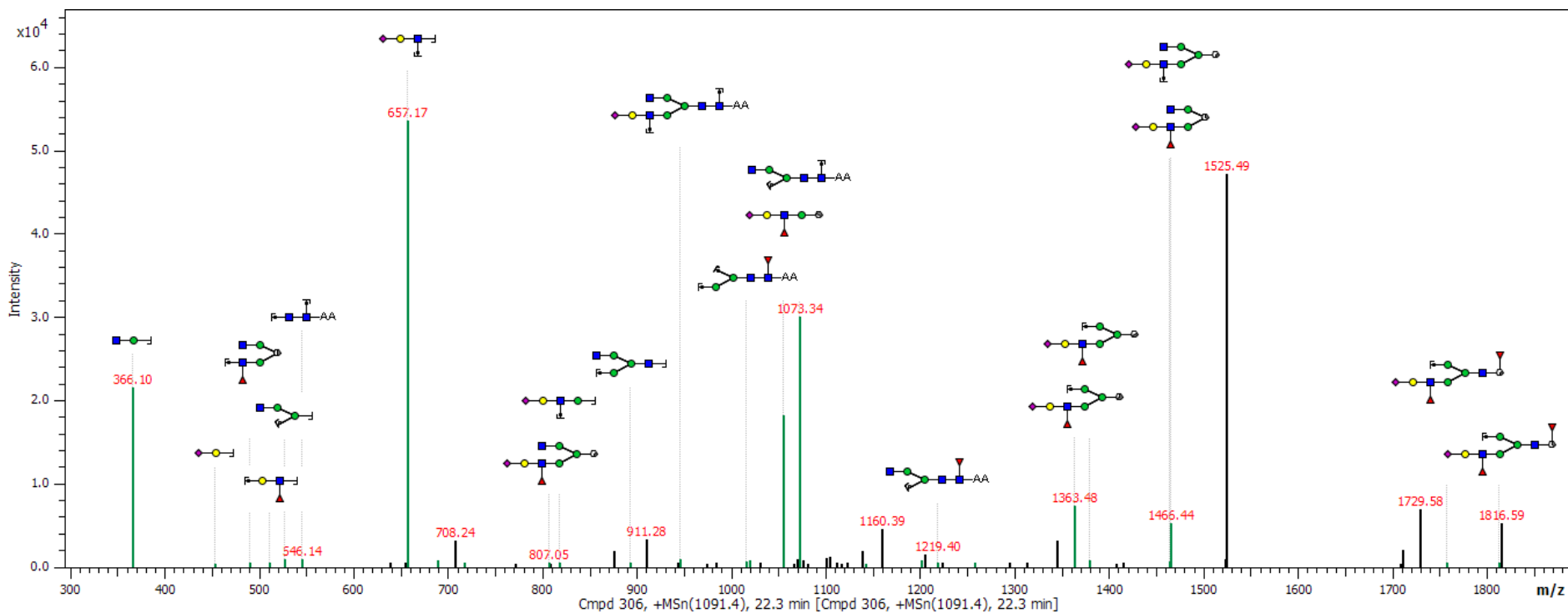
Project path: /N-glycans cancer/25143/comp_25143_01.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25143_01.d/comp_25143_01.mgf

Parent m/z: 1092.4089 2+ **Score:** 32.026

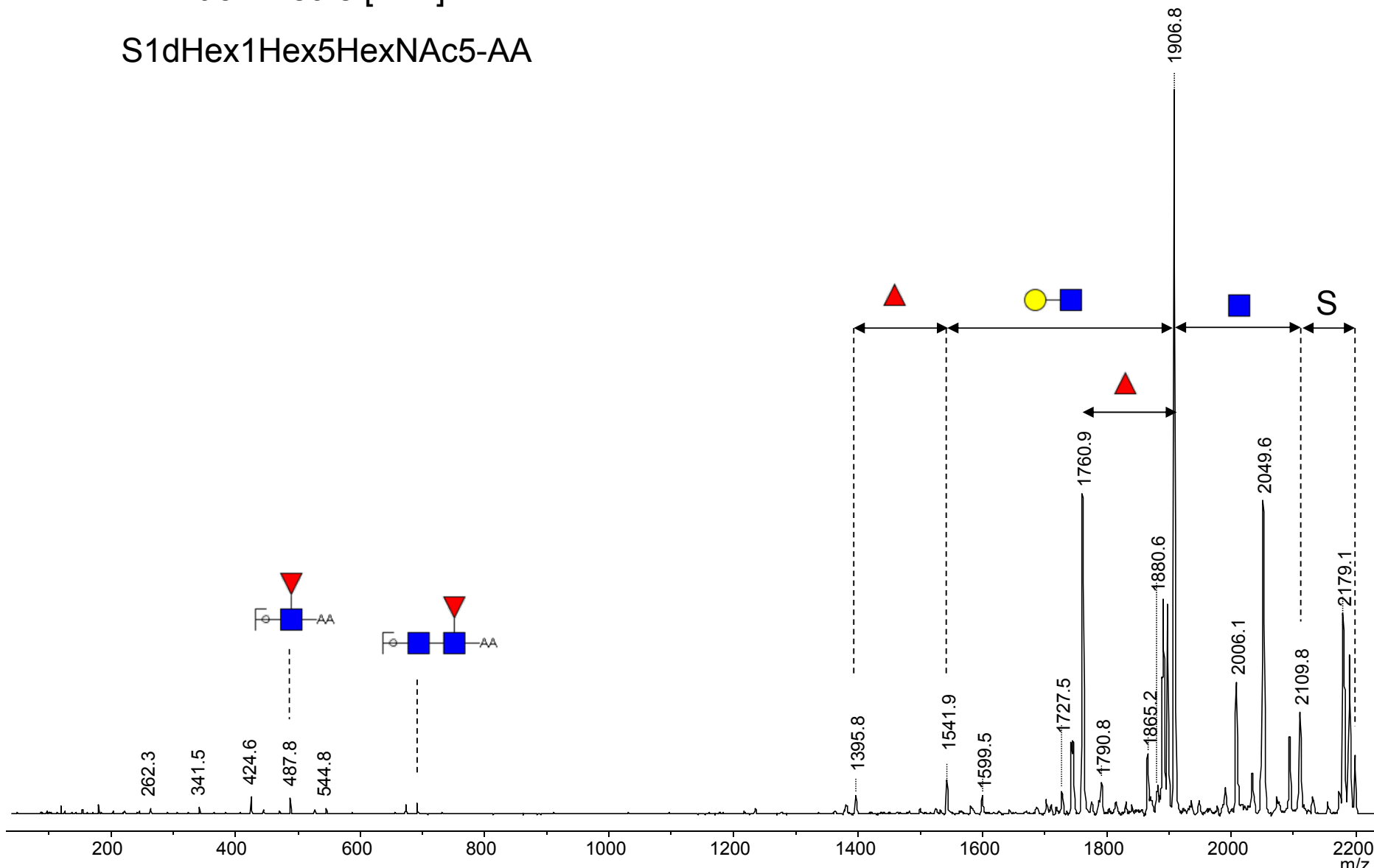
Composition: Hex4HexNAc4NeuAc1dHex2-AA **Intensity coverage [%]:** 0.61

Accession: 29191 **Fragment coverage [%]:** 0.17



Spectrum 100

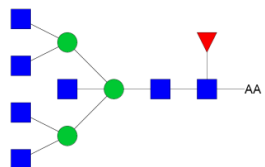
Lift of 2189.8 [M-H]⁻
S1dHex1Hex5HexNAc5-AA



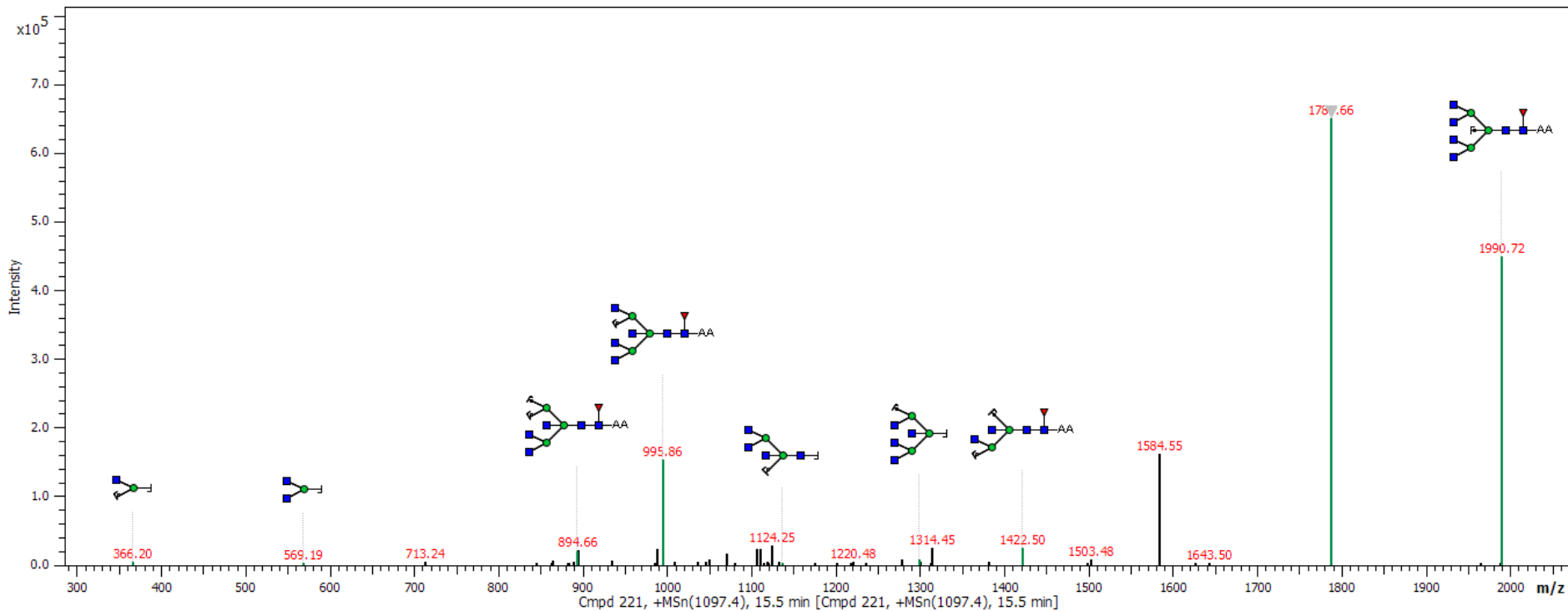


Glycan Search Report

Glycan: 15



Project path:	/N-glycans cancer/25145/comp_25145.mgf		
MS data:	K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25145_02.d/comp_25145.mgf		
Parent m/z:	1097.4250 2+	Score:	47.190
Composition:	Hex3HexNAc7dHex1-AA	Intensity coverage [%]:	0.74
Accession:	3033	Fragment coverage [%]:	0.30

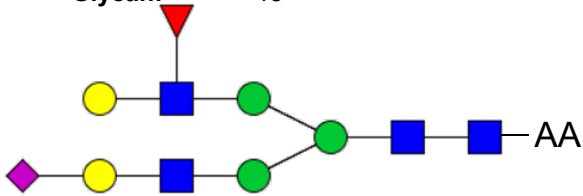


Spectrum 102

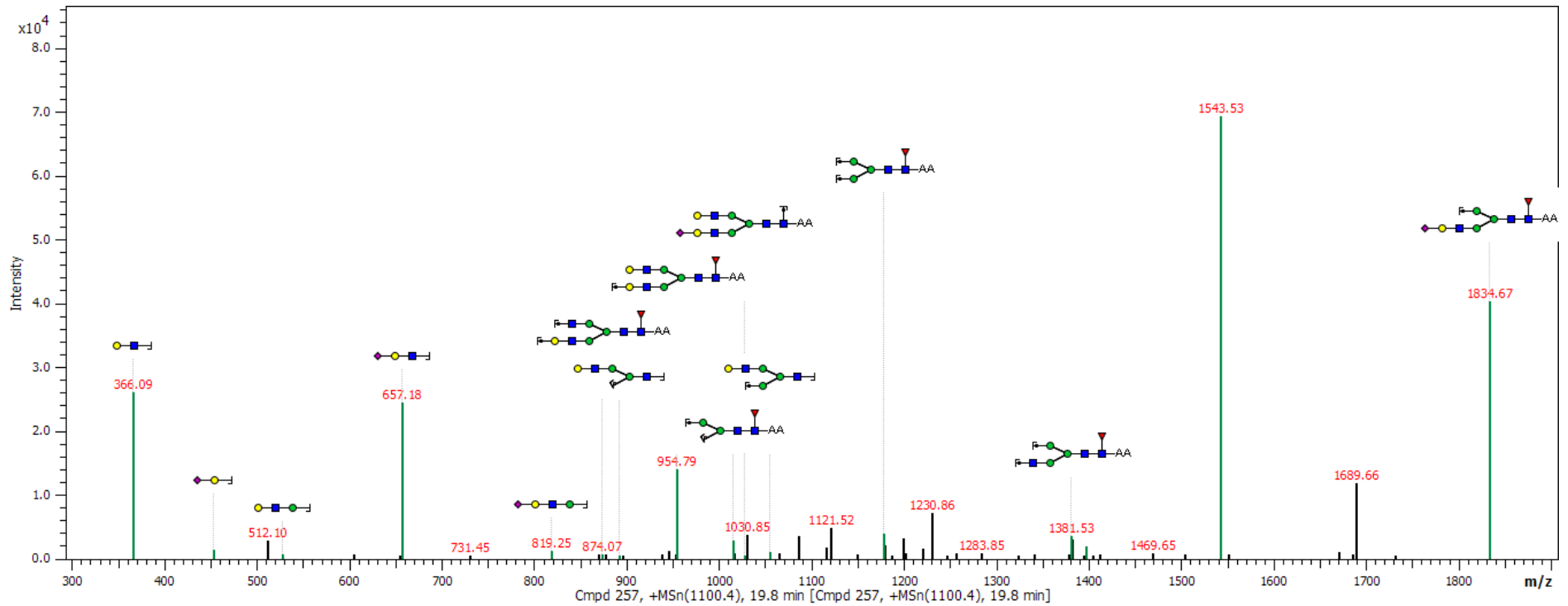


Glycan Search Report

Glycan: 18



Project path: /N-glycans cancer/25148/comp_25148.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf
Parent m/z: 1100.4064 2+ **Score:** 57.543
Composition: Hex5HexNAc4NeuAc1dHex1-AA **Intensity coverage [%]:** 0.75
Accession: **Fragment coverage [%]:** 0.44

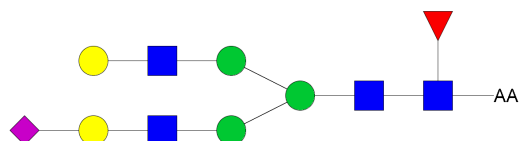




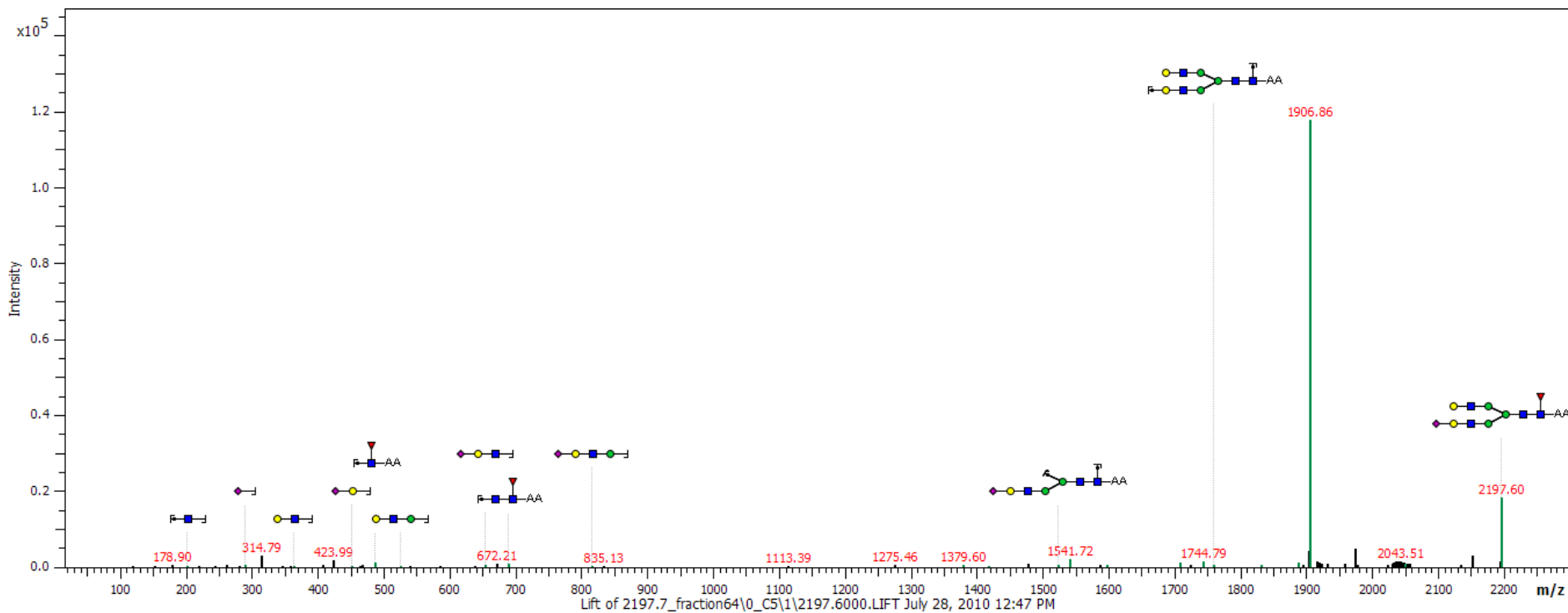
Spectrum 103

Glycan Search Report

Glycan: 3



Project path: /N-glycans cancer/Lift spectra/CombinedLIFT
MS data: c:/documents and settings/ciabalog/desktop/new folder/lift of 2197.7_fraction64/0_c5/1/2197.6000.lift/ 1sref/pdata/1/1r
Parent m/z: 2197.7909 -1 **Score:** 63.053
Composition: Hex5HexNAc4NeuAc1dHex1-AA **Intensity coverage [%]:** 0.78
Accession: 36273 **Fragment coverage [%]:** 0.51

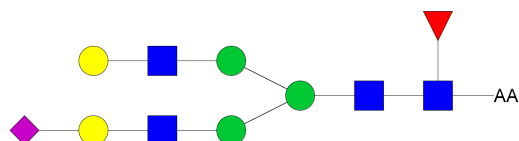


Spectrum 104

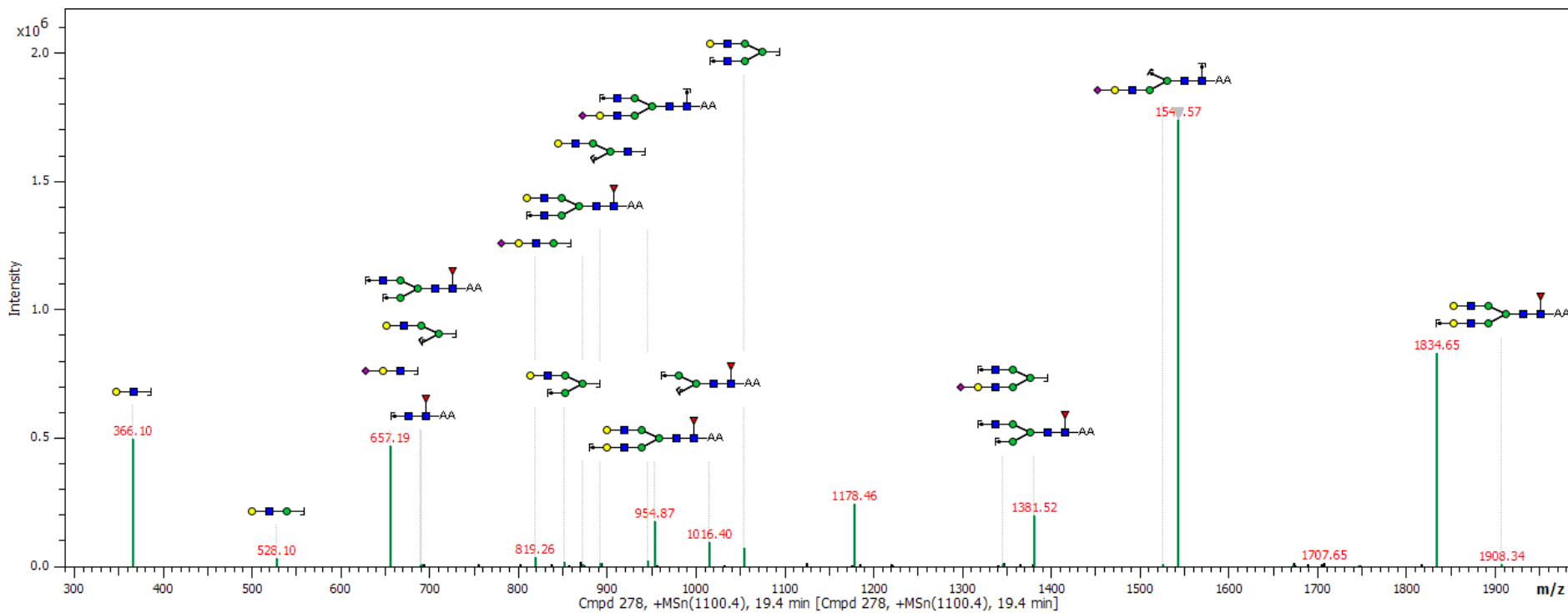


Glycan Search Report

Glycan: 2



Project path: /N-glycans cancer/25147/comp_25147.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25147_02.d/comp_25147.mgf
Parent m/z: 1100.4064 2+ **Score:** 76.225
Composition: Hex5HexNAc4NeuAc1dHex1-AA **Intensity coverage [%]:** 0.96
Accession: 36273 **Fragment coverage [%]:** 0.61

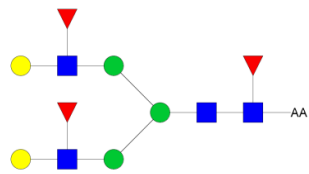


Spectrum 105



Glycan Search Report

Glycan: 5



Project path: /N-glycans cancer/Lift spectra/CombinedLIFT

MS data: c:/documents and settings/ciabalog/desktop/new folder/lift of 2198.7_fraction68/0_c9/1/2198.7000.lift/1sref/pdata/1/1r

Parent m/z: 2198.8113 -1

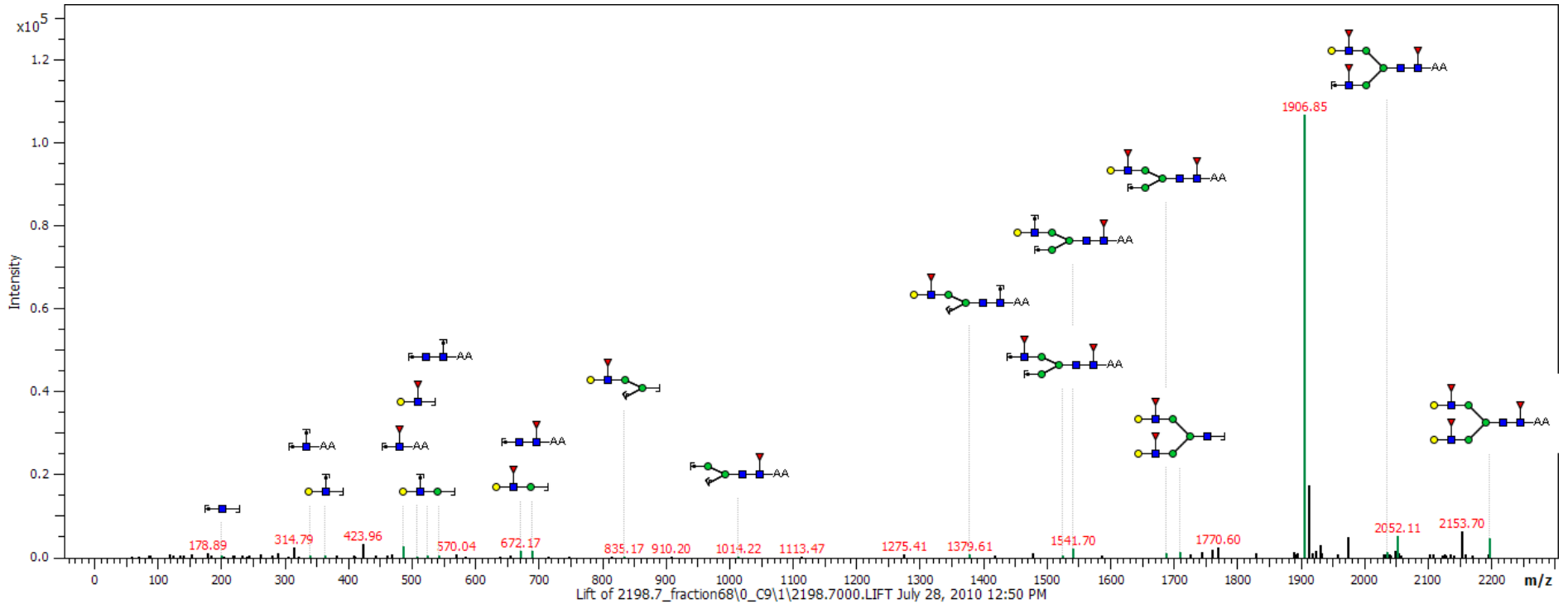
Score: 60.225

Composition: Hex5HexNAc4dHex3-AA

Intensity coverage [%]: 0.63

Accession: 36245

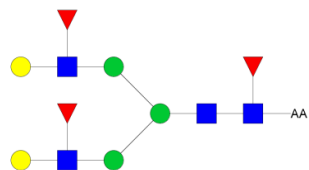
Fragment coverage [%]: 0.58



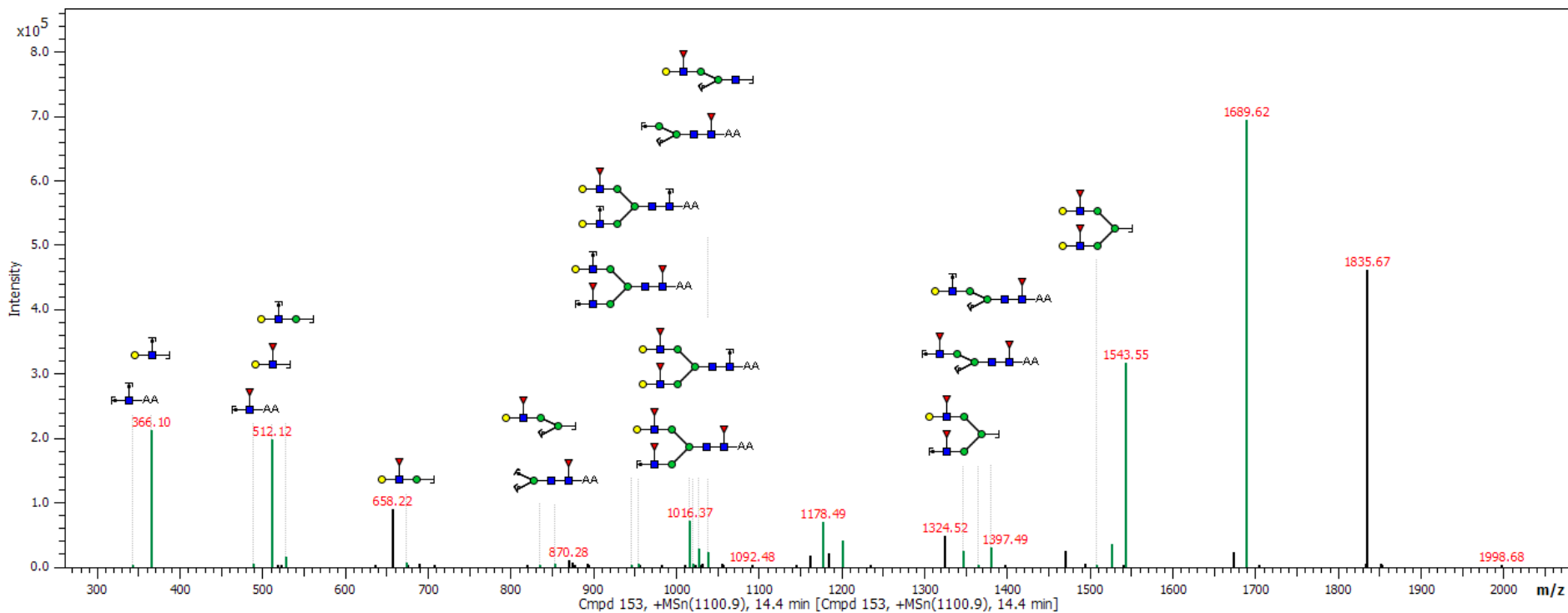


Glycan Search Report

Glycan: 12

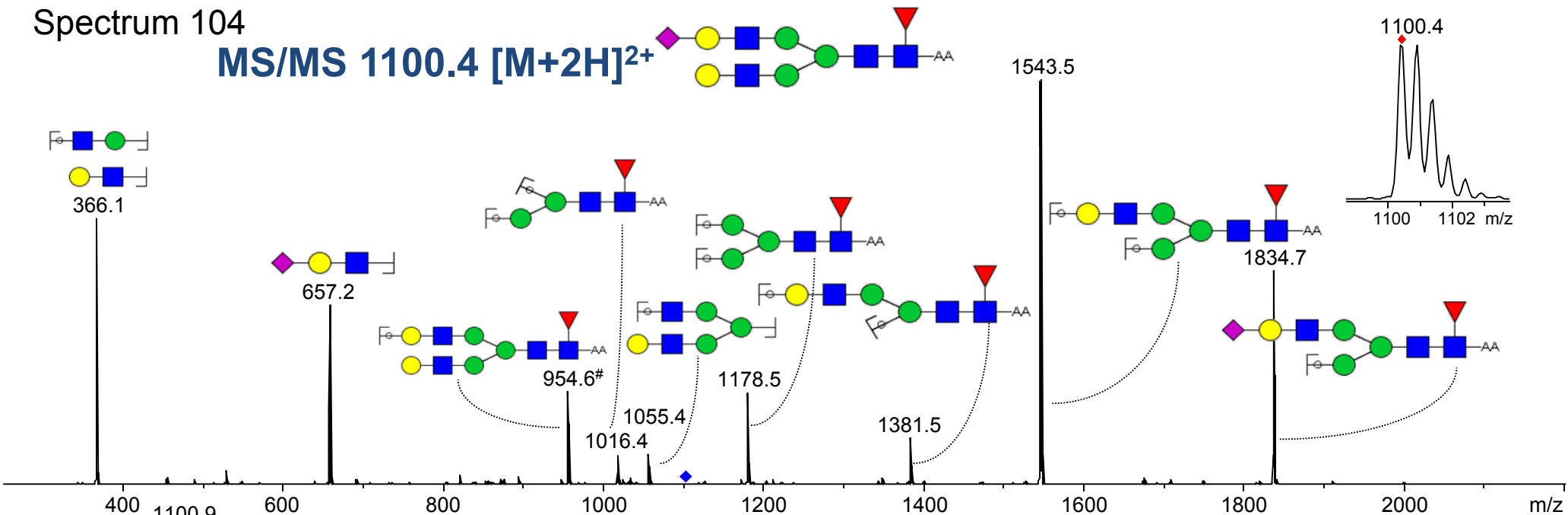


Project path: /N-glycans cancer/25148/comp_25148.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf
Parent m/z: 1100.9166 2+ **Score:** 69.786
Composition: Hex5HexNAc4dHex3-AA **Intensity coverage [%]:** 0.68
Accession: 36245 **Fragment coverage [%]:** 0.71

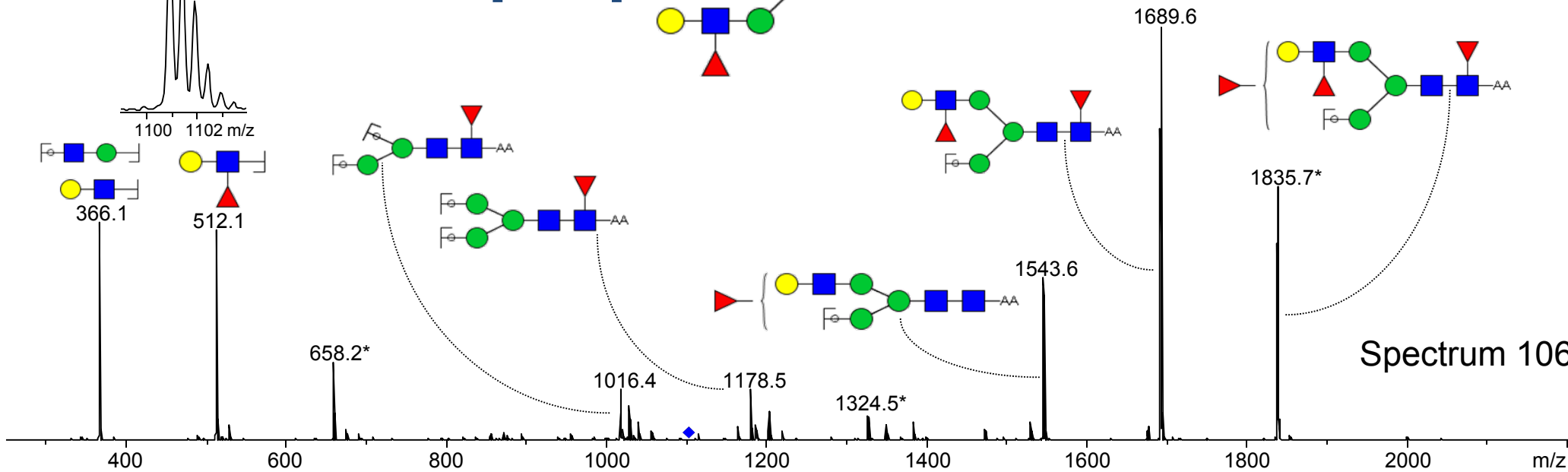


Spectrum 104

MS/MS 1100.4 [M+2H]²⁺



MS/MS 1100.9 [M+2H]²⁺



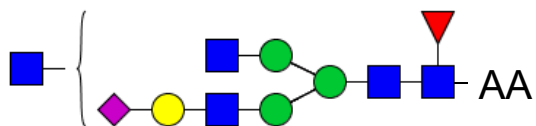
Spectrum 106



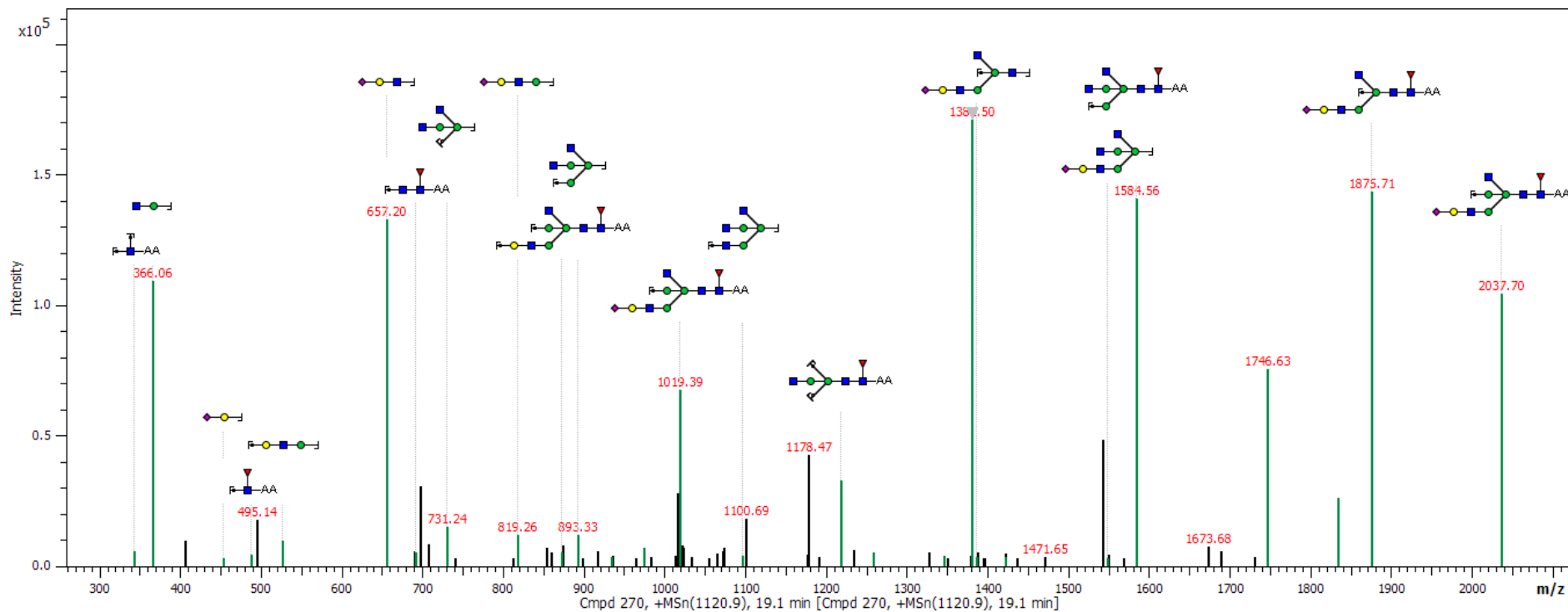
Spectrum 107

Glycan Search Report

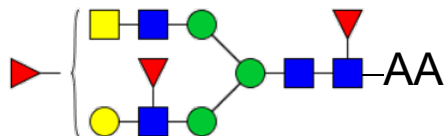
Glycan: 3



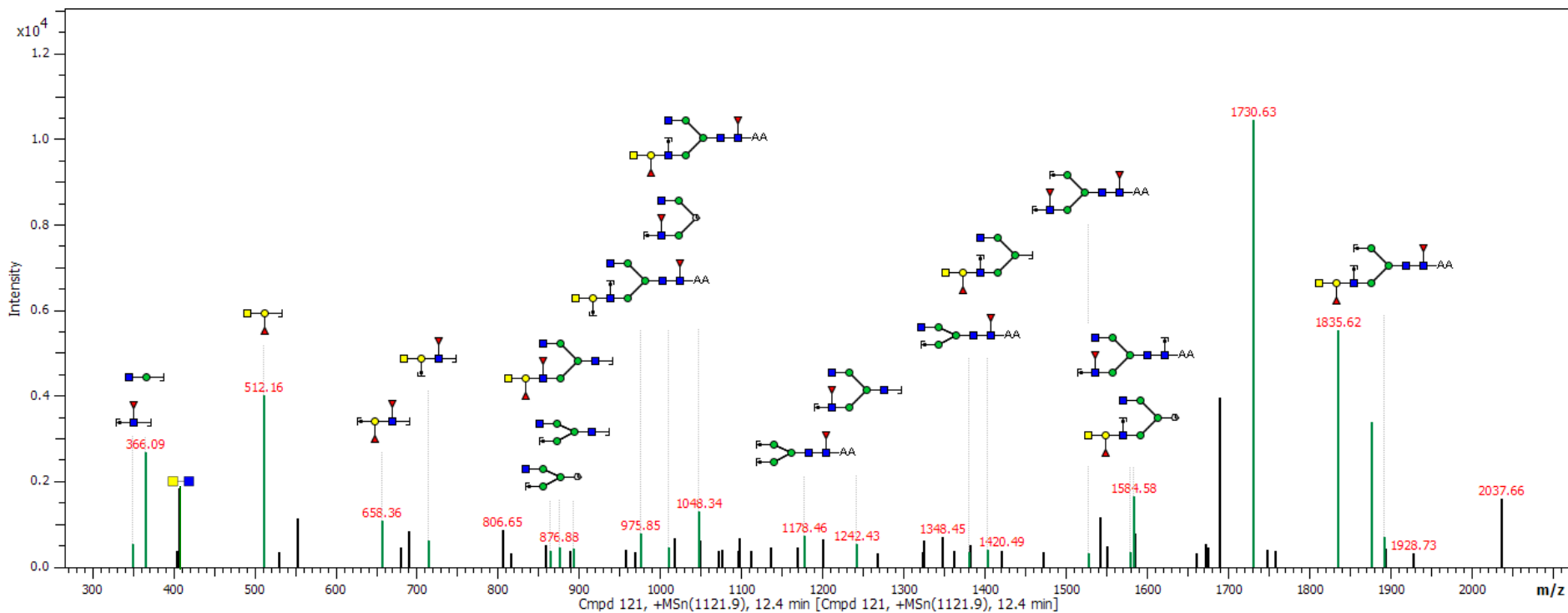
Project path: /N-glycans cancer/25147/comp_25147.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25147_02.d/comp_25147.mgf
Parent m/z: 1120.9197 2+ **Score:** 71.202
Composition: Hex4HexNAc5NeuAc1dHex1-AA **Intensity coverage [%]:** 0.74
Accession: 36229 **Fragment coverage [%]:** 0.68



Glycan: 39



Project path: /N-glycans cancer/25148/comp_25148.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf
Parent m/z: 1121.4299 2+ **Score:** 33.906
Composition: Hex4HexNAc5dHex3-AA **Intensity coverage [%]:** 0.57
Accession: 35814 **Fragment coverage [%]:** 0.20

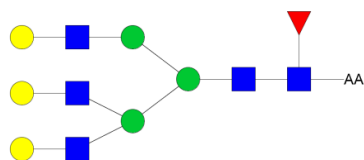




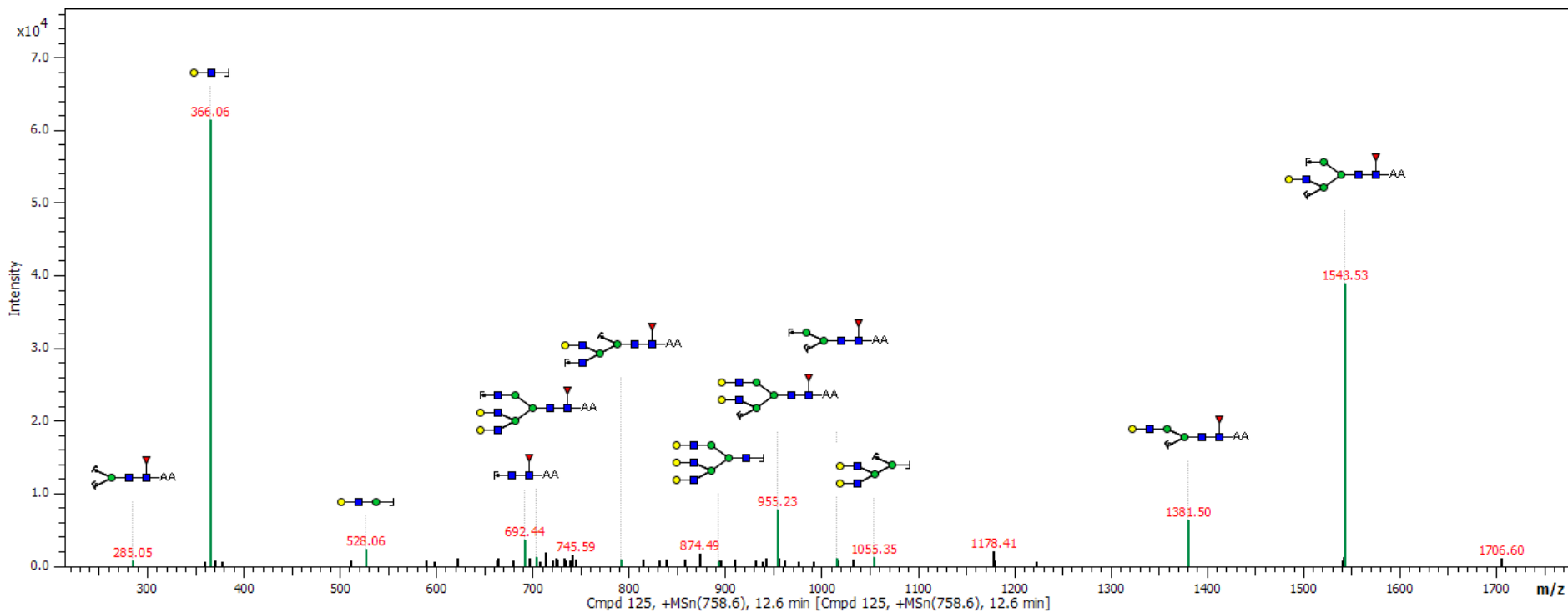
Spectrum 109

Glycan Search Report

Glycan: 25

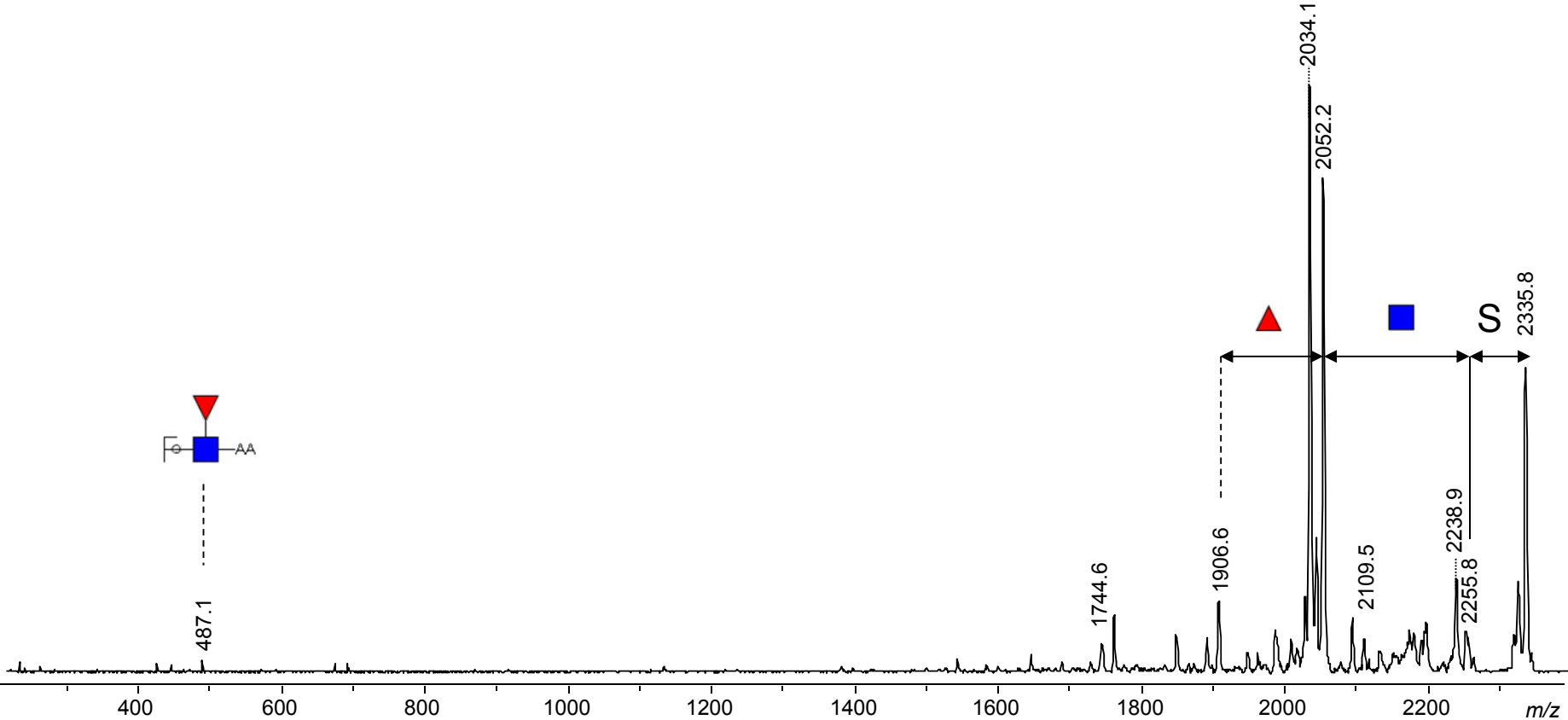


Project path: /N-glycans cancer/25148/comp_25148.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf
Parent m/z: 758.6189 3+ **Score:** 52.446
Composition: Hex6HexNAc5dHex1-AA **Intensity coverage [%]:** 0.76
Accession: 36108 **Fragment coverage [%]:** 0.36



Spectrum 110

Lift of 2335.6 [M-H]⁻
SdHex2Hex5HexNAc5-AA

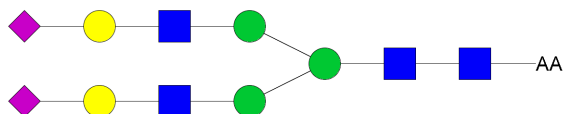




Spectrum 111

Glycan Search Report

Glycan: 2



Project path: /N-glycans cancer/25148/comp_25148.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf

Parent m/z: 782.2858 3+

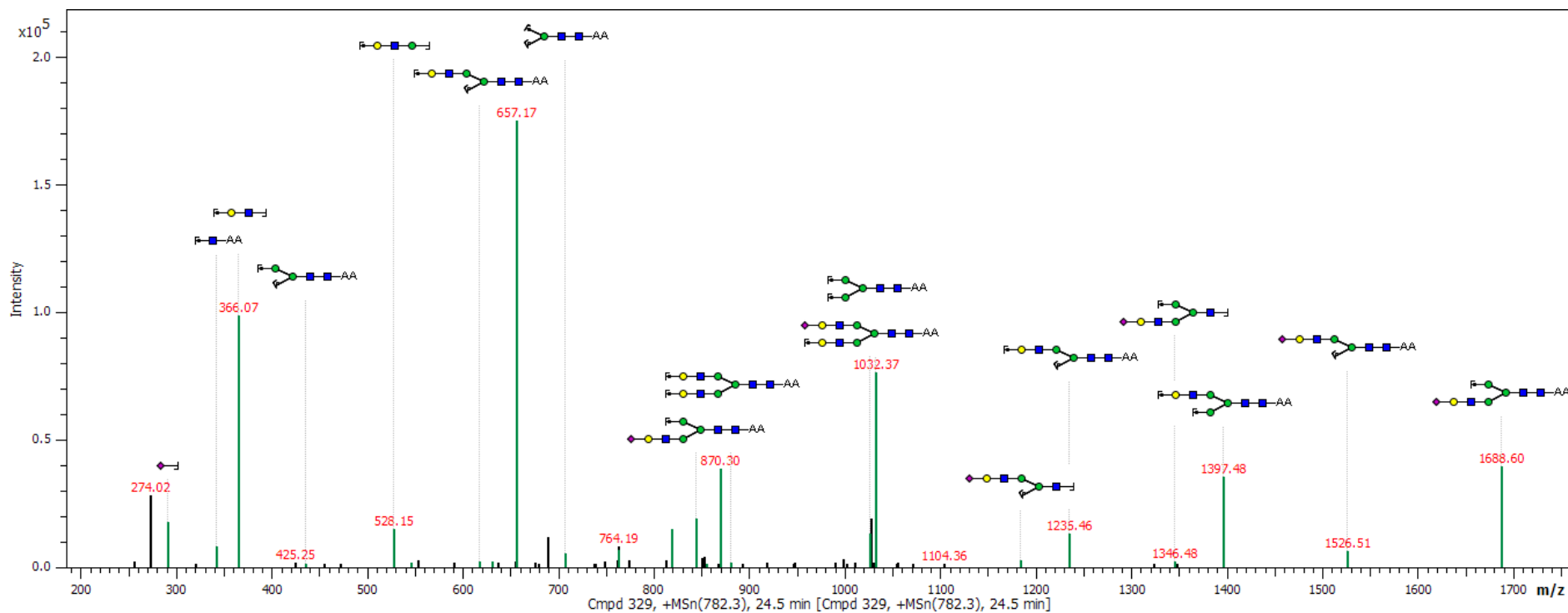
Score: 79.524

Composition: Hex5HexNAc4NeuAc2-AA

Intensity coverage [%]: 0.80

Accession: 32146

Fragment coverage [%]: 0.79

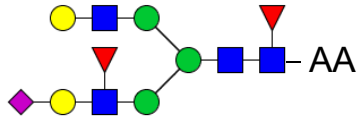


Spectrum 112

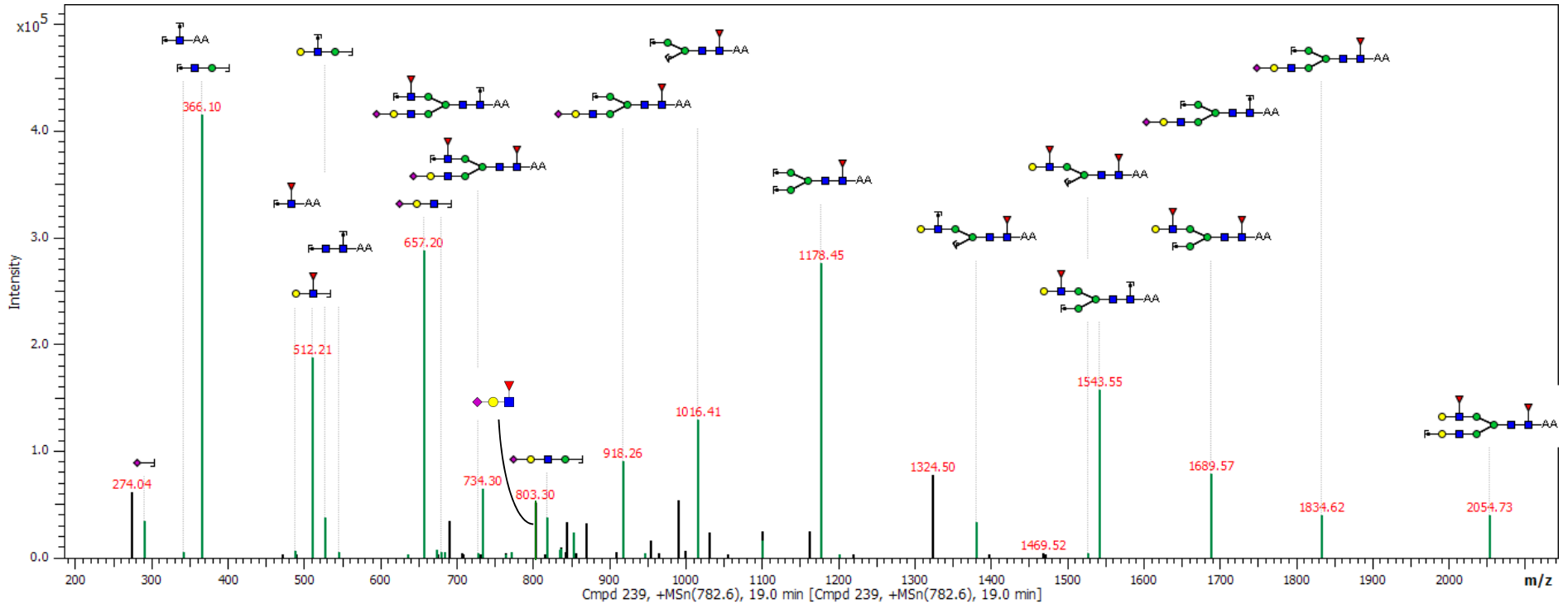


Glycan Search Report

Glycan: 5



Project path: /N-glycans cancer/25148/comp_25148.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf
Parent m/z: 782.6260 3+ **Score:** 75.526
Composition: Hex5HexNAc4NeuAc1dHex2-AA **Intensity coverage [%]:** 0.78
Accession: **Fragment coverage [%]:** 0.73

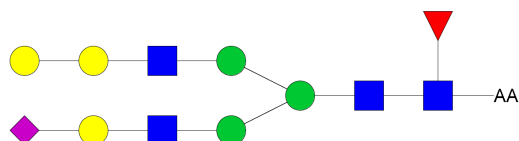


Spectrum 113

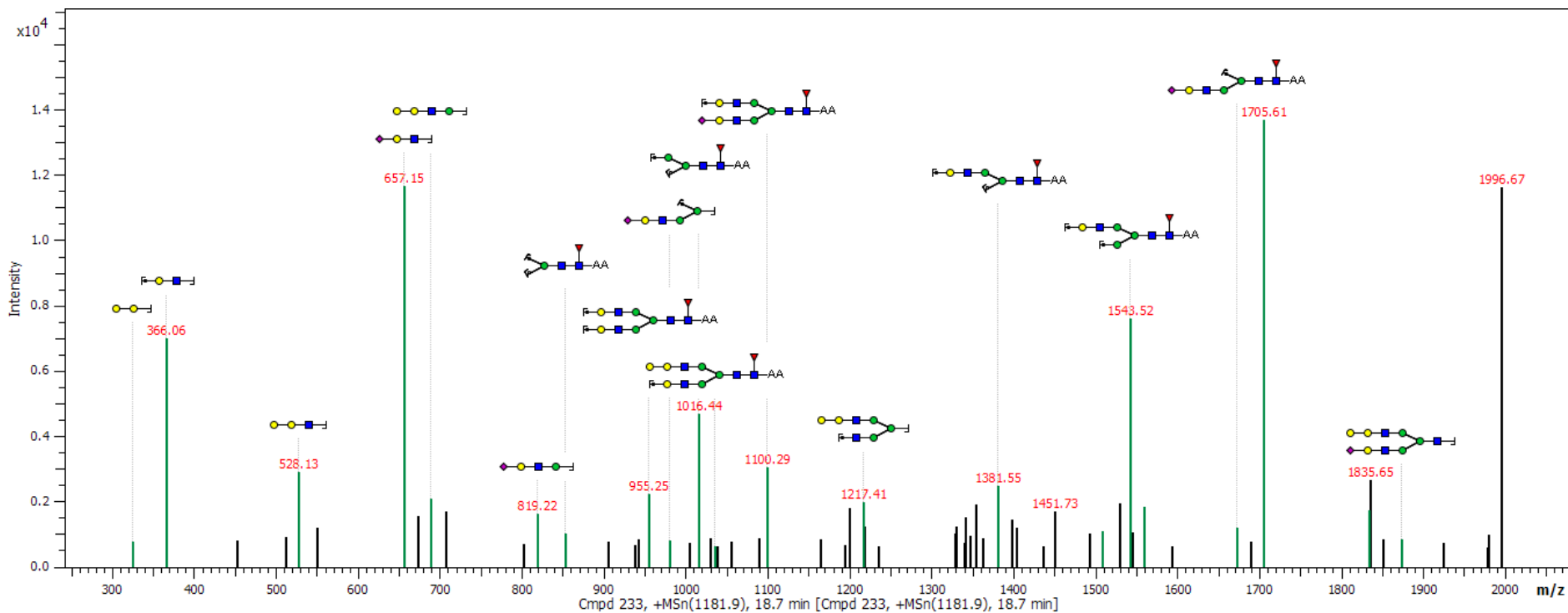


Glycan Search Report

Glycan: 27

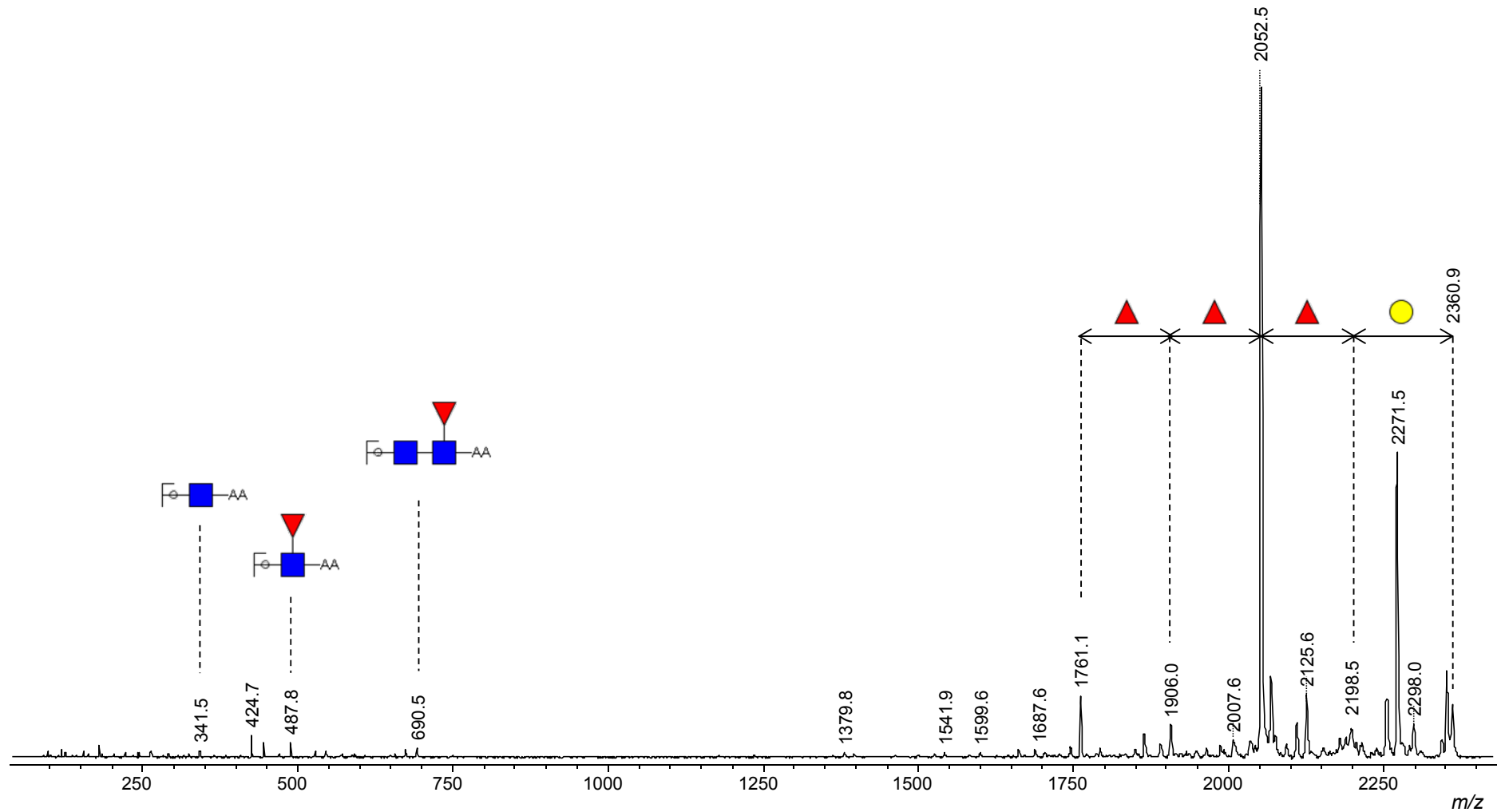


Project path: /N-glycans cancer/25148/comp_25148.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf
Parent m/z: 1181.4328 2+ **Score:** 49.693
Composition: Hex6HexNAc4NeuAc1dHex1-AA **Intensity coverage [%]:** 0.56
Accession: 36289 **Fragment coverage [%]:** 0.44



Spectrum 114

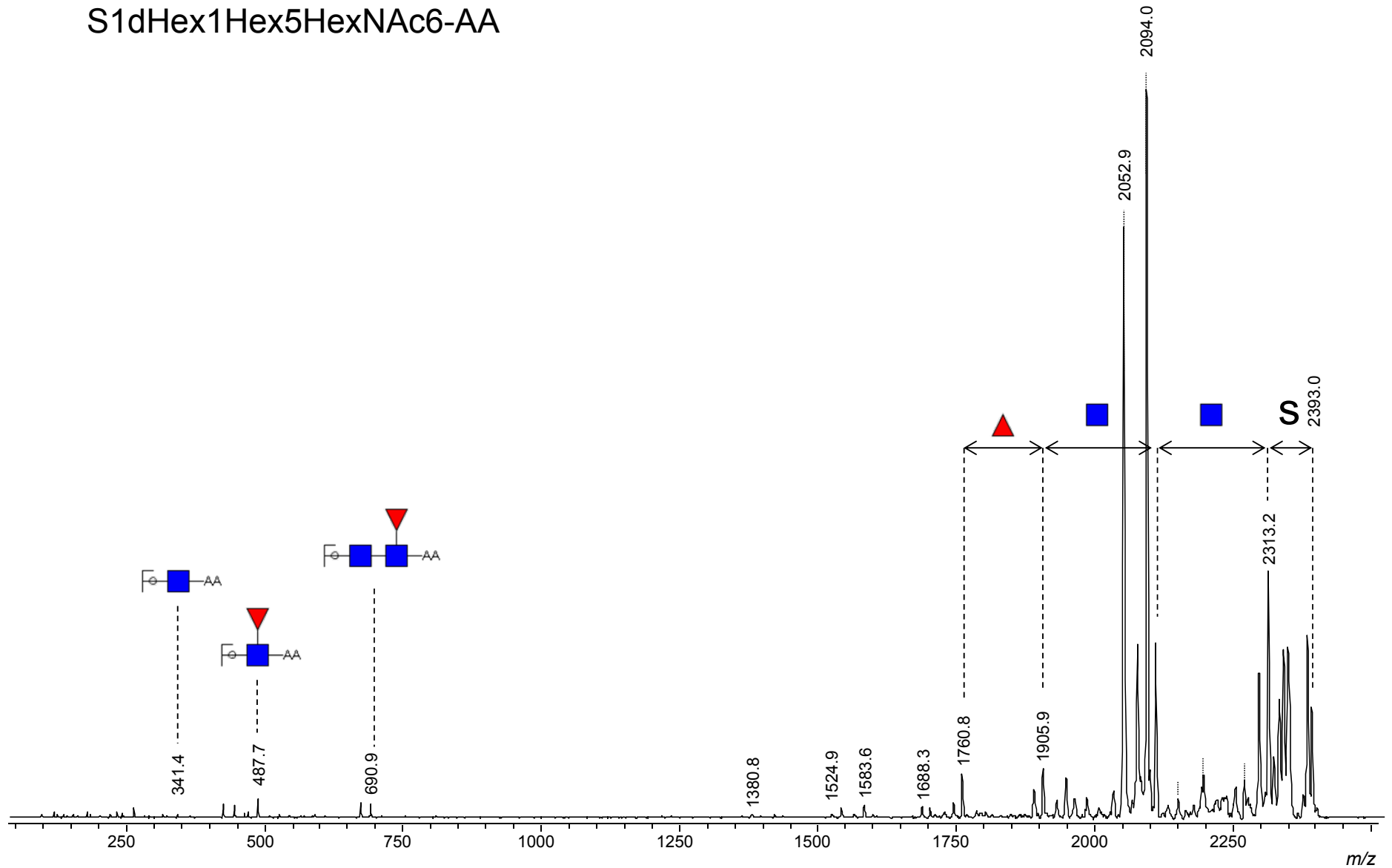
LIFT of 2360.9
dHex3Hex6HexNAc4-AA



Spectrum 115

LIFT of 2392.95

S1dHex1Hex5HexNAc6-AA

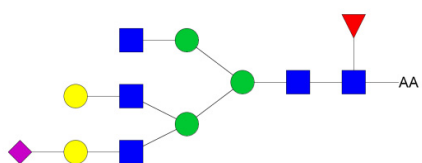


Spectrum 116

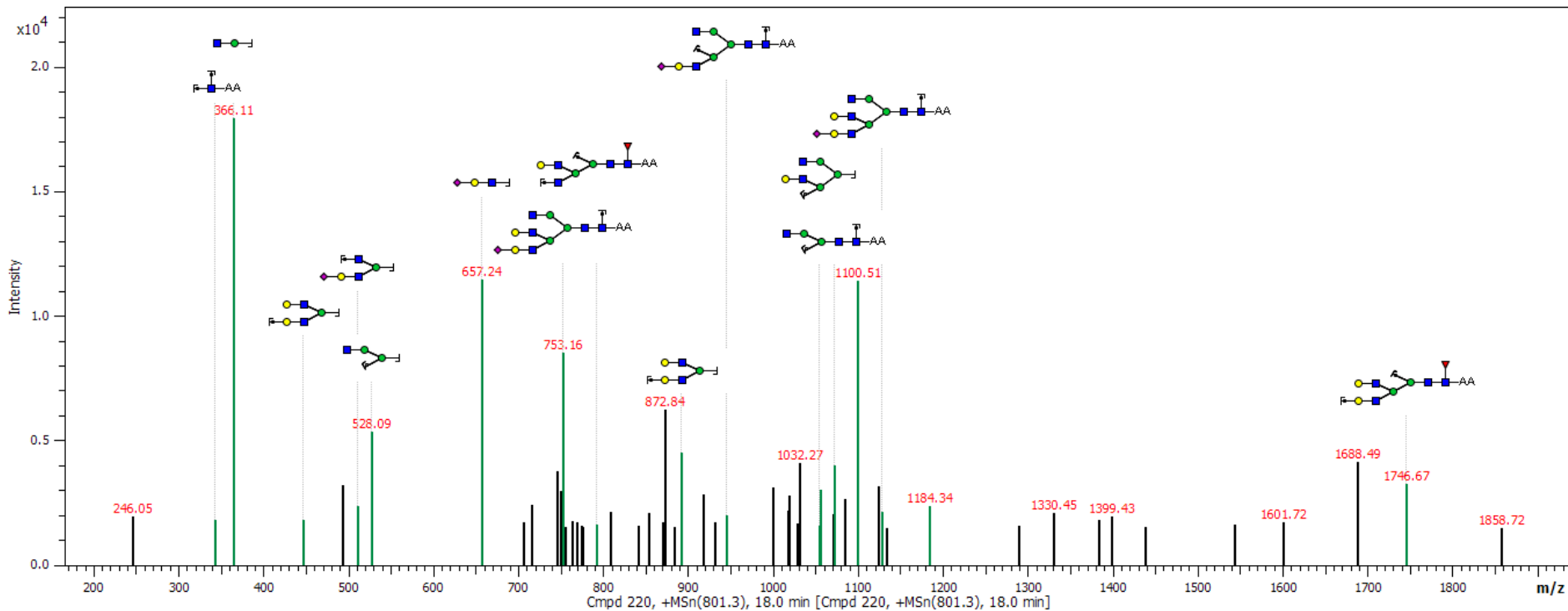


Glycan Search Report

Glycan: 31



Project path: /N-glycans cancer/25148/comp_25148.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf
Parent m/z: 801.6331 3+ **Score:** 40.173
Composition: Hex5HexNAc5NeuAc1dHex1-AA **Intensity coverage [%]:** 0.49
Accession: 36415 **Fragment coverage [%]:** 0.33

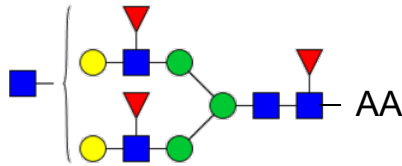


Spectrum 117



Glycan Search Report

Glycan: 7



Project path: /N-glycans cancer/25148/comp_25148.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf

Parent m/z: 1202.4563 2+

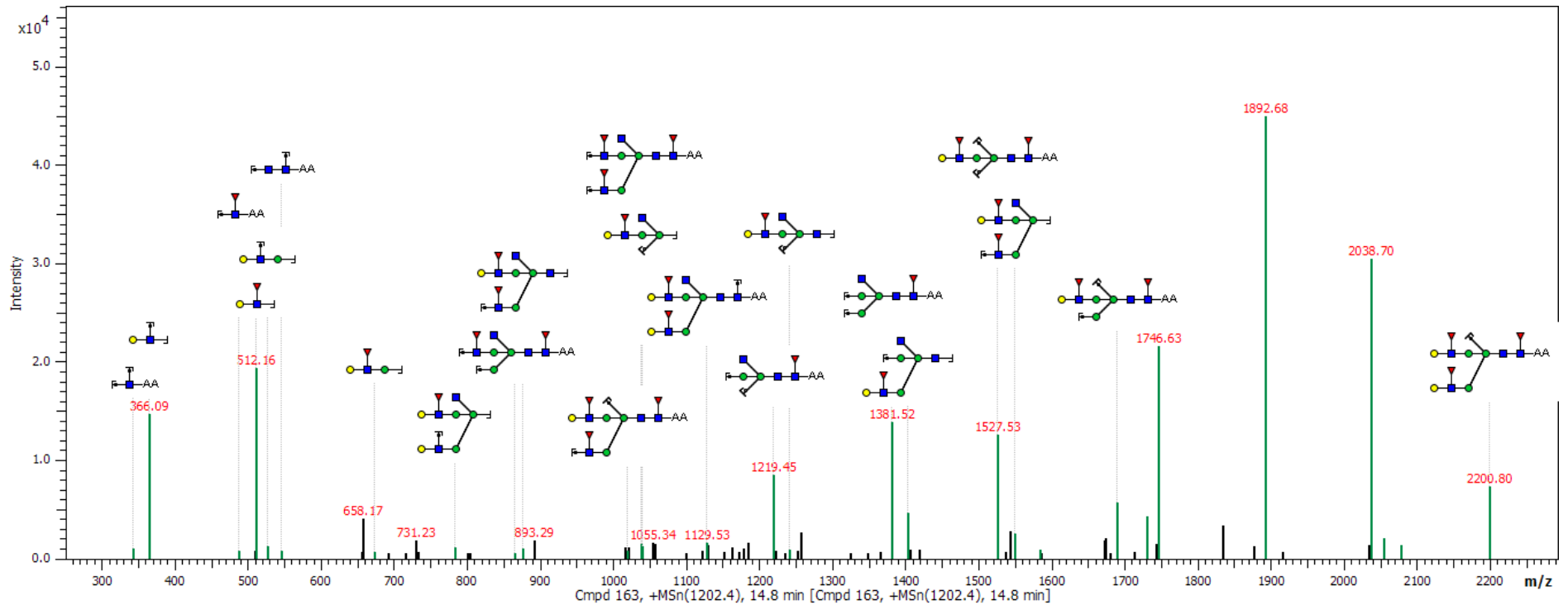
Score: 74.572

Composition: Hex5HexNAc5dHex3-AA

Intensity coverage [%]: 0.79

Accession: 36239

Fragment coverage [%]: 0.70

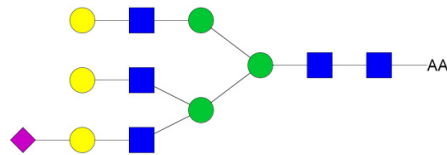


Spectrum 118

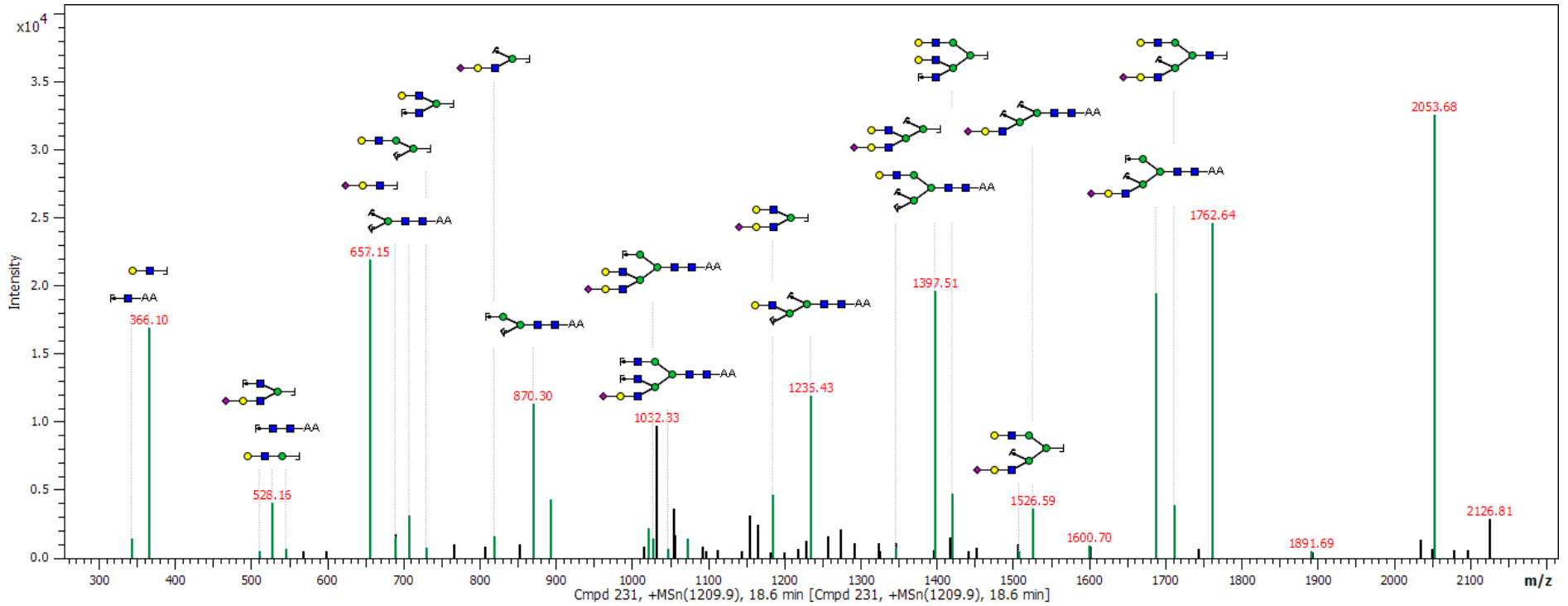


Glycan Search Report

Glycan: 10



Project path: /N-glycans cancer/25148/comp_25148.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf
Parent m/z: 1209.9435 2+ **Score:** 72.998
Composition: Hex6HexNAc5NeuAc1-AA **Intensity coverage [%]:** 0.79
Accession: 36350 **Fragment coverage [%]:** 0.67

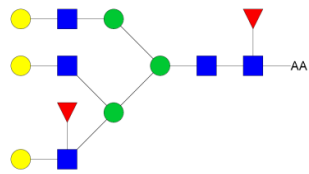


Spectrum 119

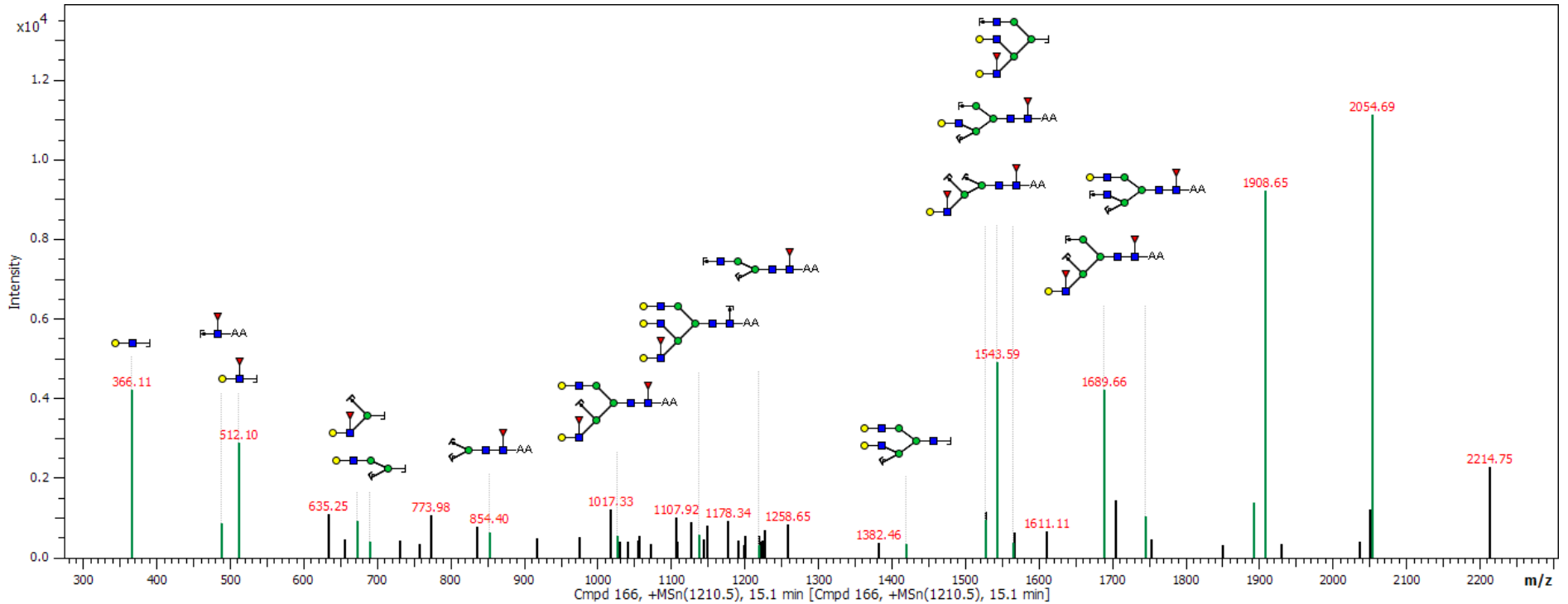


Glycan Search Report

Glycan: 24



Project path: /N-glycans cancer/25148/comp_25148.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf
Parent m/z: 1210.4537 2+ **Score:** 53.280
Composition: Hex6HexNAc5dHex2-AA **Intensity coverage [%]:** 0.63
Accession: 36260 **Fragment coverage [%]:** 0.45

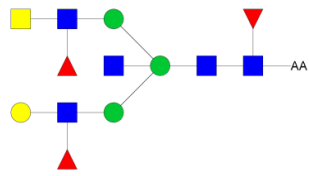


Spectrum 120

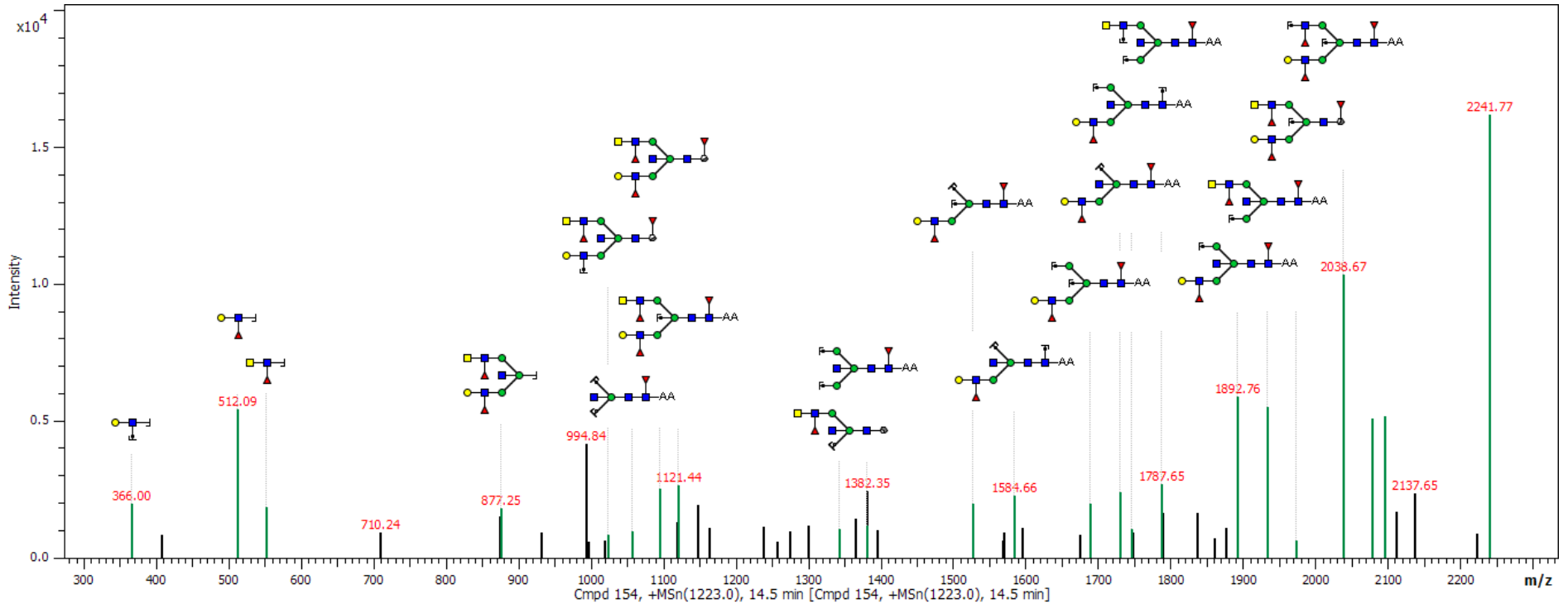


Glycan Search Report

Glycan: 41



Project path: /N-glycans cancer/25148/comp_25148.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf
Parent m/z: 1222.9696 2+ **Score:** 30.005
Composition: Hex4HexNAc6dHex3-AA **Intensity coverage [%]:** 0.66
Accession: 29530 **Fragment coverage [%]:** 0.14

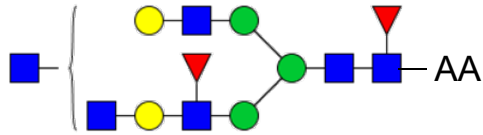


Spectrum 121



Glycan Search Report

Glycan: 20



Project path: /N-glycans cancer/25148/comp_25148.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf

Parent m/z: 820.9804 3+

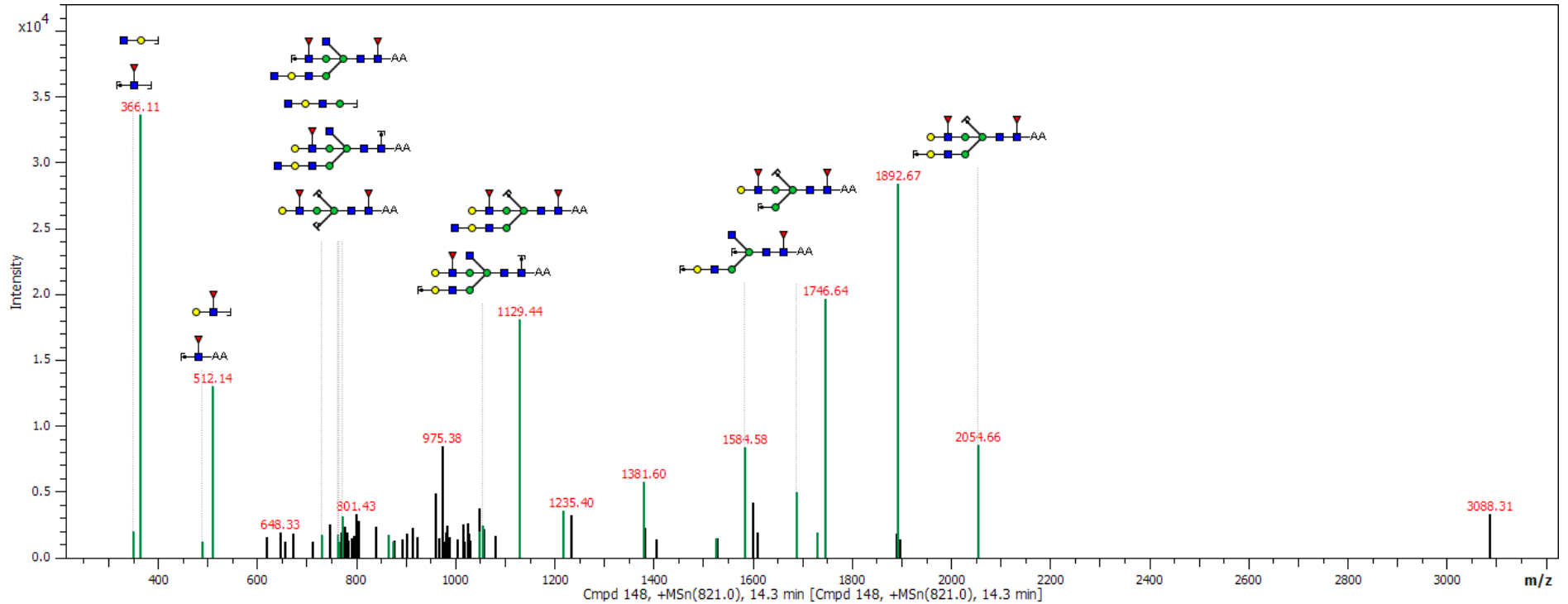
Score: 56.989

Composition: Hex5HexNAc6dHex2-AA

Intensity coverage [%]: 0.61

Accession: 36376

Fragment coverage [%]: 0.53

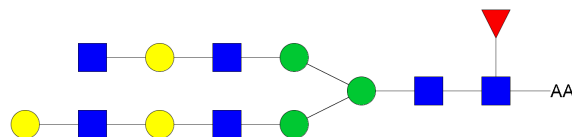




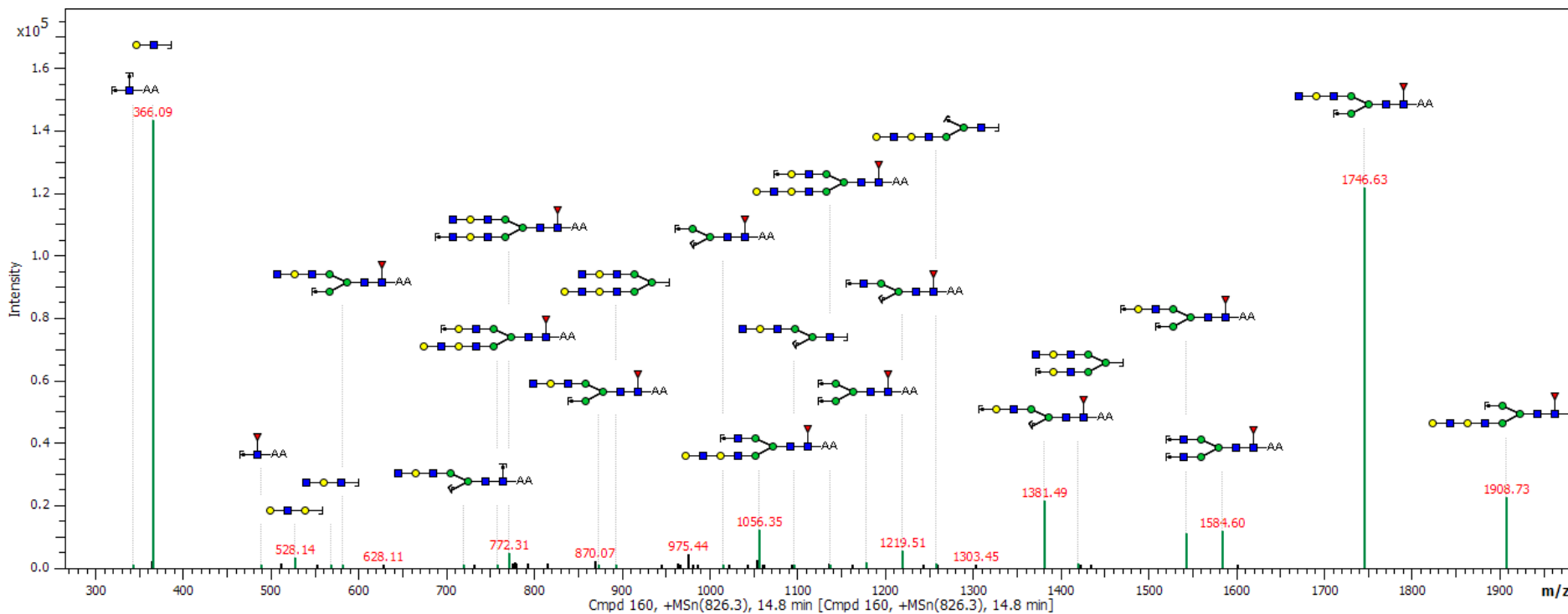
Spectrum 122

Glycan Search Report

Glycan: 3

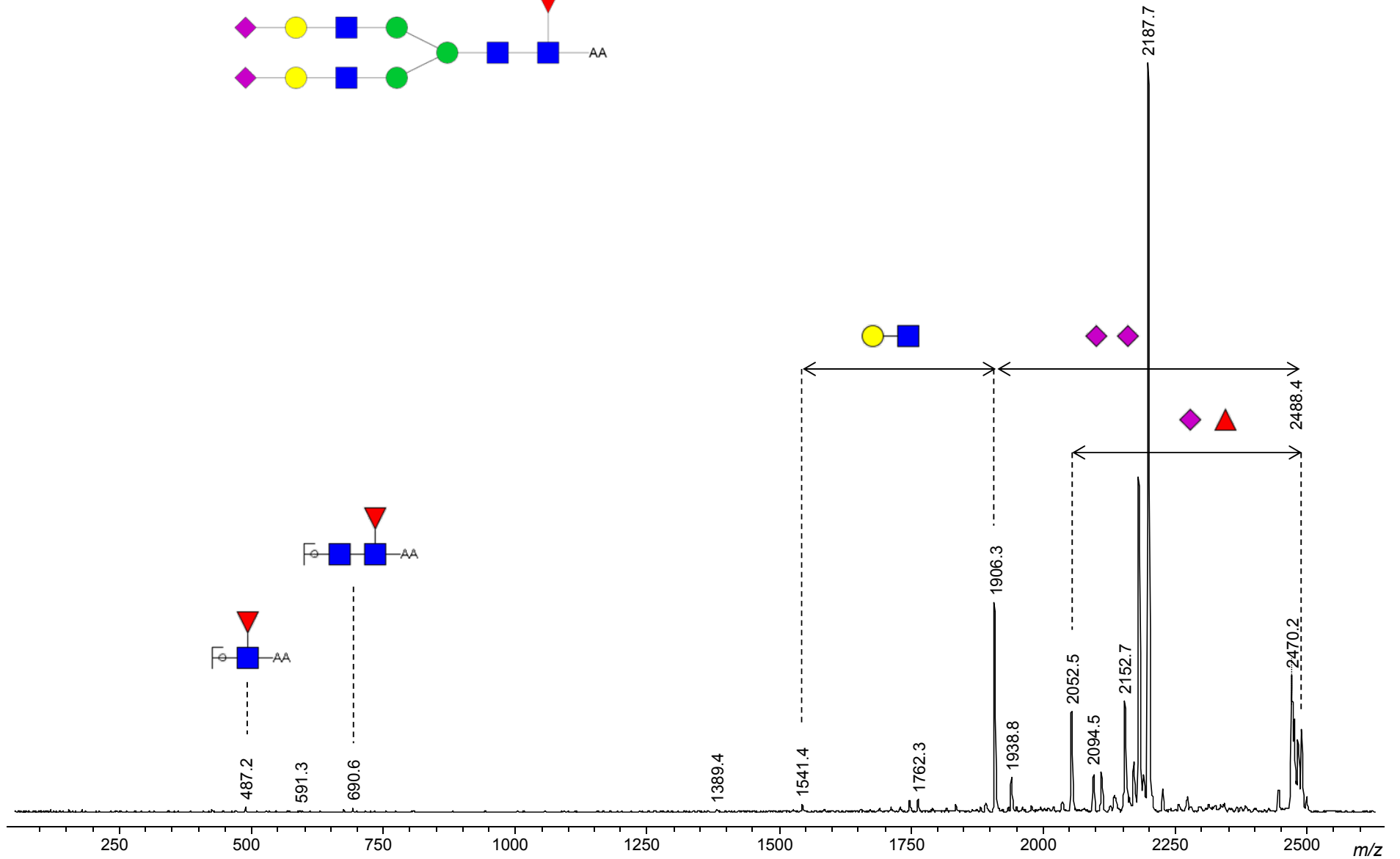
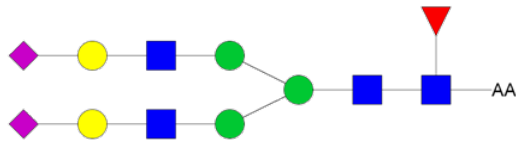


Project path: /N-glycans cancer/25148/comp_25148.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf
Parent m/z: 826.3121 3+ **Score:** 78.983
Composition: Hex6HexNAc6dHex1-AA **Intensity coverage [%]:** 0.88
Accession: 36298 **Fragment coverage [%]:** 0.71



Spectrum 123

Lift of 2488.8 [M-H]⁻
 dHex1Hex5HexNAc4Neu5Ac2-AA

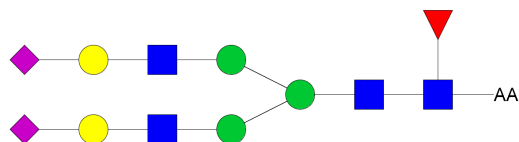




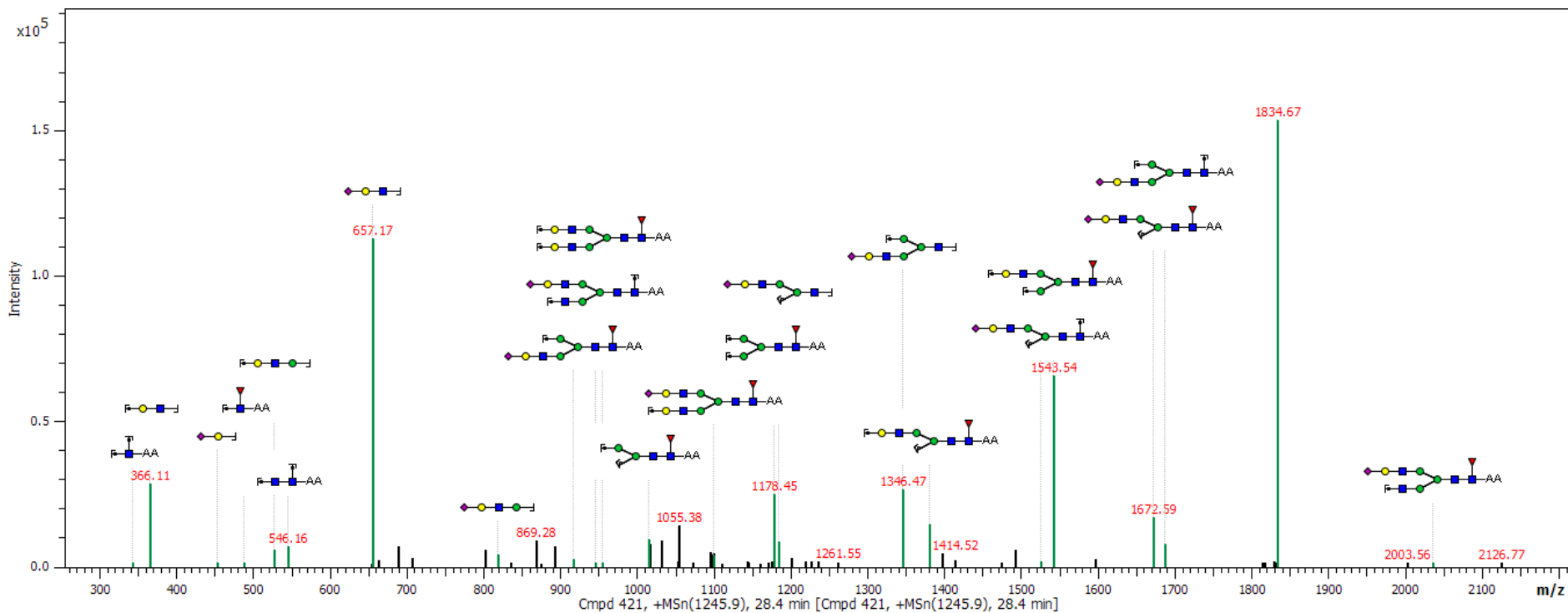
Spectrum 124

Glycan Search Report

Glycan: 13



Project path: /N-glycans cancer/25148/comp_25148.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf
Parent m/z: 1245.9541 2+ **Score:** 68.289
Composition: Hex5HexNAc4NeuAc2dHex1-AA **Intensity coverage [%]:** 0.77
Accession: 36307 **Fragment coverage [%]:** 0.61

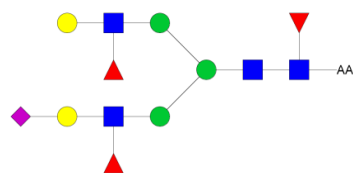




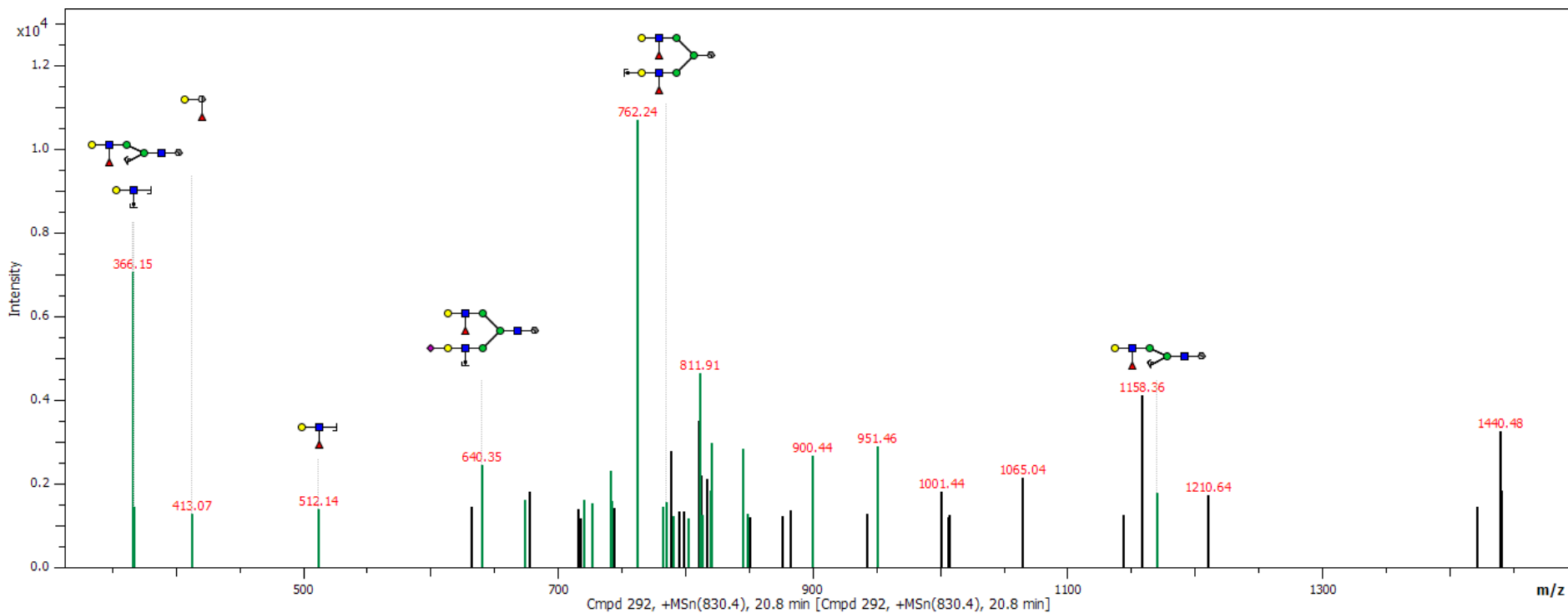
Spectrum 125

Glycan Search Report

Glycan: 15



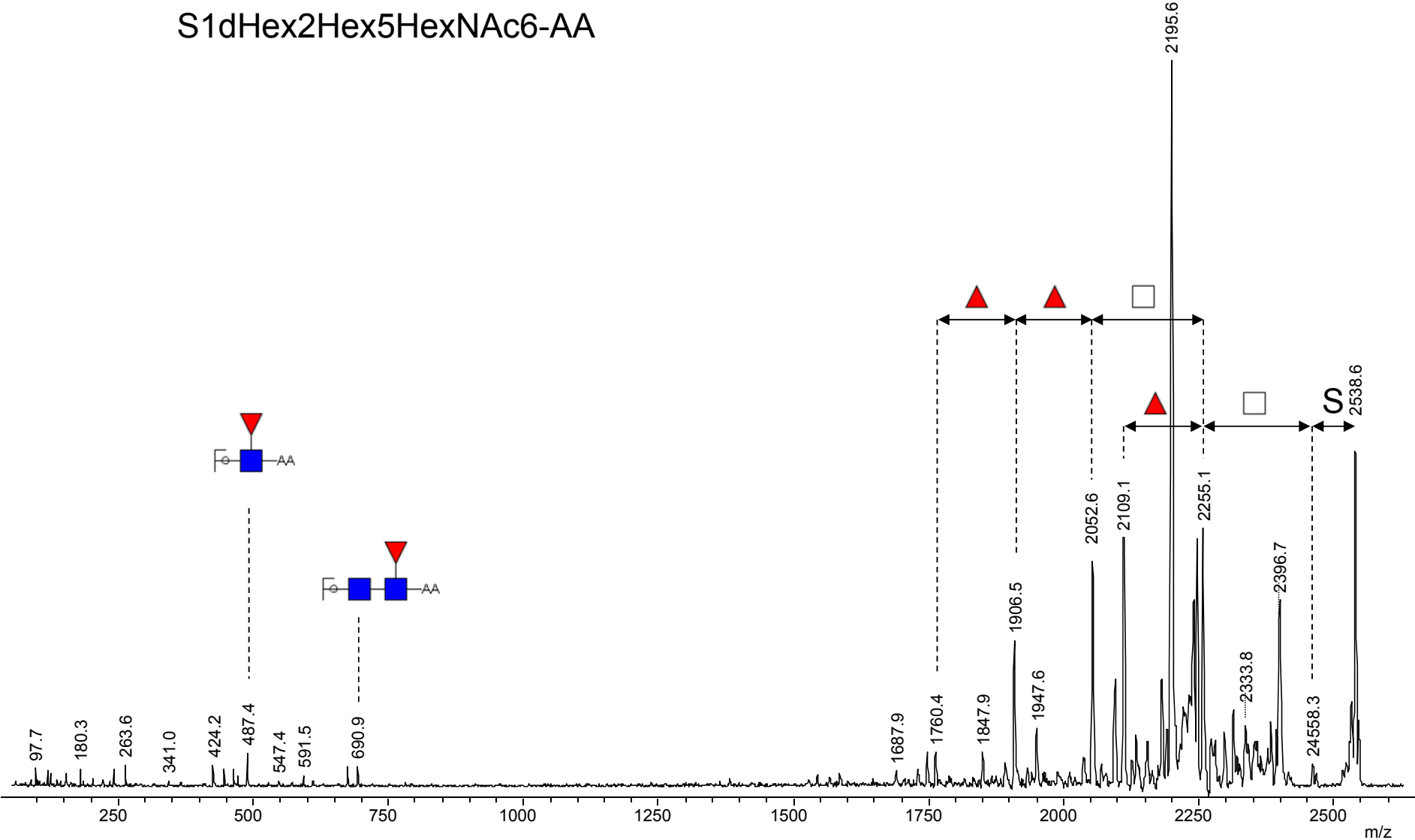
Project path: /N-glycans cancer/25142/comp_25142_01.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25142_01.d/comp_25142_01.mgf
Parent m/z: 831.3119 3+ **Score:** 26.917
Composition: Hex5HexNAc4NeuAc1dHex3-AA **Intensity coverage [%]:** 0.58
Accession: 14007 **Fragment coverage [%]:** 0.13



Spectrum 126

Lift of 2538.6[M-H]⁻

S1dHex2Hex5HexNAc6-AA

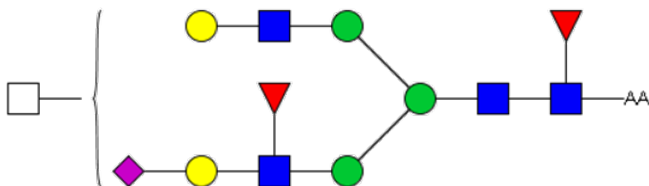




Spectrum 127

Glycan Search Report

Glycan: 26



Project path: /N-glycans cancer/25148/comp_25148.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf

Parent m/z: 850.3191 3+

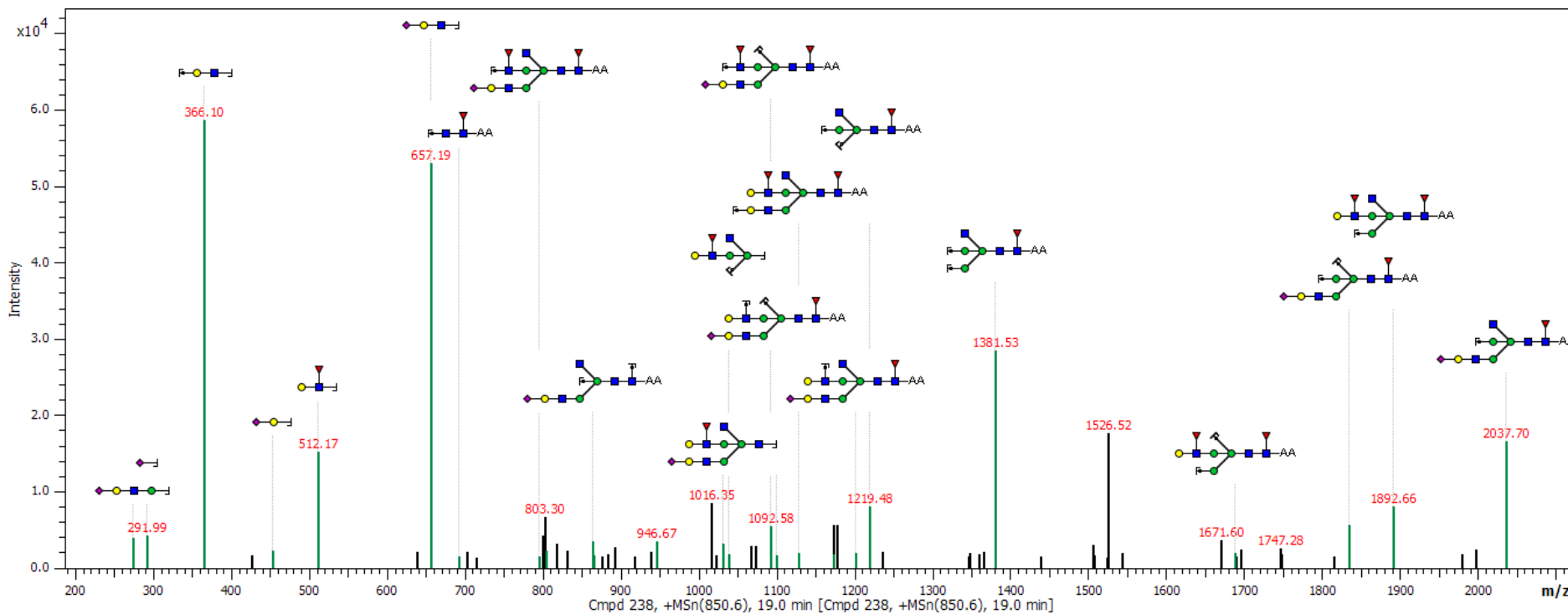
Score: 52.119

Composition: Hex5HexNAc5NeuAc1dHex2-AA

Intensity coverage [%]: 0.66

Accession:

Fragment coverage [%]: 0.41

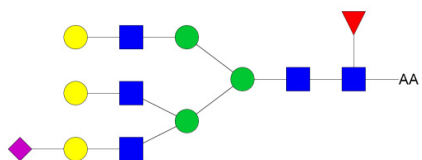




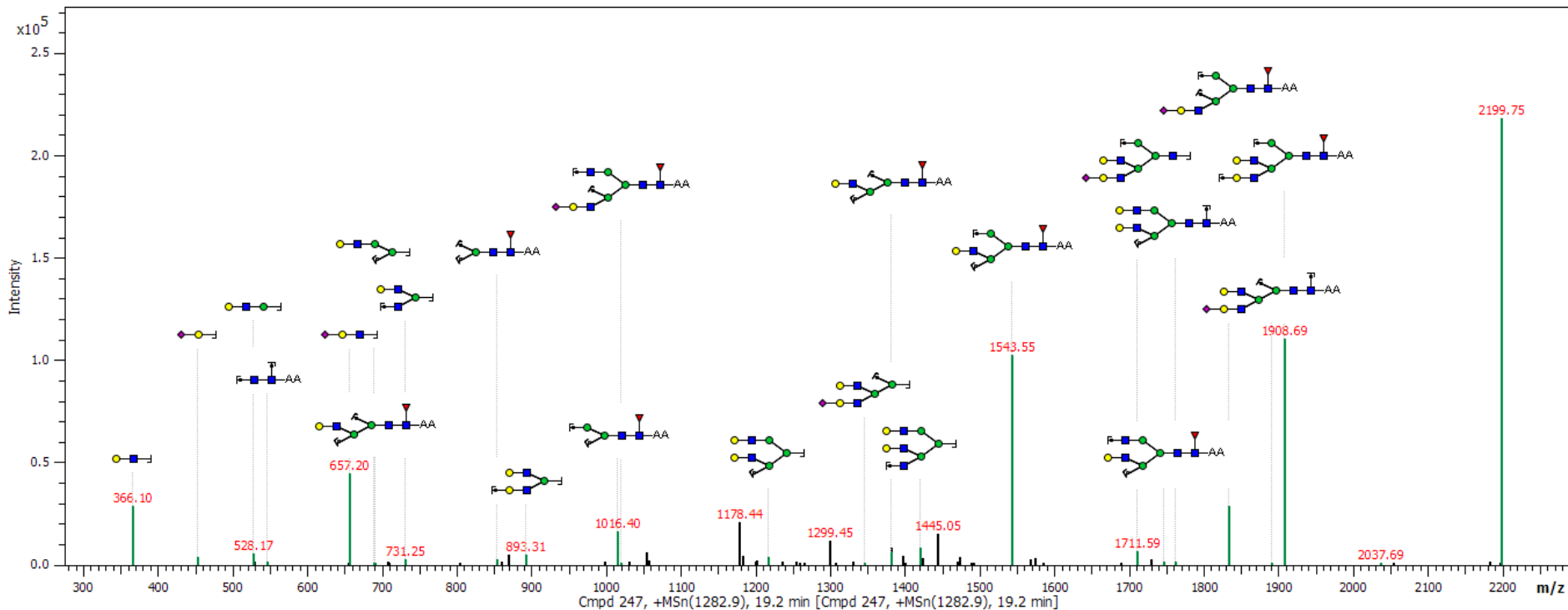
Spectrum 128

Glycan Search Report

Glycan: 14



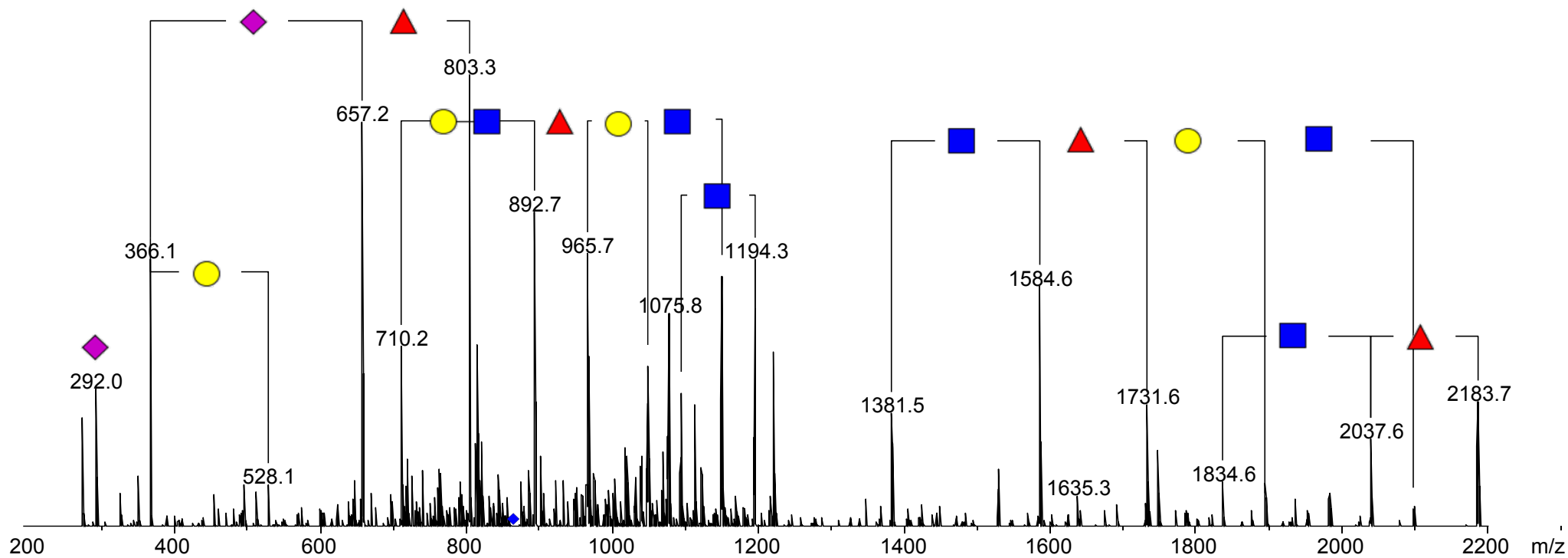
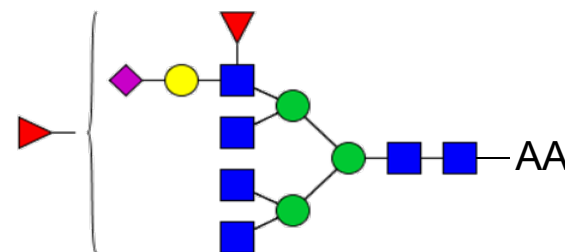
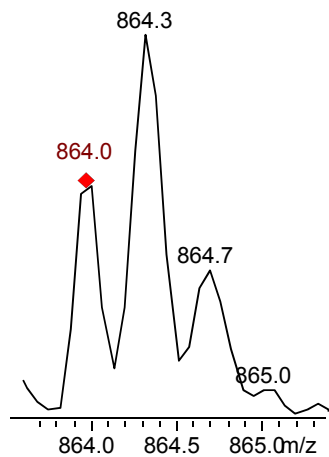
Project path: /N-glycans cancer/25148/comp_25148.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf
Parent m/z: 1282.9725 2+ **Score:** 66.069
Composition: Hex6HexNAc5NeuAc1dHex1-AA **Intensity coverage [%]:** 0.82
Accession: 36262 **Fragment coverage [%]:** 0.53



Spectrum 129

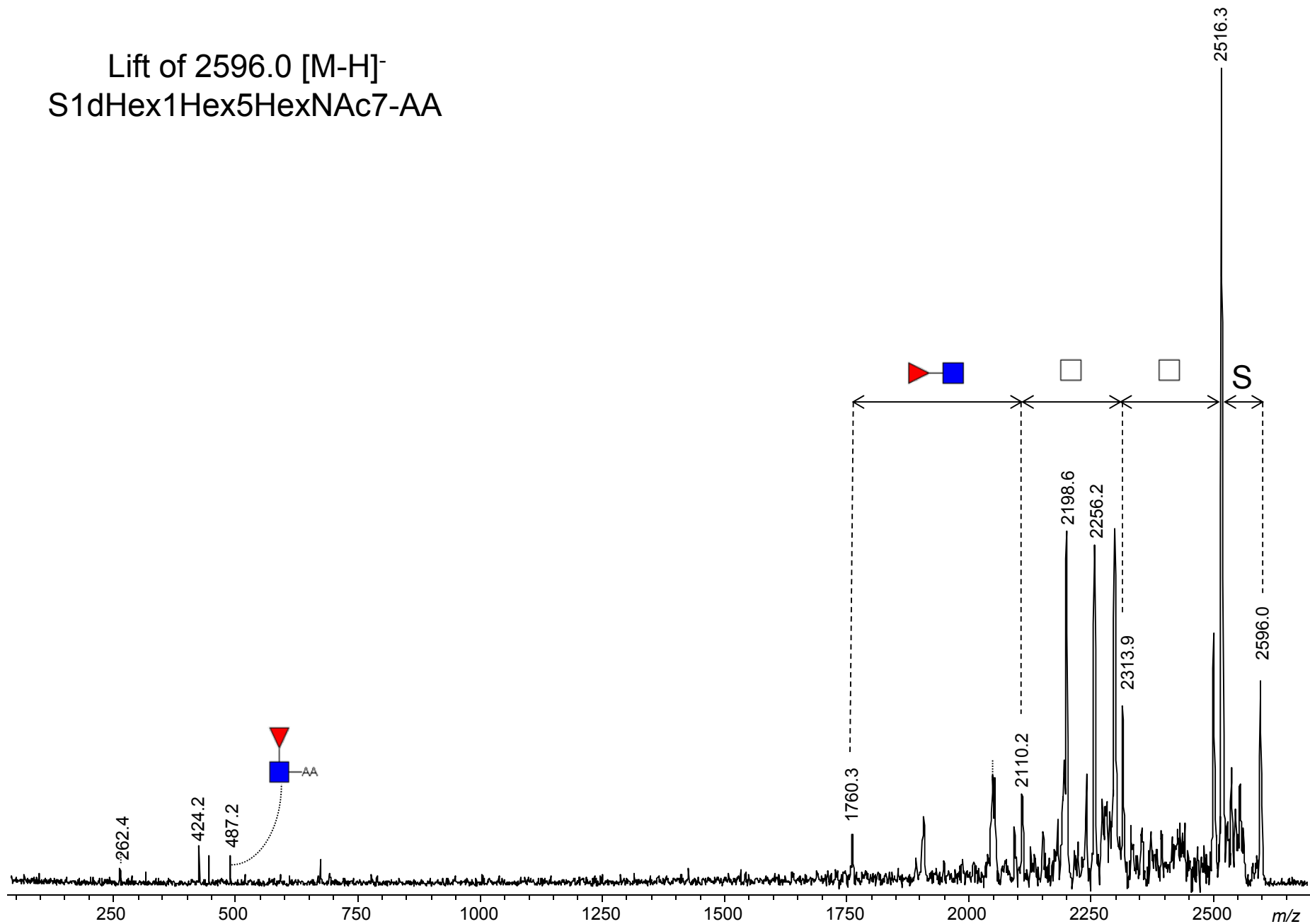
ESI MS/MS of [864.0 +3H]³⁺

dHex2Hex4HexNAc6Neu5Ac1-AA



Spectrum 130

Lift of 2596.0 [M-H]⁻
S1dHex1Hex5HexNAc7-AA

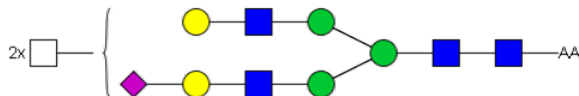




Spectrum 131

Glycan Search Report

Glycan: 21



Project path: /N-glycans cancer/25148/comp_25148.mgf

MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf

Parent m/z: 869.3263 3+

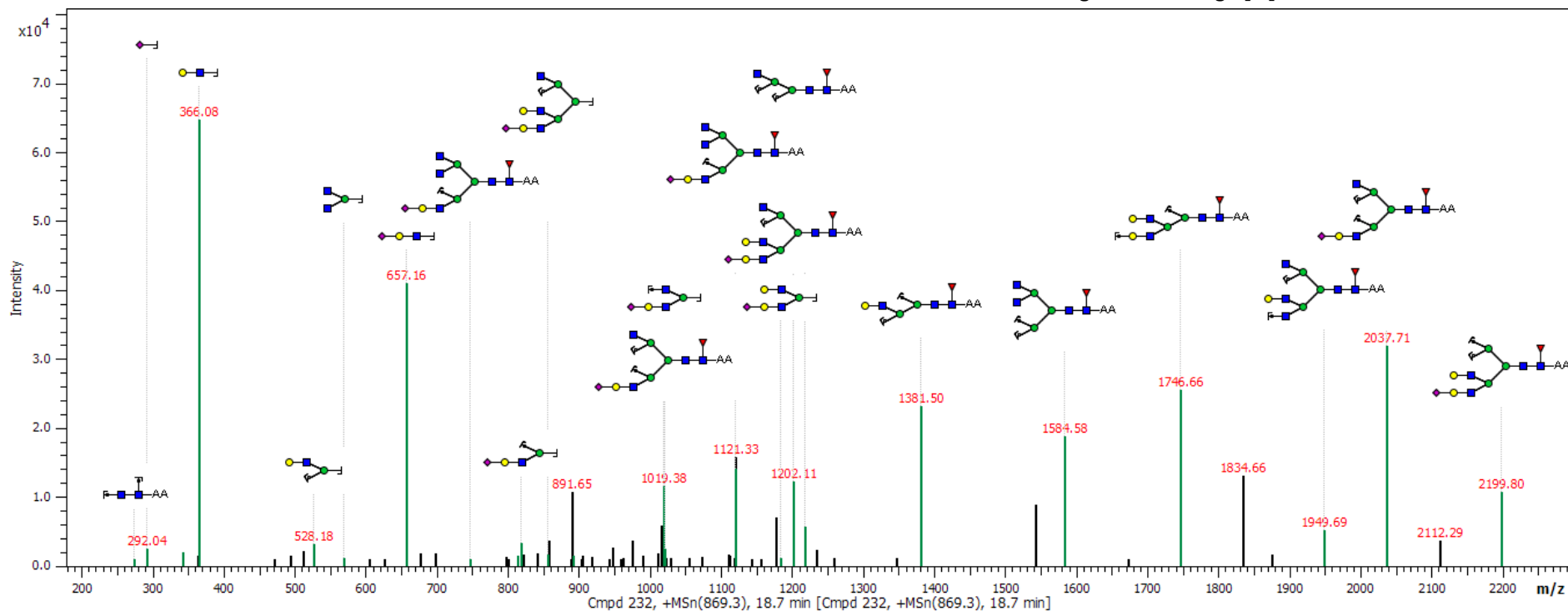
Score: 55.577

Composition: Hex5HexNAc6NeuAc1dHex1-AA

Intensity coverage [%]: 0.68

Accession: 36128

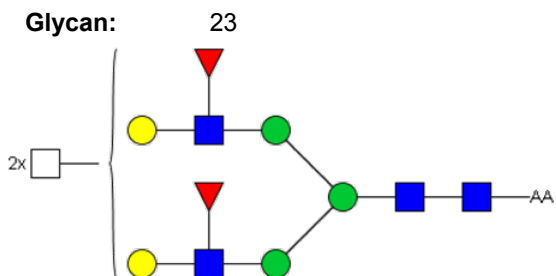
Fragment coverage [%]: 0.45



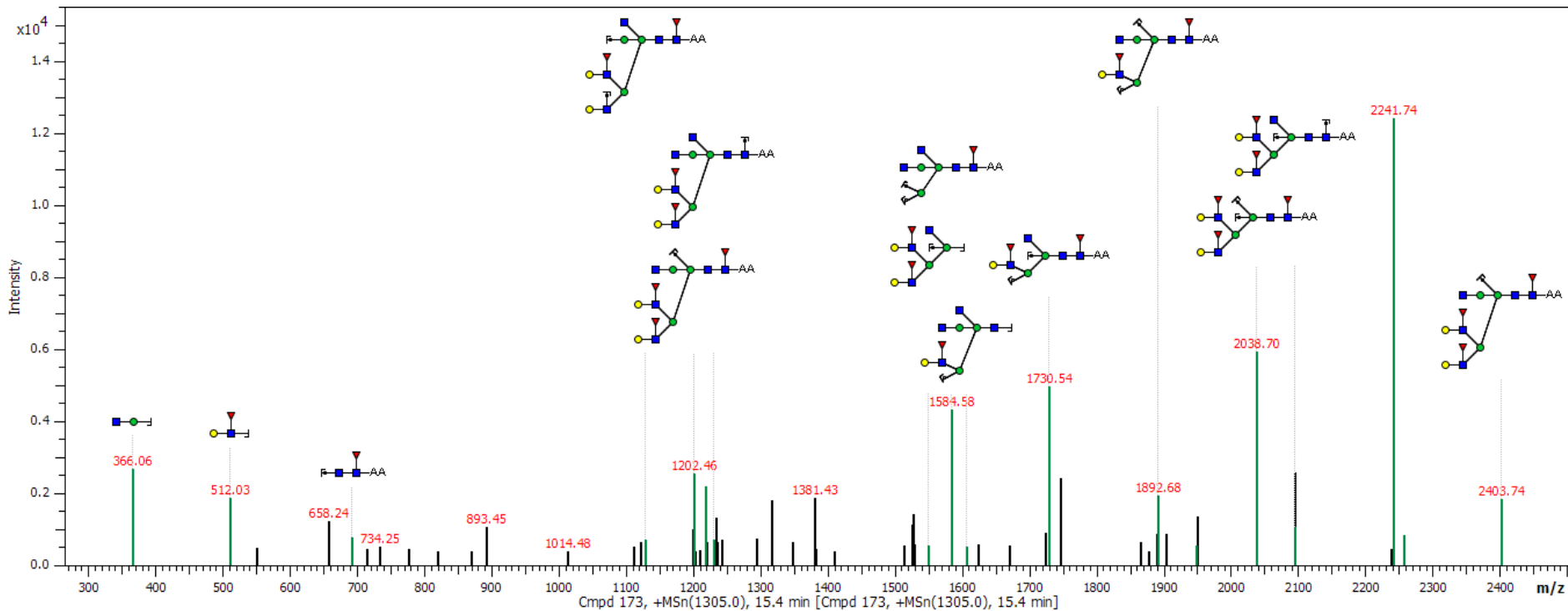


Spectrum 132

Glycan Search Report

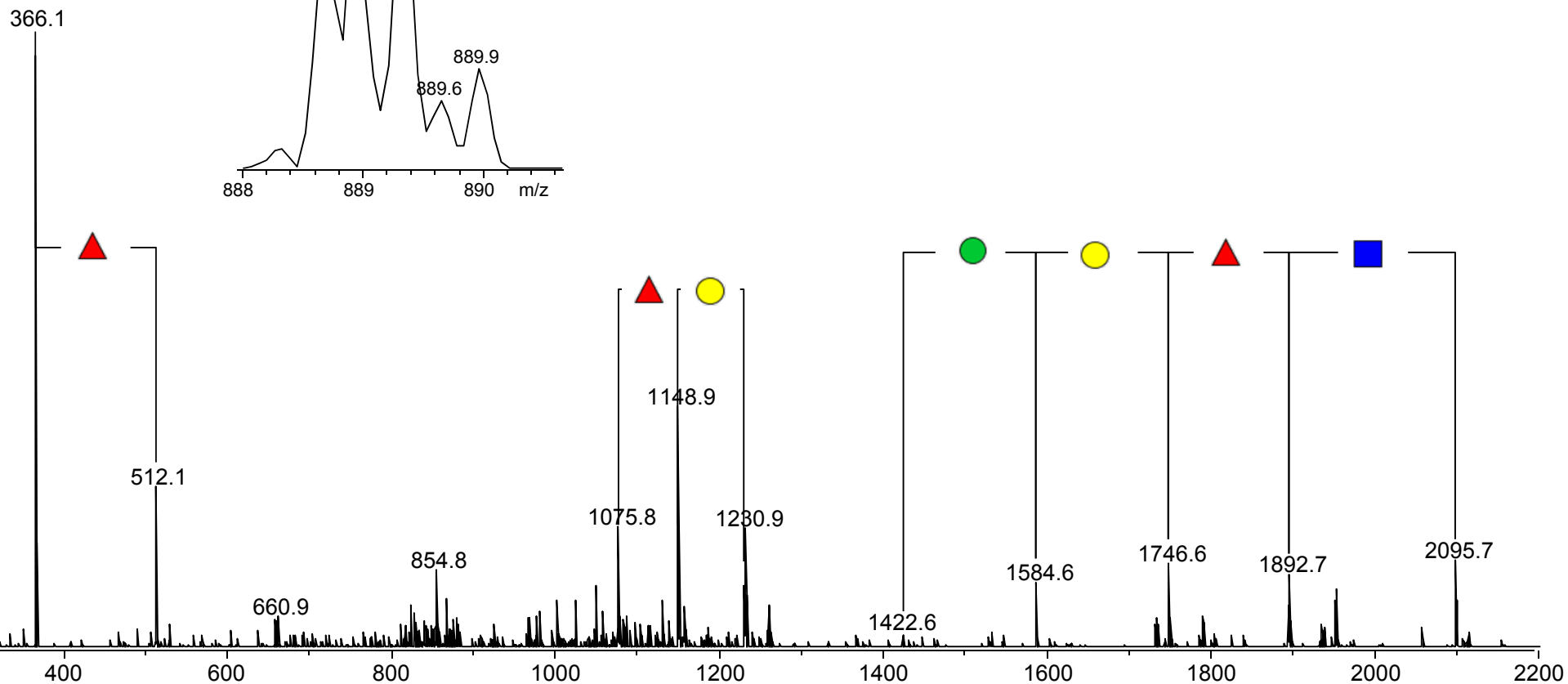
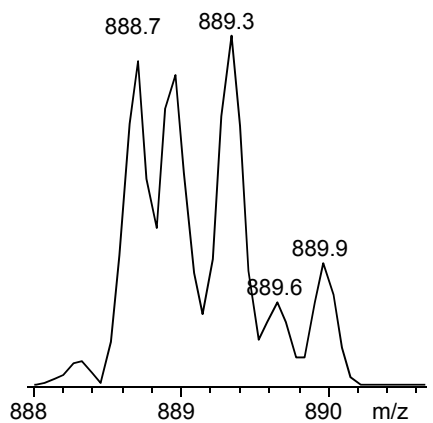
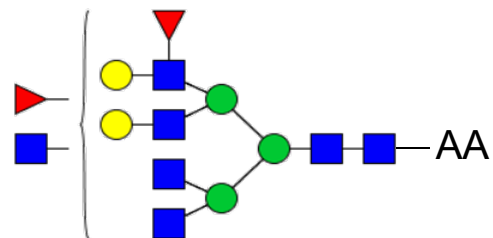


Project path: /N-glycans cancer/25148/comp_25148.mgf
MS data: K:/Cancer-CCR/N-glycans raw data_MS/LC-MS of the discriminators/25148_02.d/comp_25148.mgf
Parent m/z: 1303.9960 2+ **Score:** 54.112
Composition: Hex5HexNAc6dHex3-AA **Intensity coverage [%]:** 0.59
Accession: 36219 **Fragment coverage [%]:** 0.50

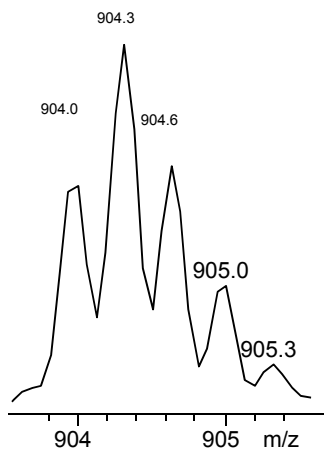


Spectrum 133

ESI MS/MS of $[888.7 + 3H]^{3+}$
dHex2Hex5HexNAc7-AA

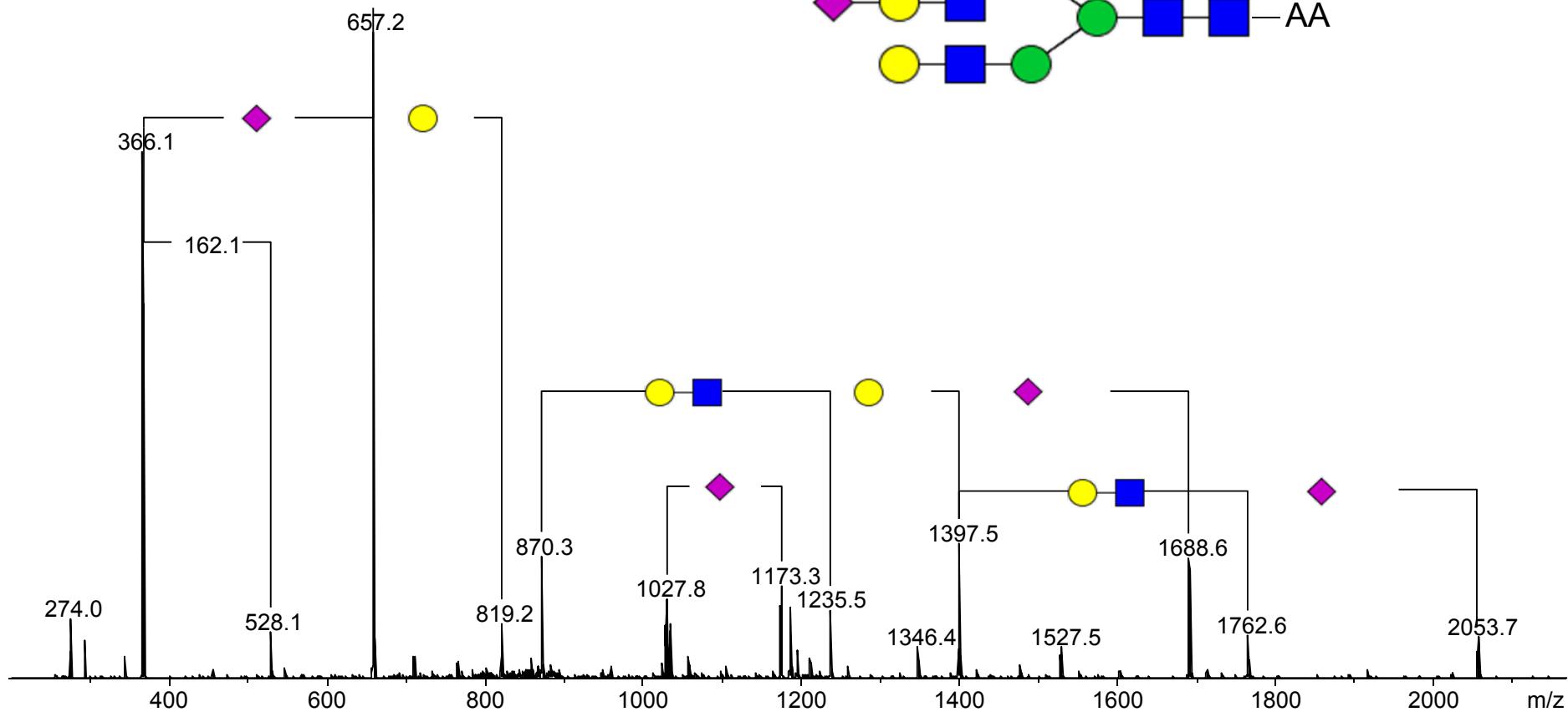
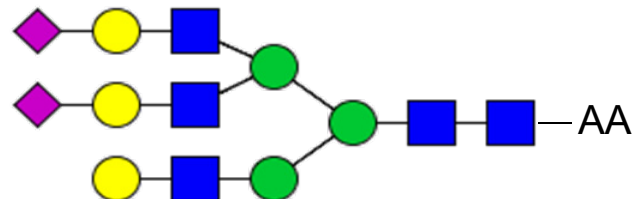


Spectrum 134



ESI MS/MS of [904.0 + 3H]³⁺

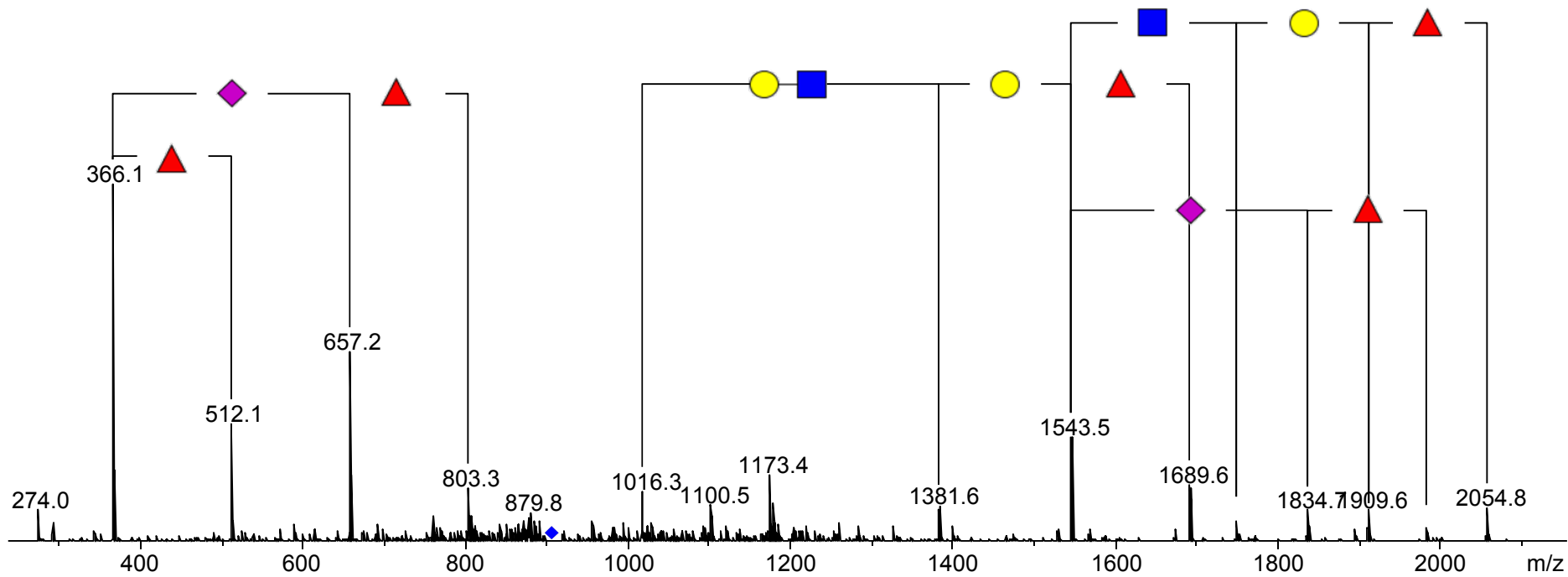
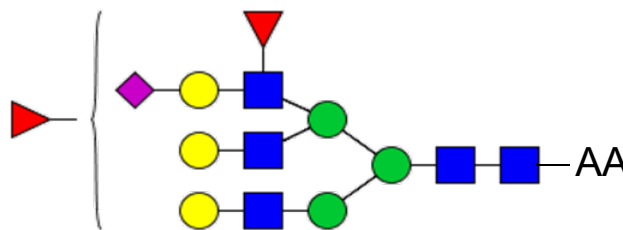
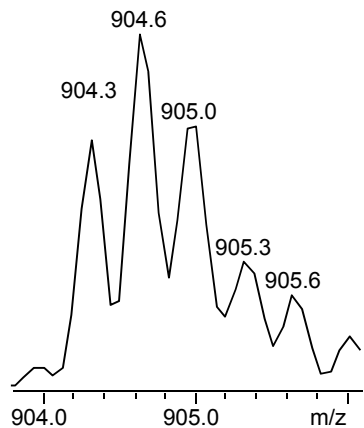
Hex6HexNAc5Neu5Ac2-AA



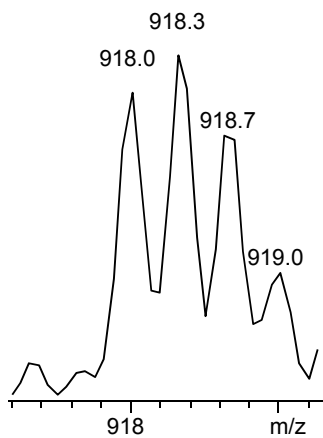
Spectrum 135

ESI MS/MS of $[904.3 + 3H]^{3+}$

dHex2Hex6HexNAc5Neu5Ac1-AA

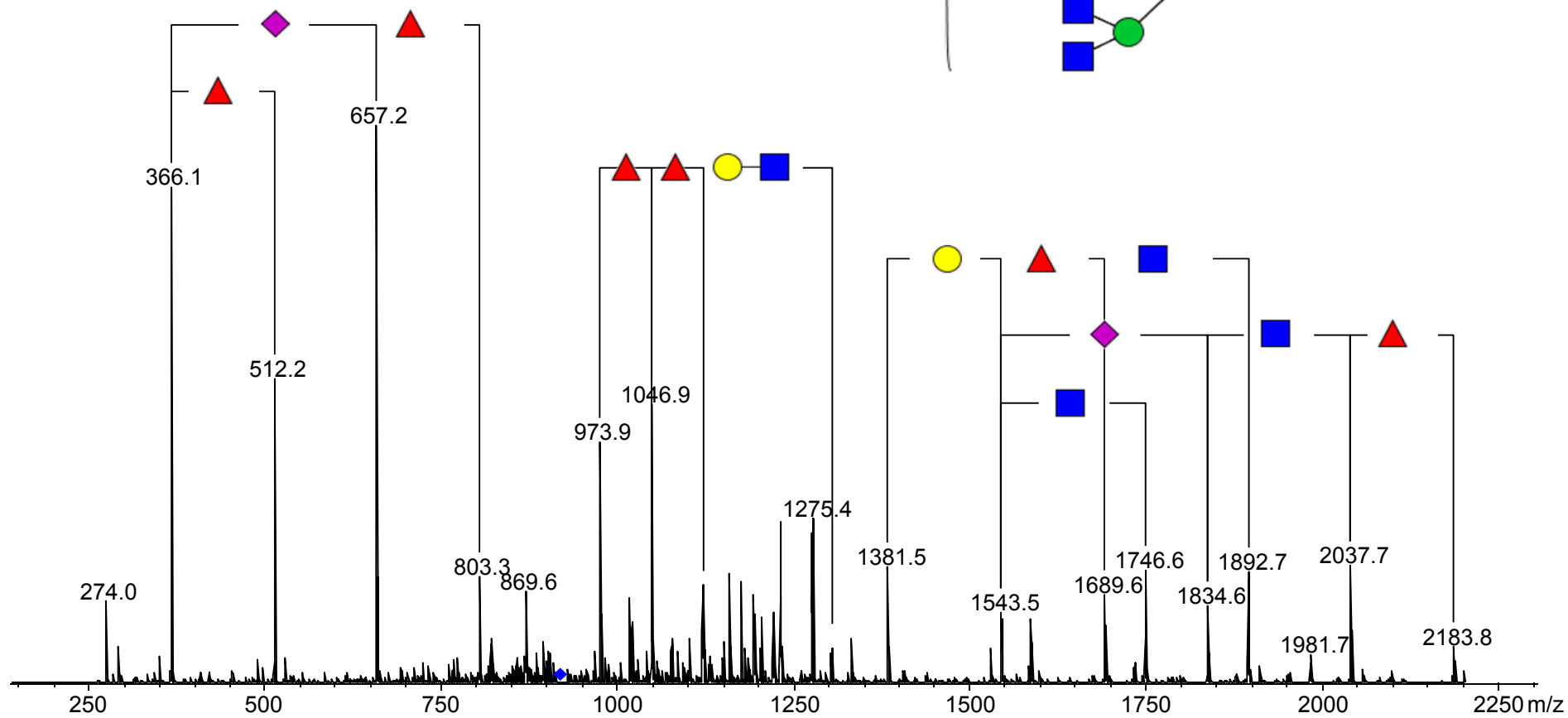
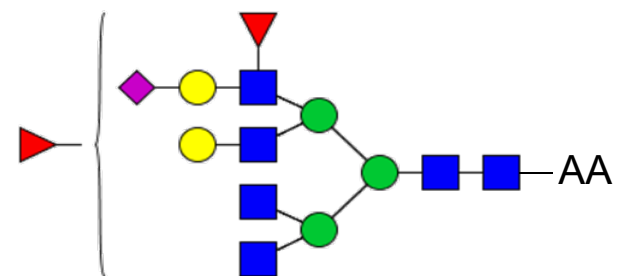


Spectrum 136

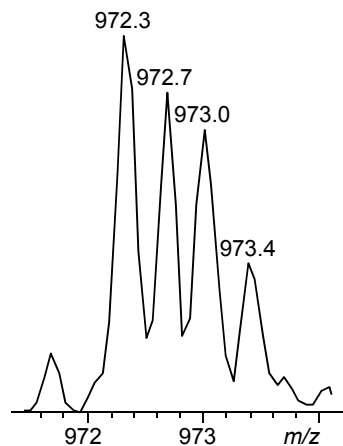


ESI MS/MS of $[918.0 + 3H]^{3+}$

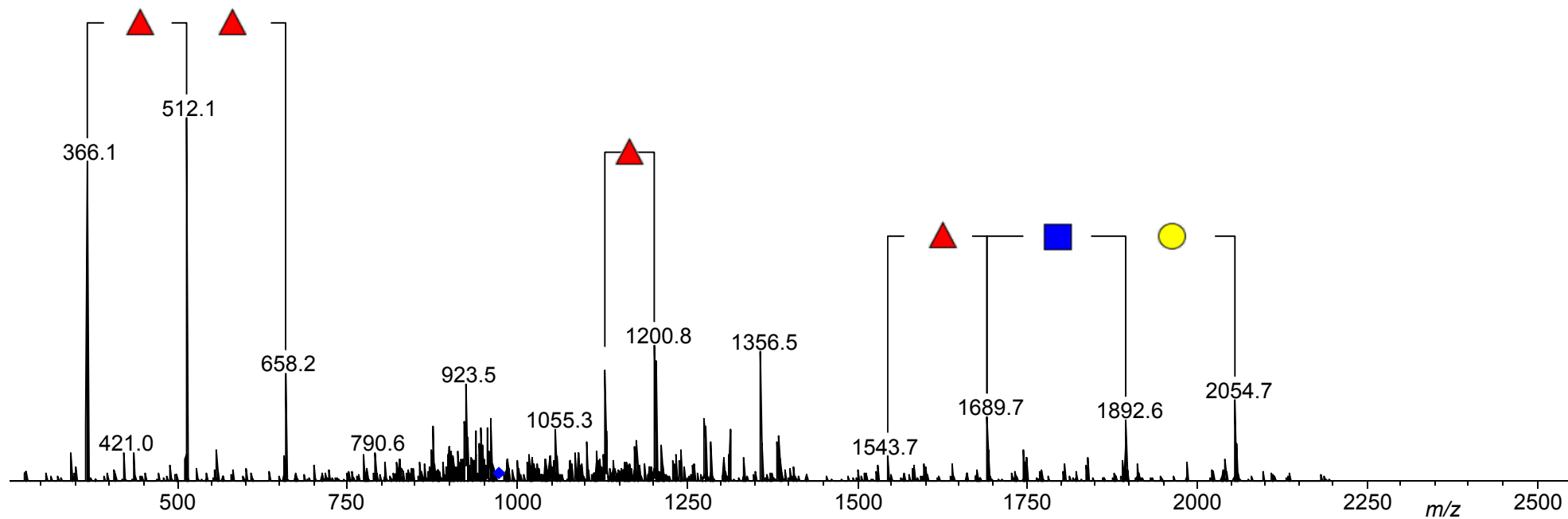
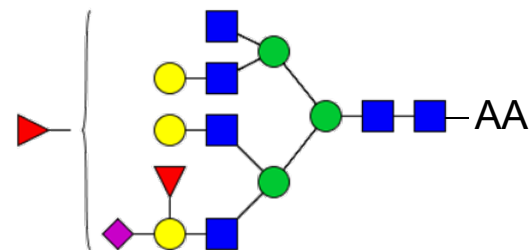
dHex2Hex5HexNAc6Neu5Ac1-AA



Spectrum 137

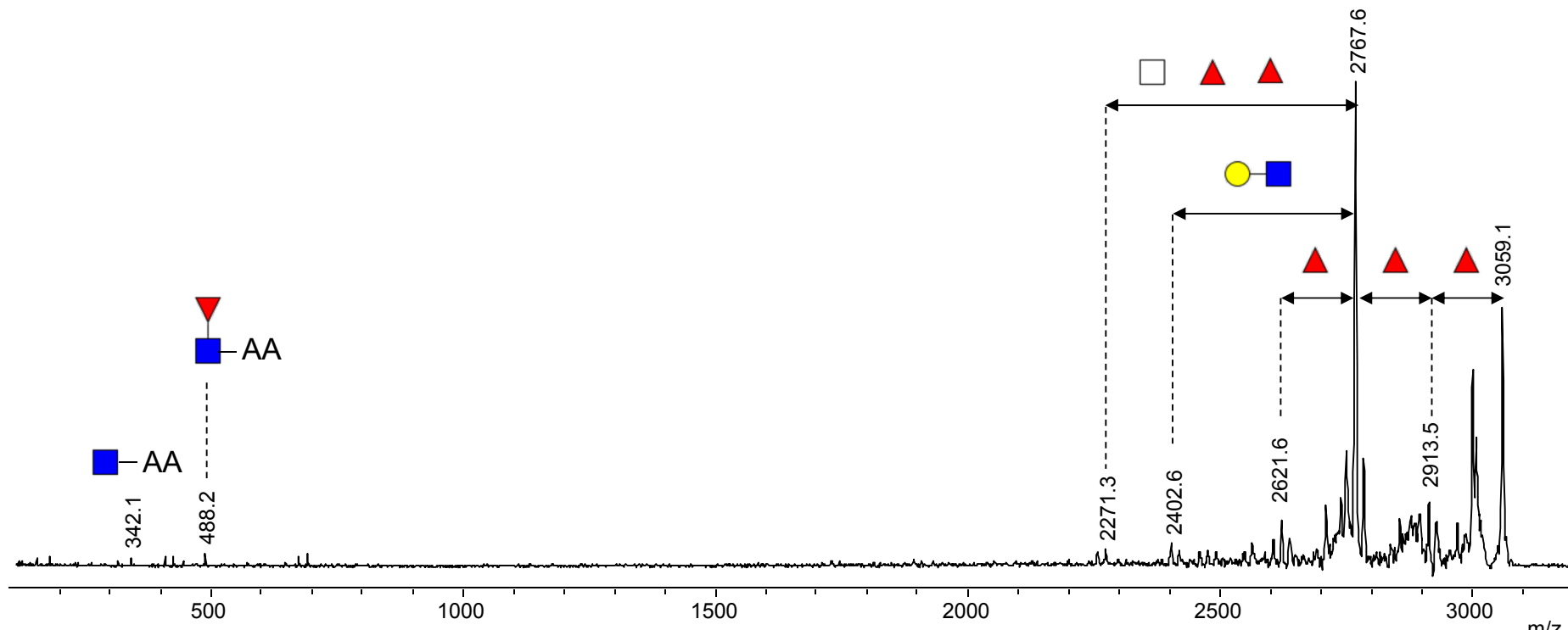


ESI MS/MS of $[972.3+3H]^{3+}$
dHex2Hex6HexNAc6Neu5Ac1-AA

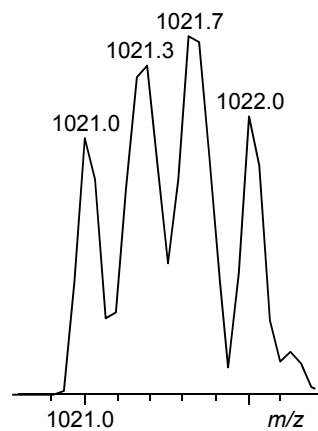


Spectrum 138

Lift of 3059.1 [M-H]⁻
dHex5Hex6HexNAc6-AA

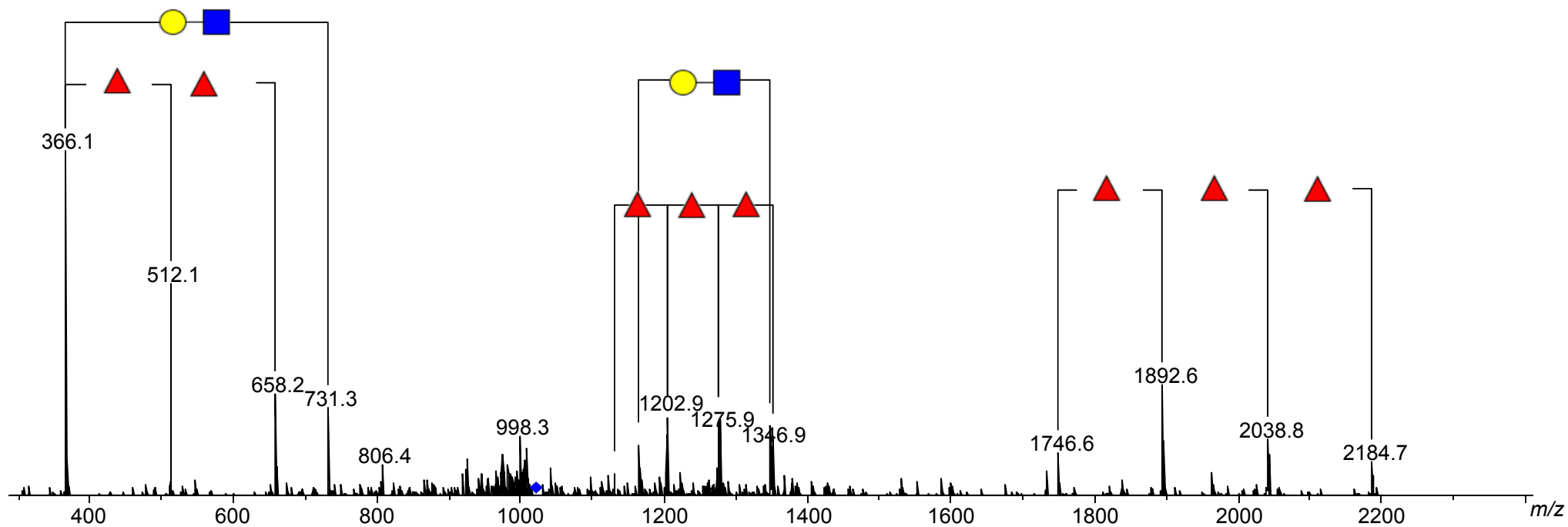
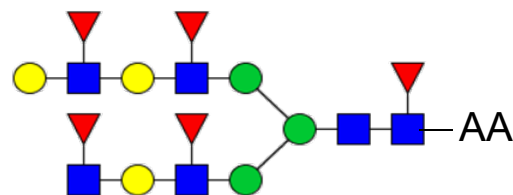


Spectrum 139



ESI MS/MS of $[1021.0 + 3H]^{3+}$

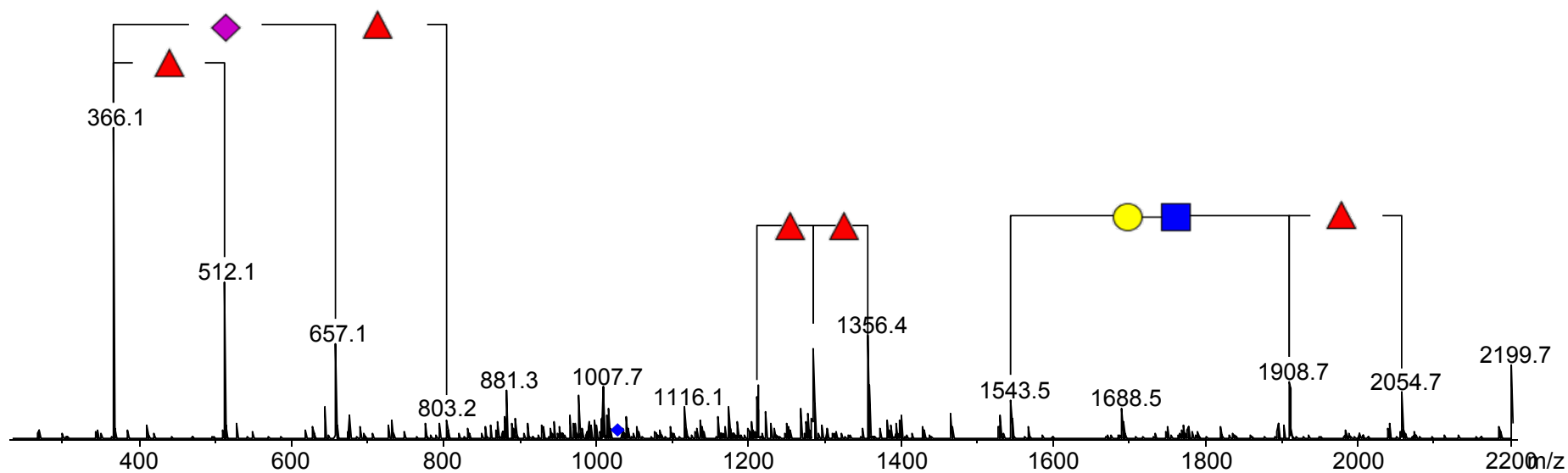
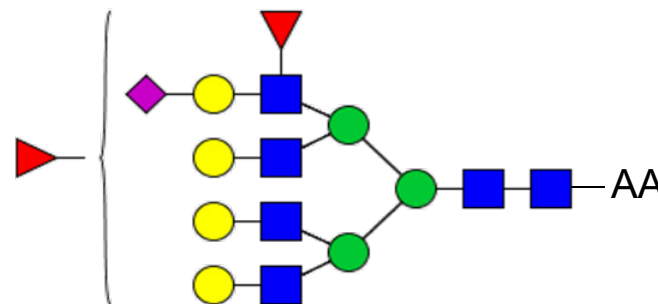
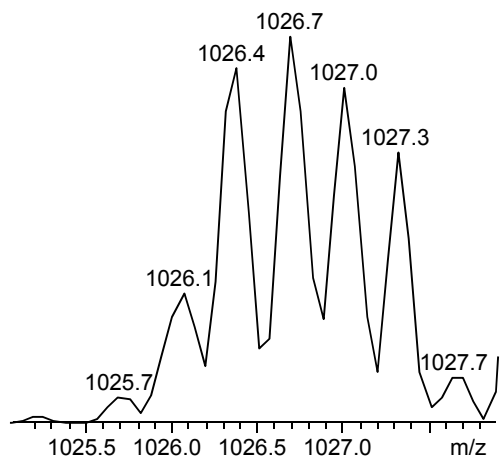
dHex5Hex6HexNAc6-AA



Spectrum 140

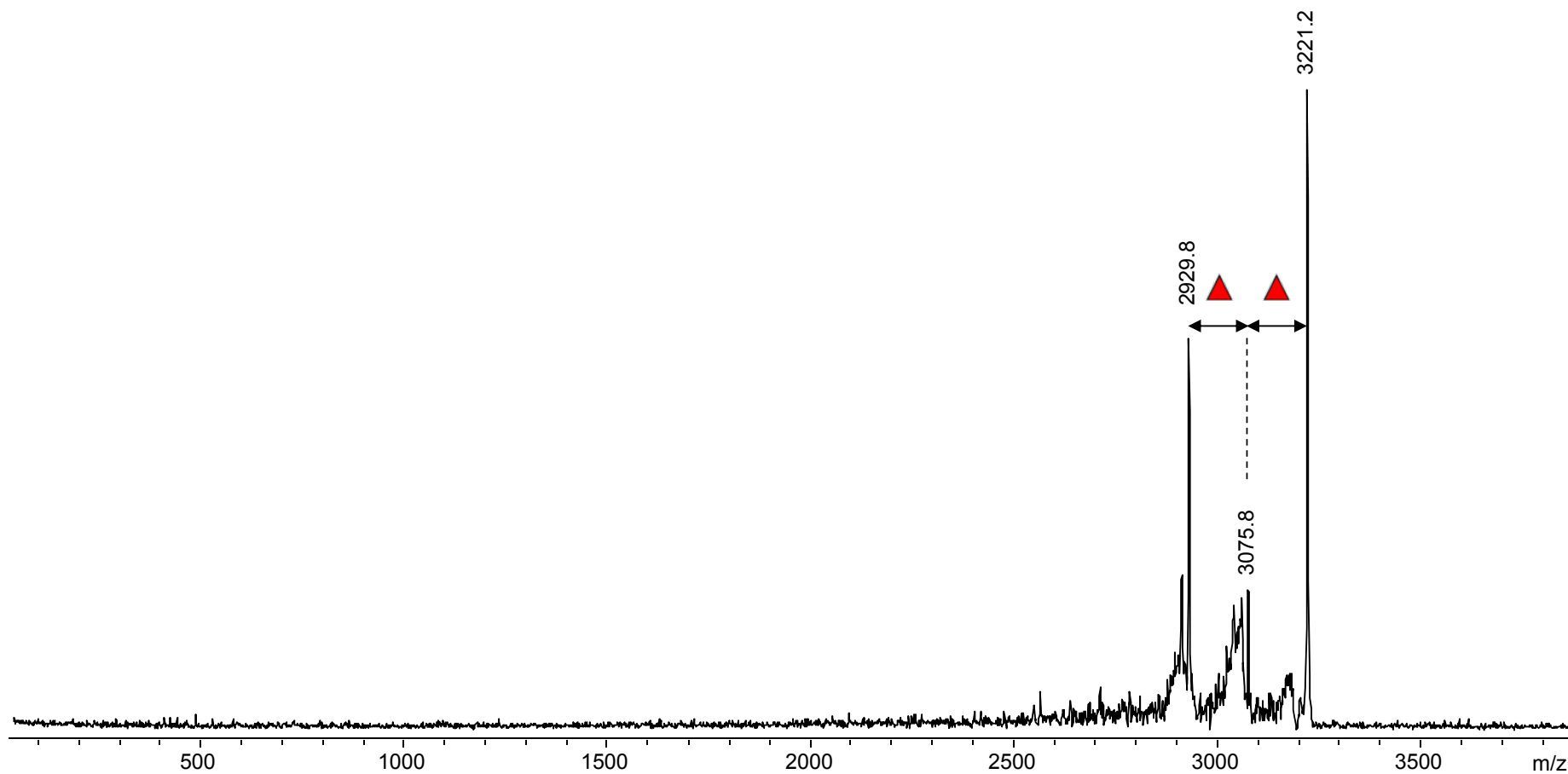
ESI MS/MS of [1026.1 +3H]³⁺

dHex2Hex7HexNAc6Neu5Ac1-AA

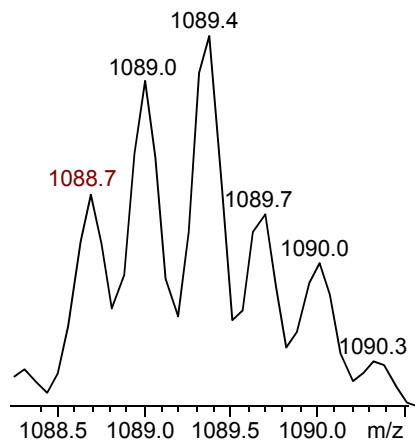


Spectrum 141

Lift of 3221.2 [M-H]⁻
dHex5Hex7HexNAc6-AA

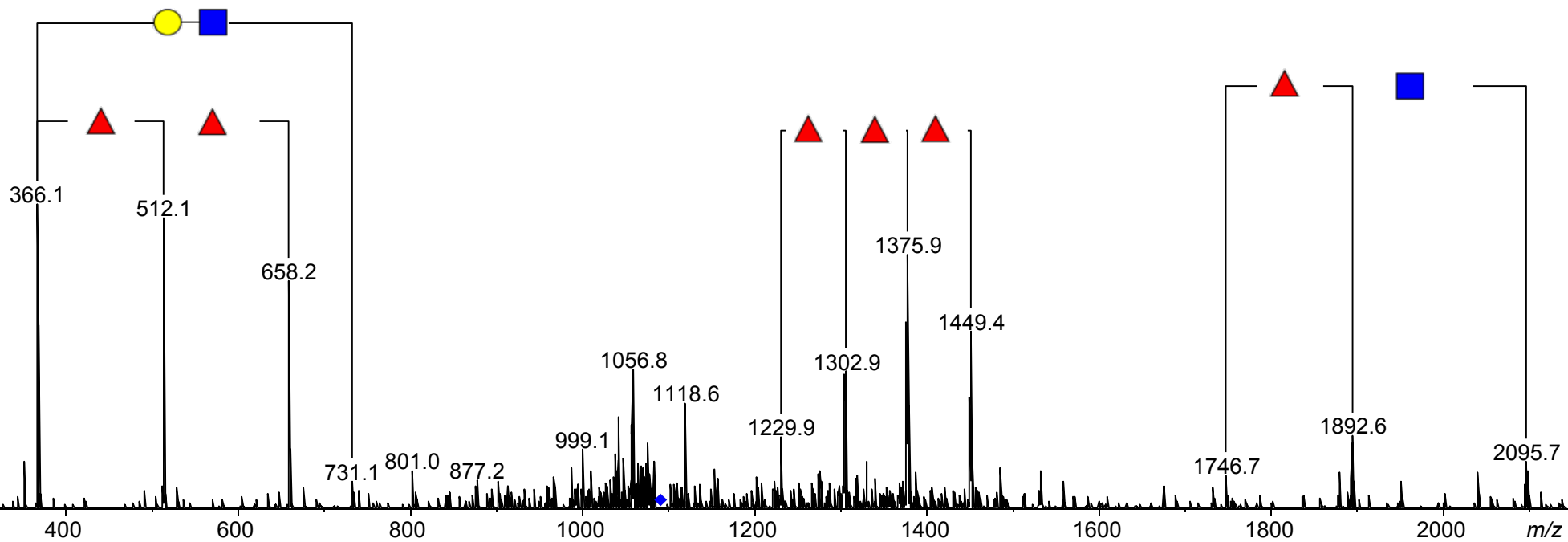
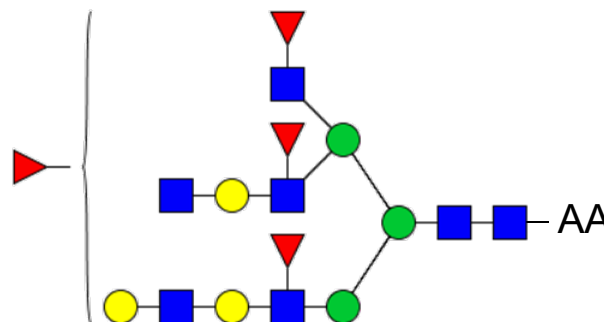


Spectrum 142



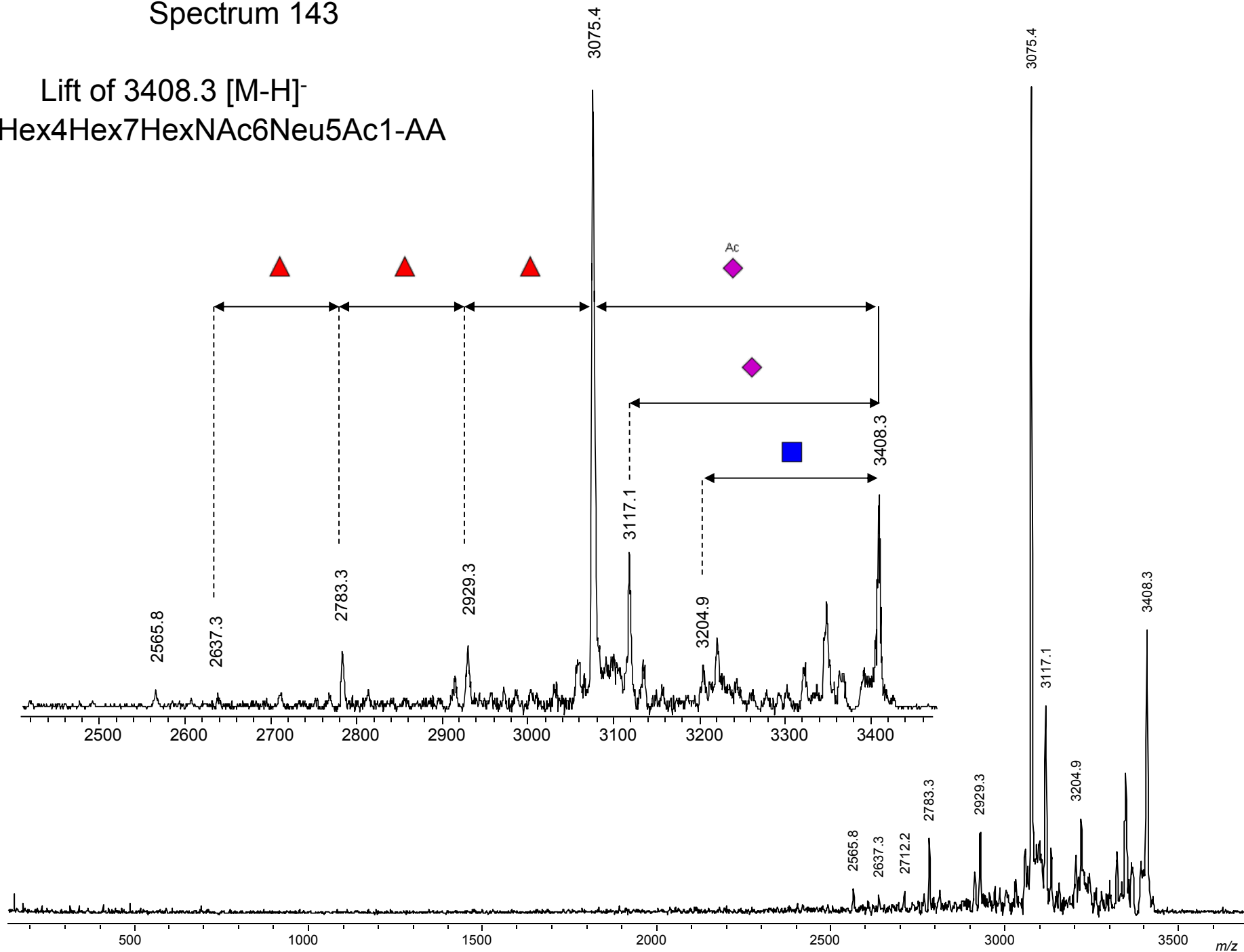
ESI MS/MS of [1088.7 + 3H]³⁺

dHex5Hex6HexNAc7-AA



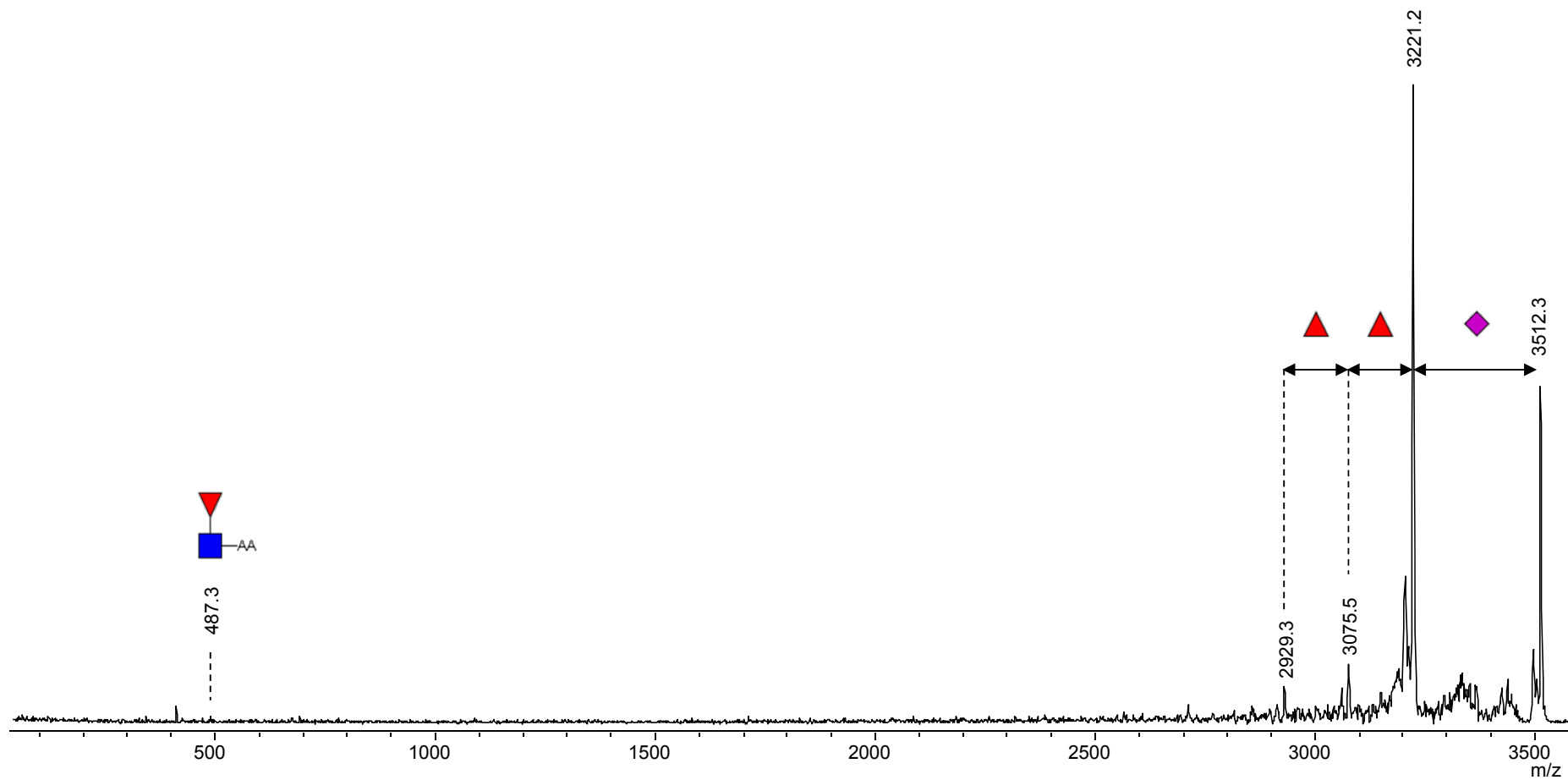
Spectrum 143

Lift of 3408.3 [M-H]⁻
Ac1dHex4Hex7HexNAc6Neu5Ac1-AA



Spectrum 144

Lift of 3512.2 [M-H]⁻
dHex5Hex7HexNAc6Neu5Ac1-AA



Spectrum 145

Lift of 3715.6 [M-H]⁻
dHex5Hex7HexNAc7Neu5Ac1-AA

