

Supplementary Data 1:

Ion Mobility-Tandem Mass Spectrometry of Mucin-type O-Glycans

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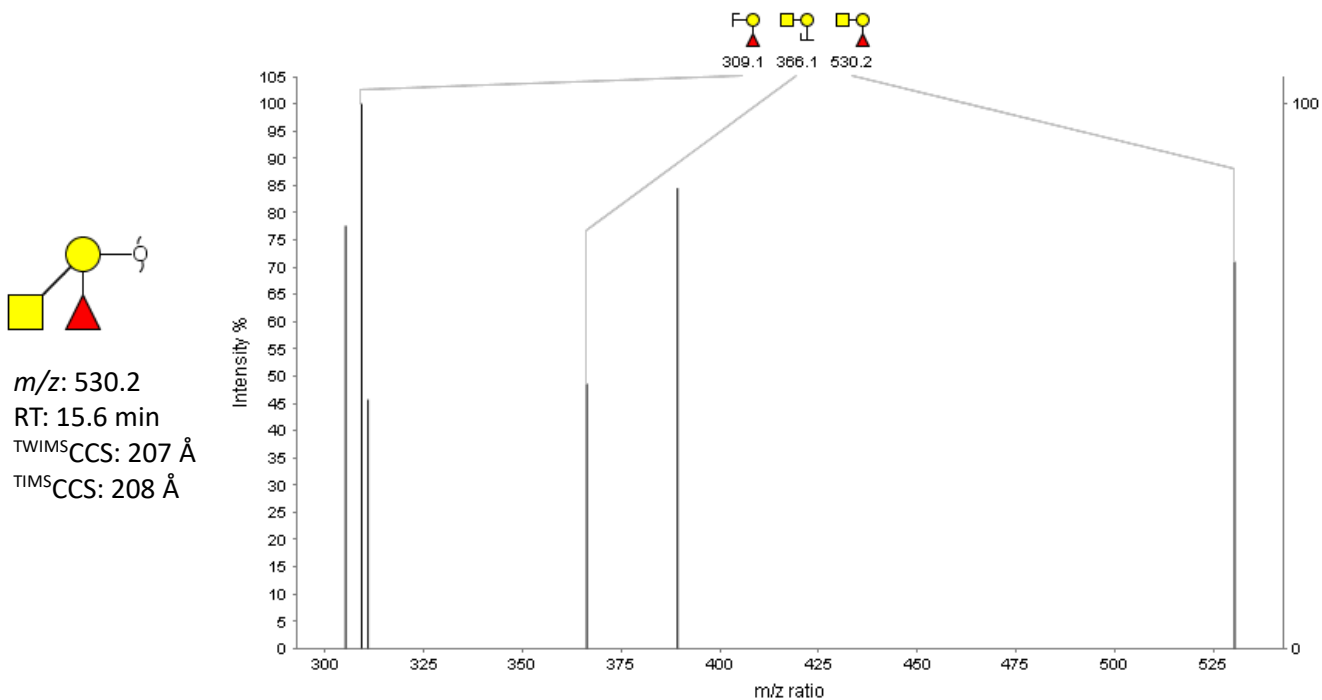
*email: kevin.pagel@fu-berlin.de

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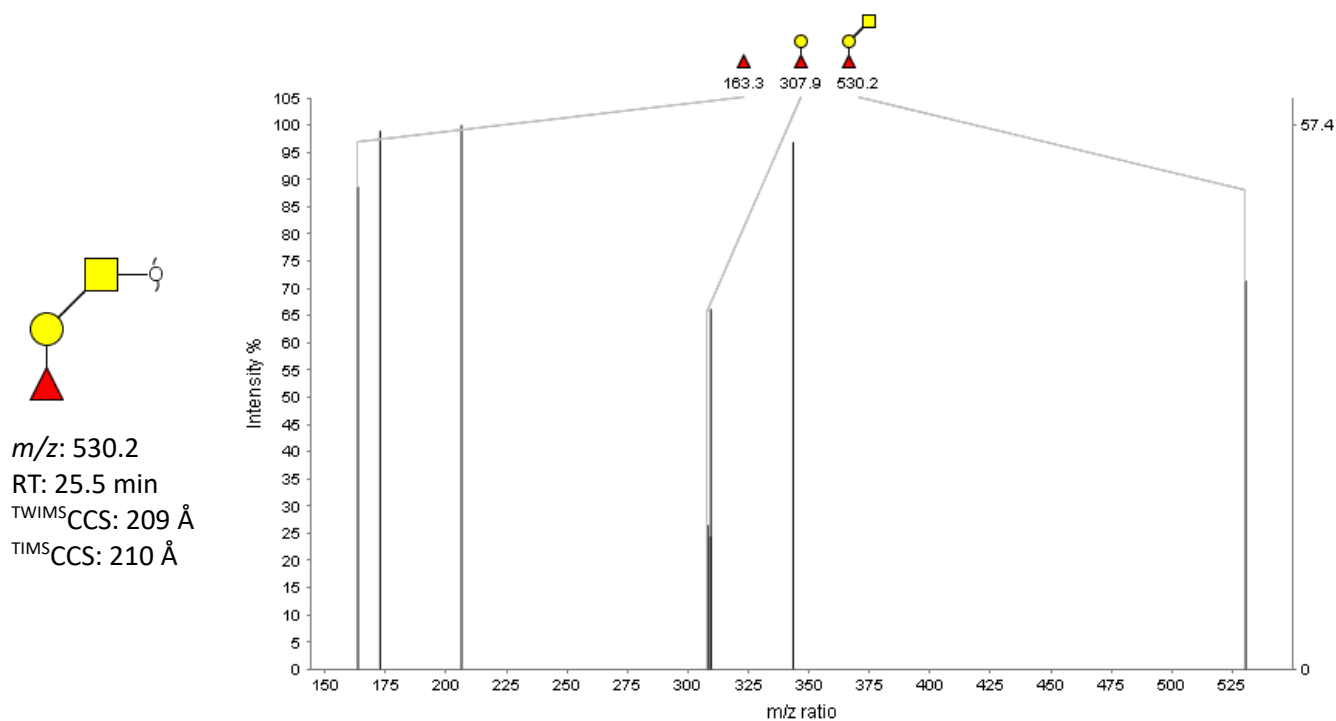
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I. Annotated MS/MS spectra of O-glycans in *porcine* gastric mucins

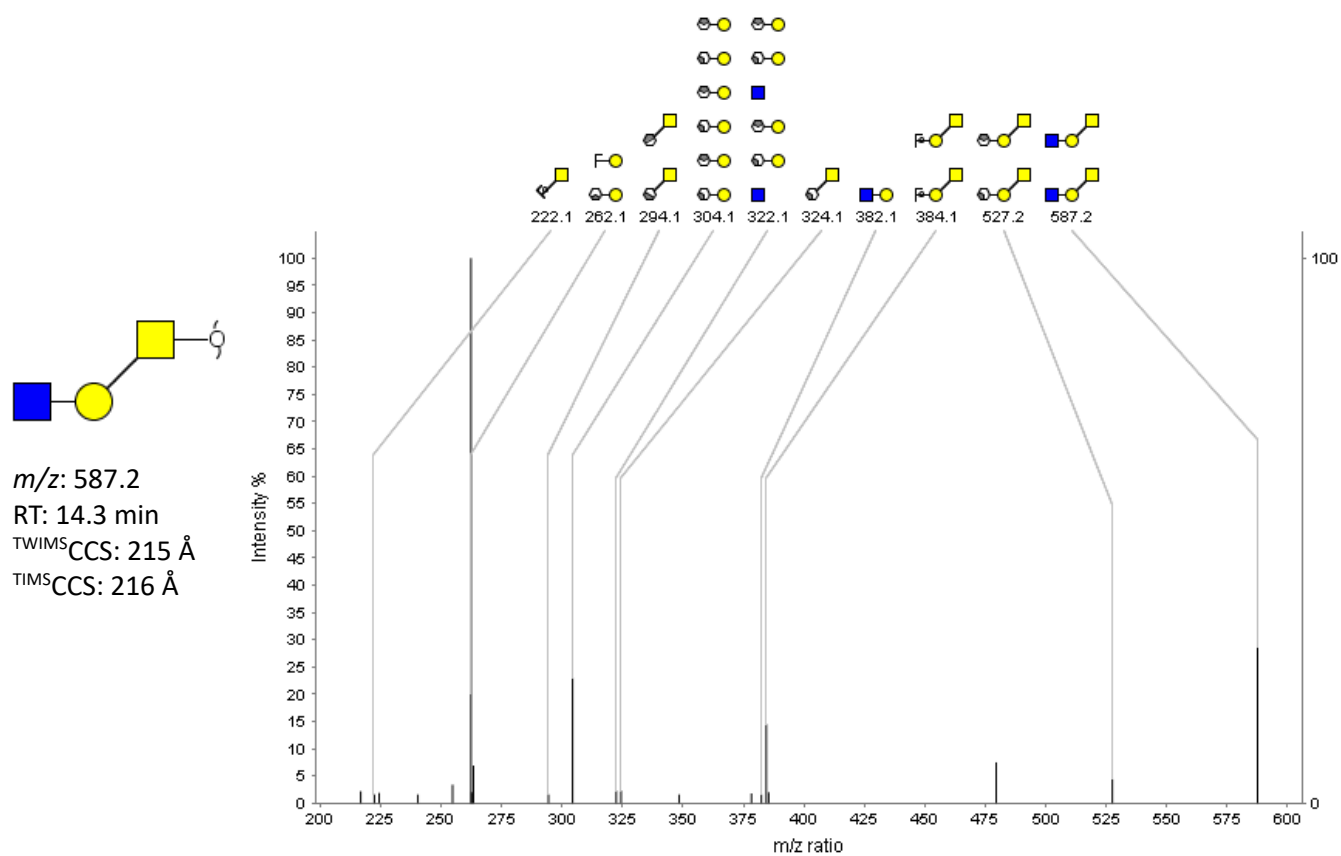
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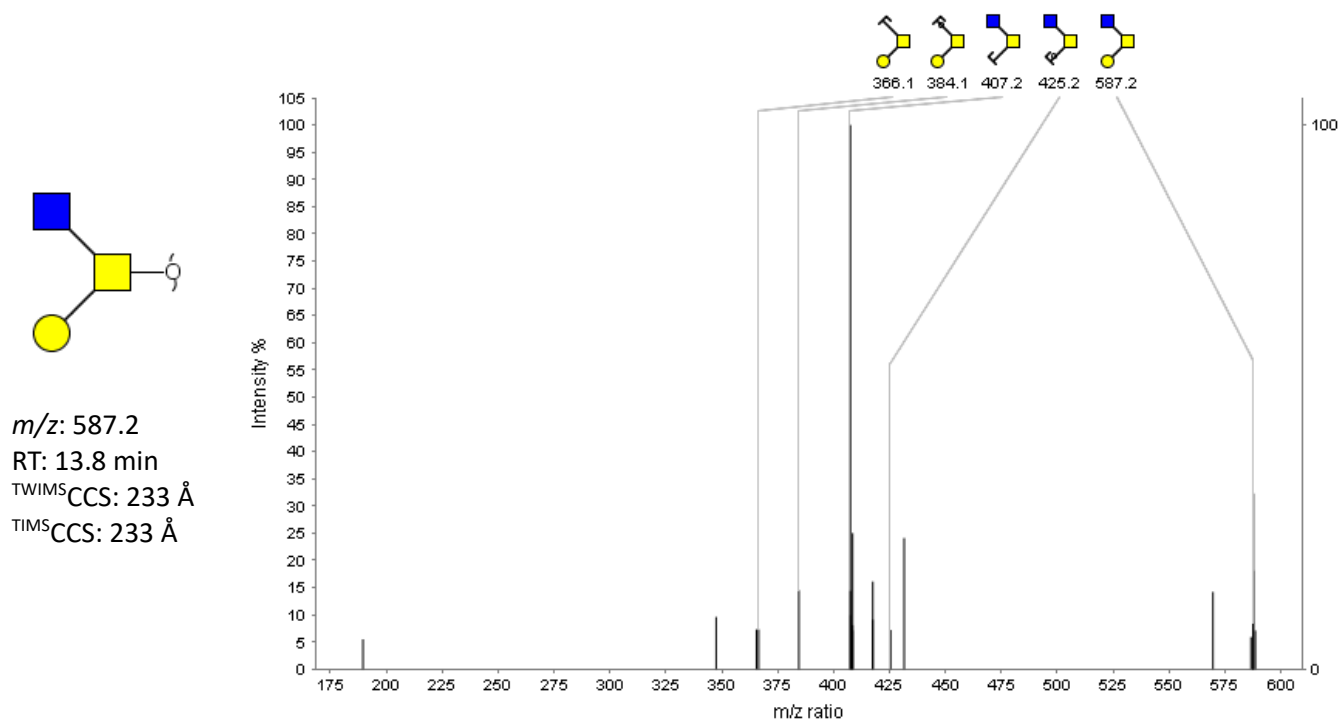
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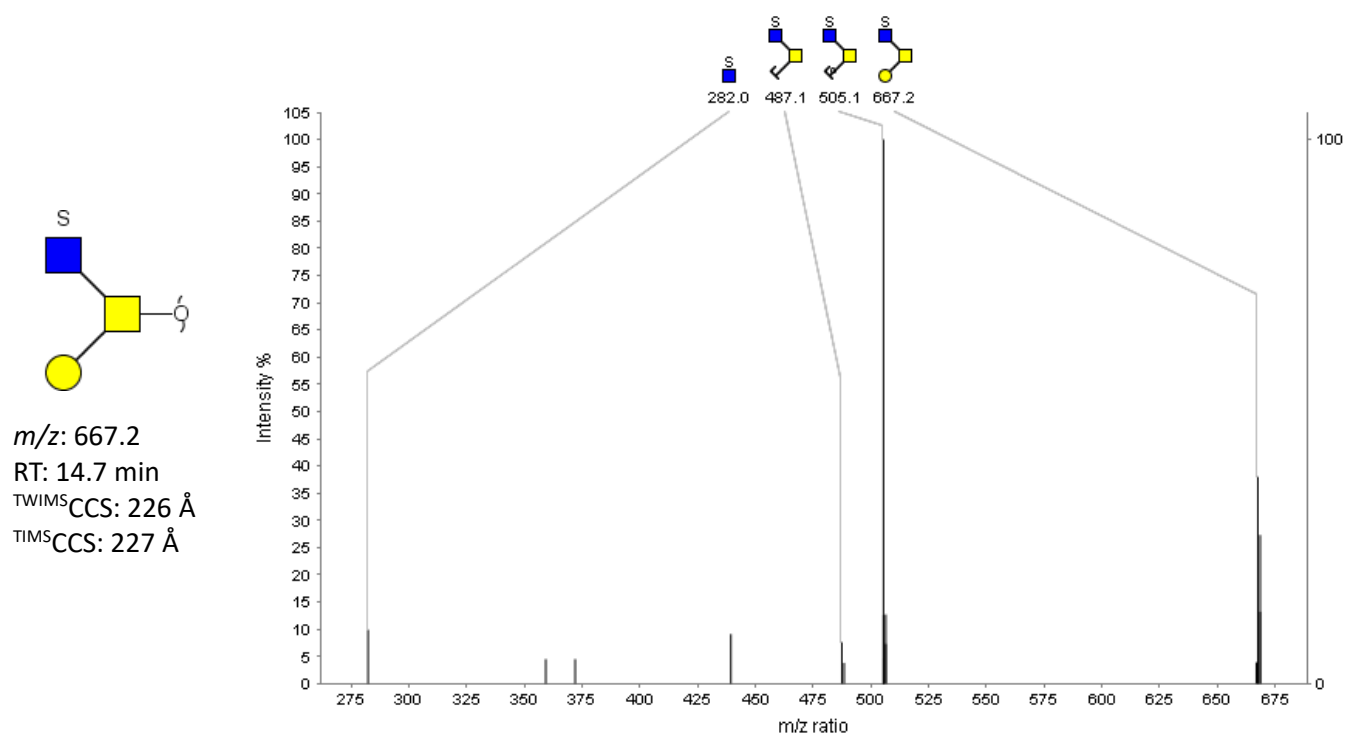
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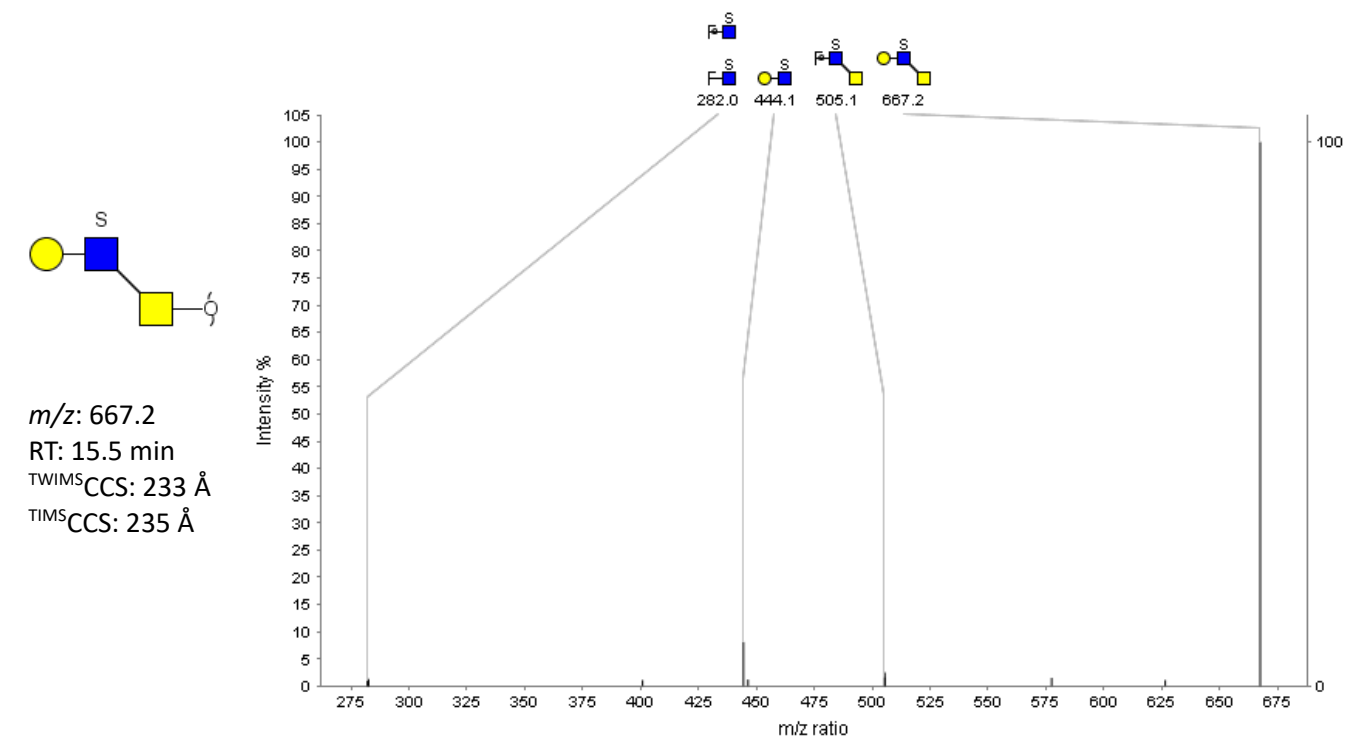
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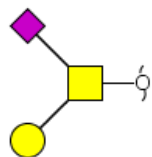
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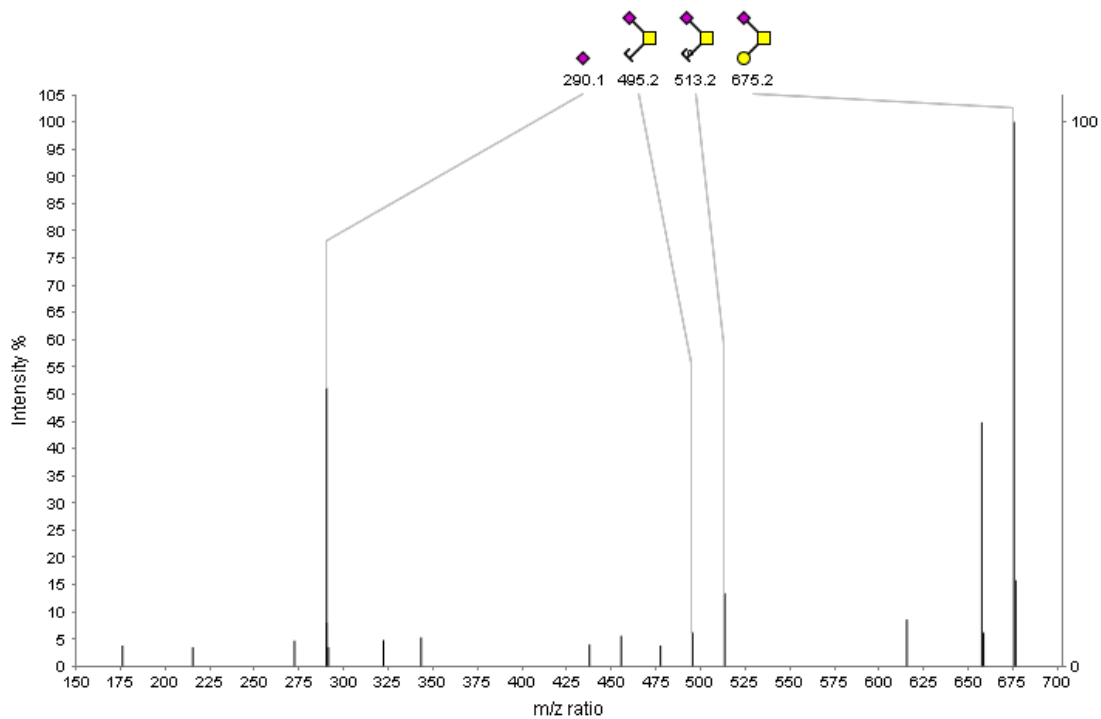
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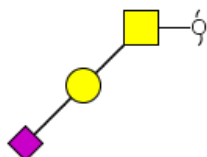
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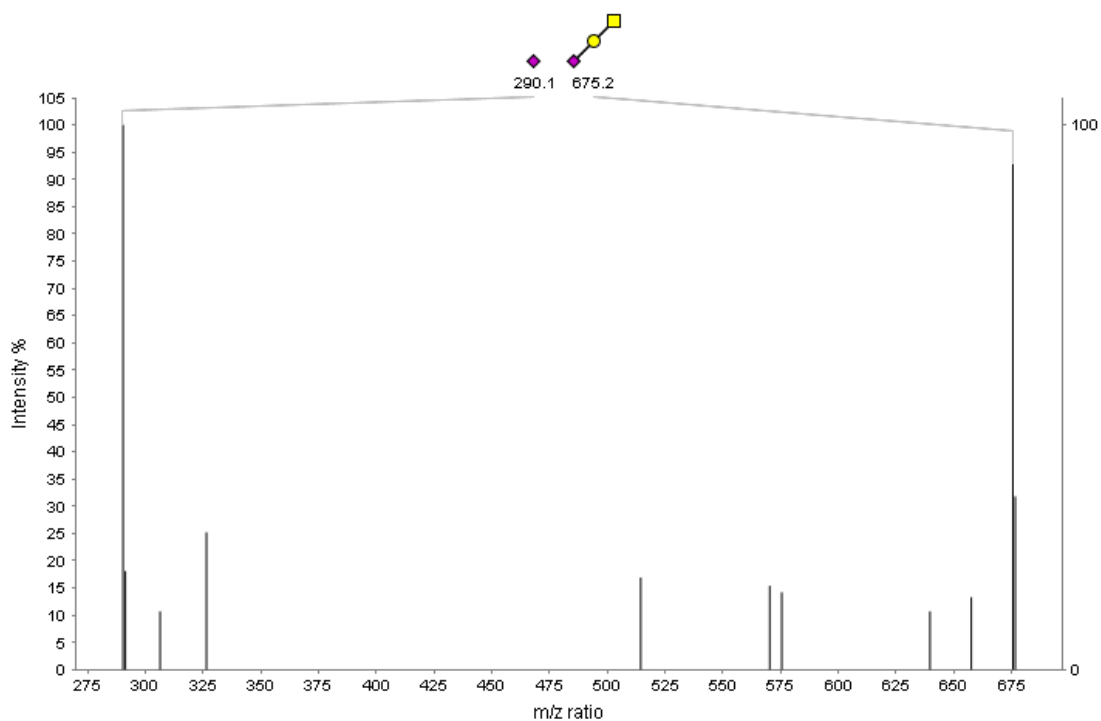
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 TIMS CCS: 246 Å



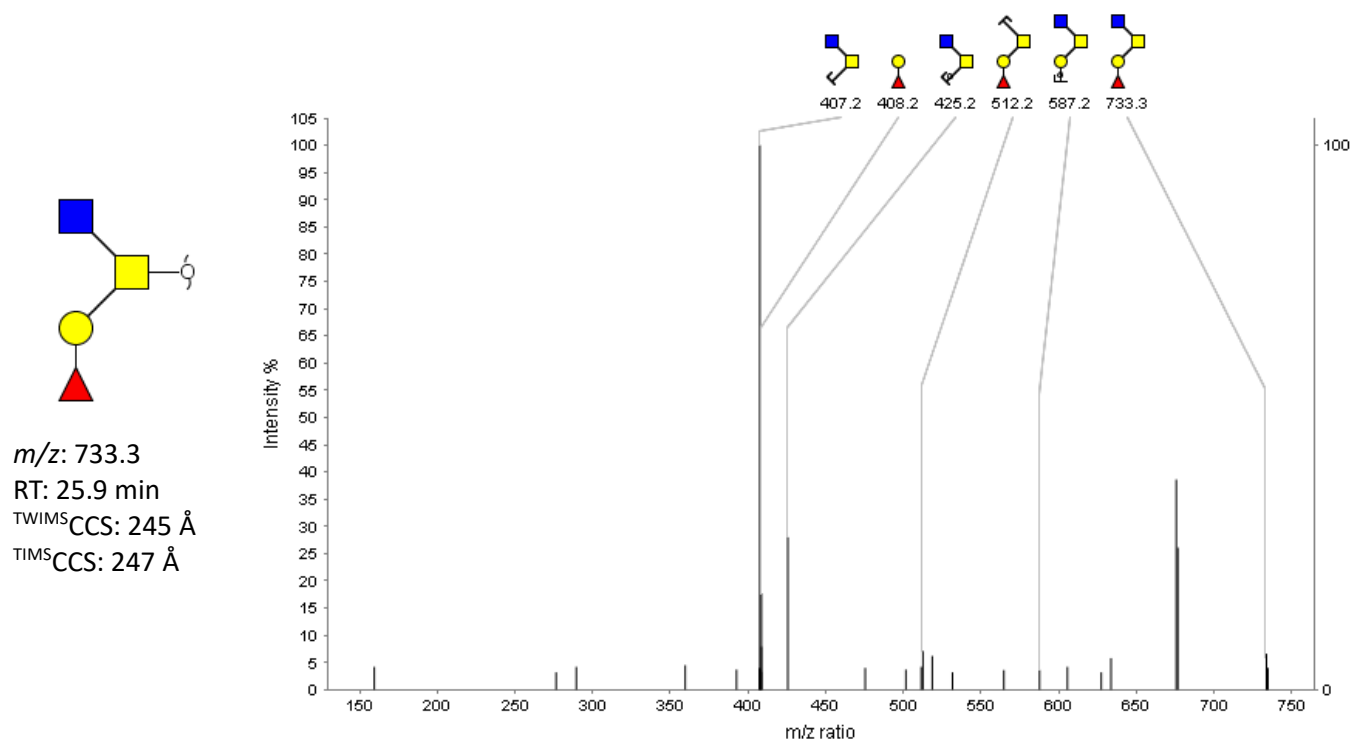
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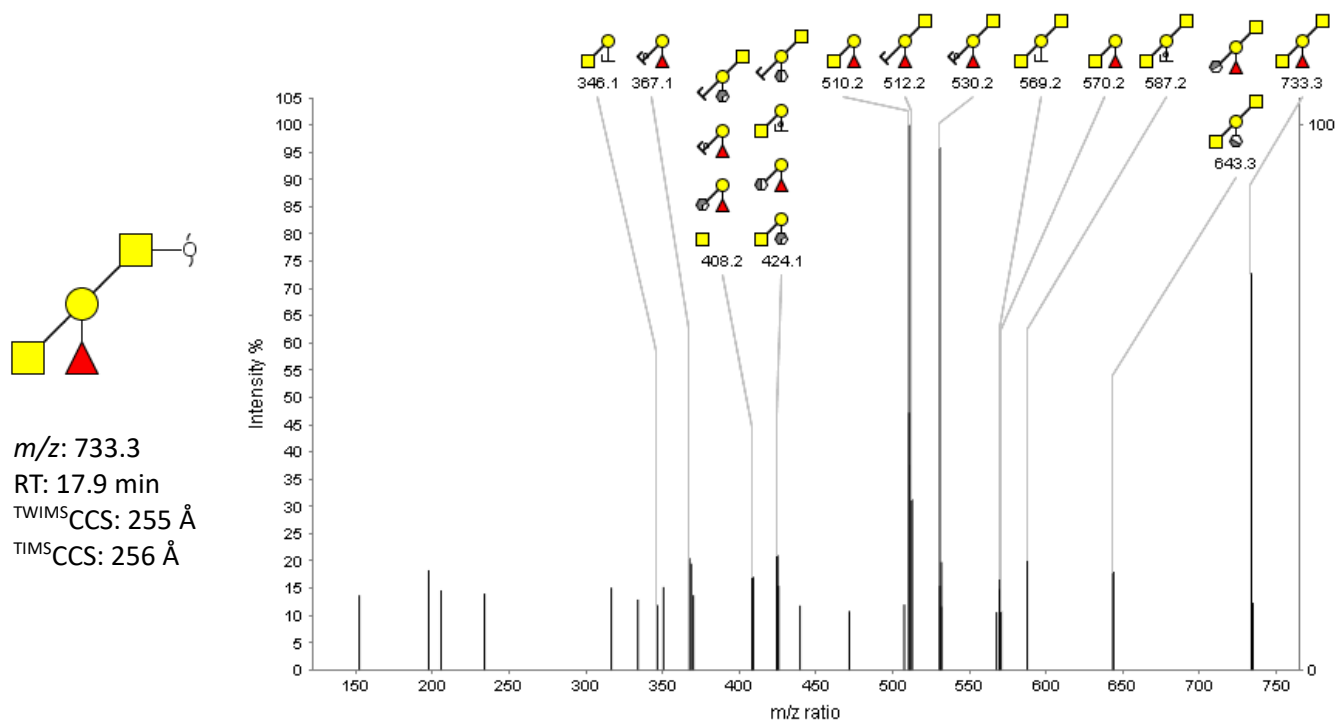
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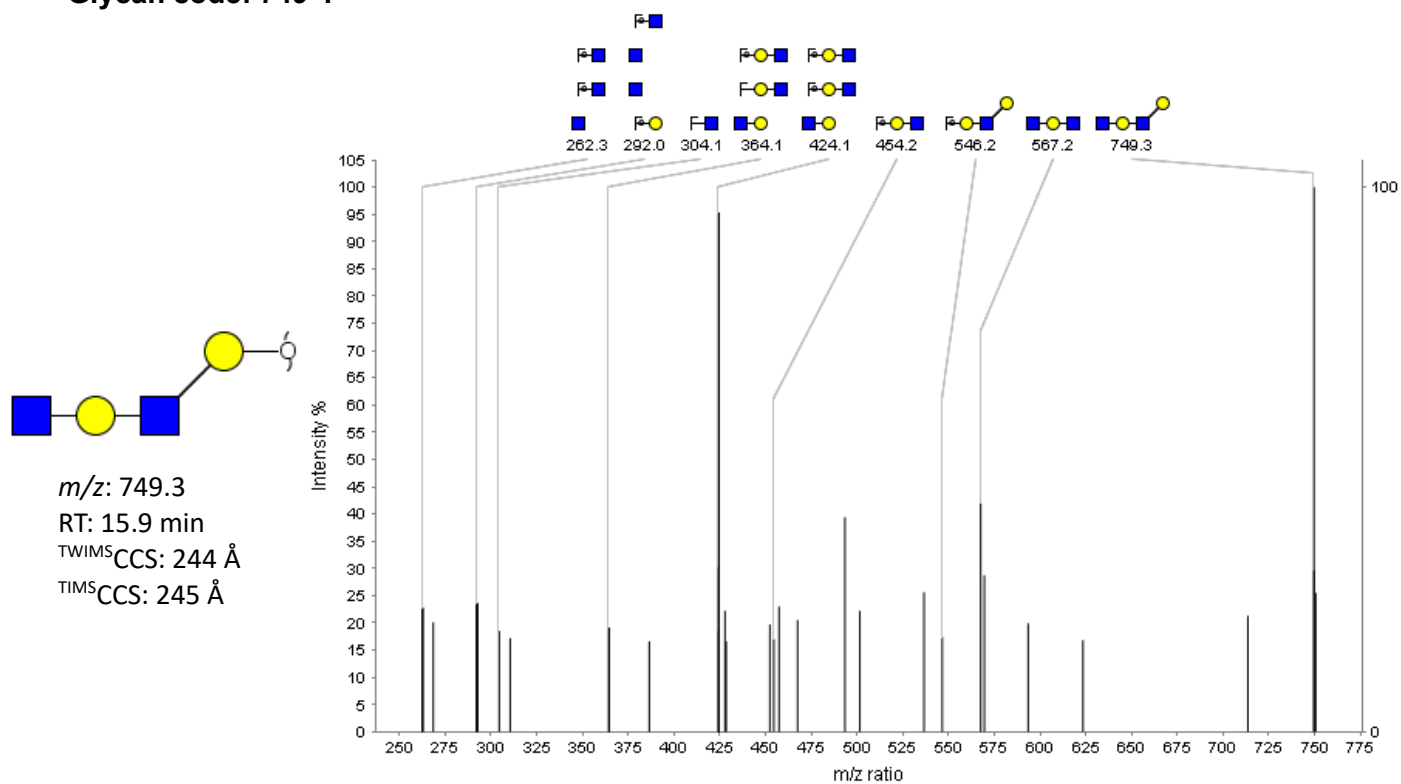
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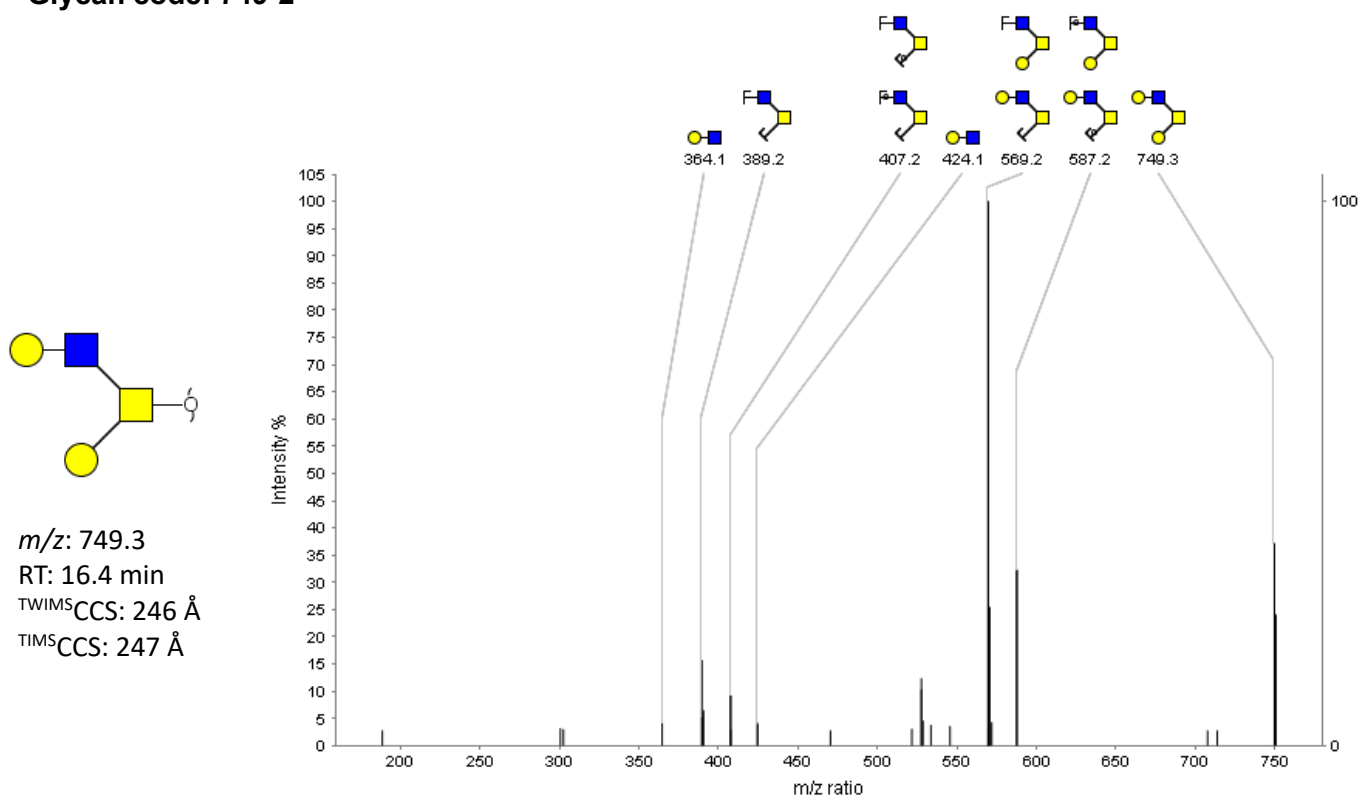
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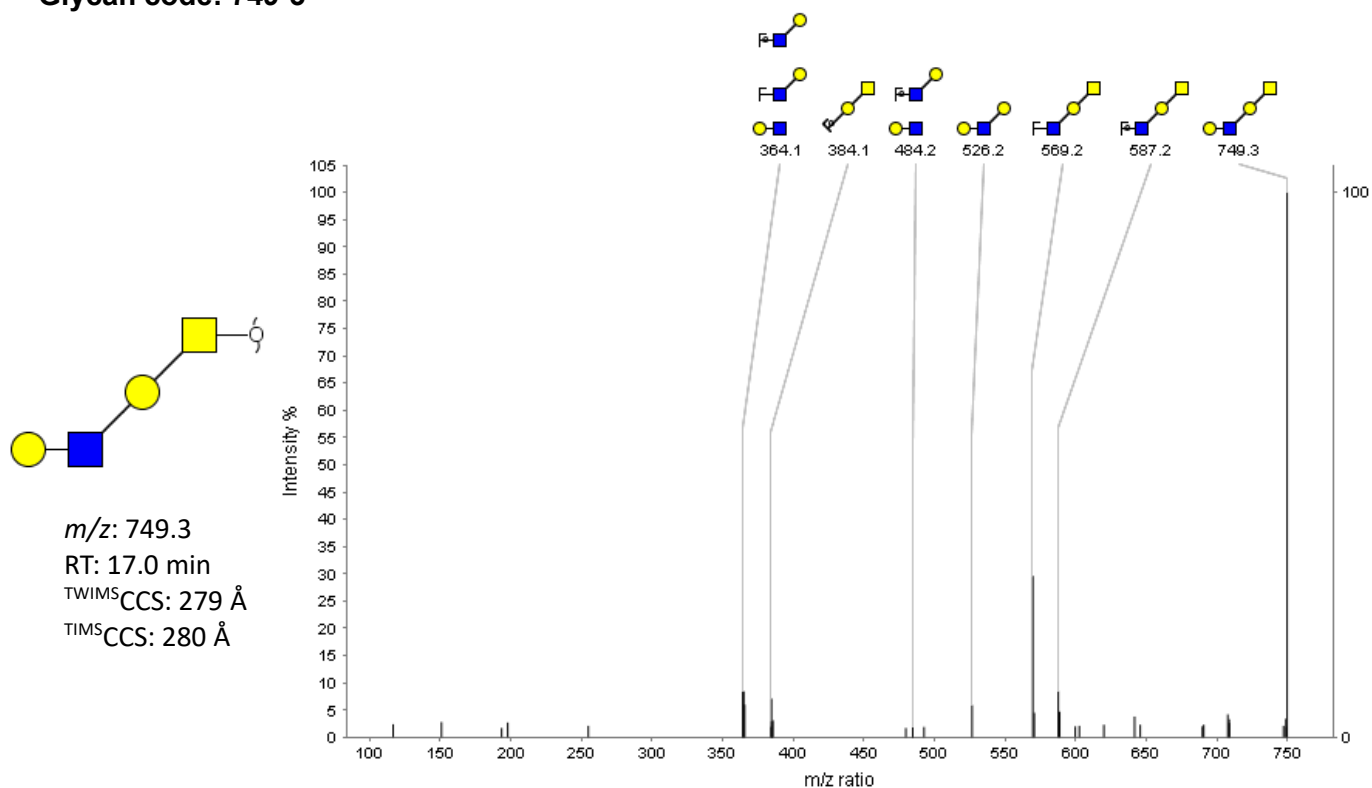
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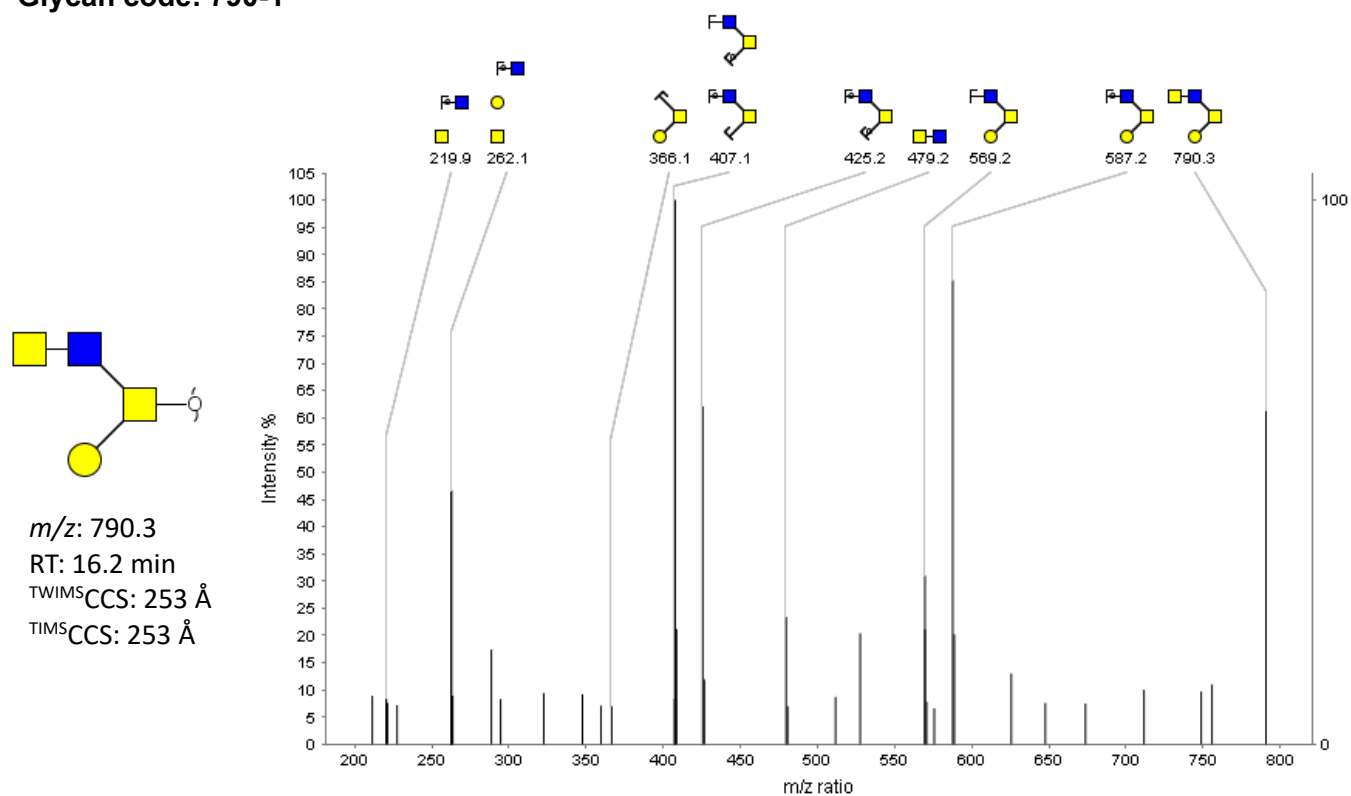
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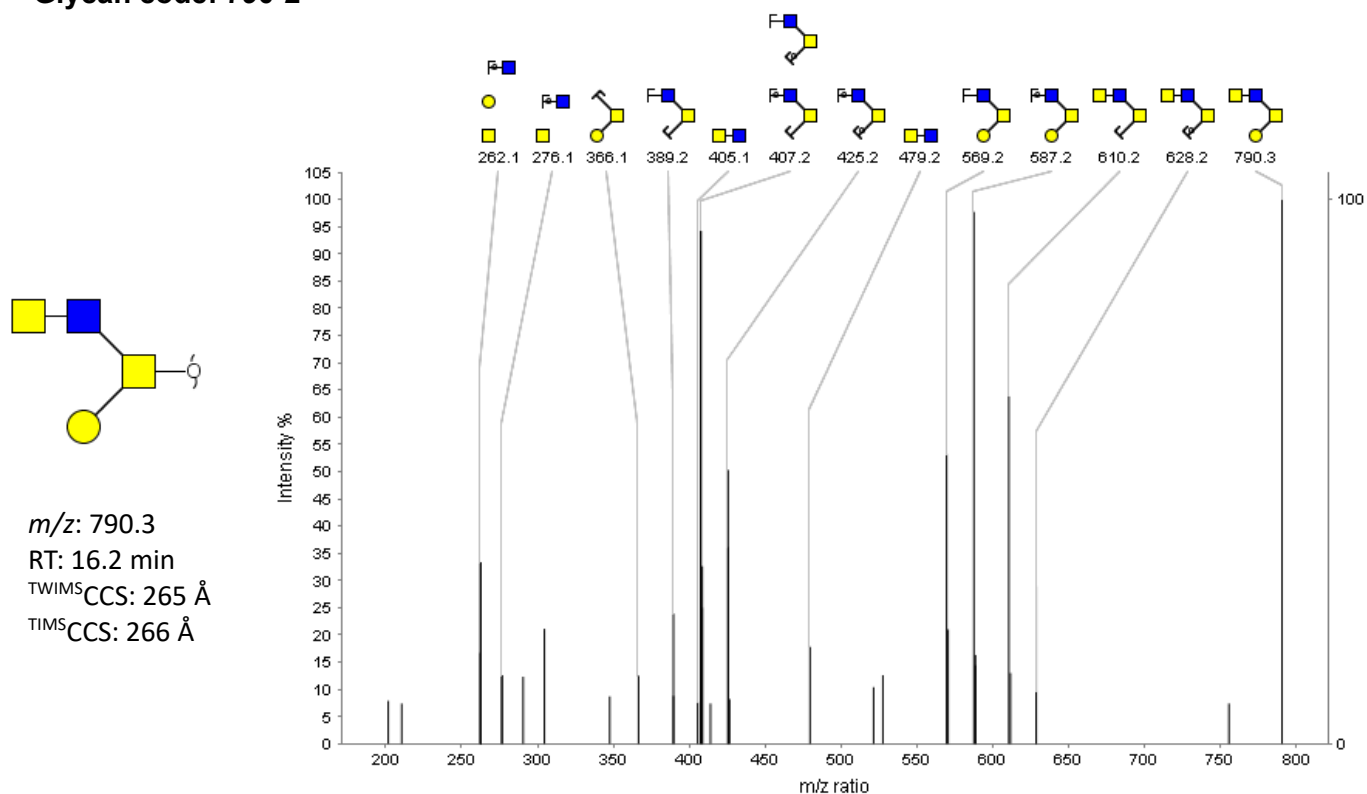
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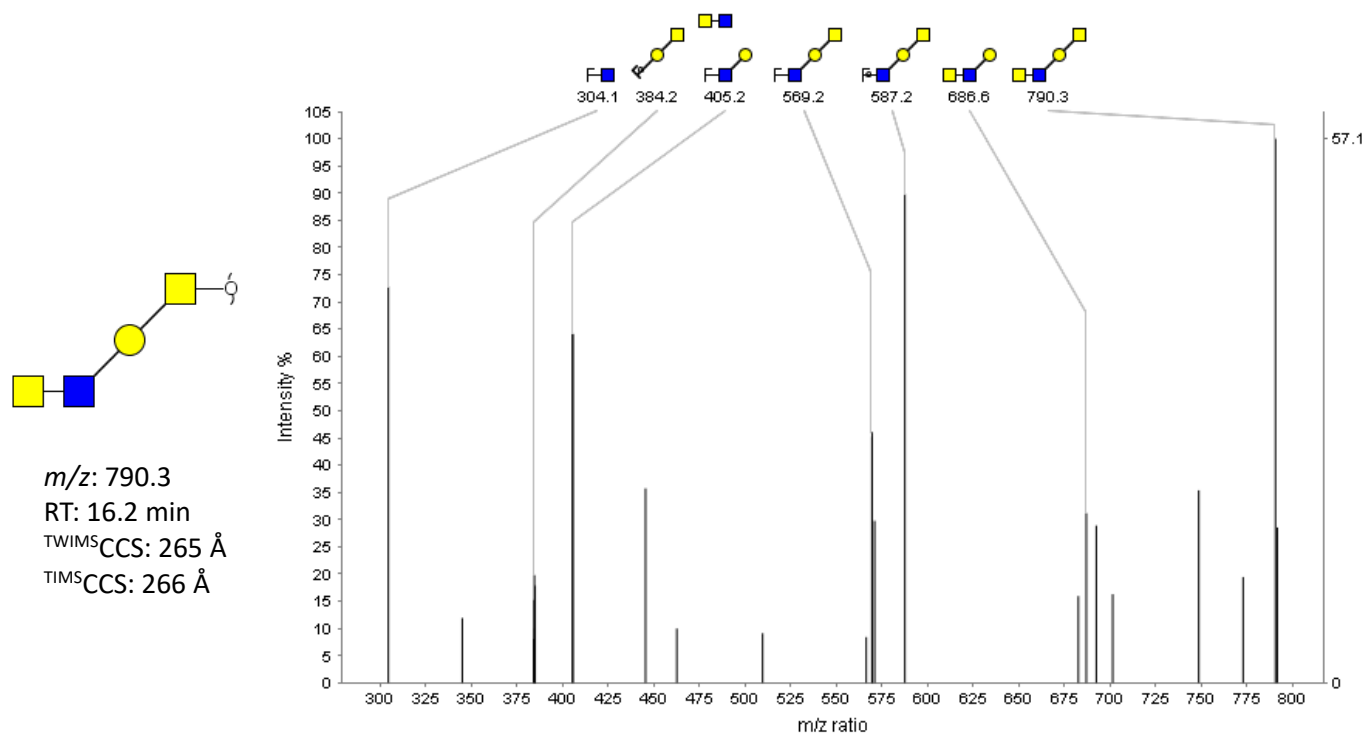
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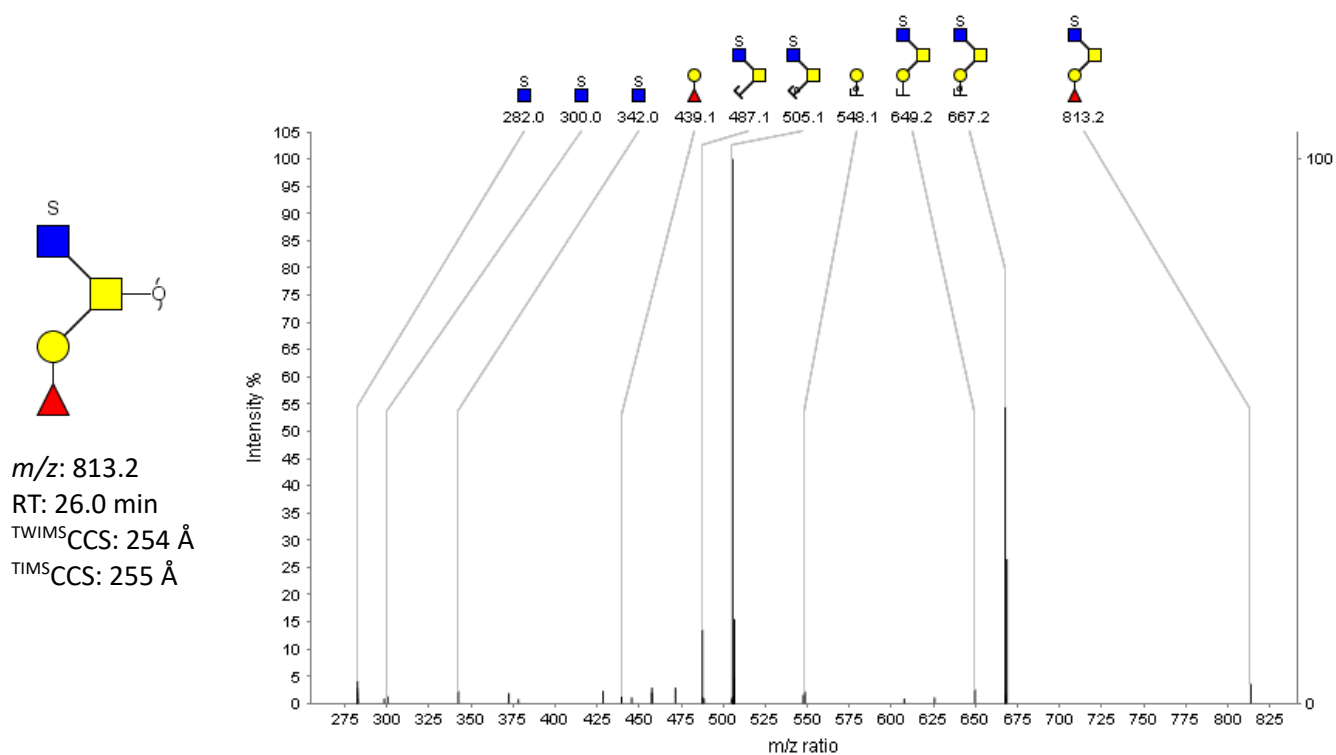
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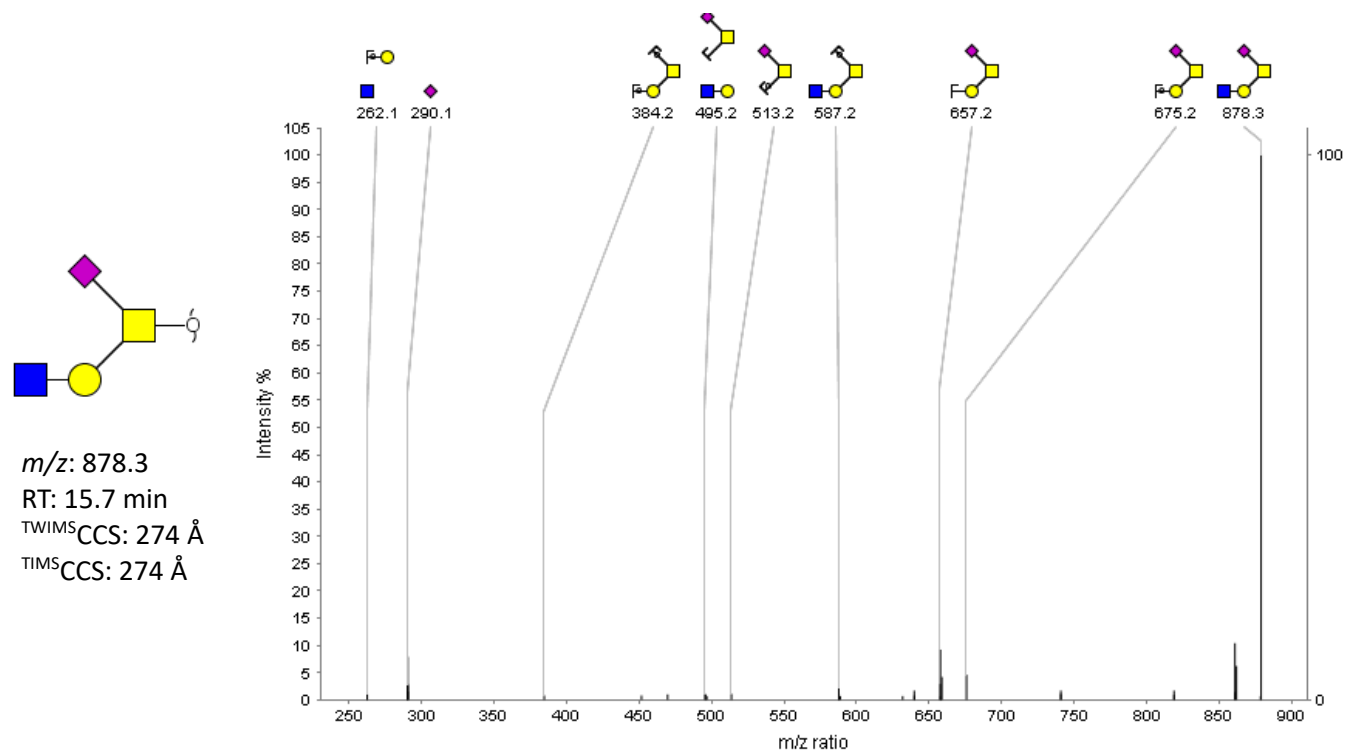
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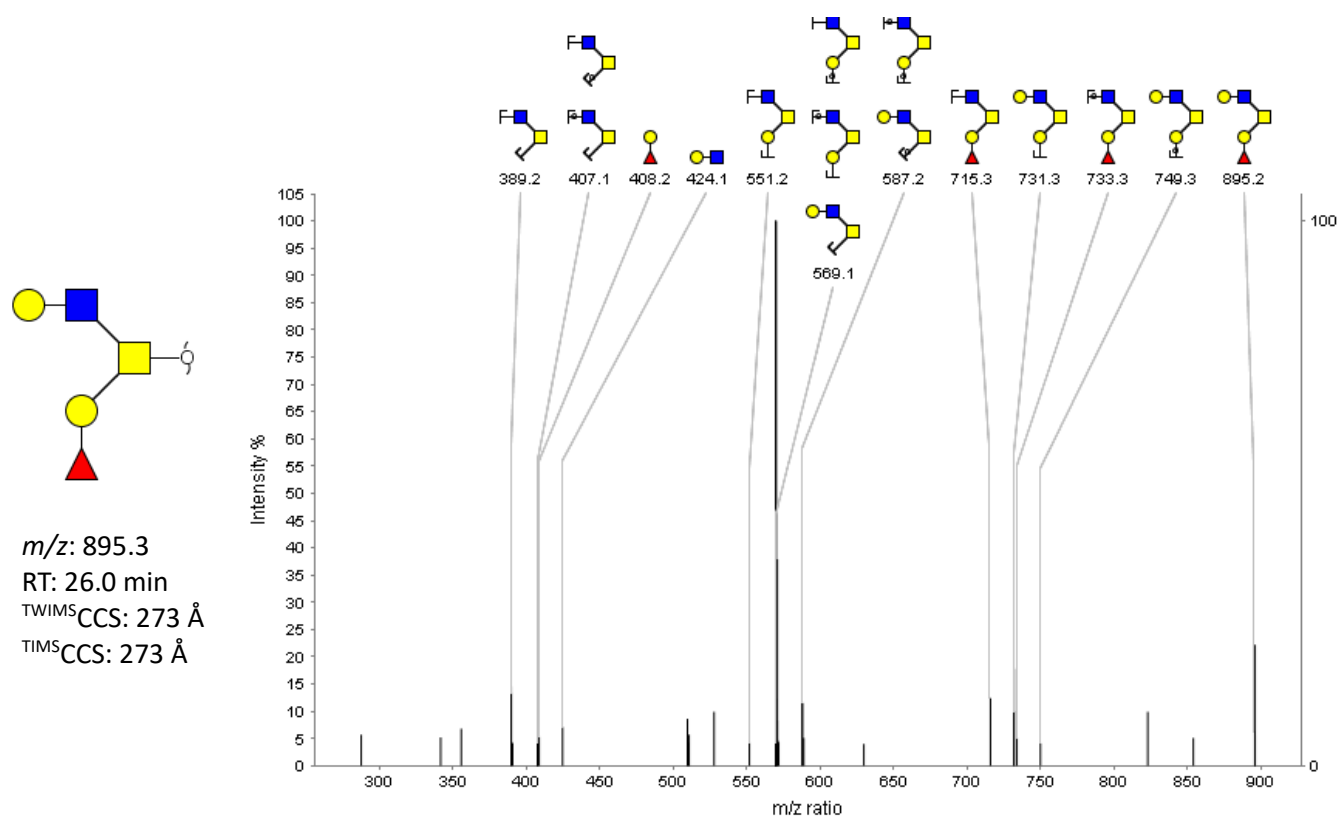
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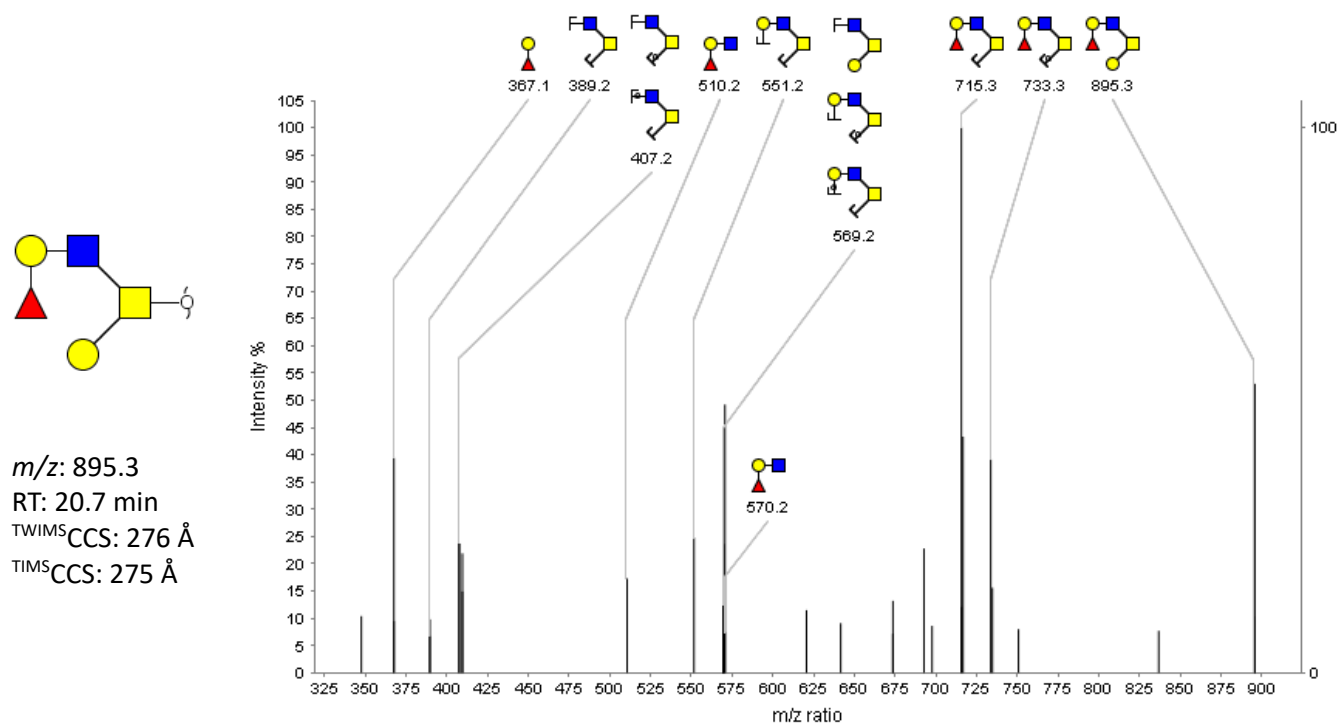
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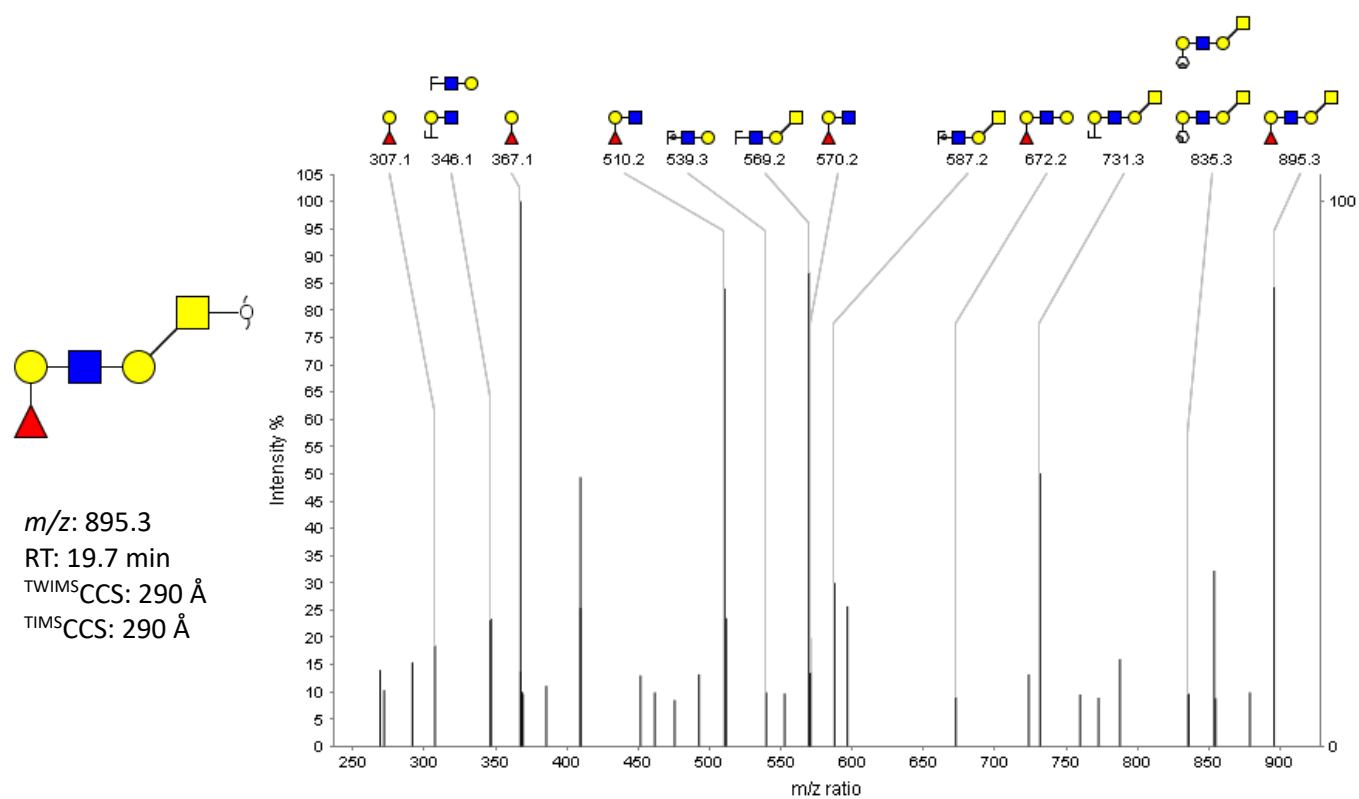
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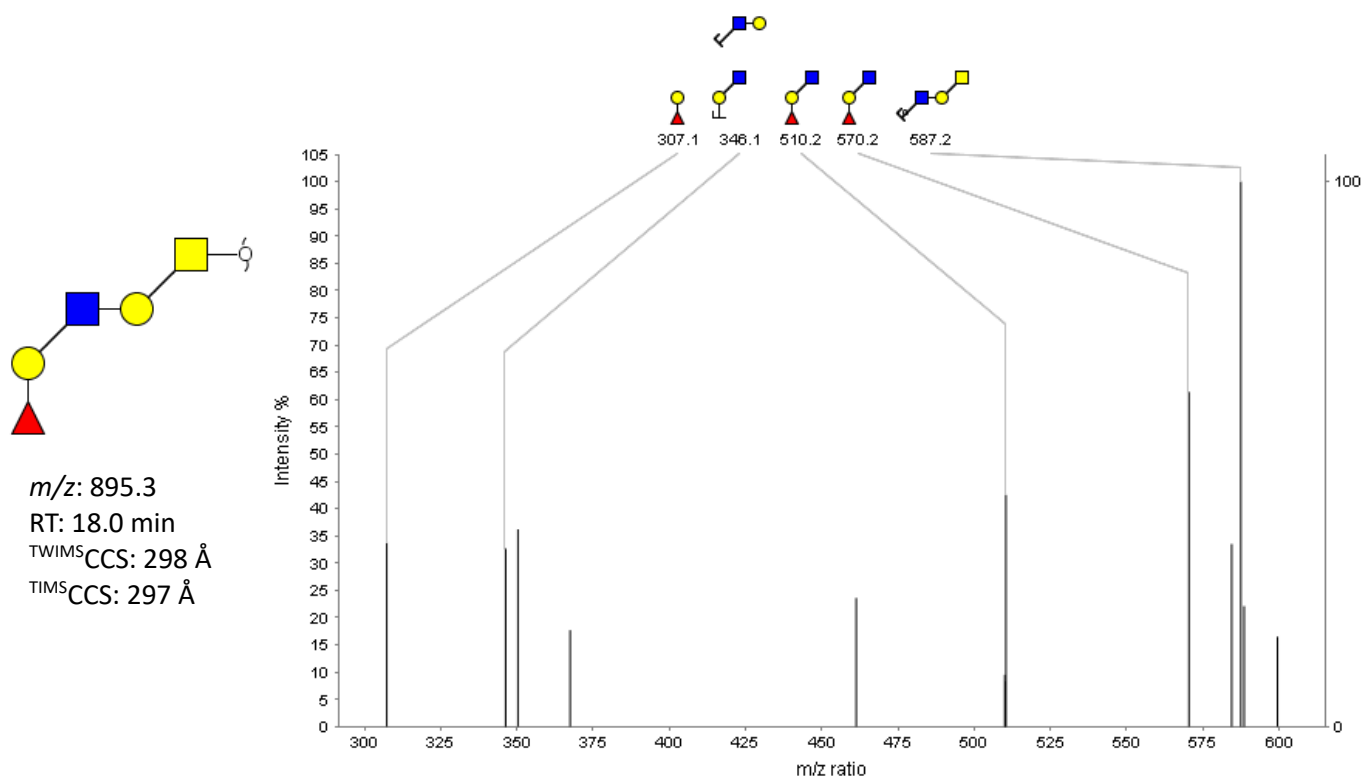
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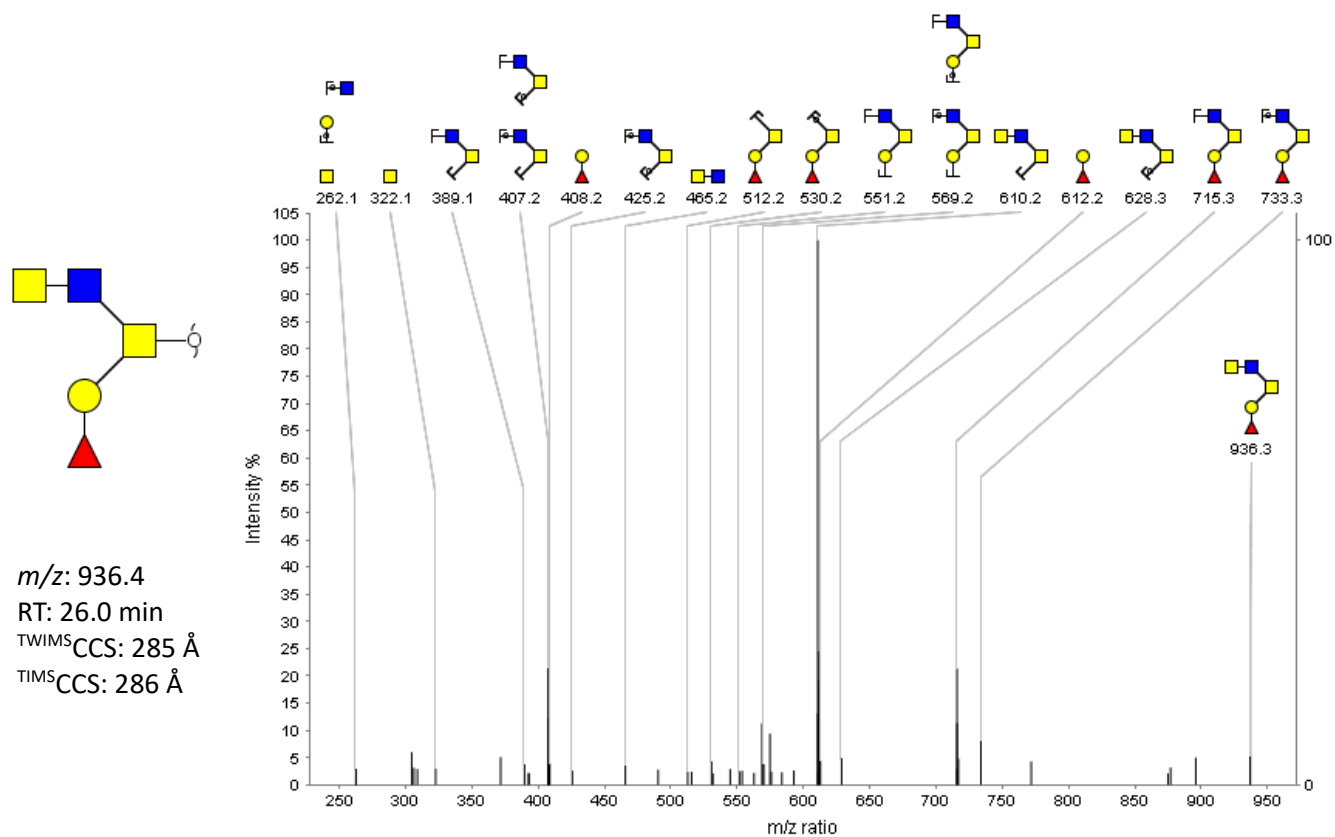
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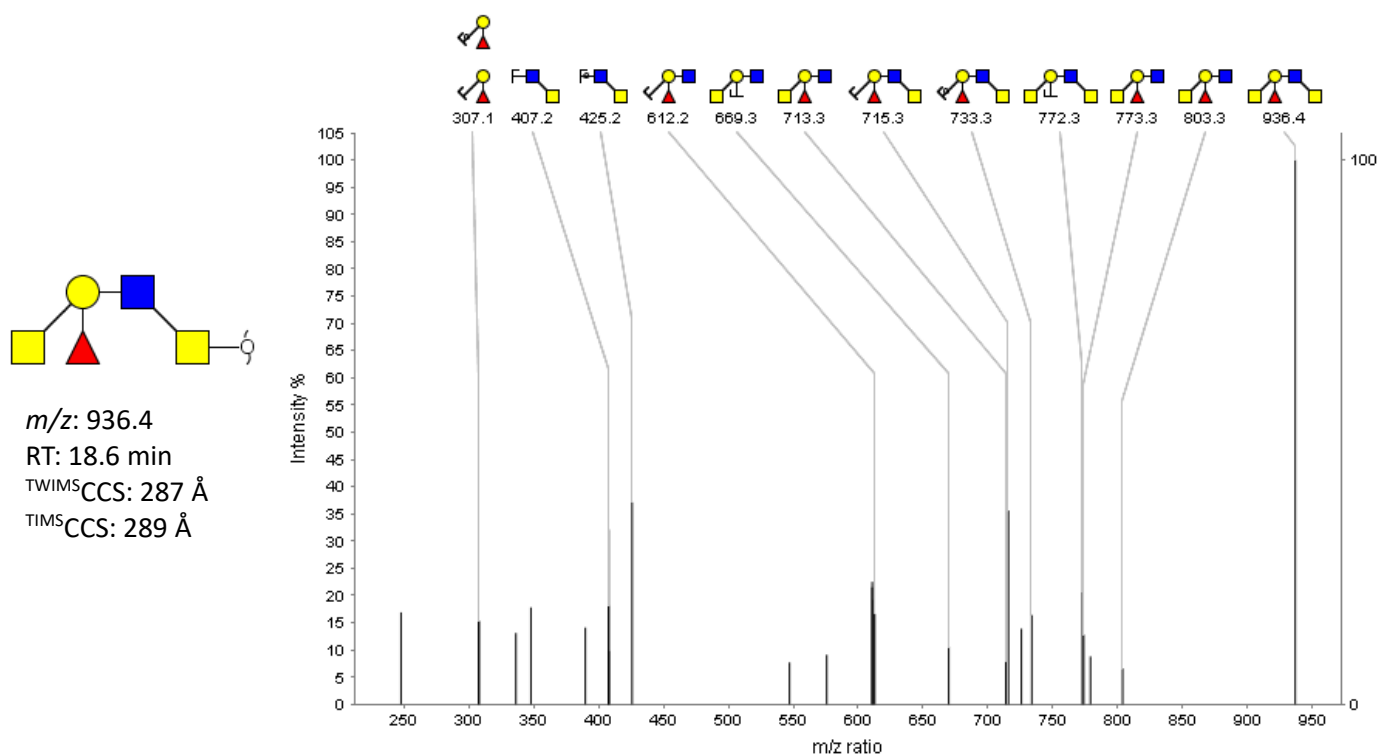
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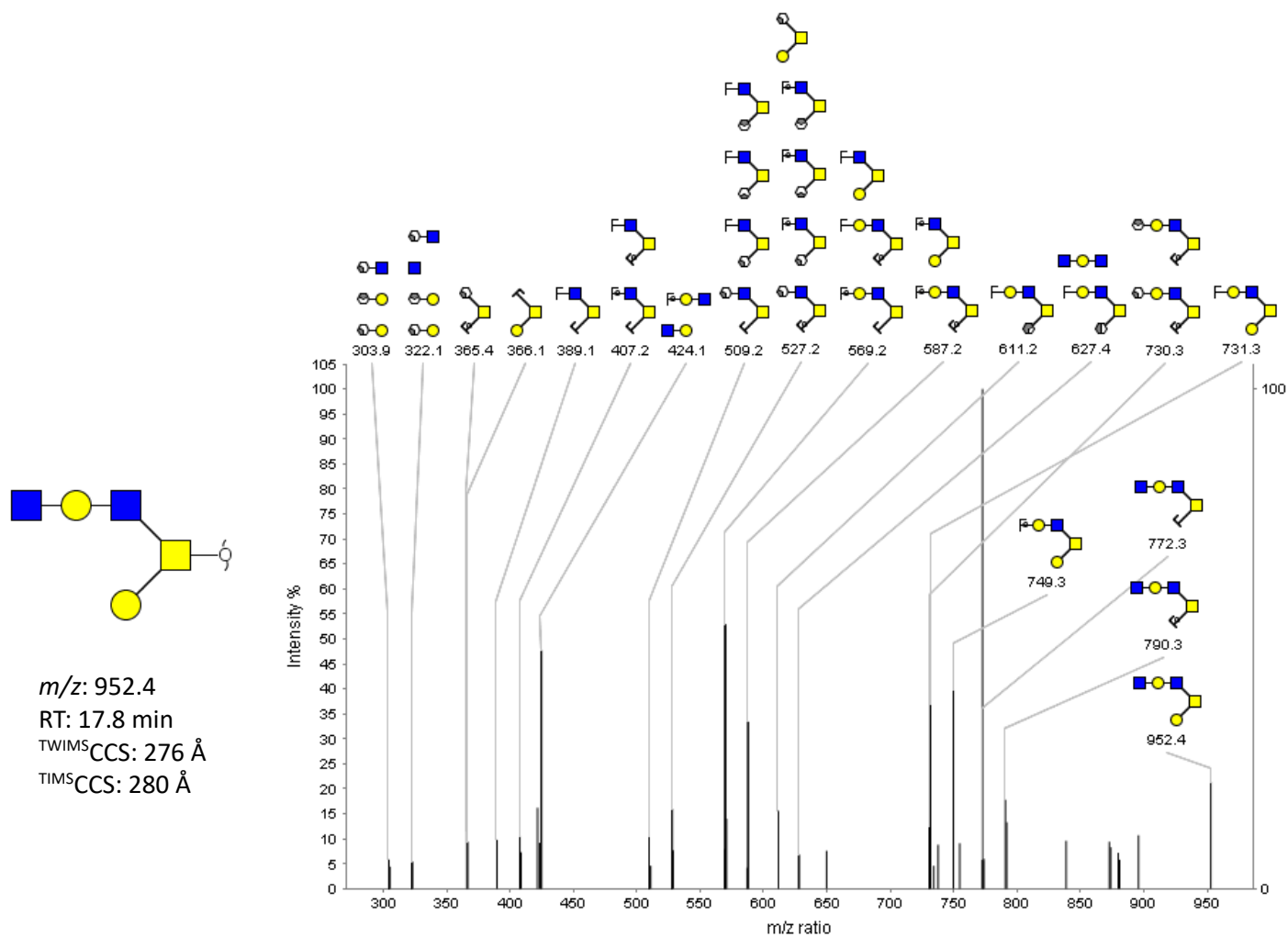
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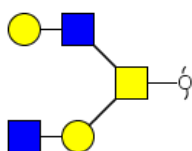
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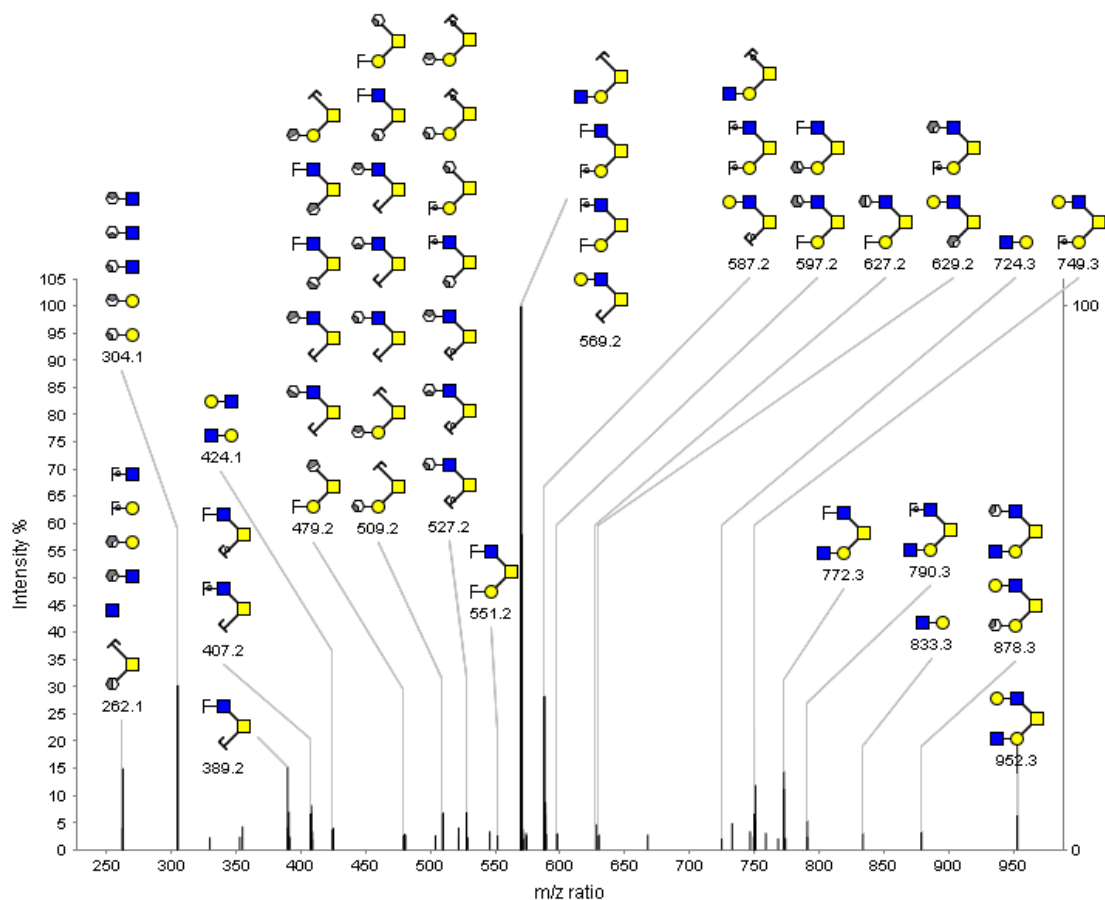
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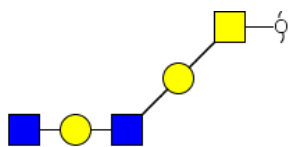
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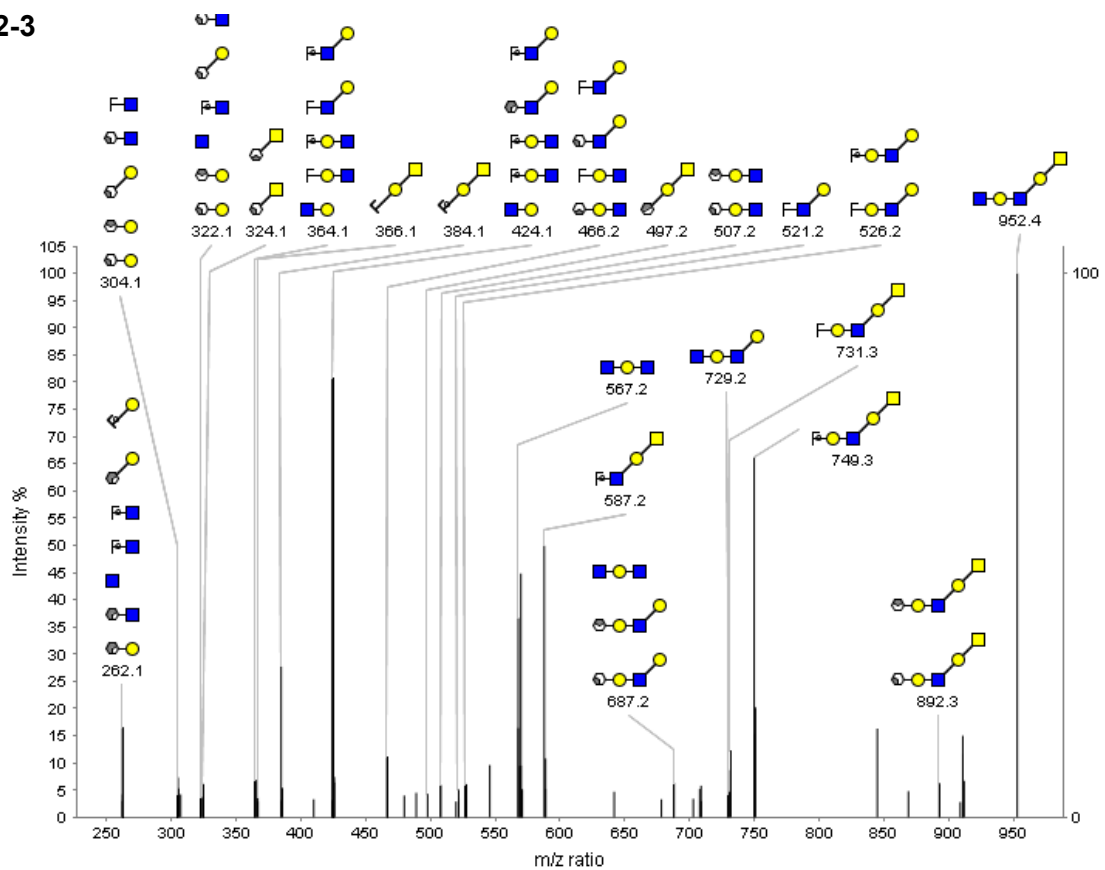
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RT: 17.8 min
TWIMS CCS: 282 Å
TIMS CCS: 285 Å



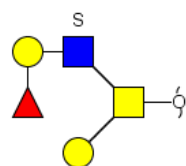
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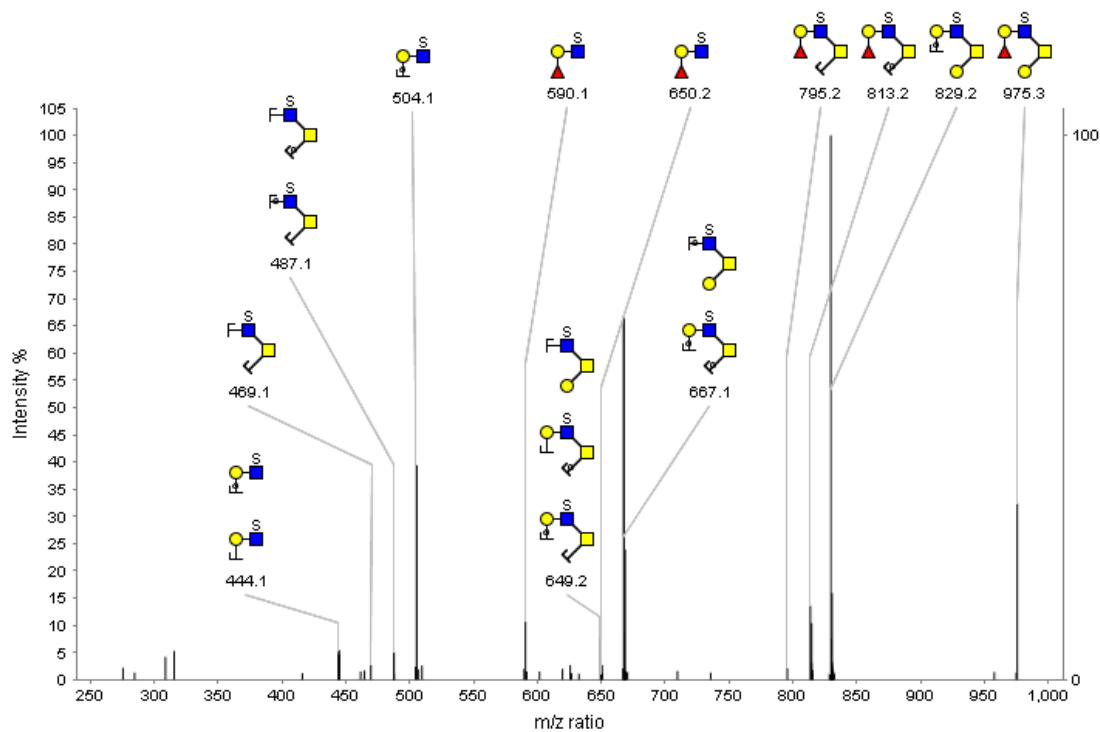
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RT: 17.4 min
TWIMS CCS: 295 Å
TIMS CCS: 295 Å



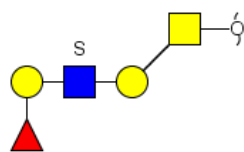
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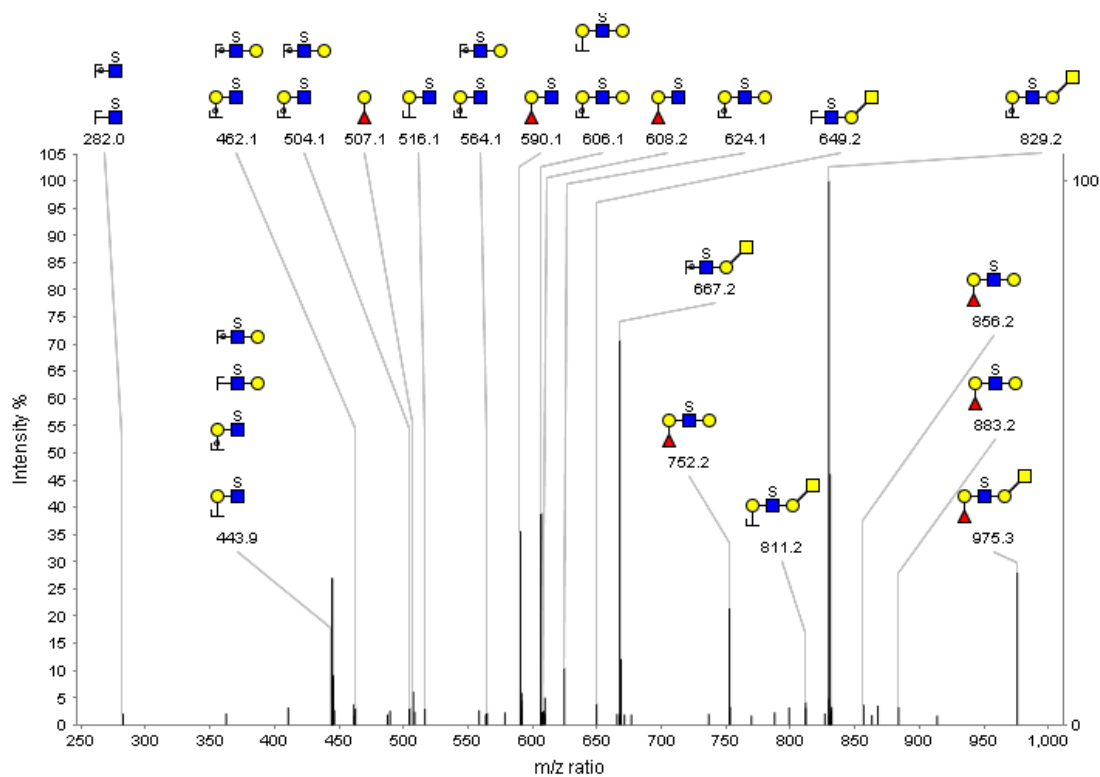
m/z : 975.3
 TWIMS CCS: n.d.
 TIMS CCS: 287 Å



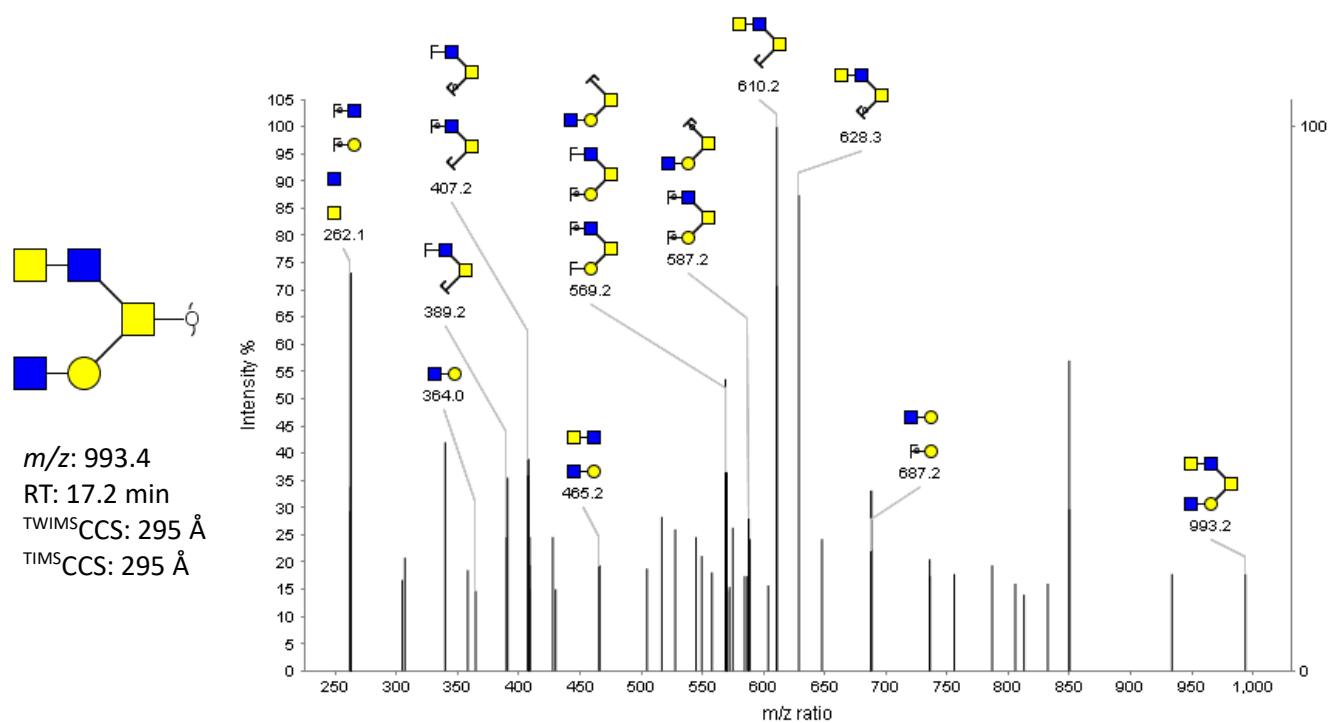
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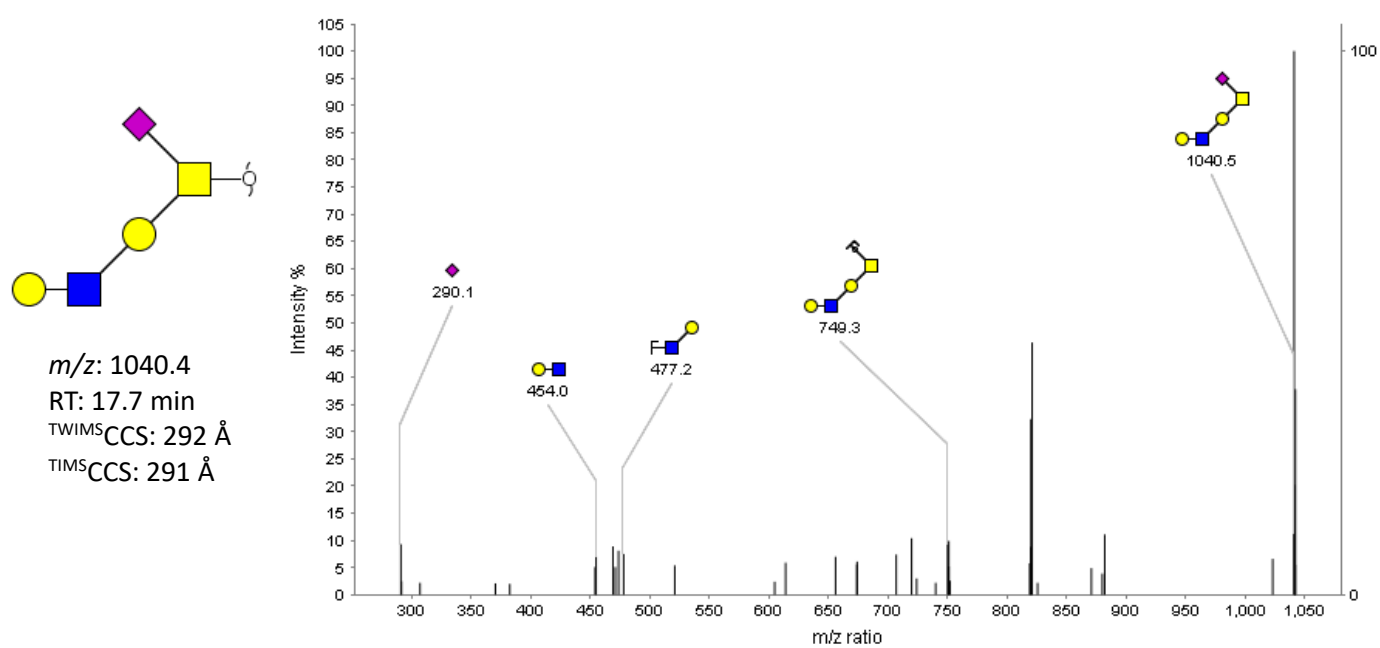
m/z : 952.4
 RT: 17.3 min
 TWIMS CCS: 303 Å
 TIMS CCS: 302 Å



Glycan code: 993-1



Glycan code: 1040-1



11-1

Mass spectrum of compound **11-1**. The x-axis represents the mass-to-charge ratio (m/z) from 300 to 1050, and the y-axis represents the relative intensity from 0 to 100%.

Key peaks and their corresponding chemical structures (shown above the peaks) are labeled:

- m/z 307.1, 325.1, 367.1, 389.2
- m/z 407.2
- m/z 510.2, 512.2
- m/z 551.2
- m/z 569.1, 570.2
- m/z 715.3 (Base Peak)
- m/z 733.1
- m/z 877.3
- m/z 1041.4

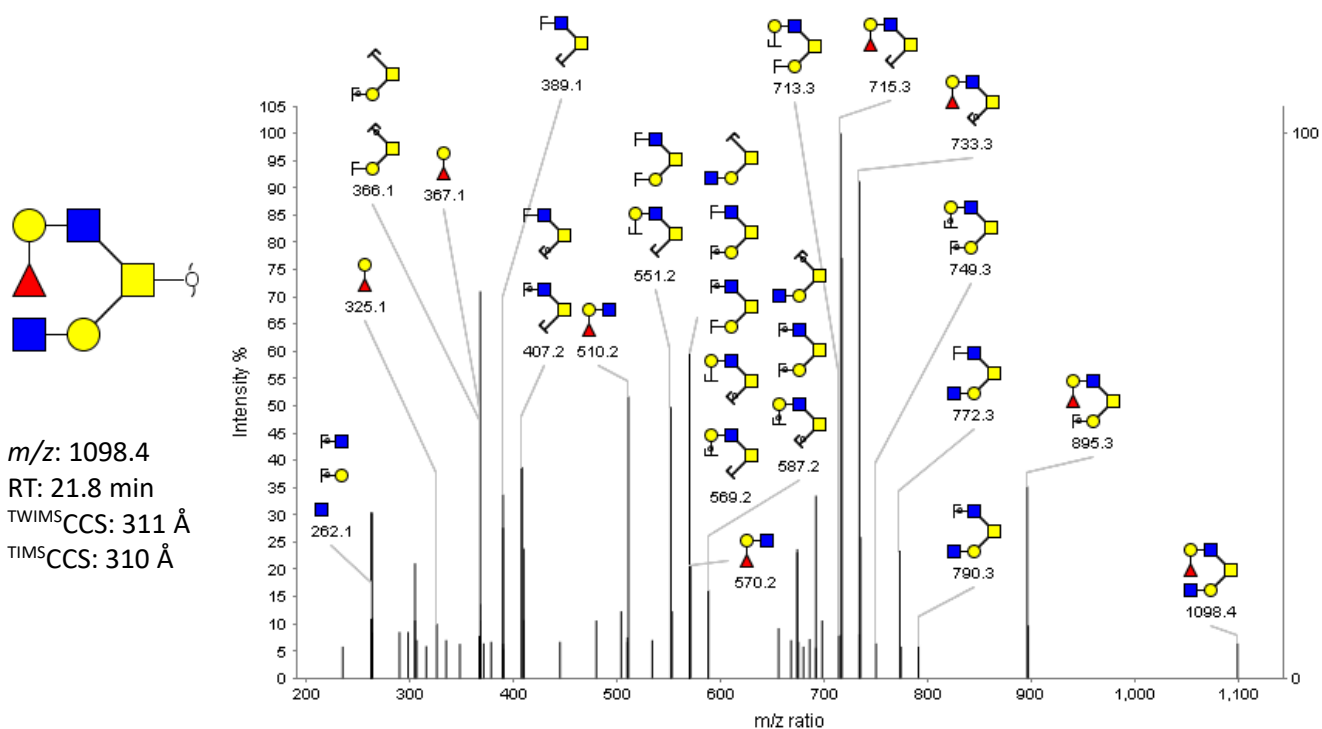
Mass spectrum of compound 10 showing relative intensity (%) versus m/z ratio. The base peak is at m/z 569.0. Numerous peaks are labeled with their m/z values and corresponding chemical structures.

Chemical structures shown above the peaks include various substituted benzene rings, often with a fluorine atom (F) and a trifluoromethyl group (CF₃), and a trifluoromethyl ether group (OCF₃).

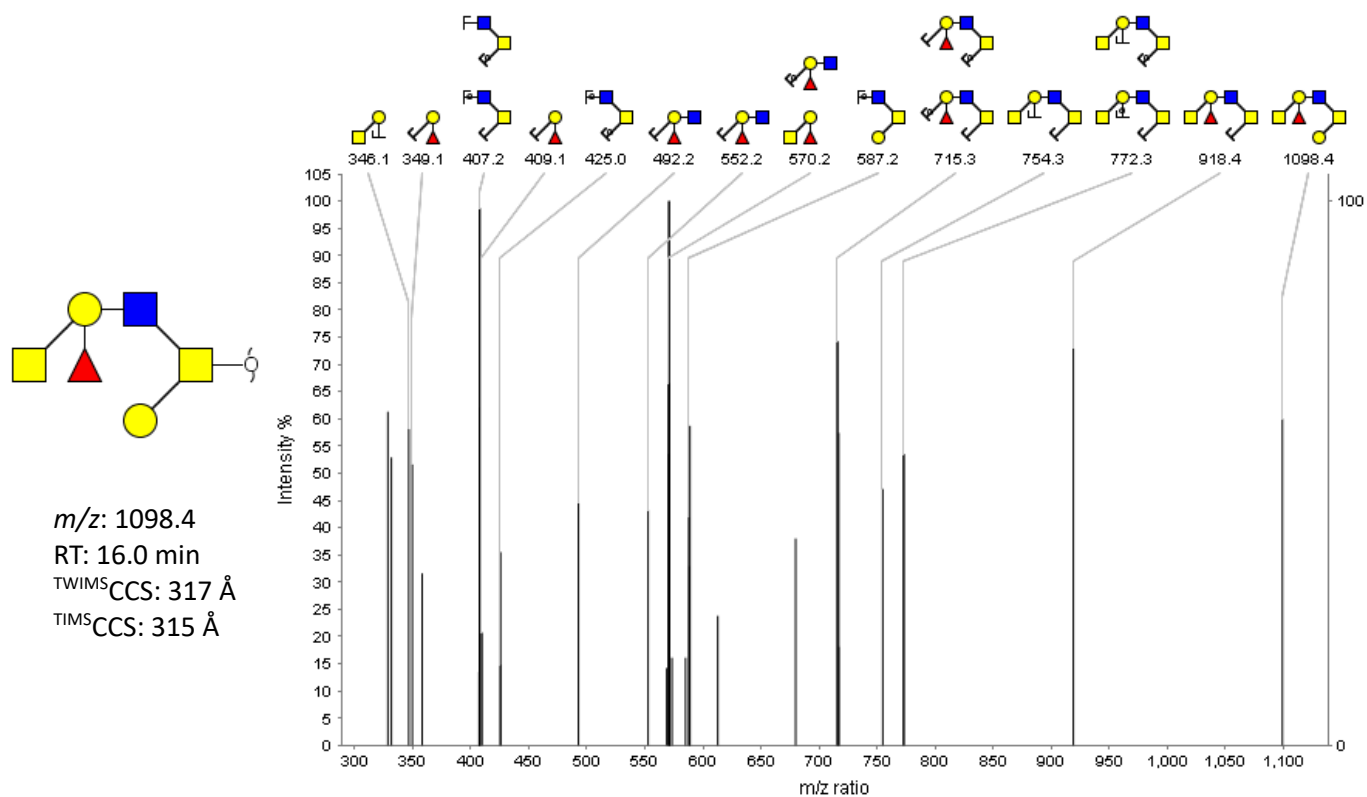
Key peaks and their m/z values:

- 303.1
- 364.1
- 366.2
- 384.1
- 389.2
- 406.0
- 407.2
- 408.2
- 424.1
- 425.1
- 449.2
- 509.1
- 512.2
- 526.9
- 527.2
- 551.2
- 567.2
- 569.0
- 587.2
- 611.2
- 613.2
- 713.3
- 715.3
- 730.3
- 733.3
- 772.3
- 790.3
- 895.5
- 1024.4

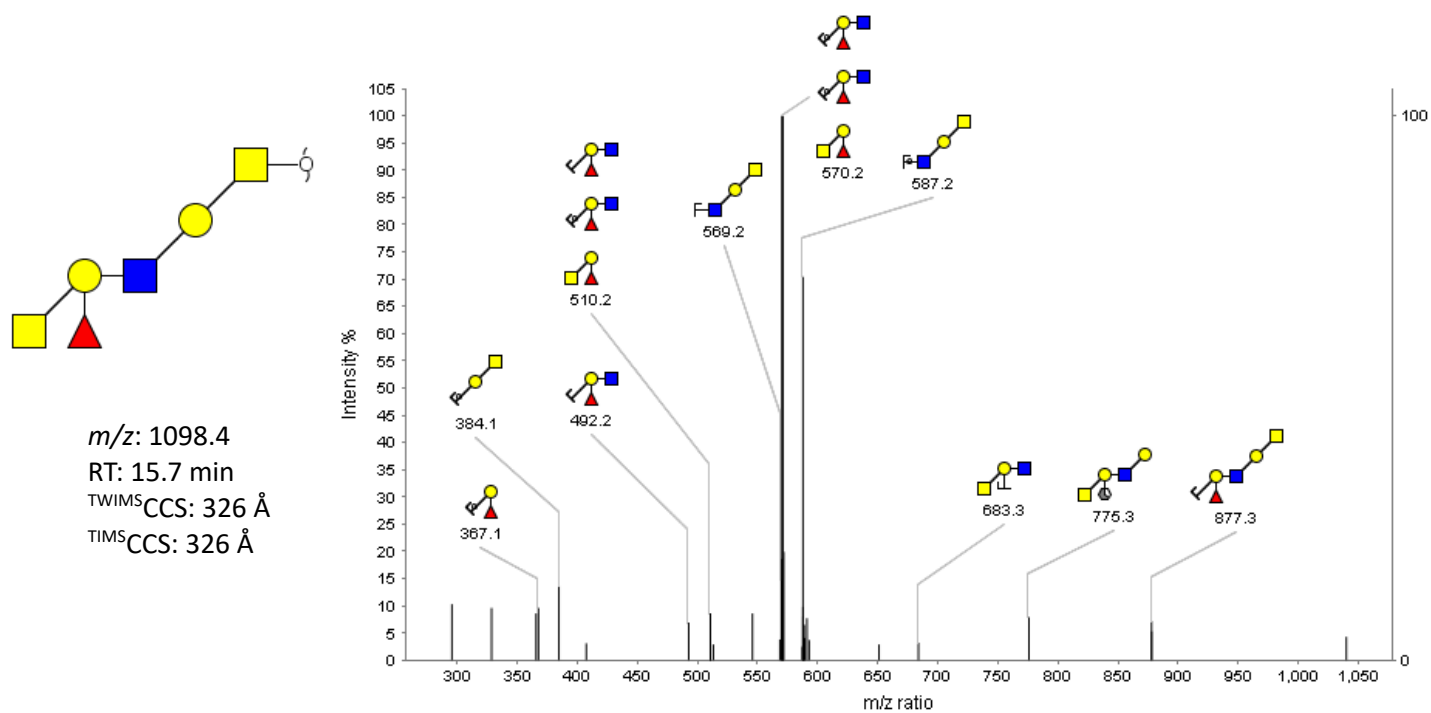
Glycan code: 1098-2



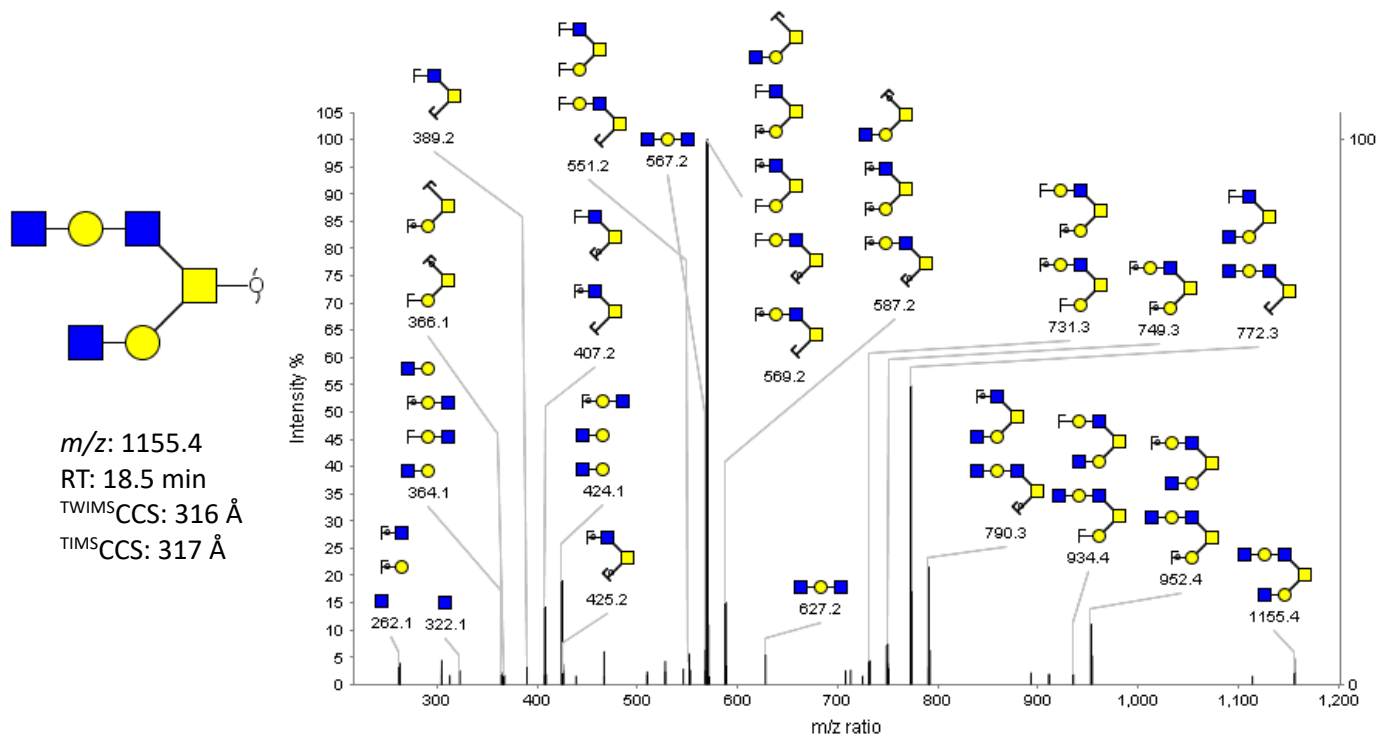
Glycan code: 1098-3



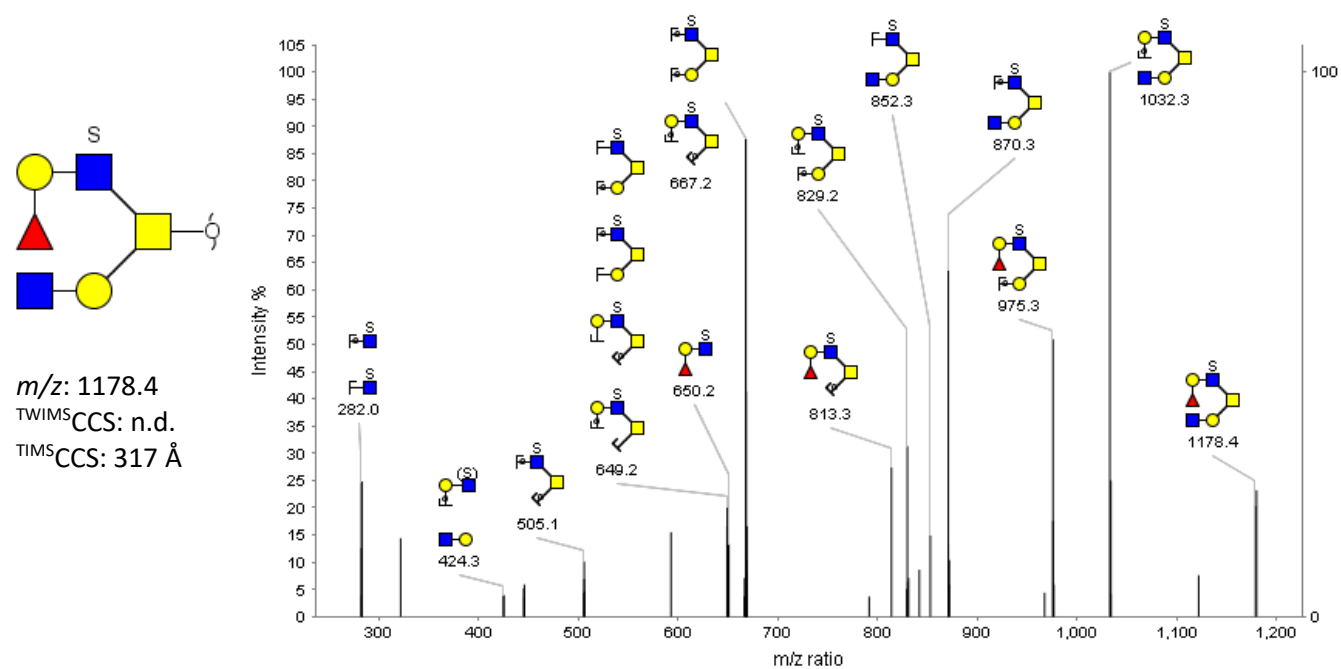
Glycan code: 1098-4



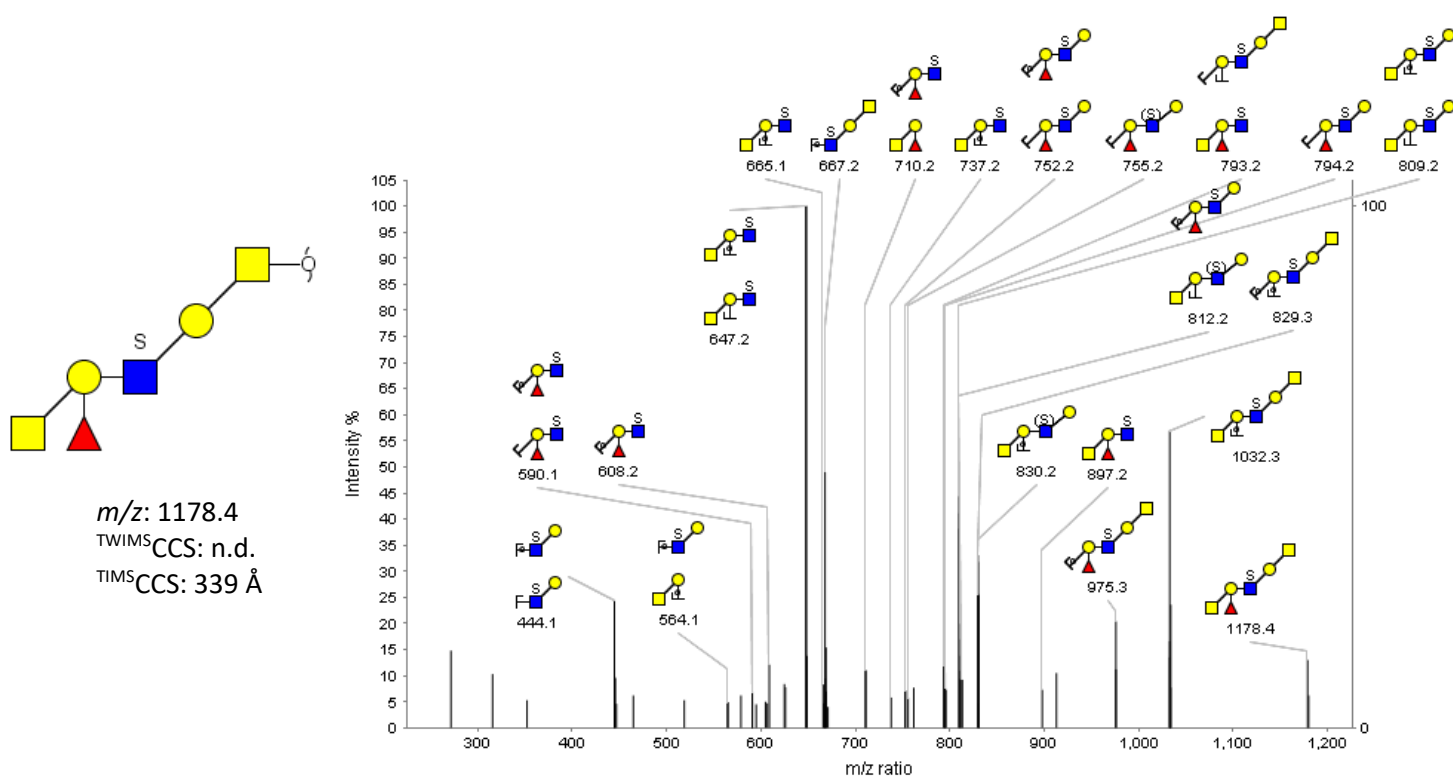
Glycan code: 1155-1



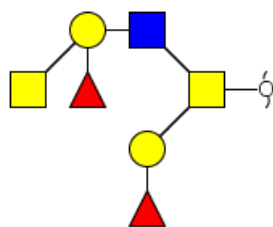
Glycan code: 1178-1



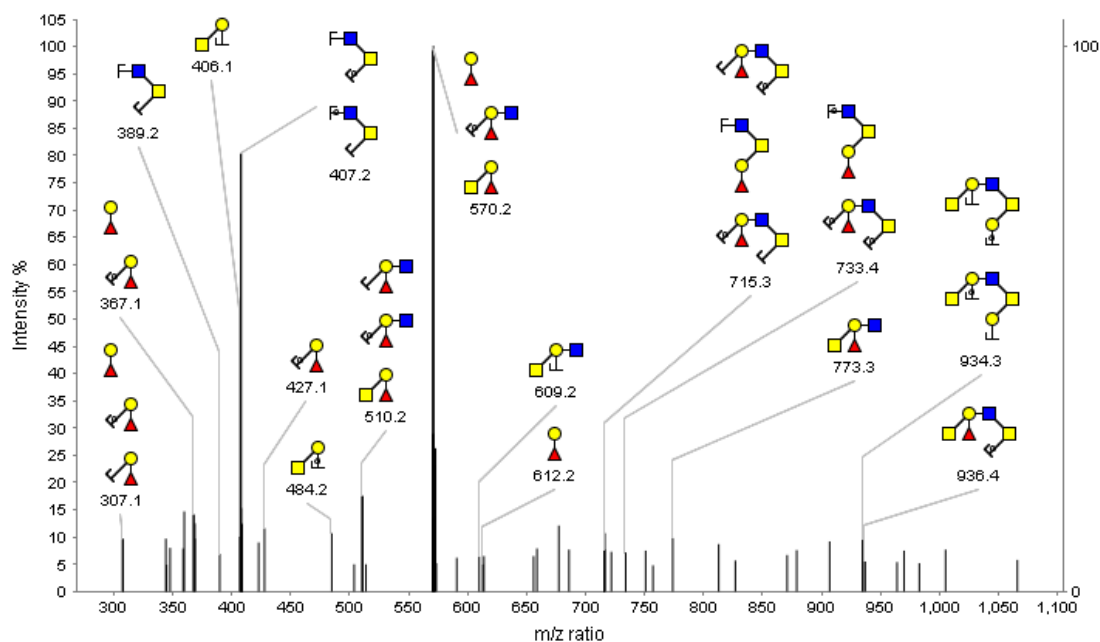
Glycan code: 1178-2



Glycan code: 621-1

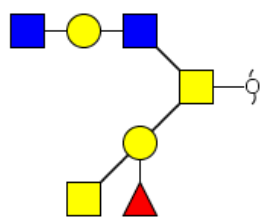


m/z : 621.7
 TWIMSCCS: n.d.
 TIMSCCS: 349 Å

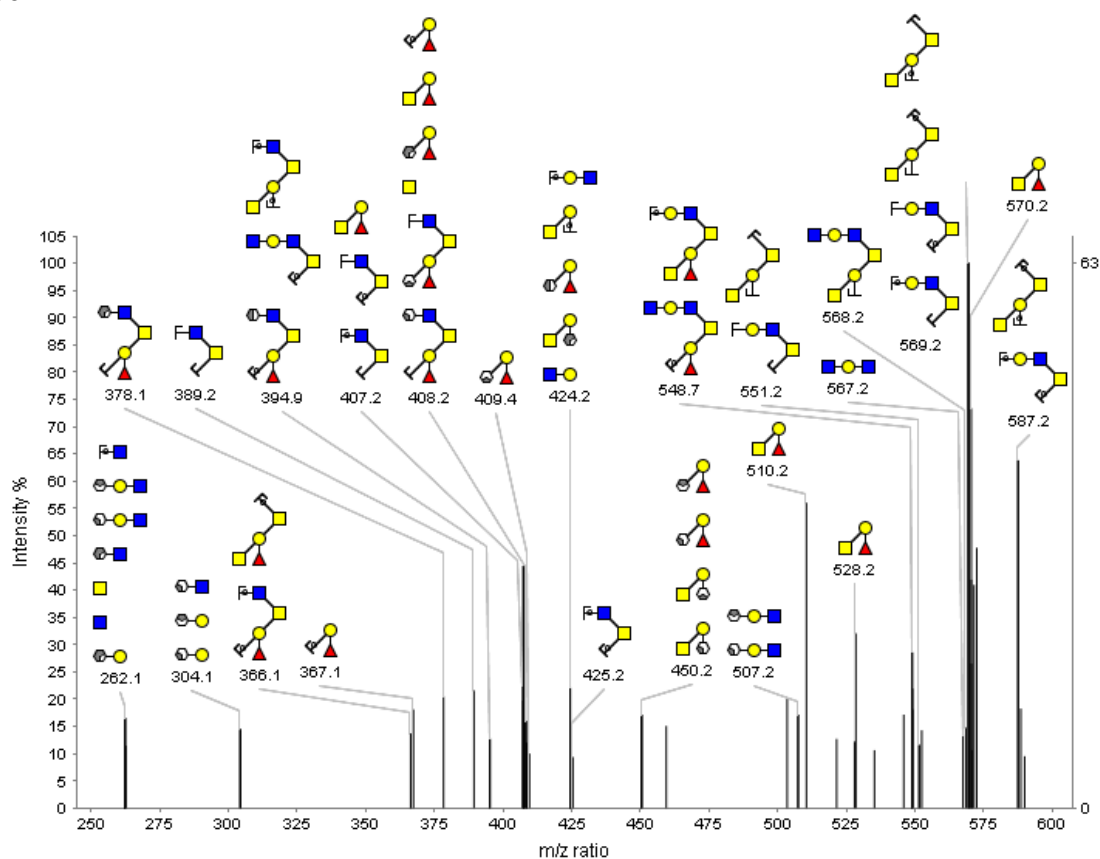


Glycan code: 650-1

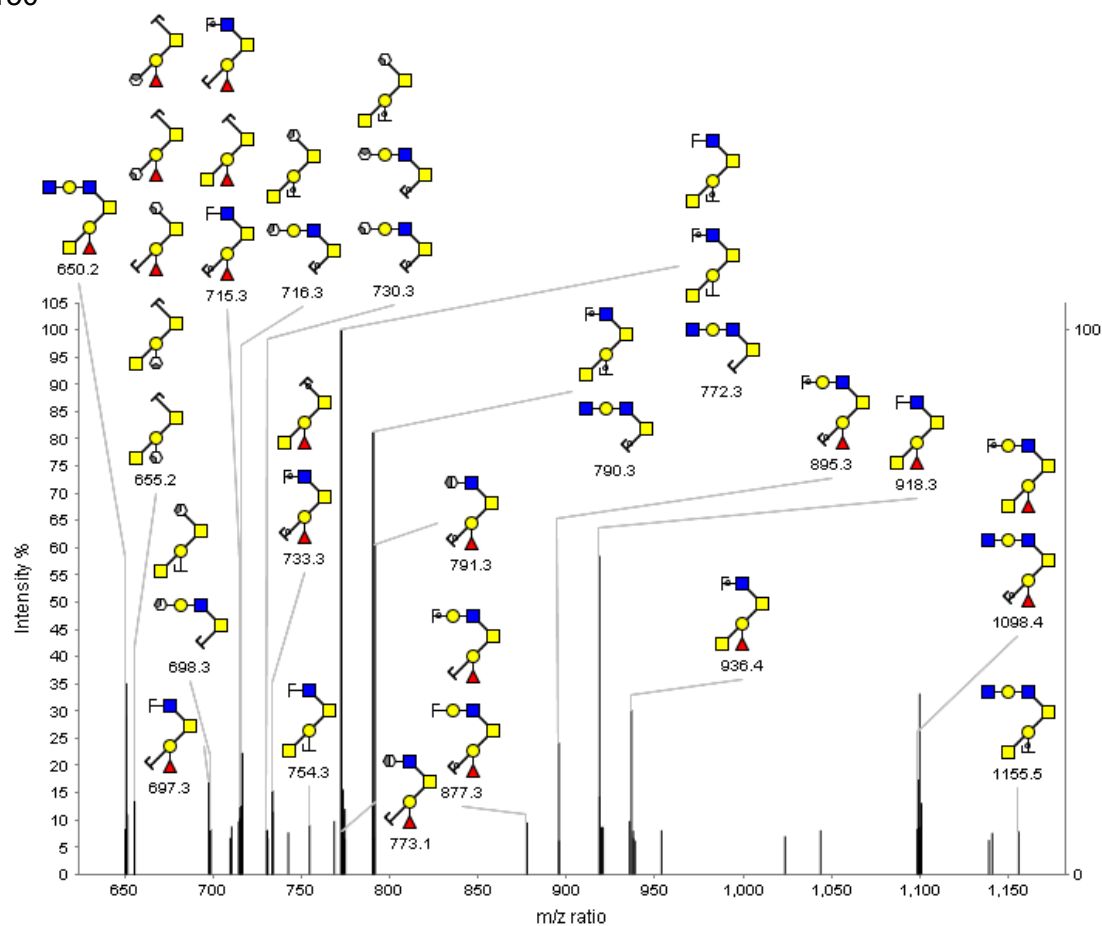
m/z range: 150-650



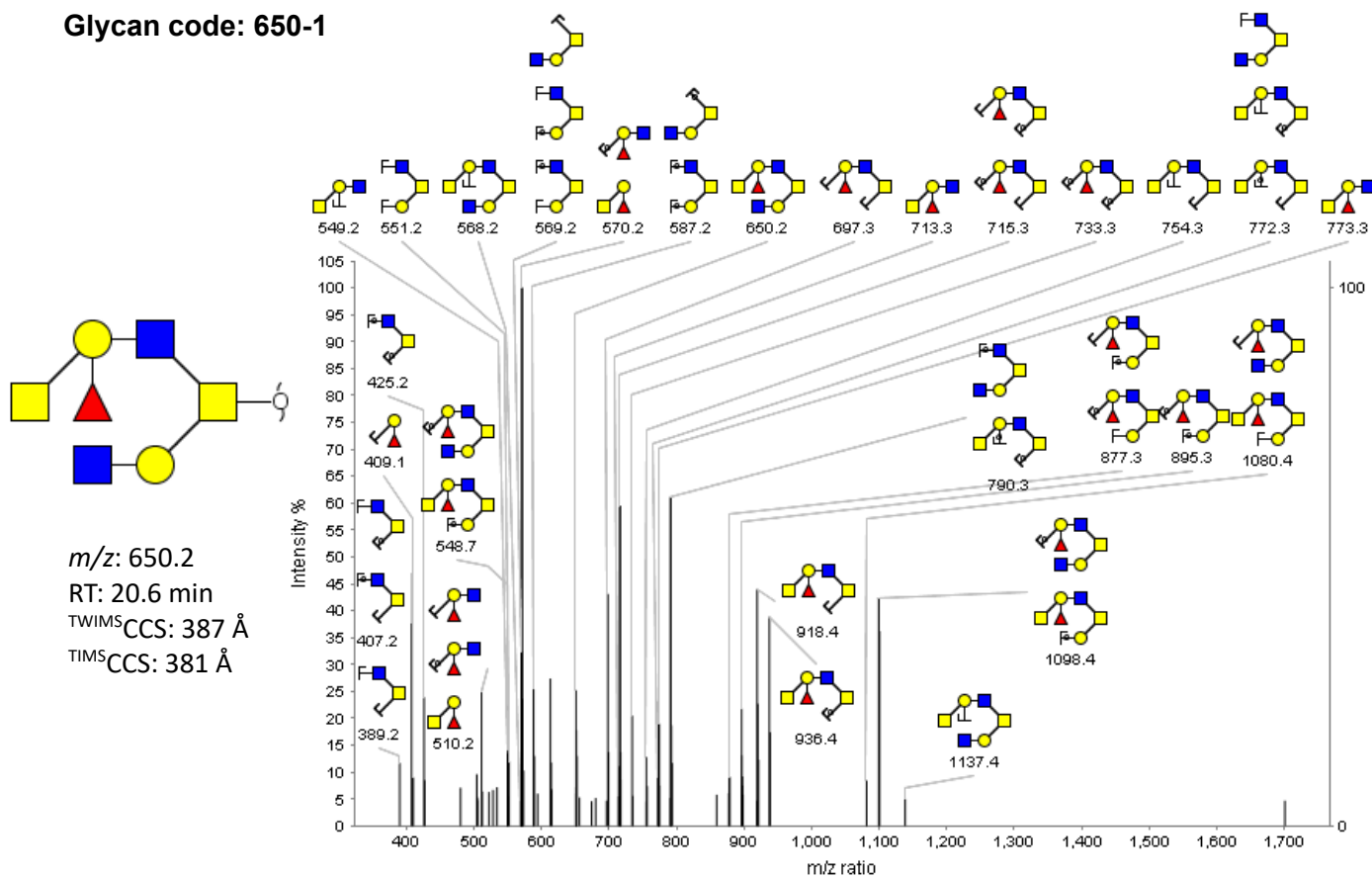
m/z : 650.2
 RT: 18.0 min
 TWIMSCCS: 364 Å
 TIMSCCS: 356 Å



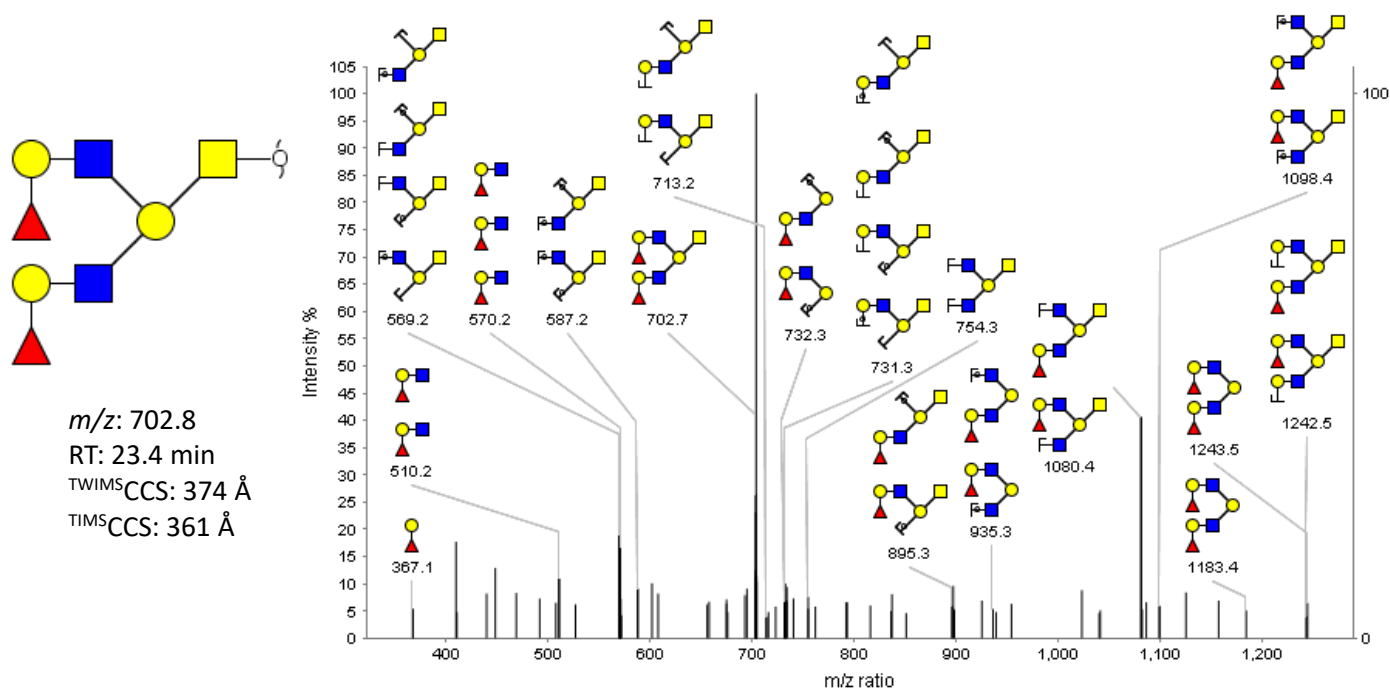
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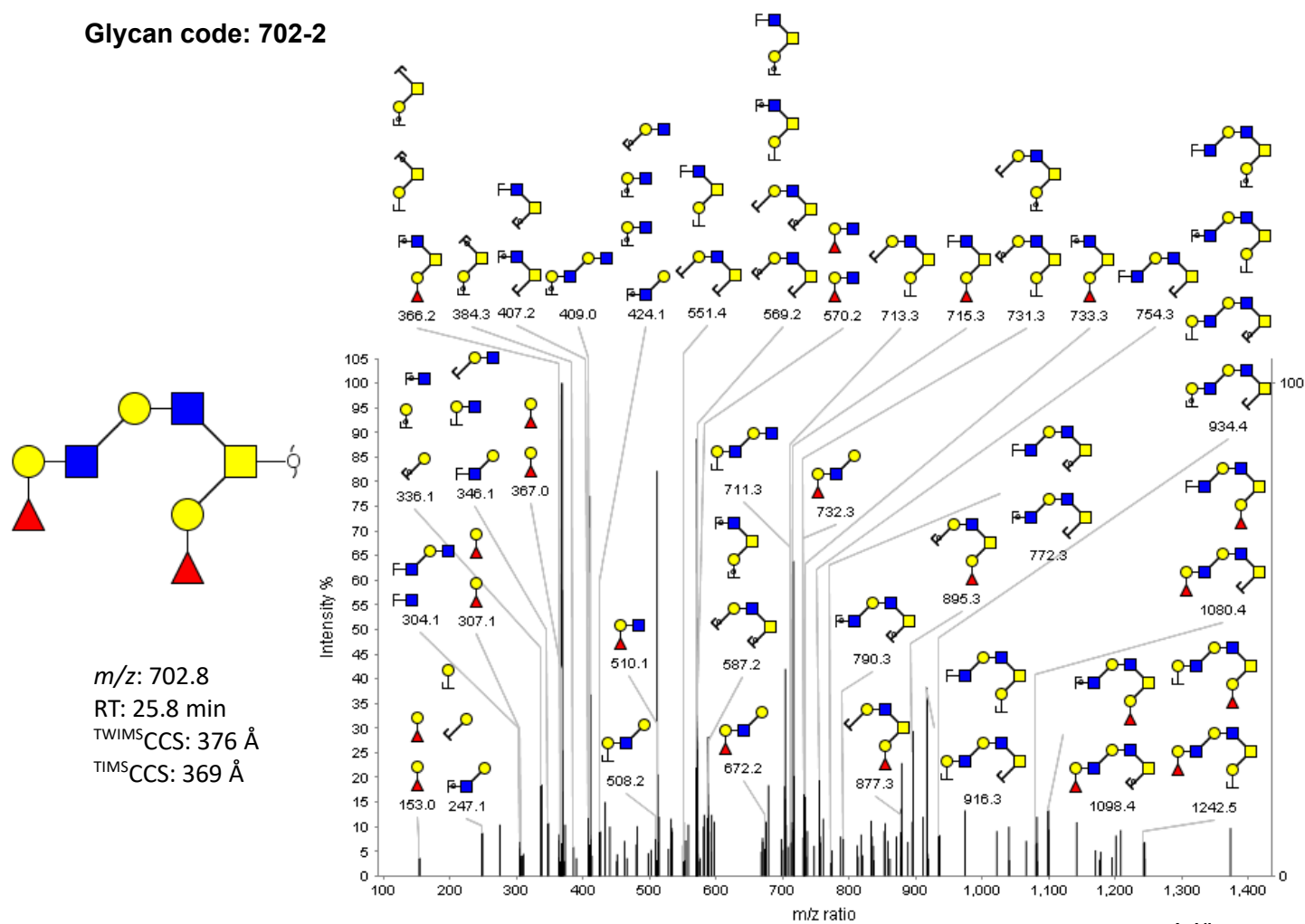
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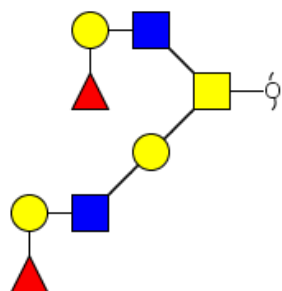
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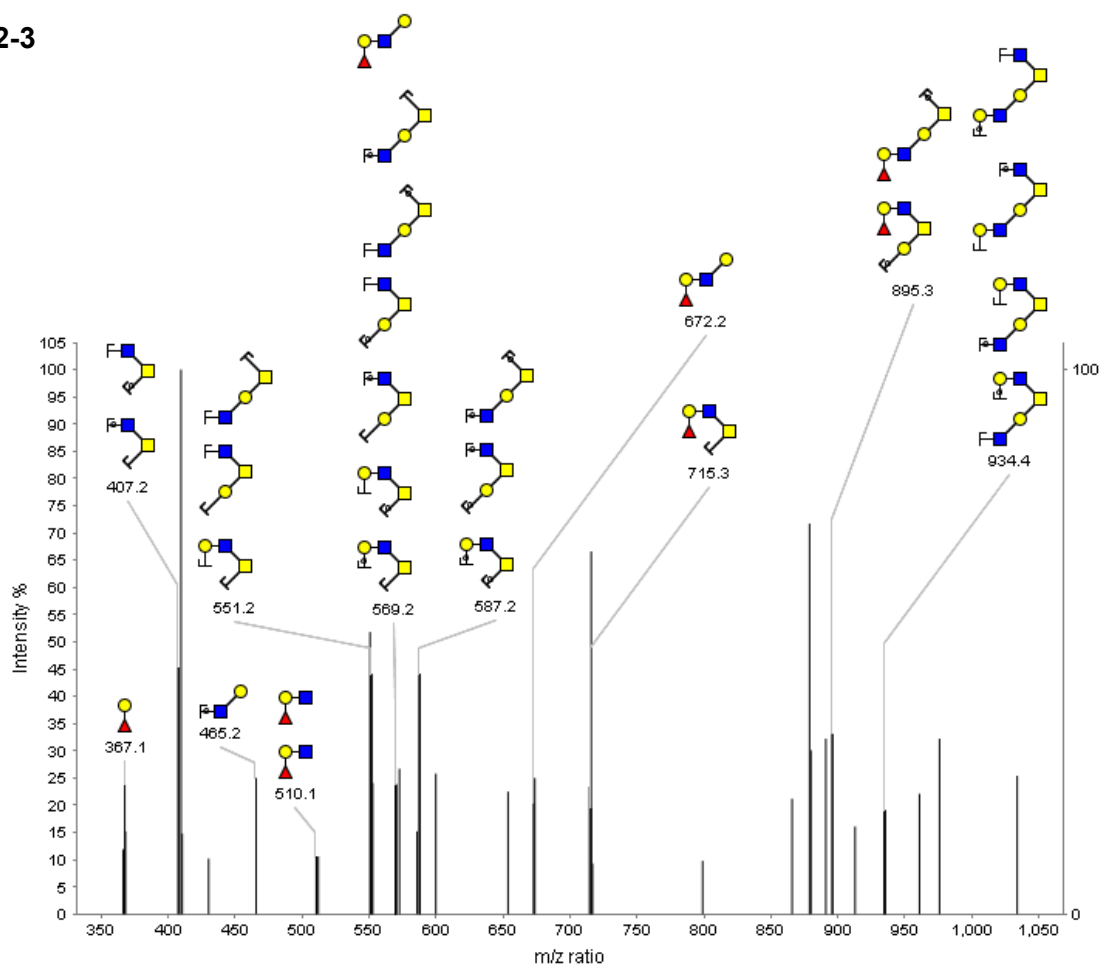
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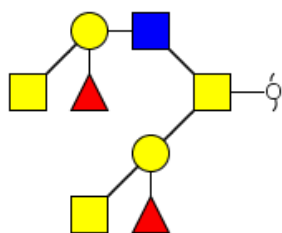
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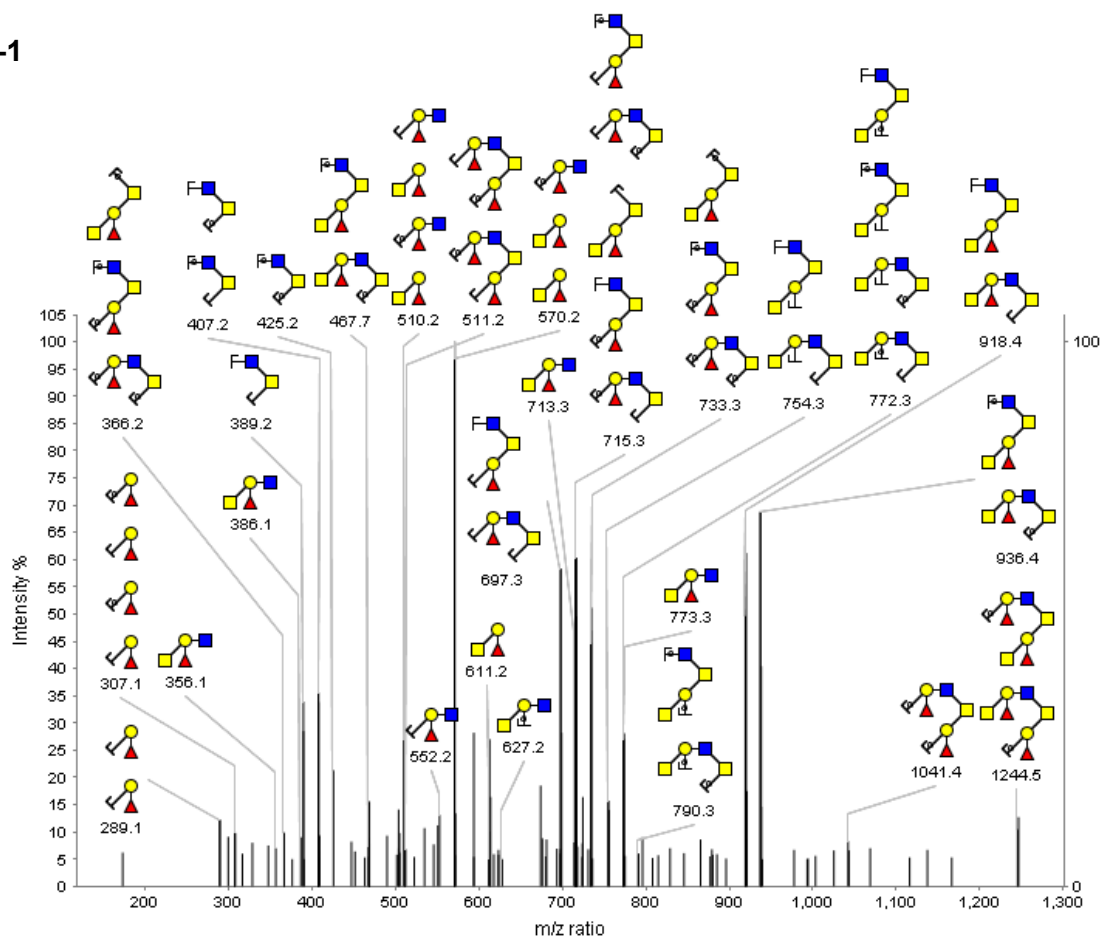
m/z : 702.8
 TWIMSCCS: n.d.
 TIMSCCS: 379 Å



Glycan code: 723-1

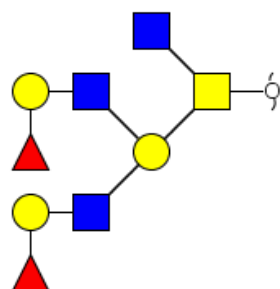


m/z : 723.3
 RT: 19.6 min
 TWIMSCCS: 372 Å
 TIMSCCS: 364 Å

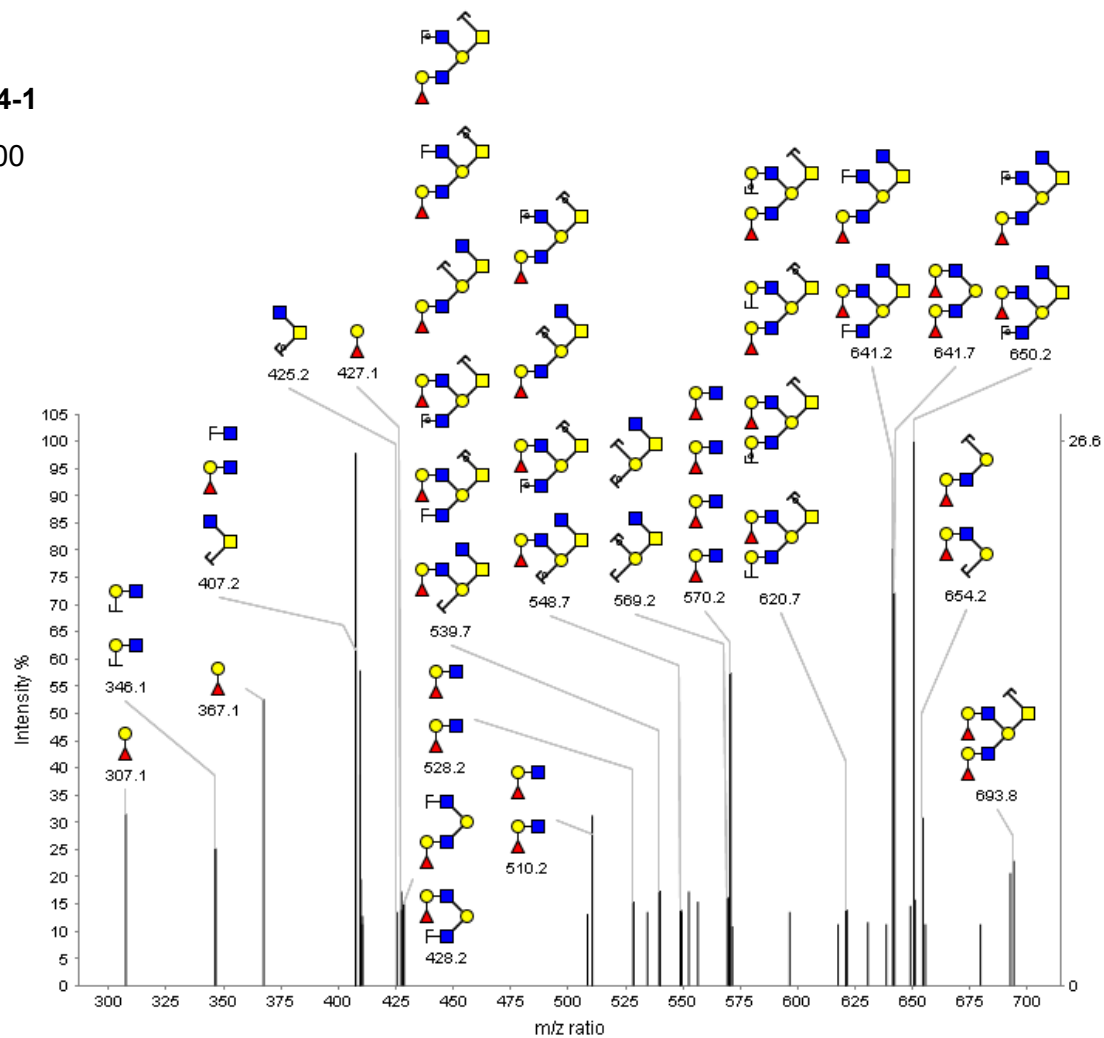


Glycan code: 804-1

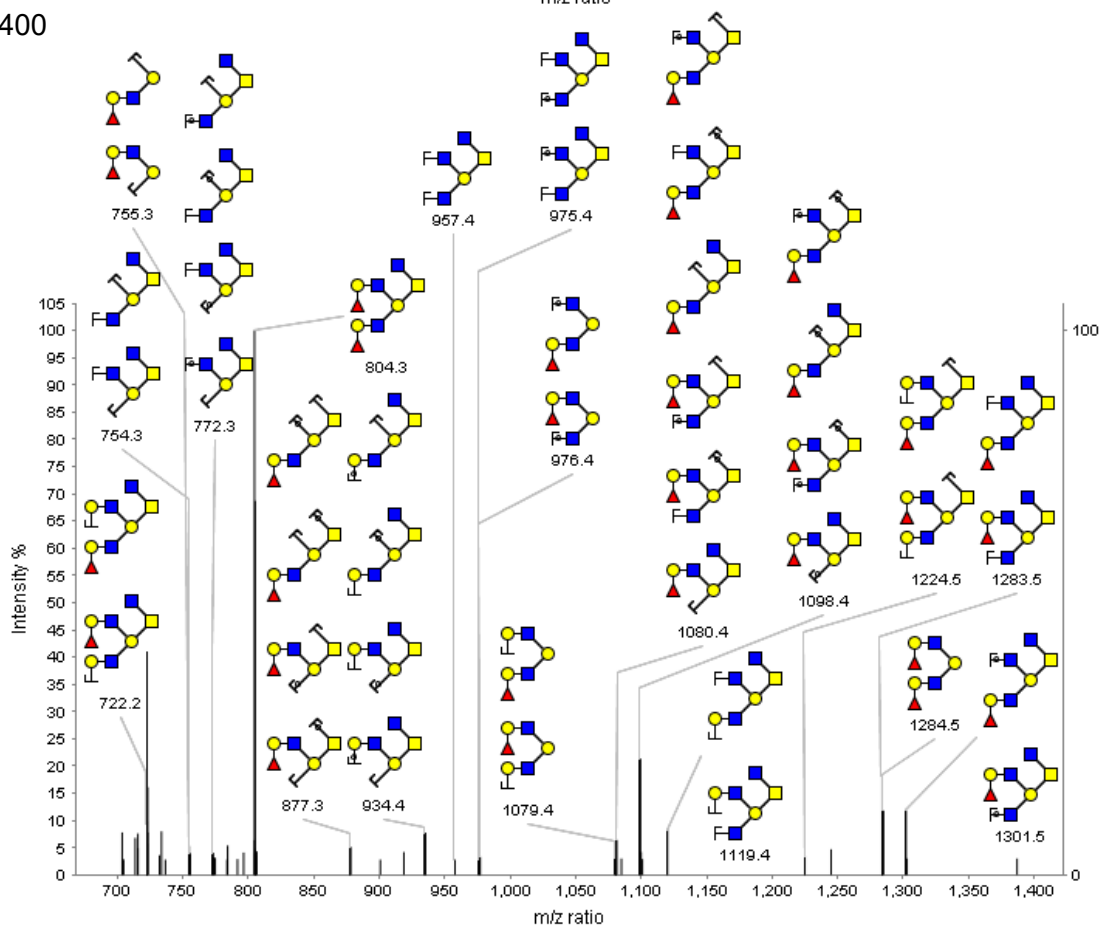
m/z range: 250-700



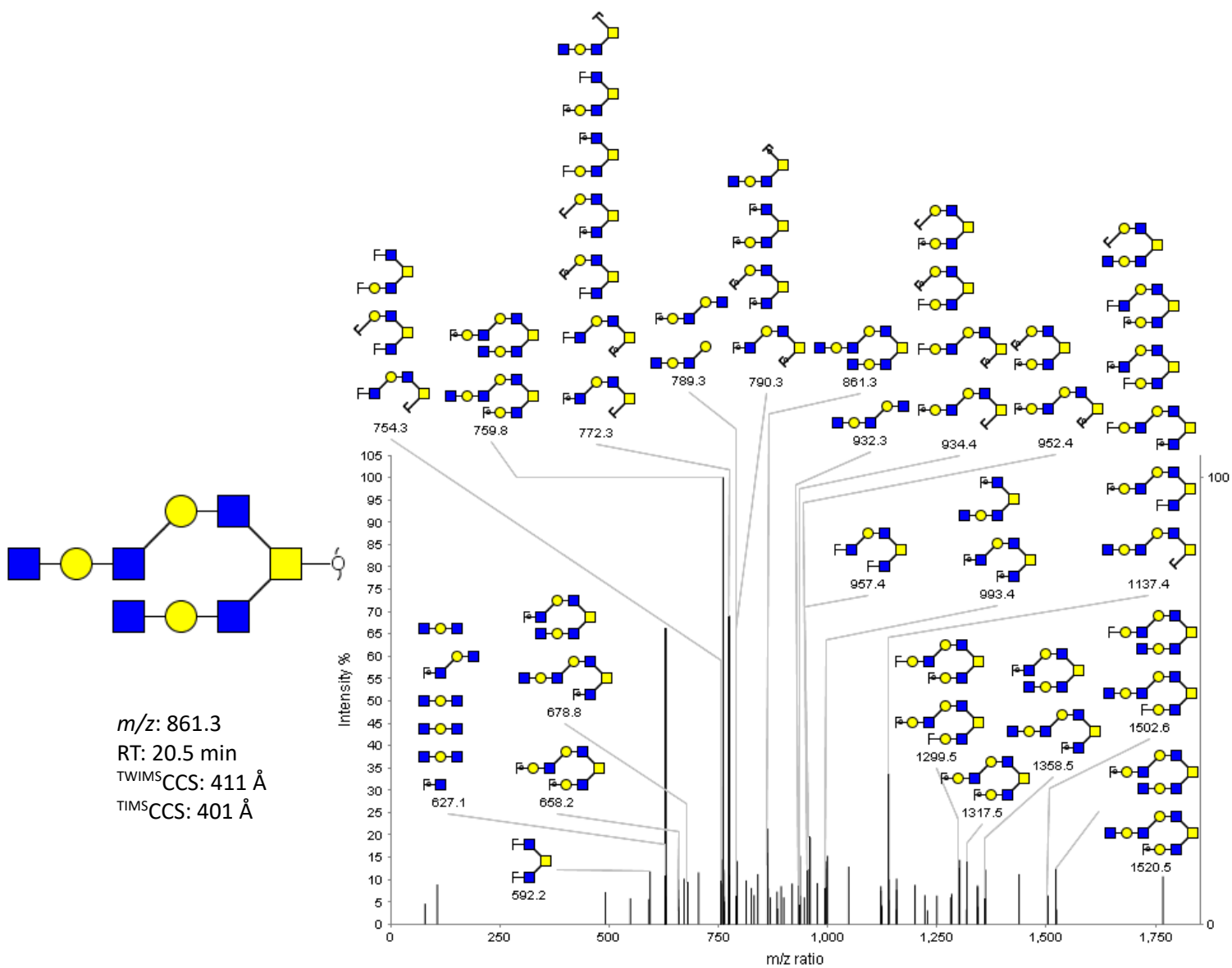
m/z: 804.3
RT: 25.7 min
TWIMS CCS: 406 Å
TIMS CCS: 399 Å



m/z range: 700-1400

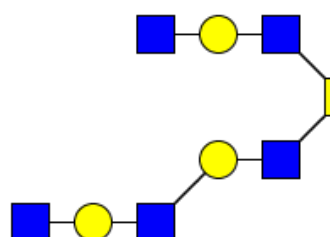


Glycan code: 861-1



Glycan code: 861-2

m/z range: 200-700

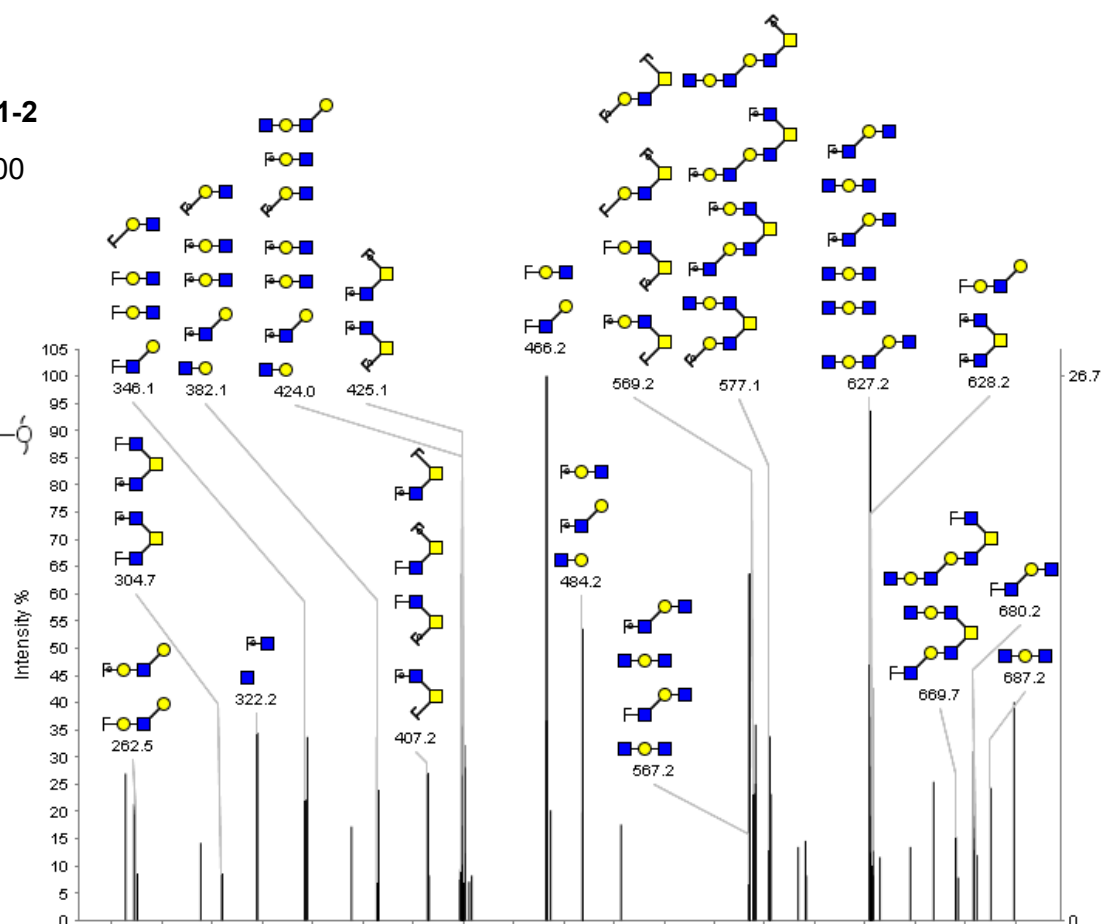


m/z: 861.3

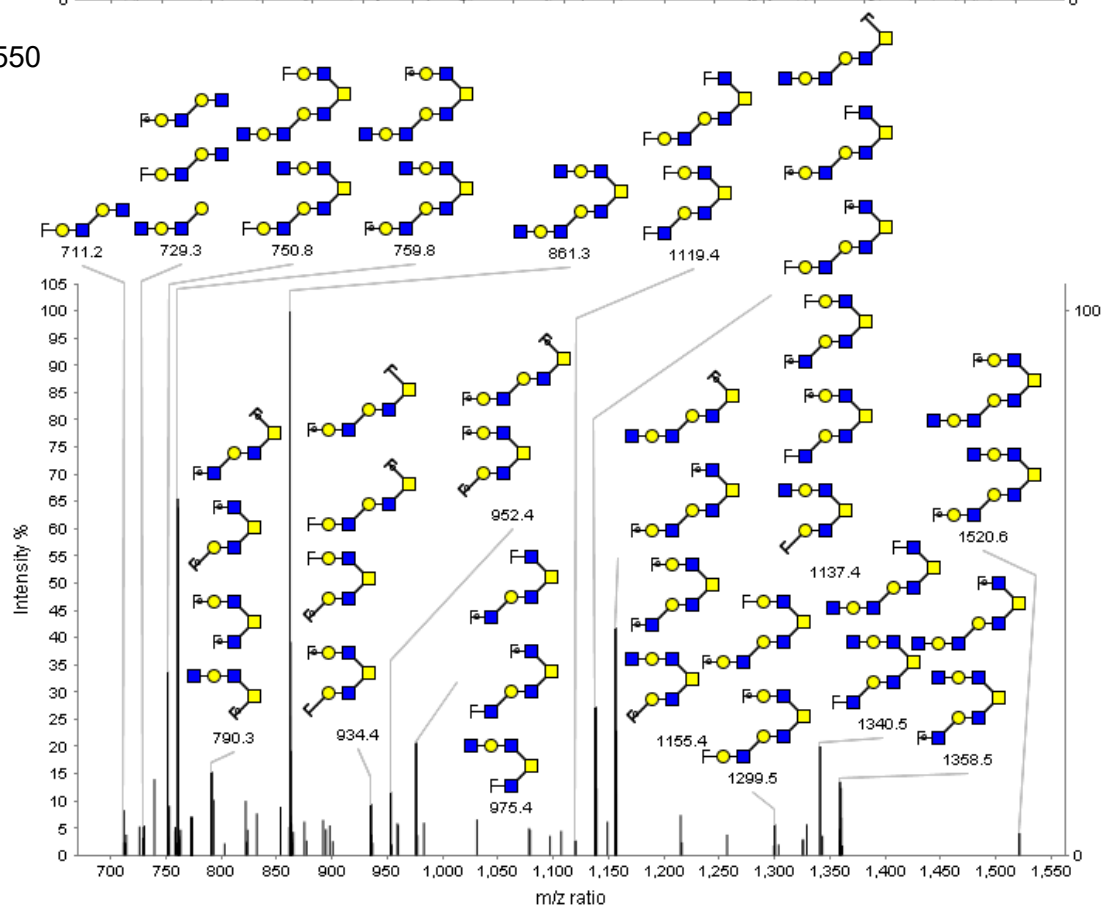
RT: 20.0 min

TWIM_{SCS}: 421 Å

TIM_{SCS}: 411 Å

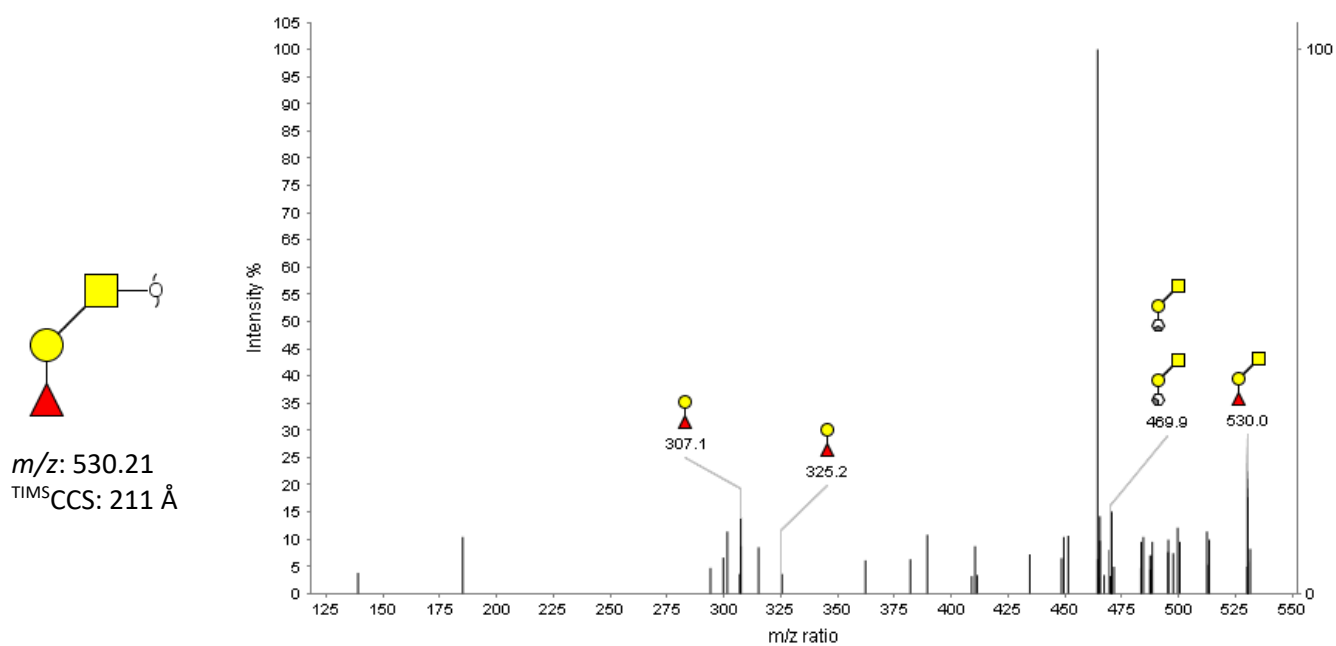


m/z range: 700-1550

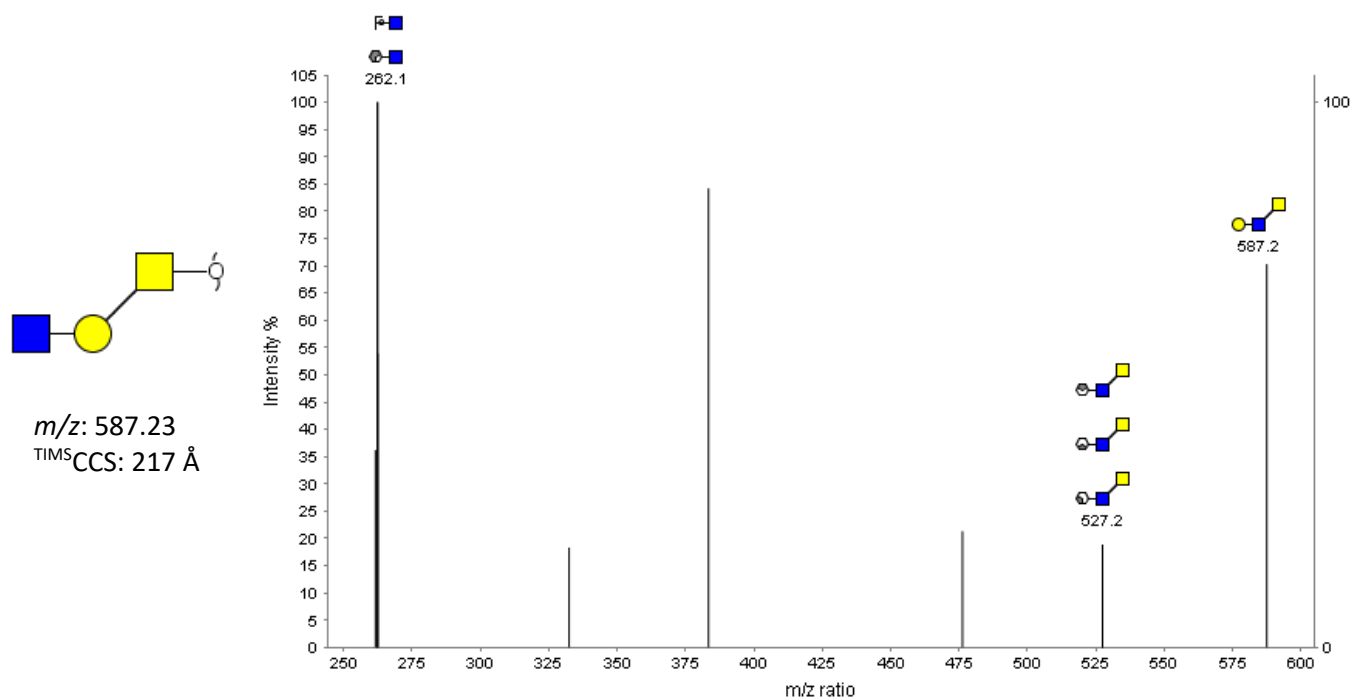


II. Annotated MS/MS spectra of O-glycans in healthy sputum

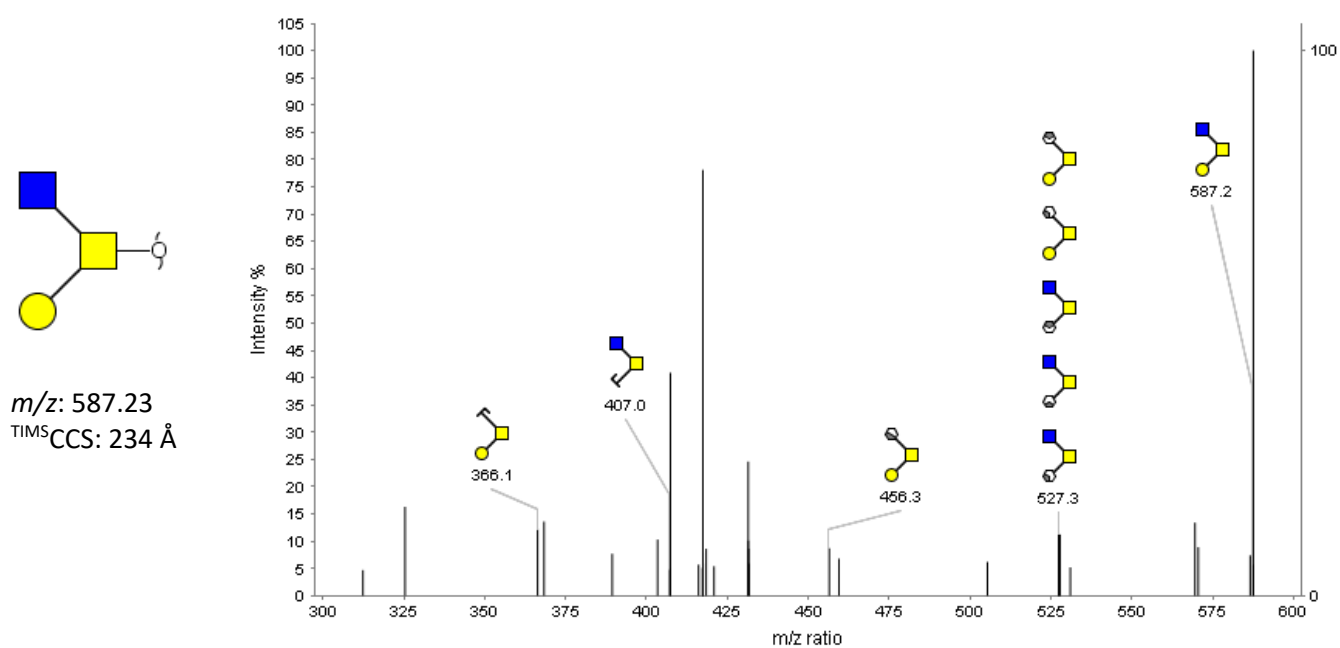
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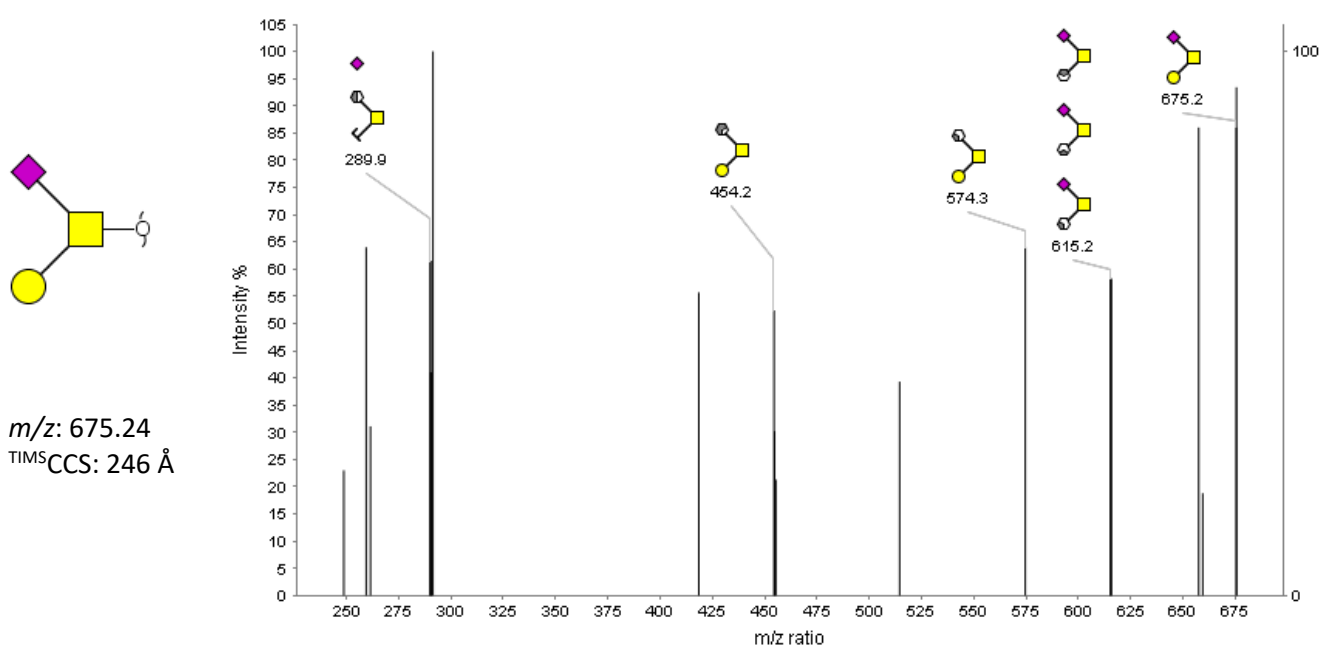
Glycan code: 587-1



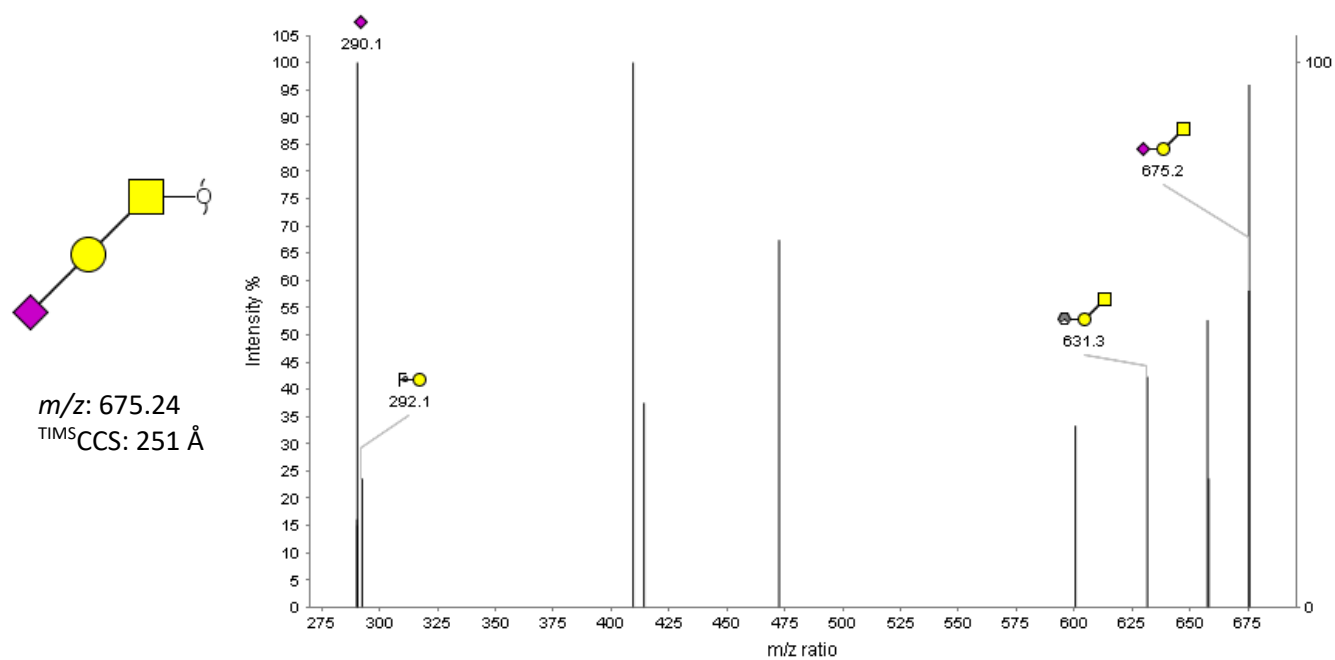
Glycan code: 587-2



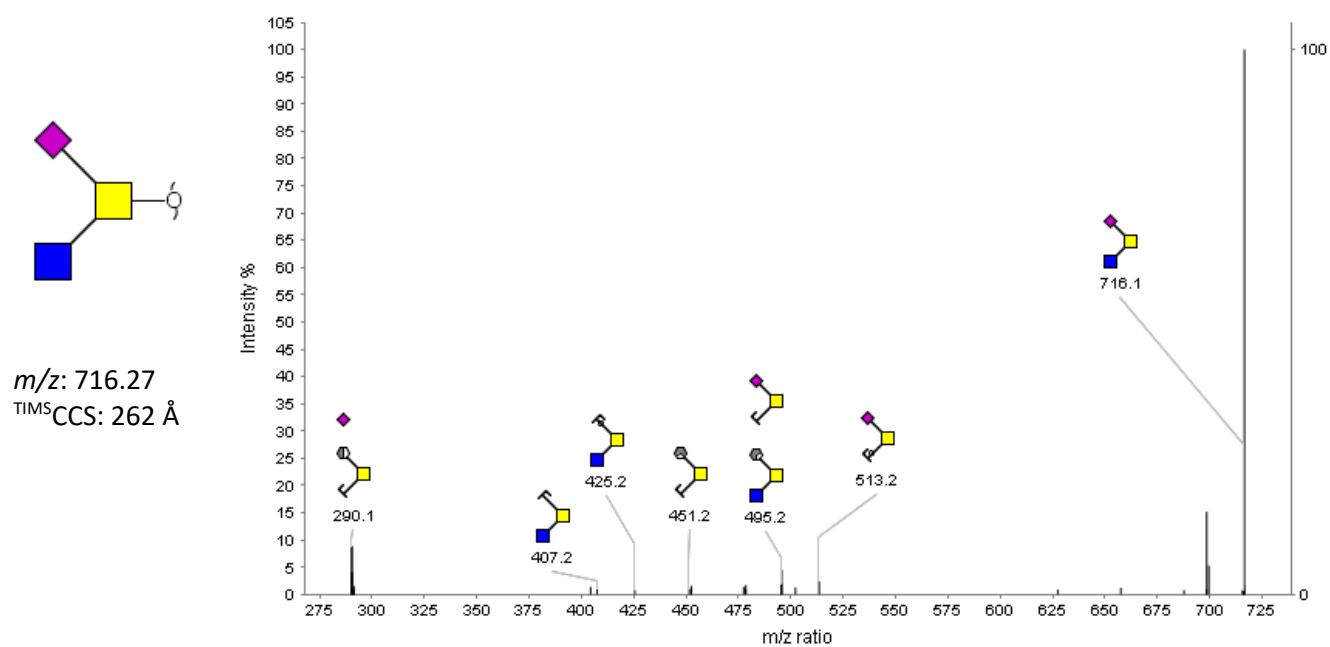
Glycan code: 675-1



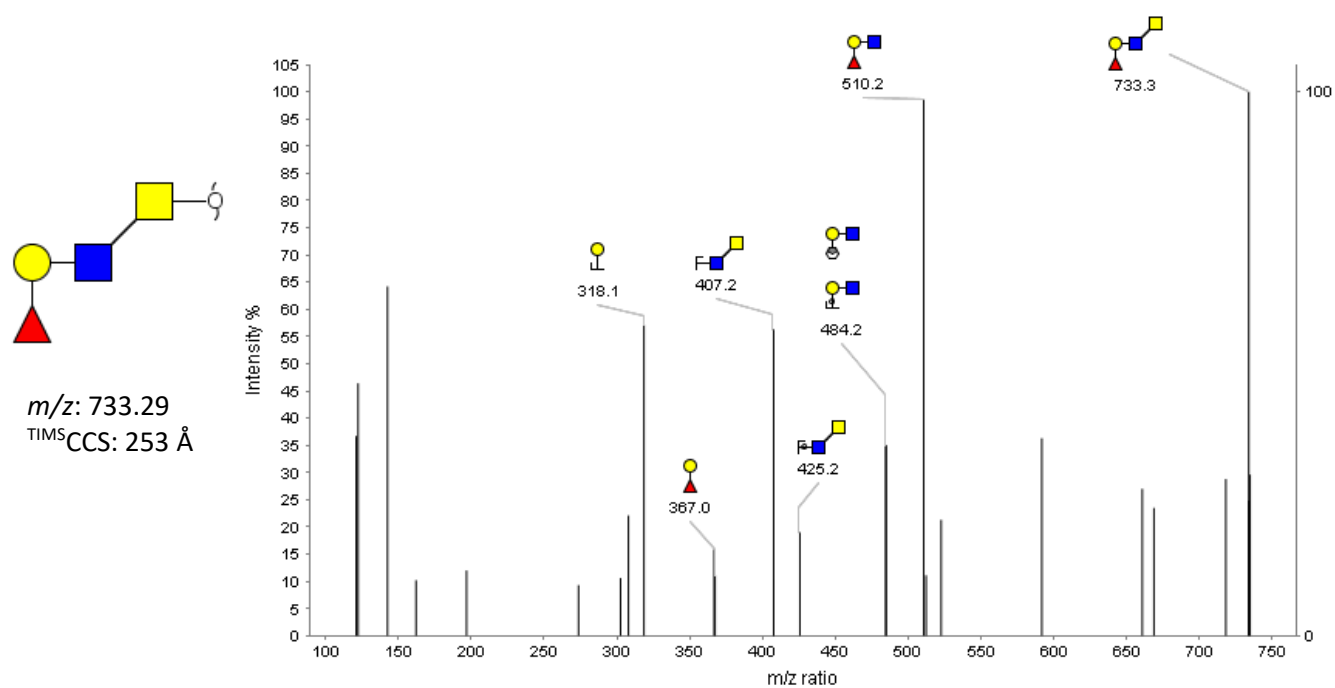
Glycan code: 675-2



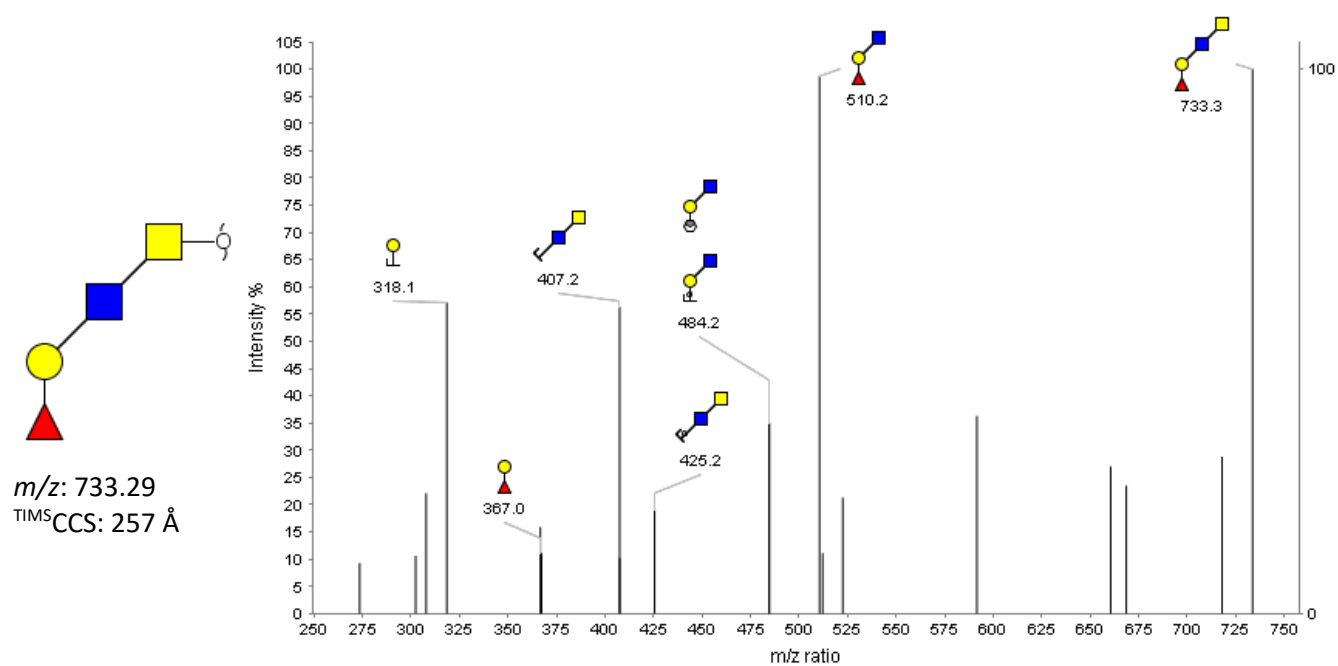
Glycan code: 716-1



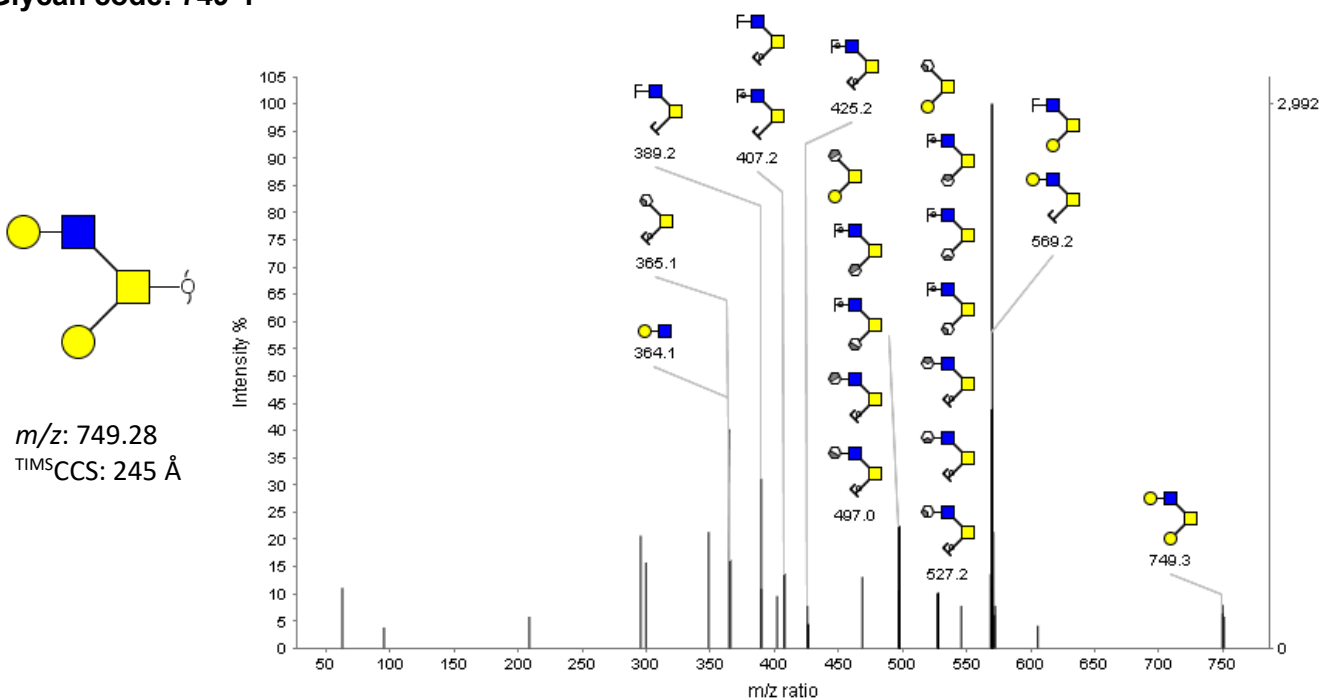
Glycan code: 733-1



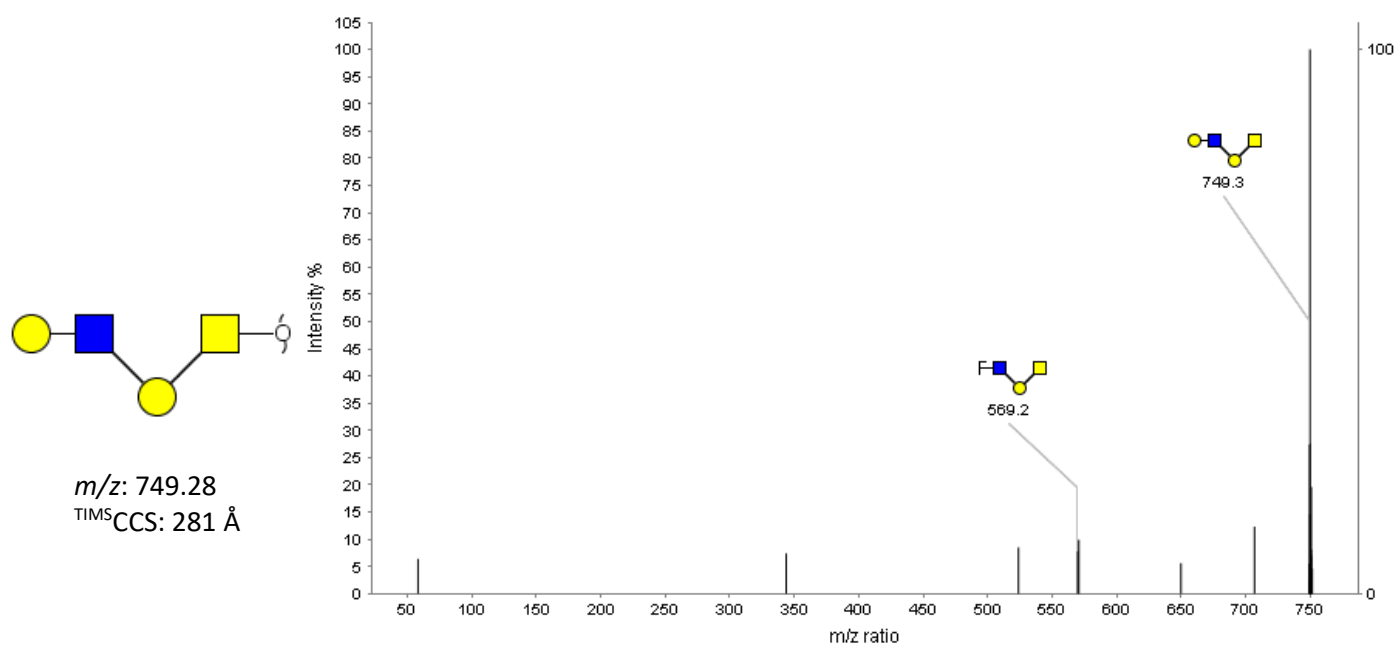
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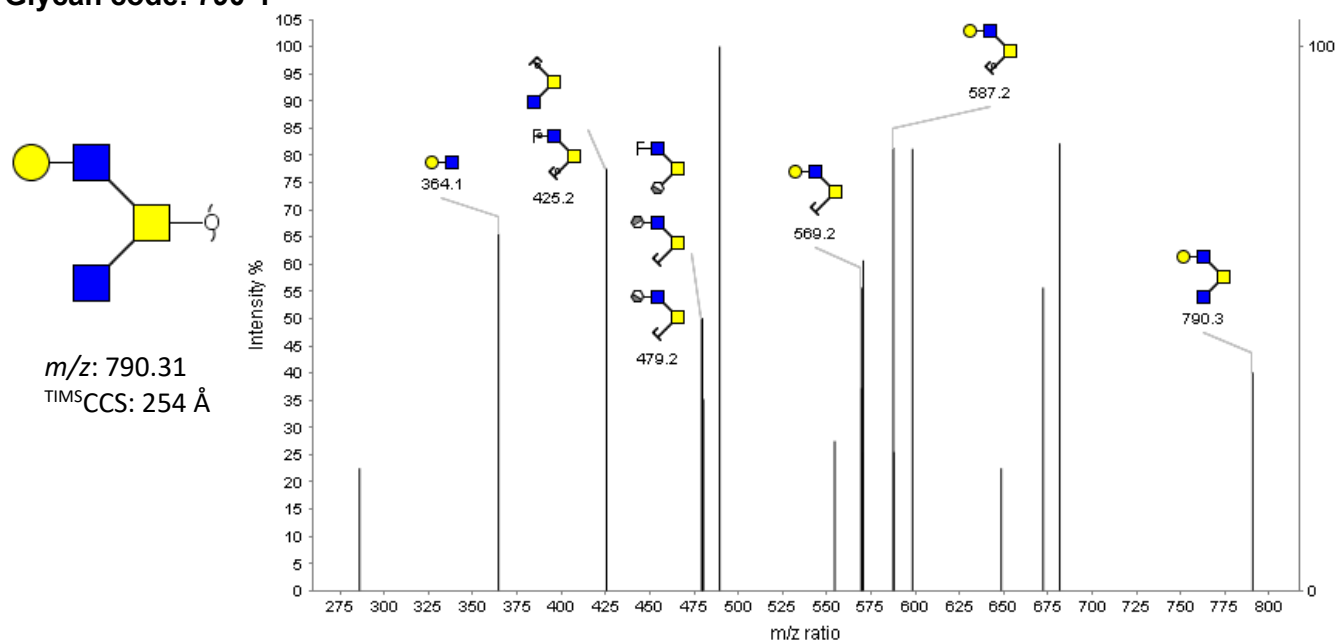
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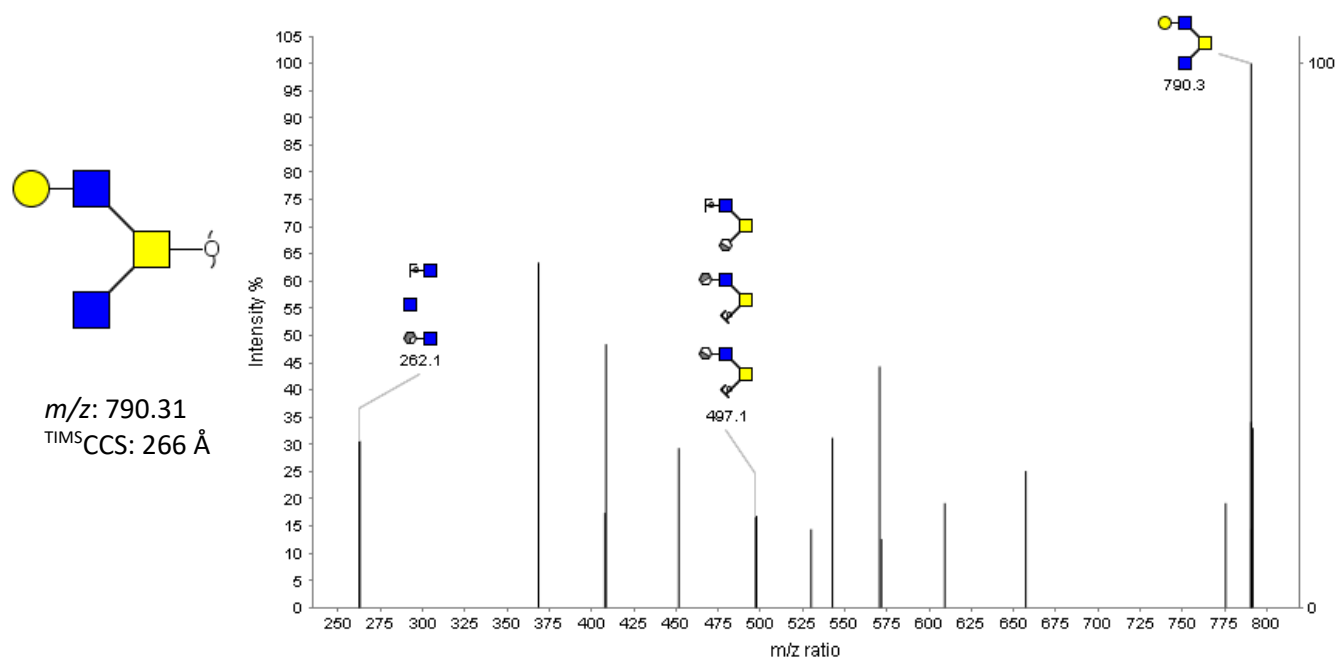
Glycan code: 749-2



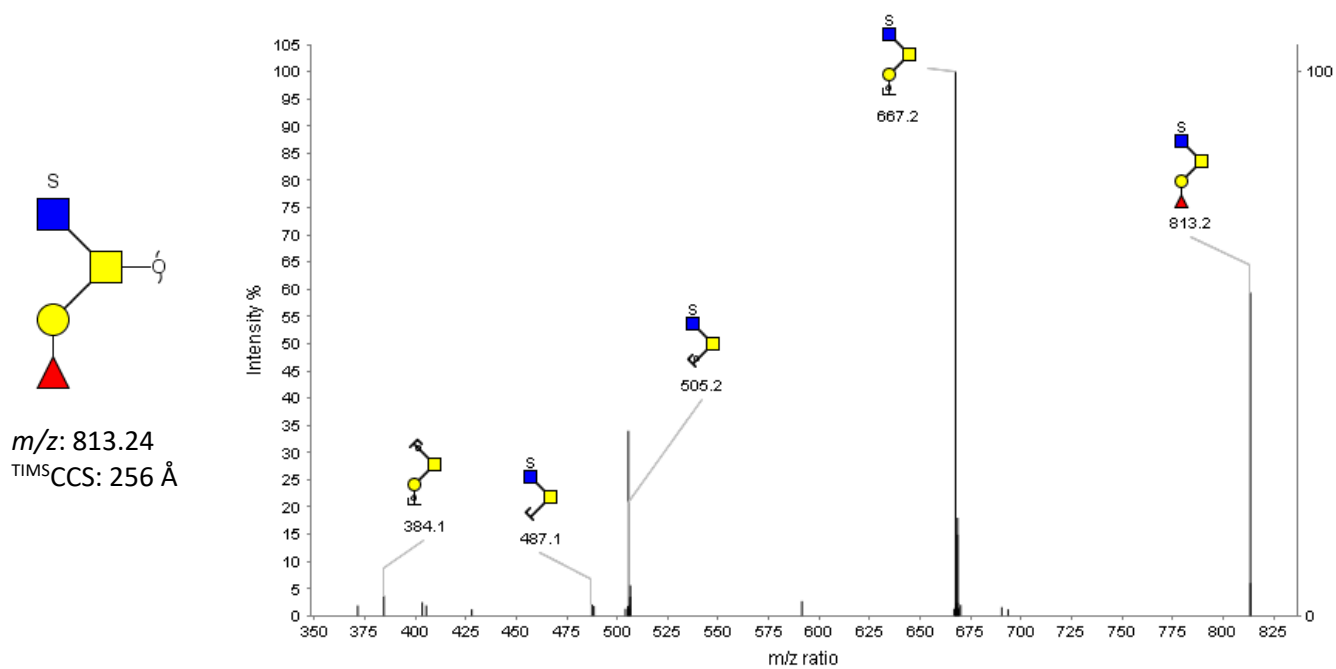
Glycan code: 790-1



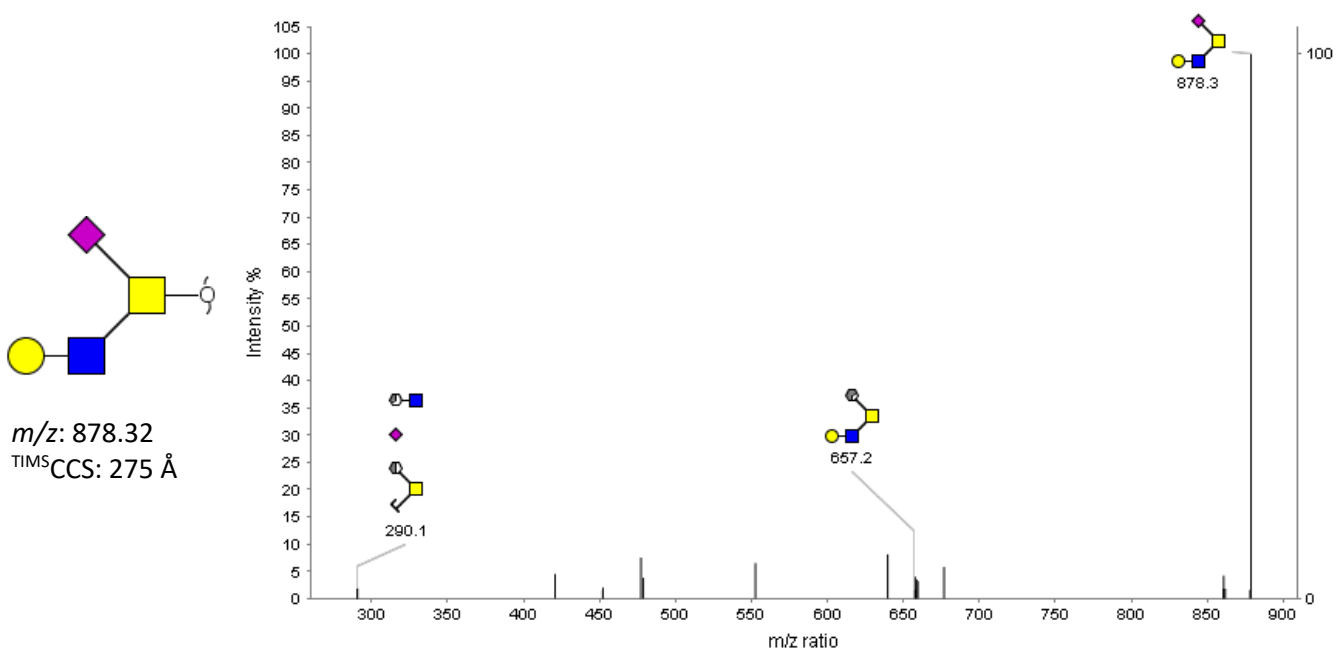
Glycan code: 790-2



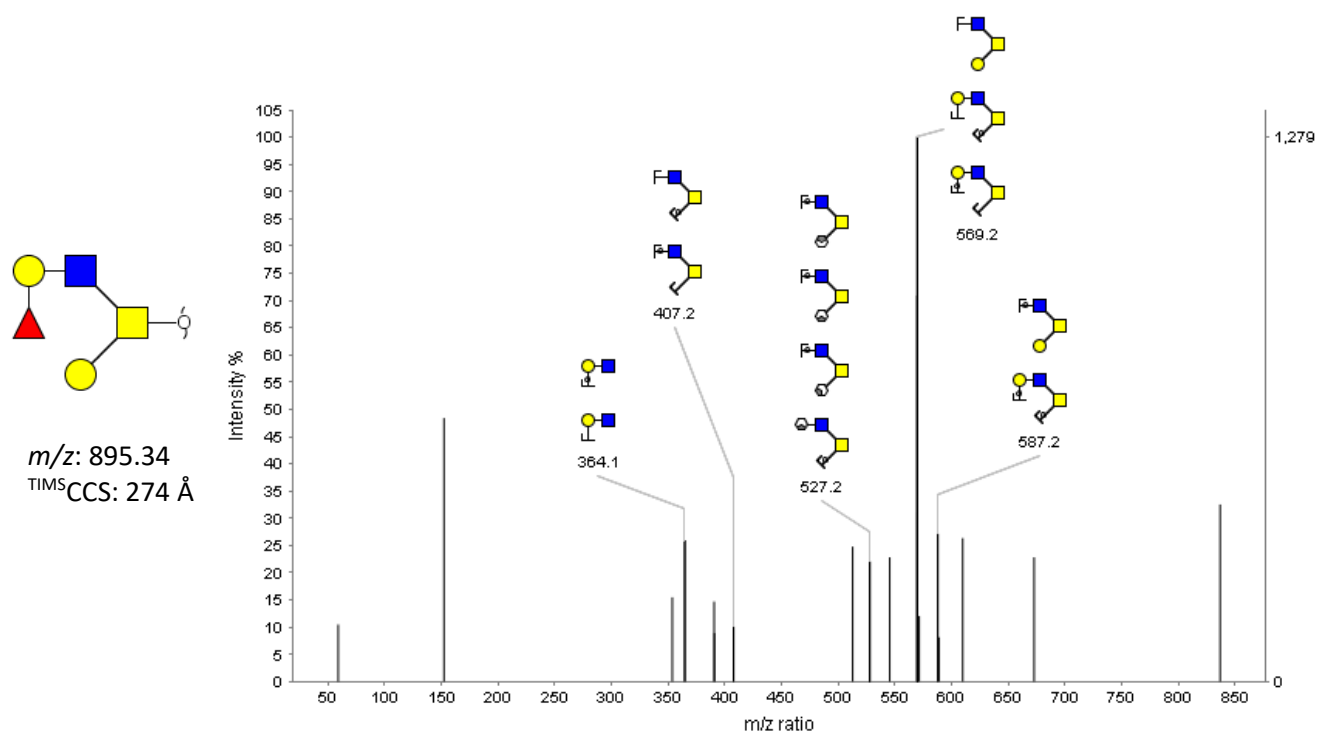
Glycan code: 813-1



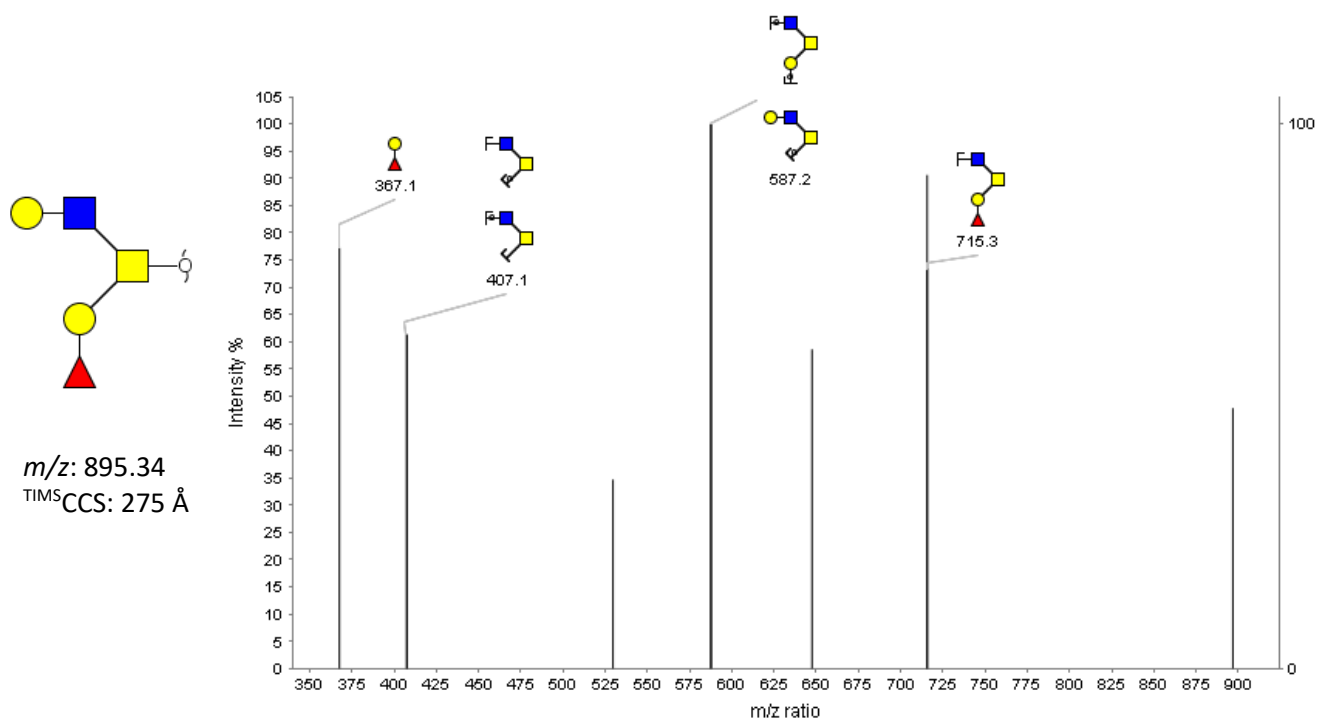
Glycan code: 878-1



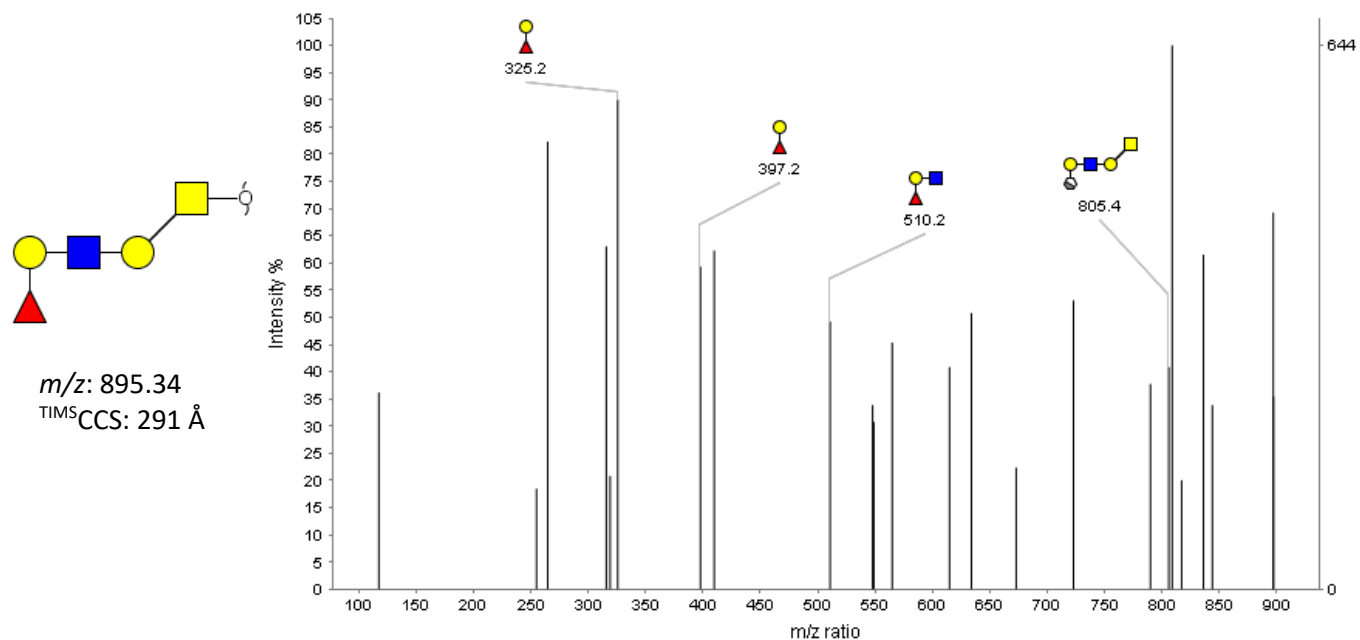
Glycan code: 895-1



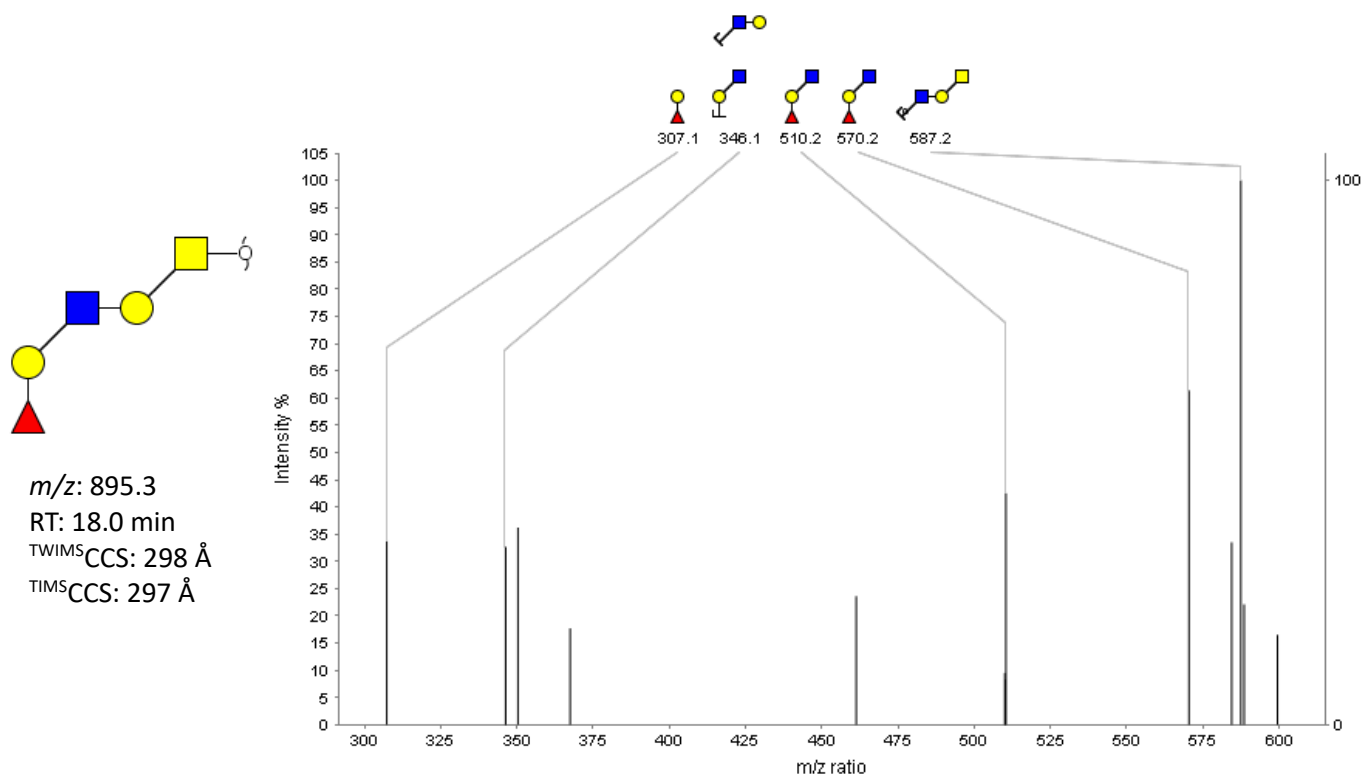
Glycan code: 895-2



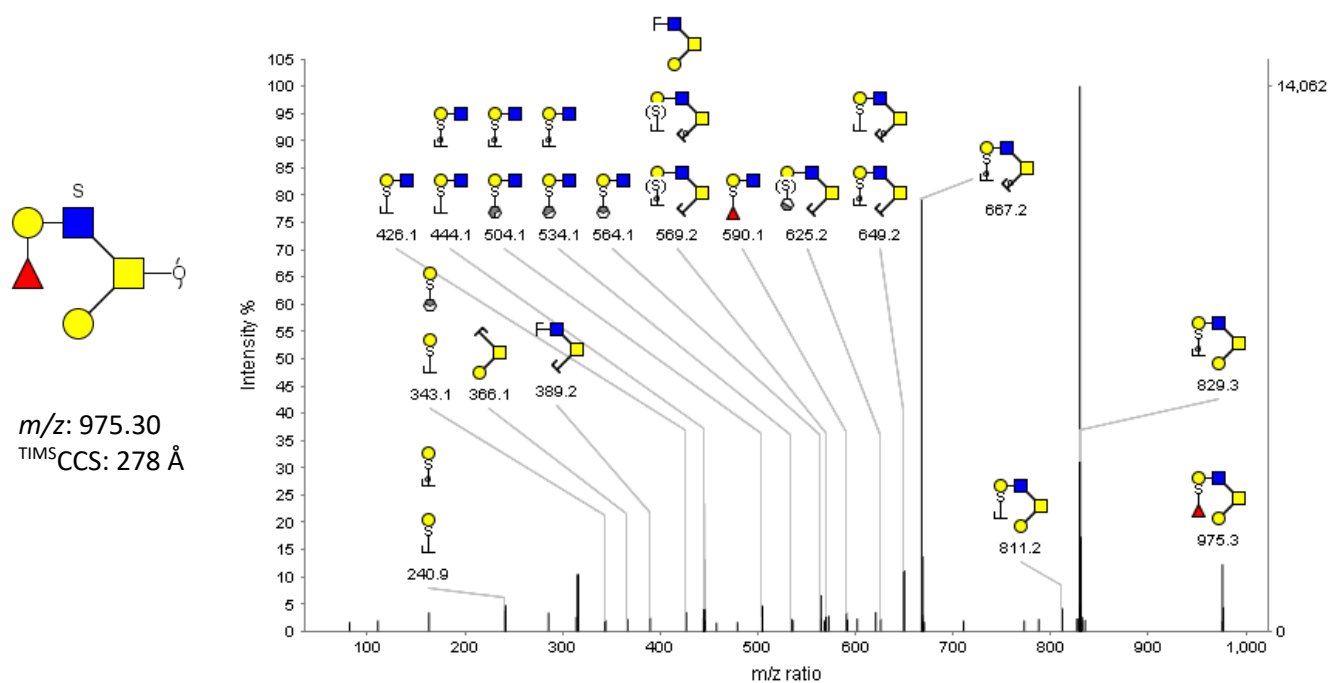
Glycan code: 895-3



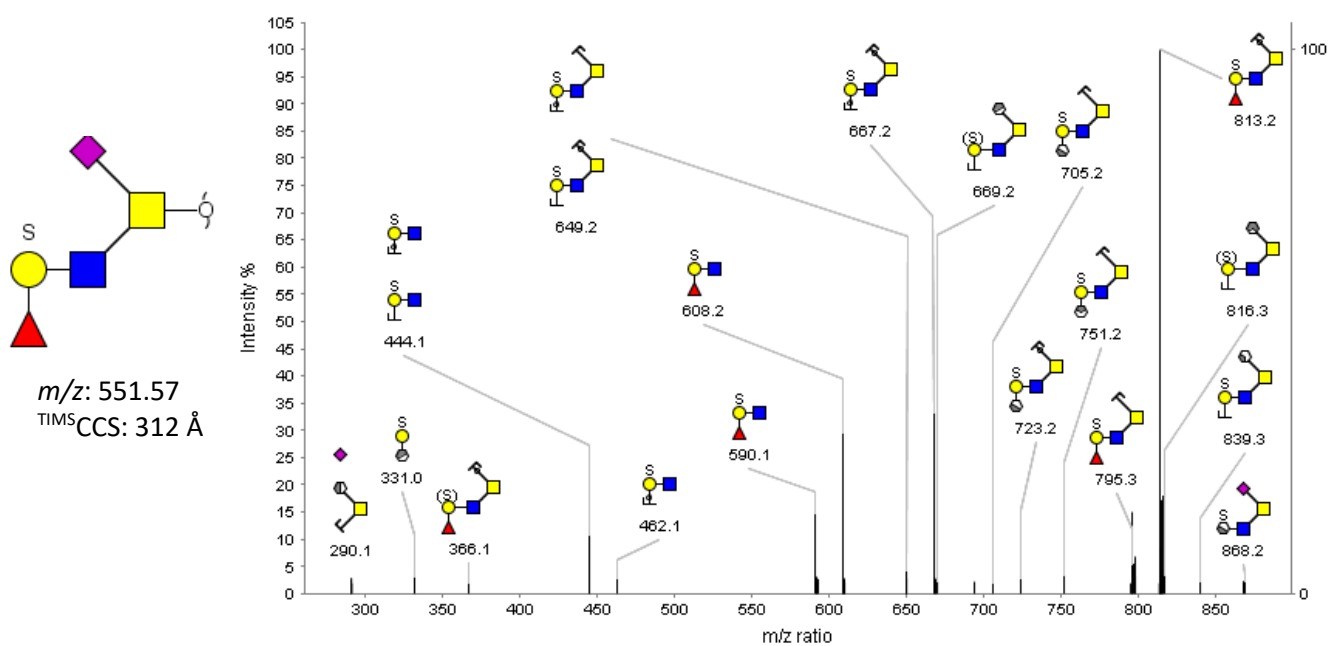
Glycan code: 895-4



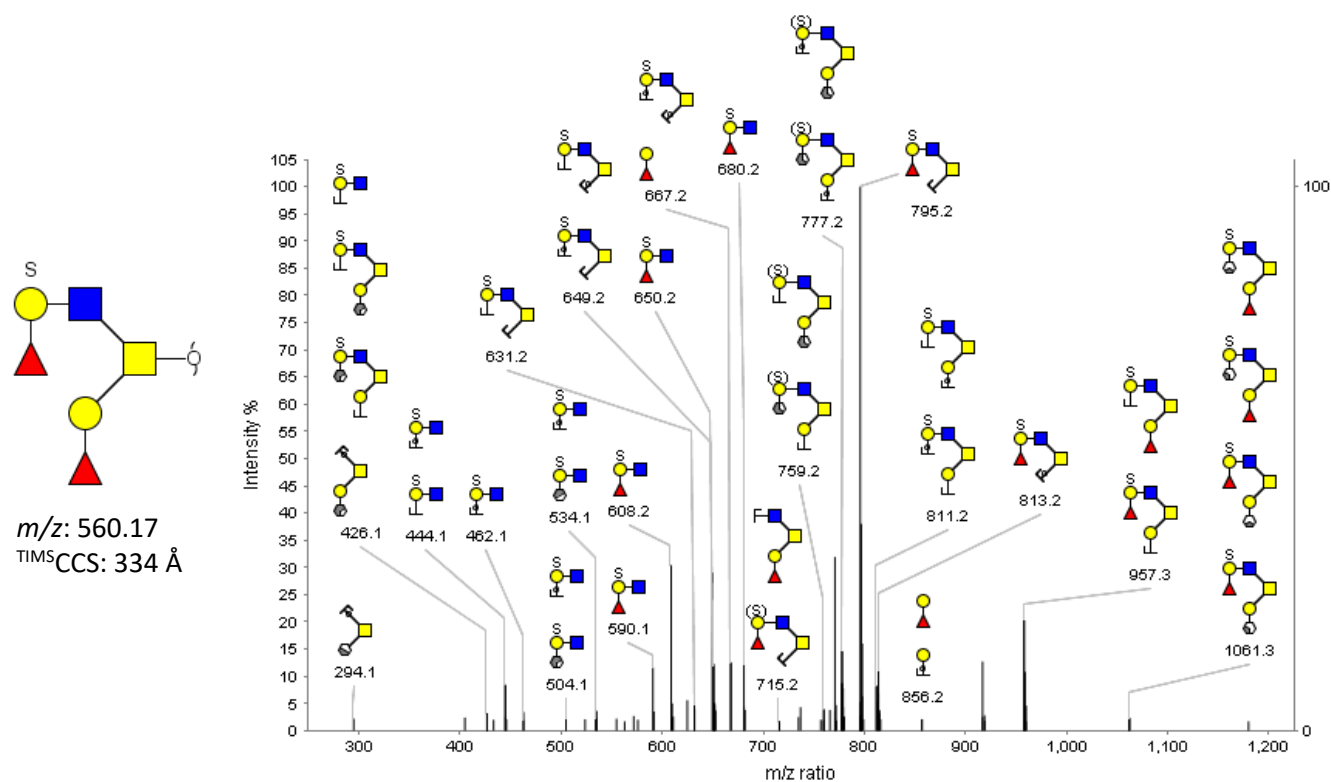
Glycan code: 975-1



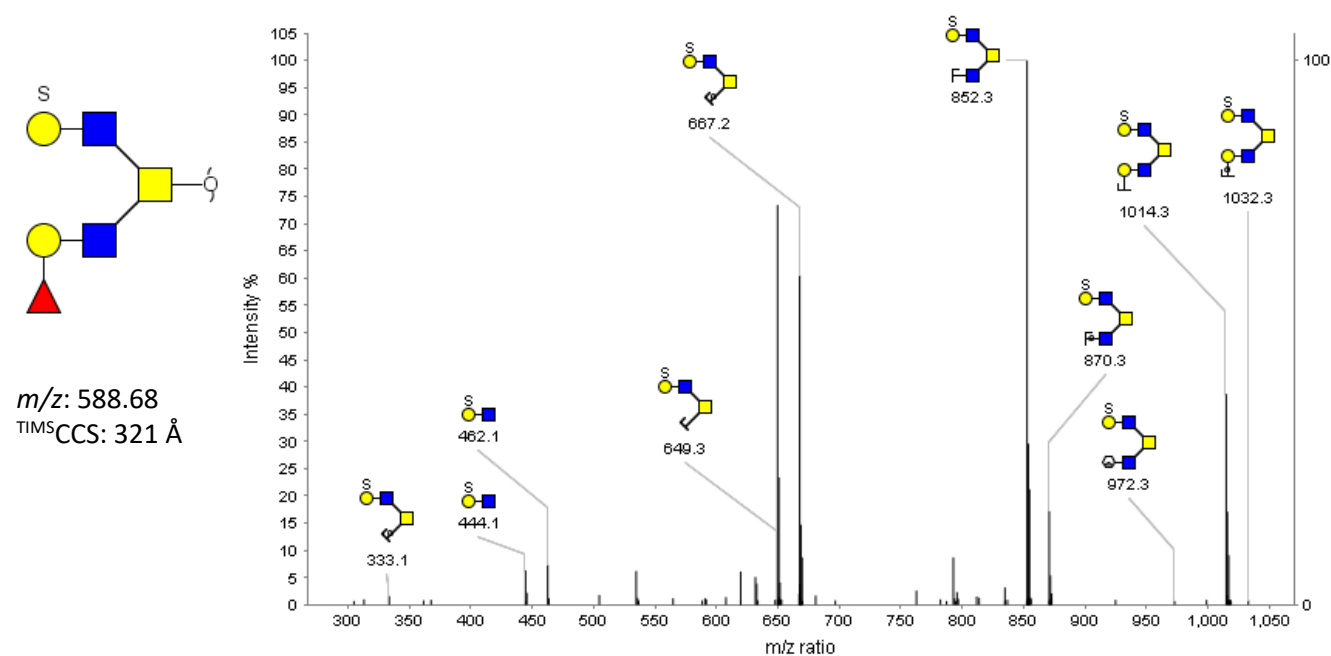
Glycan code: 551-1



Glycan code: 560-1

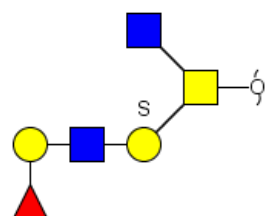


Glycan code: 588-1

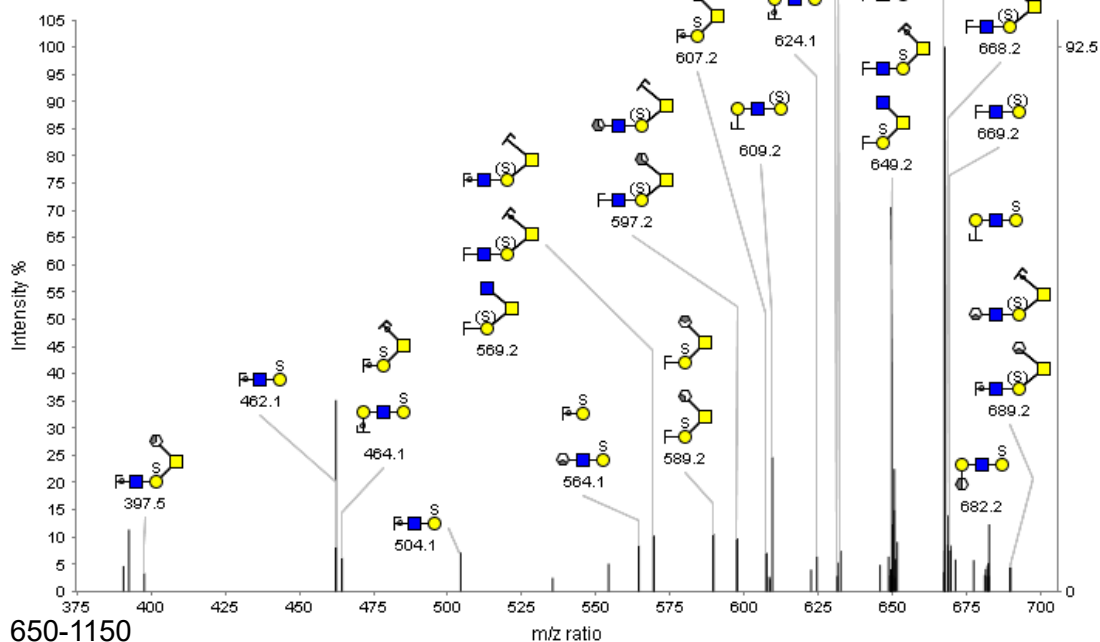


Glycan code: 588-2

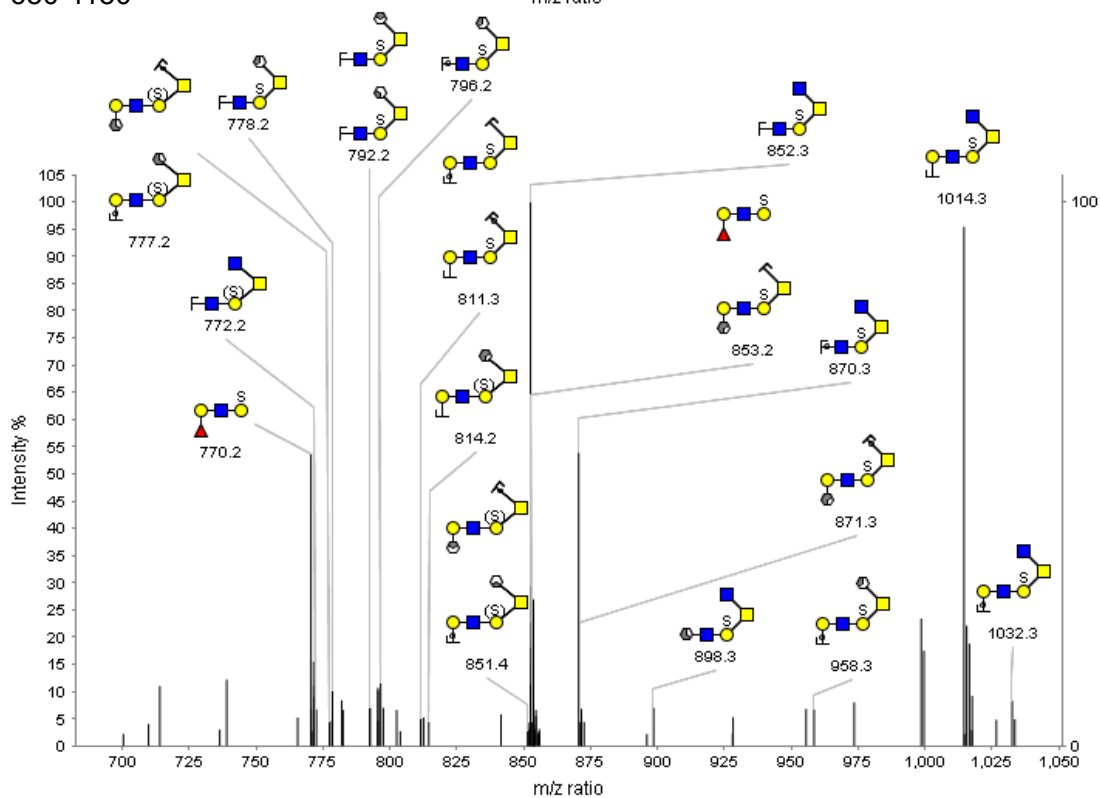
m/z range: 375-700



m/z: 588.68
TIMS CCS: 326 Å

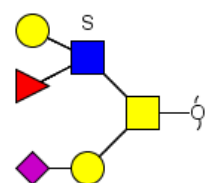


m/z range: 650-1150

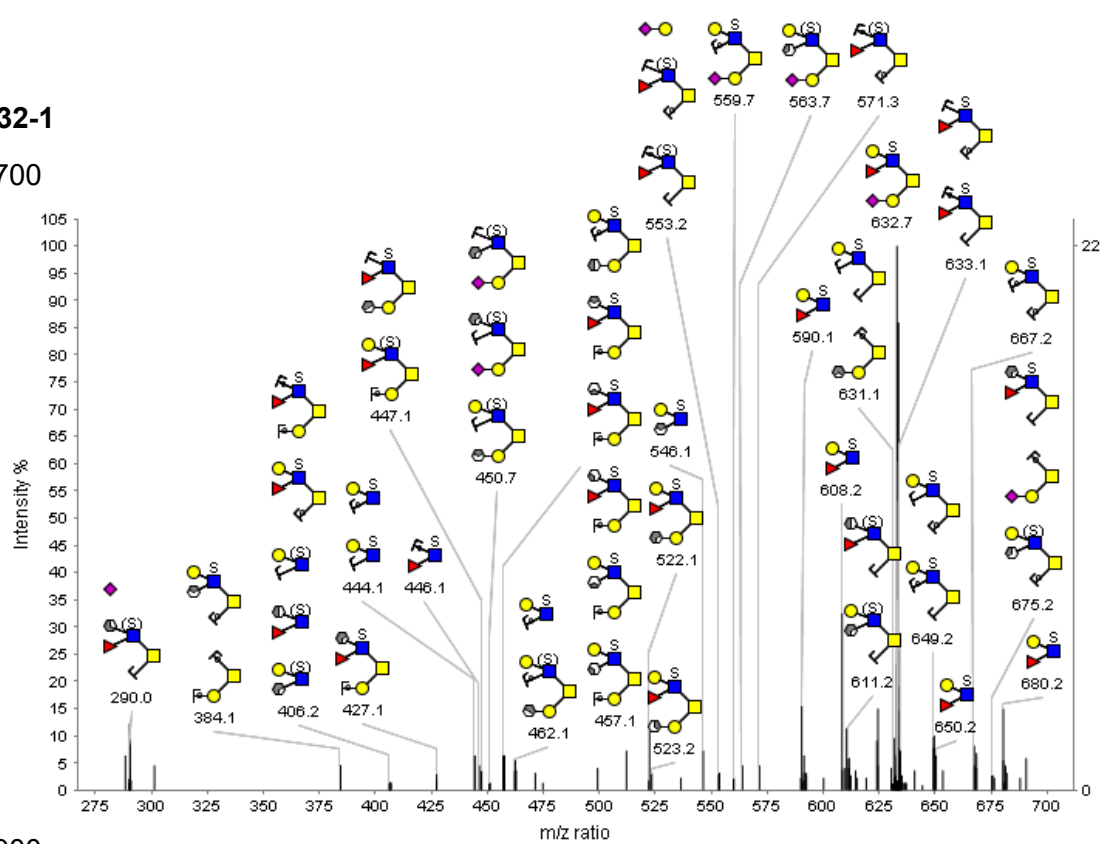


Glycan code: 632-1

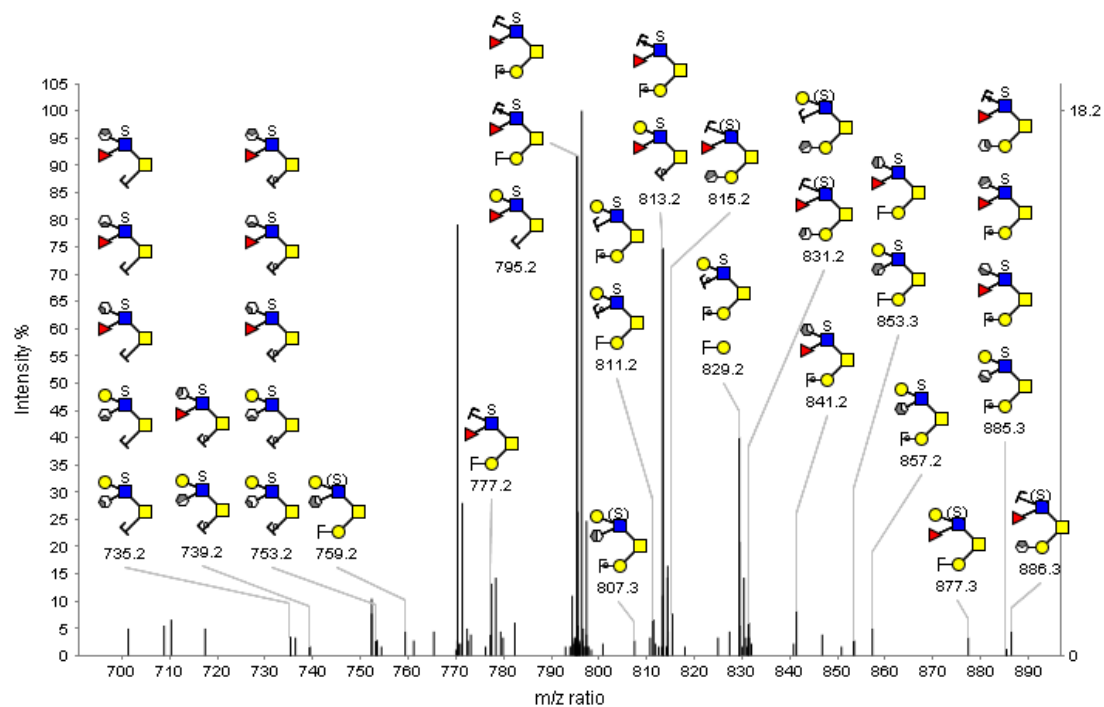
m/z range: 250-700



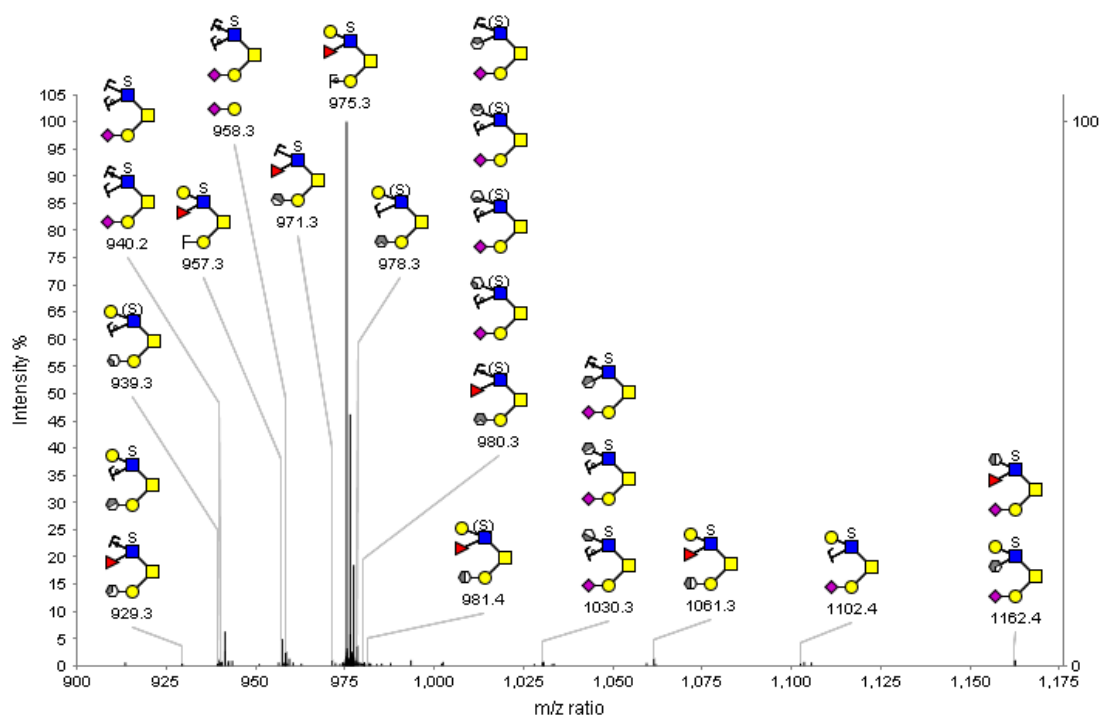
m/z: 632.69
TIMS CCS: 338 Å



m/z range: 700-900

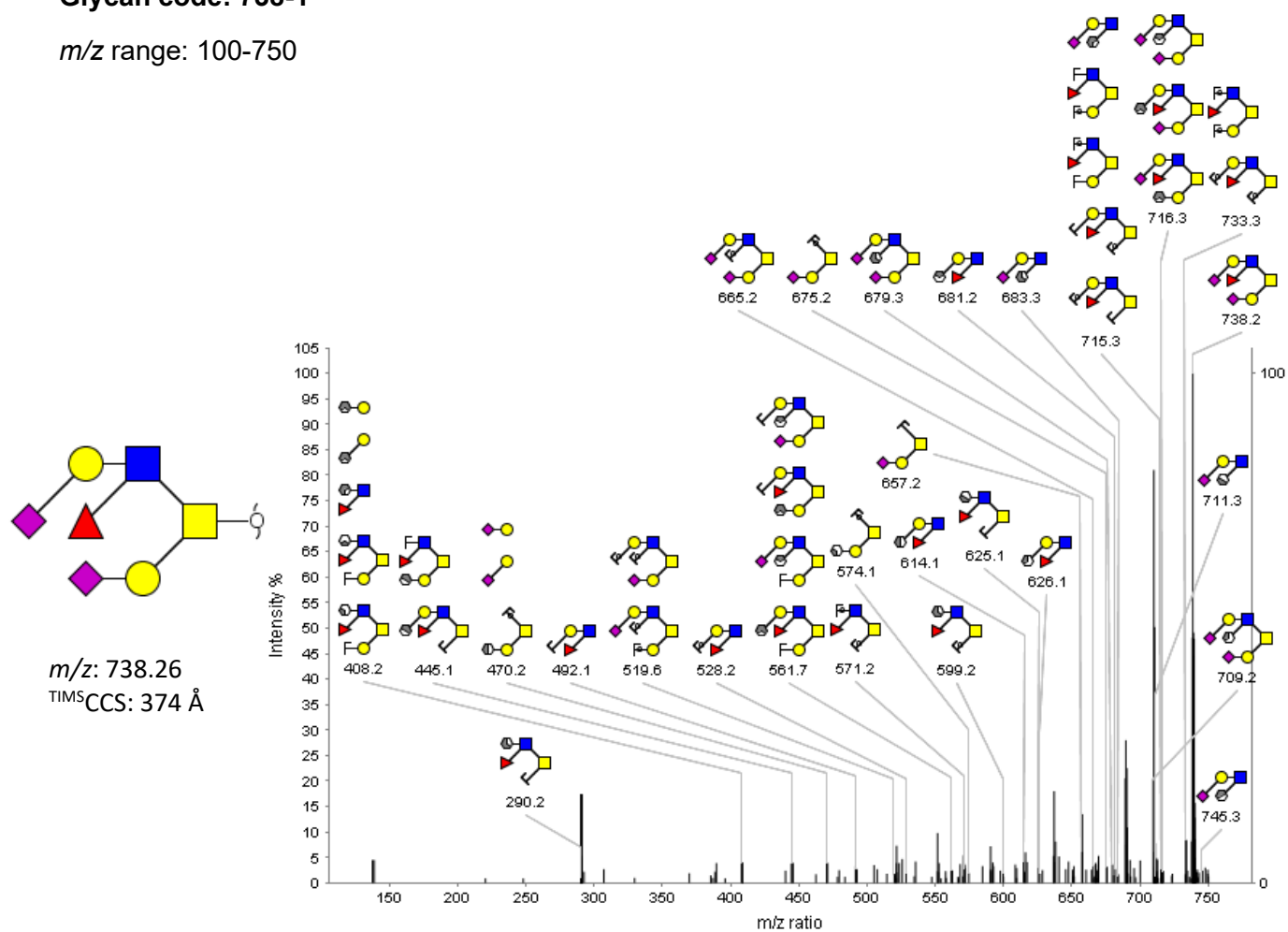


m/z range: 900-1175

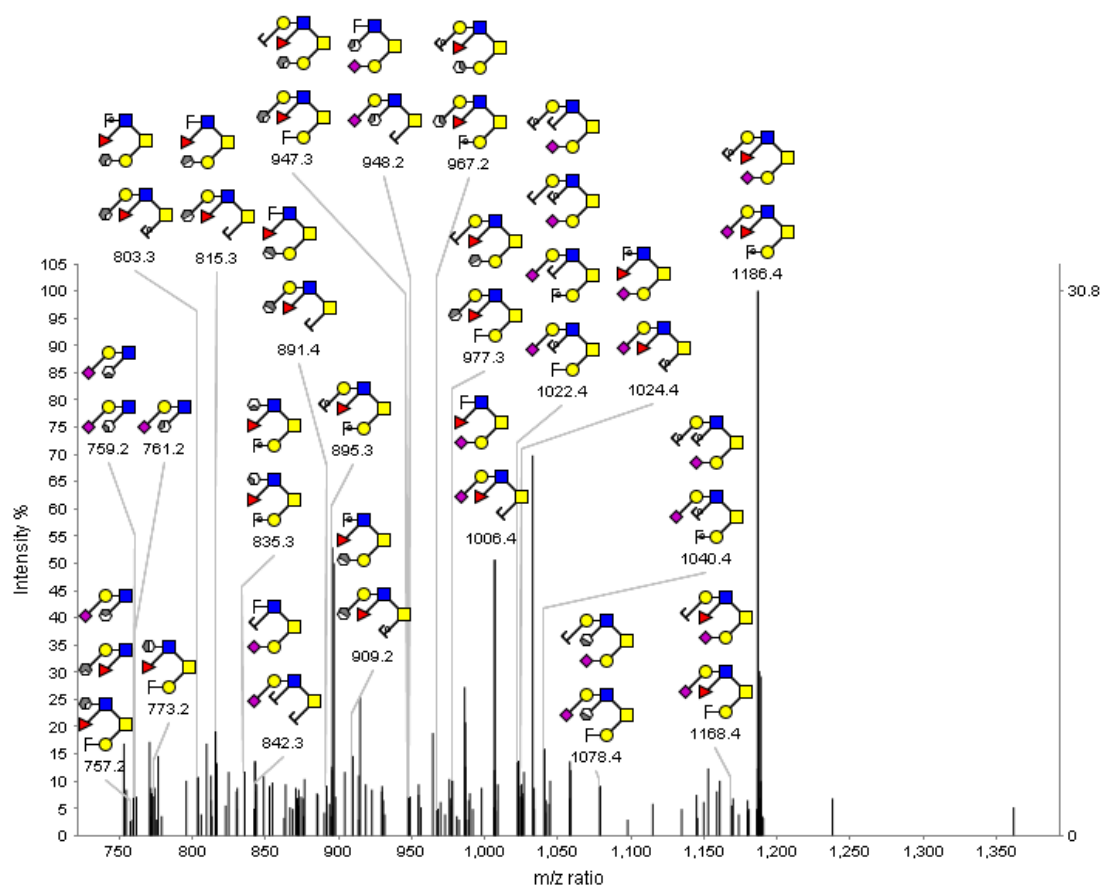


Glycan code: 738-1

m/z range: 100-750

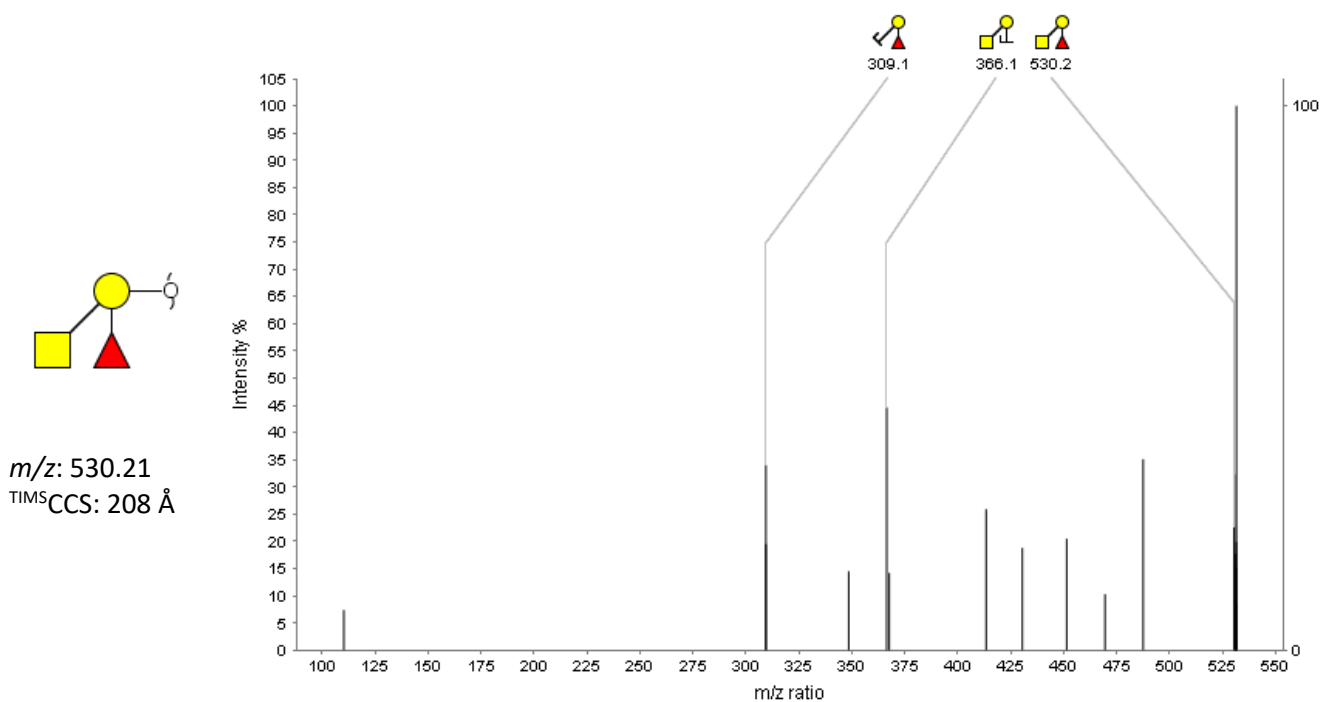


m/z range: 750-1400

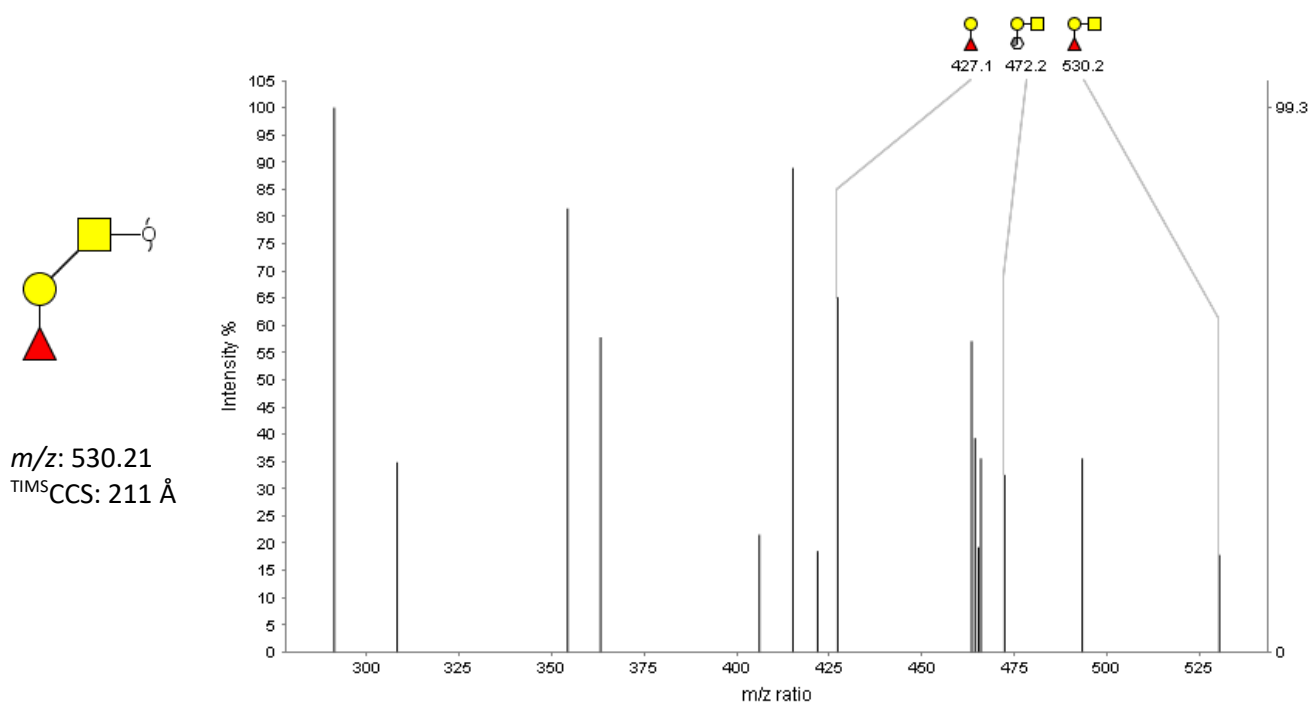


III. Annotated MS/MS spectra of O-glycans in cystic fibrosis sputum

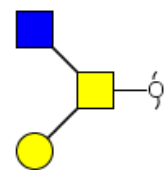
Glycan code: 530-1



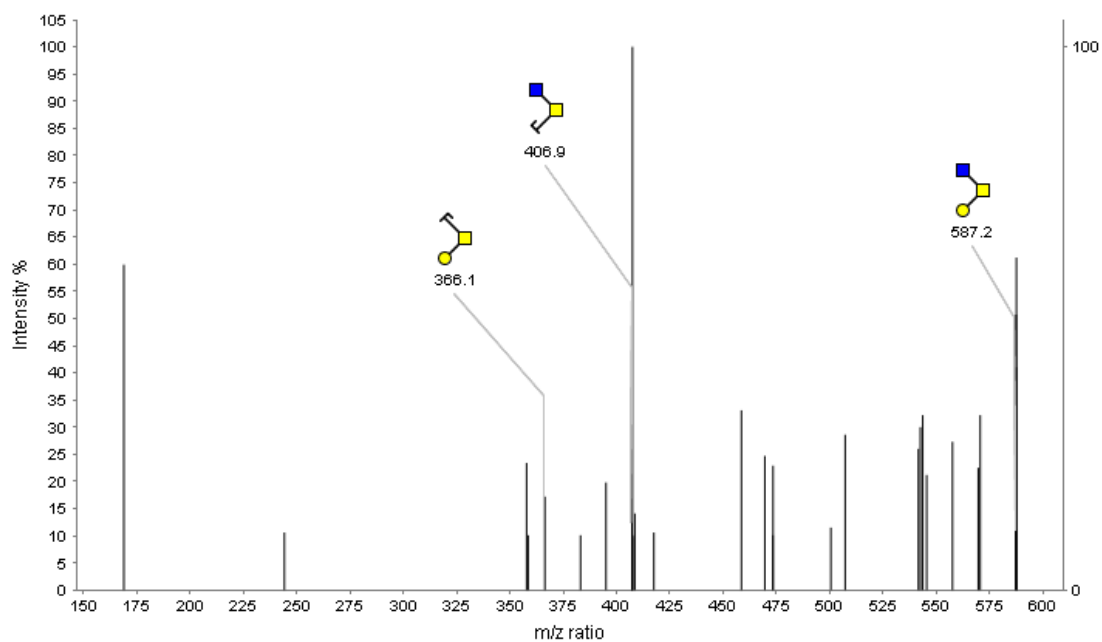
Glycan code: 530-2



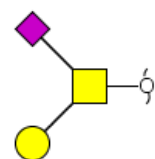
Glycan code: 587-1



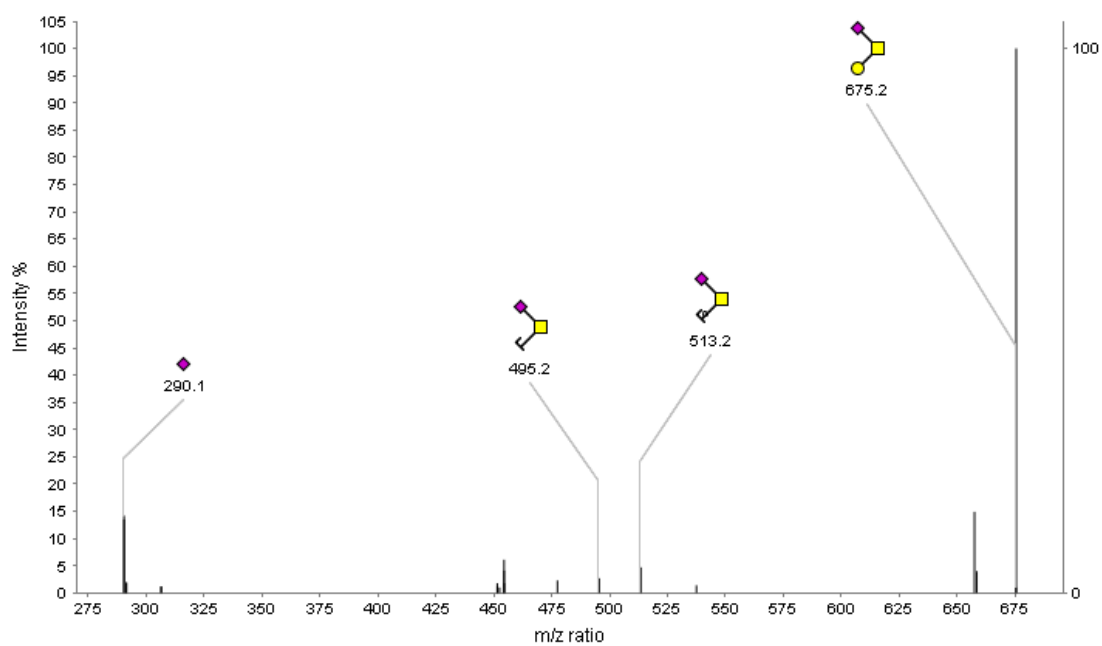
m/z : 587.23
TIMS CCS: 234 Å



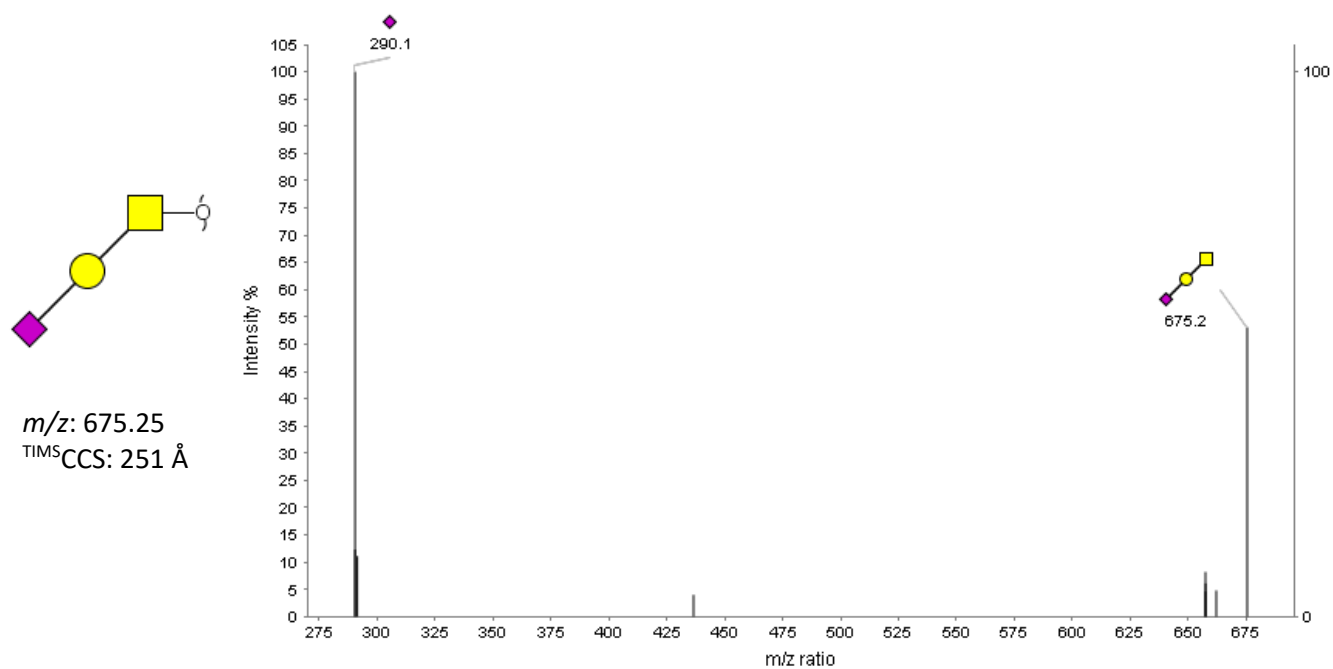
Glycan code: 675-1



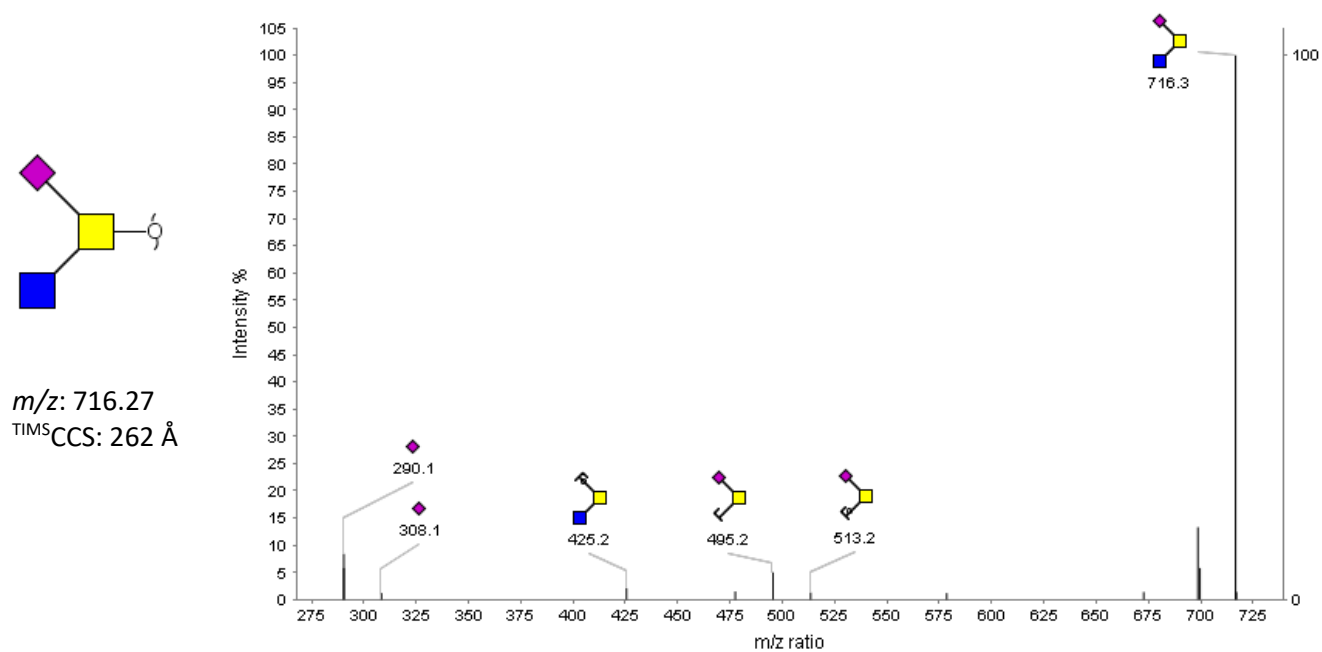
m/z : 675.25
TIMS CCS: 247 Å



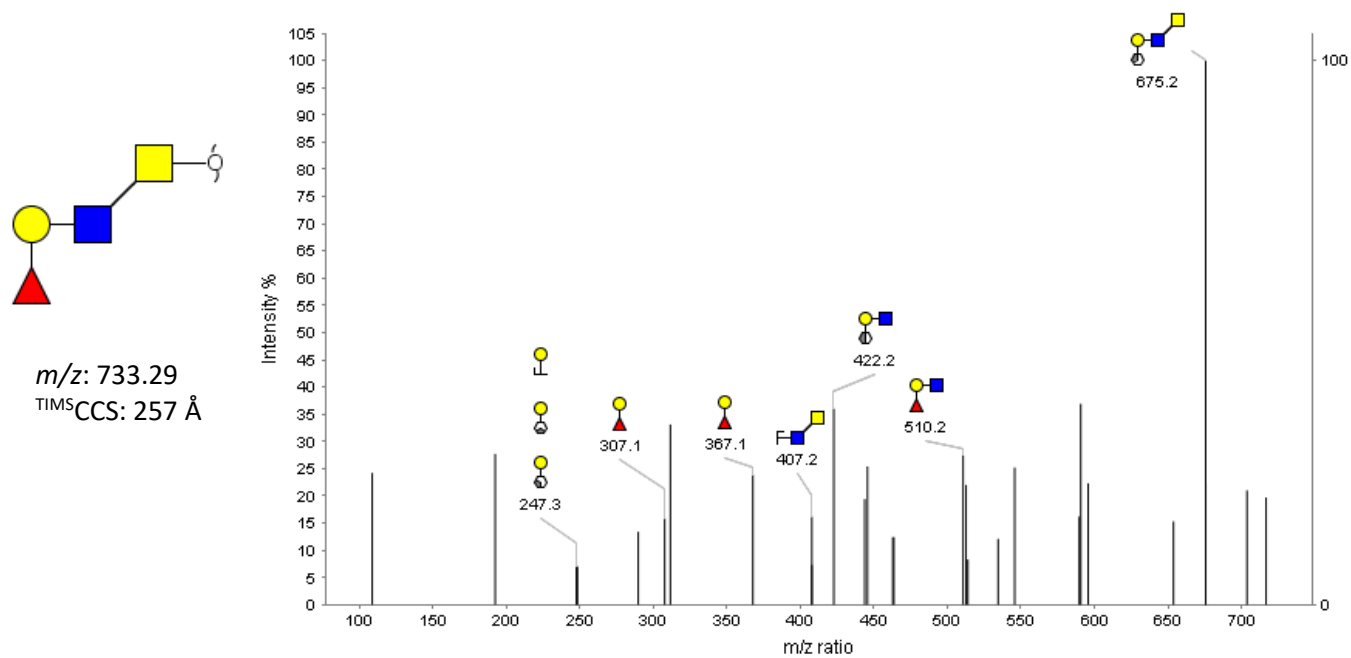
Glycan code: 675-2



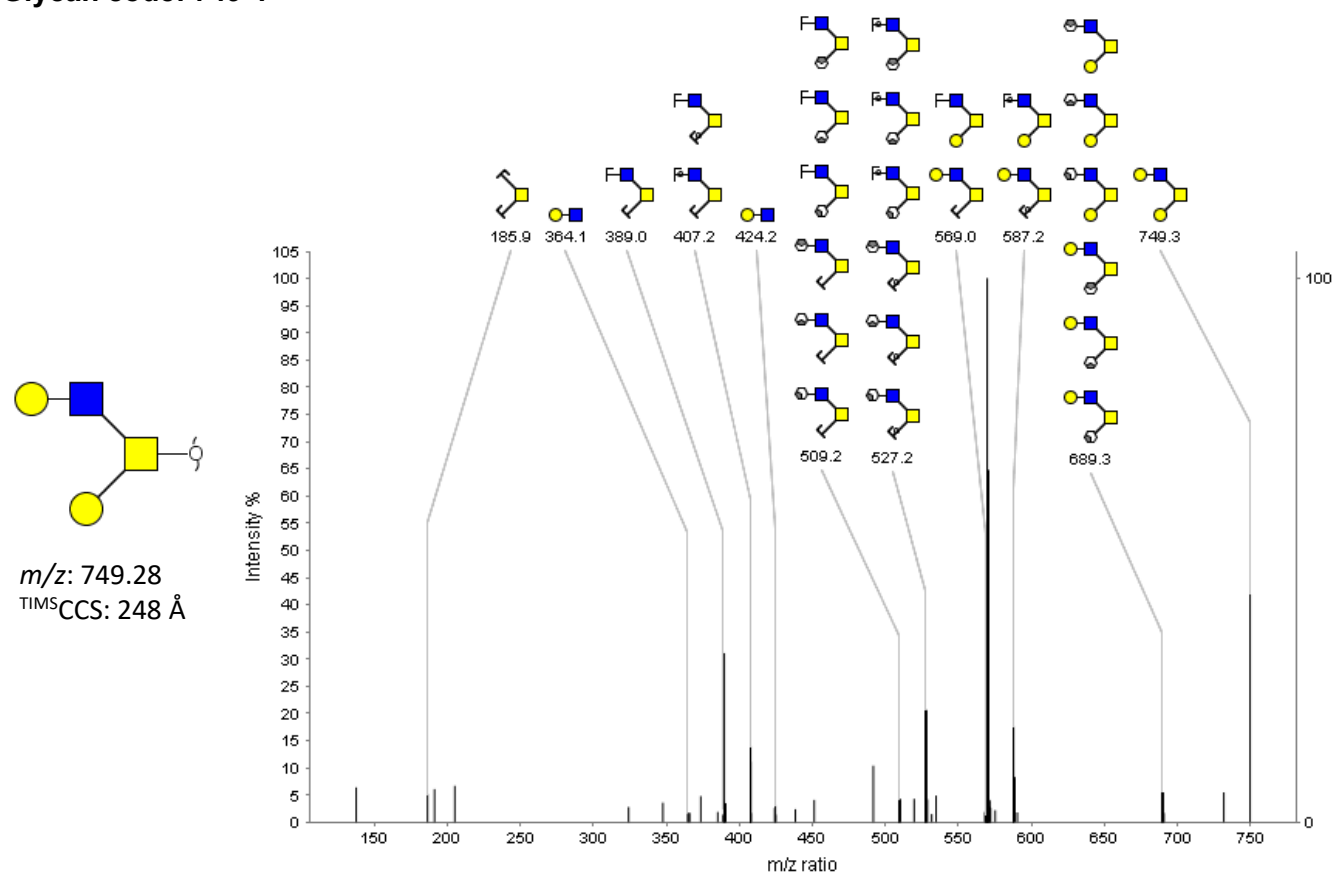
Glycan code: 716-1



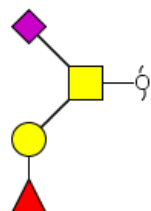
Glycan code: 733-1



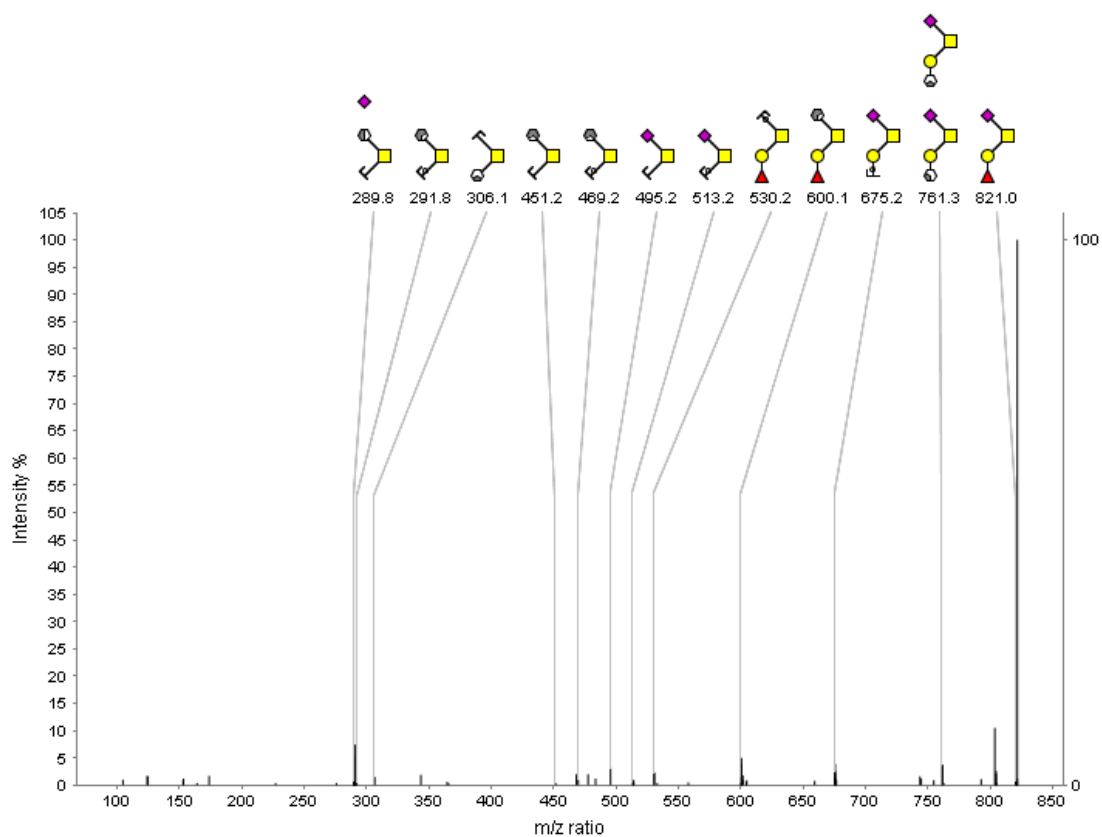
Glycan code: 749-1



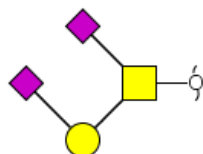
Glycan code: 821-2



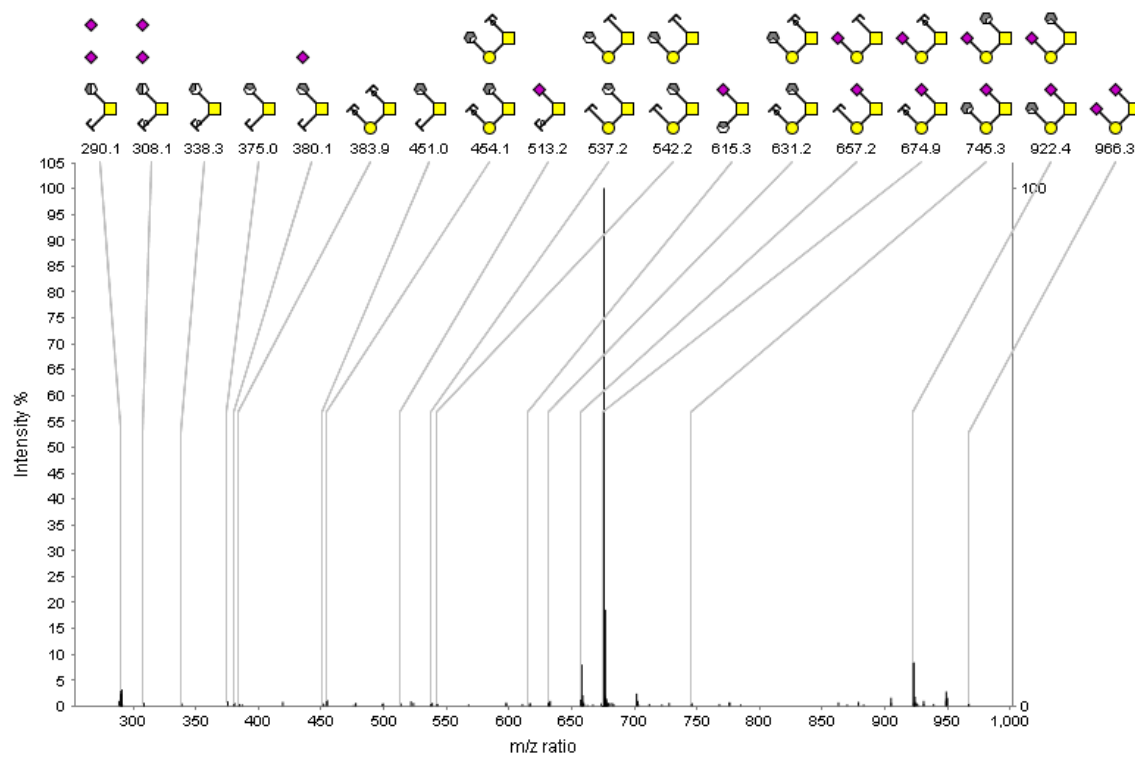
m/z : 821.30
TIMS⁺CCS: 272 Å



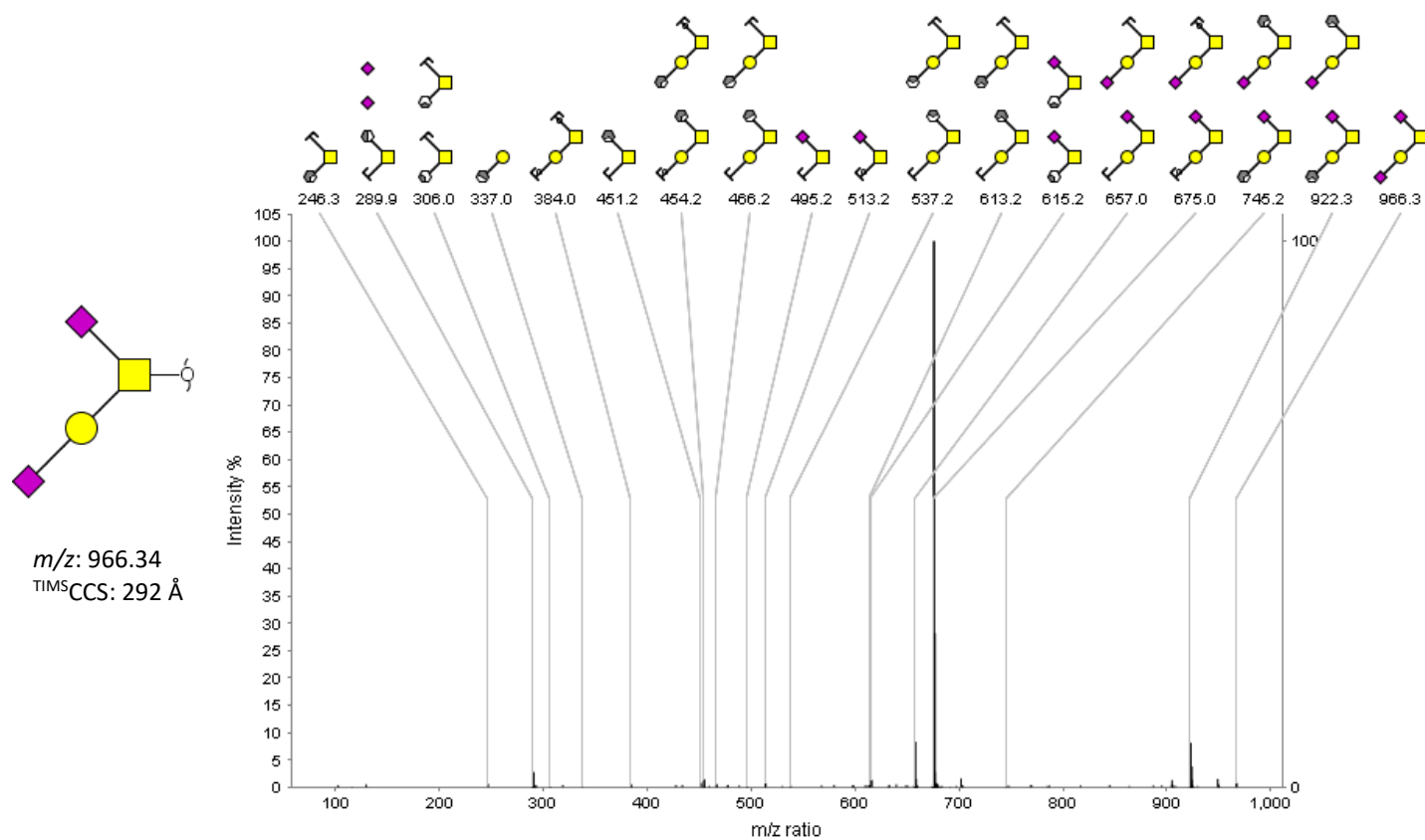
Glycan code: 966-1



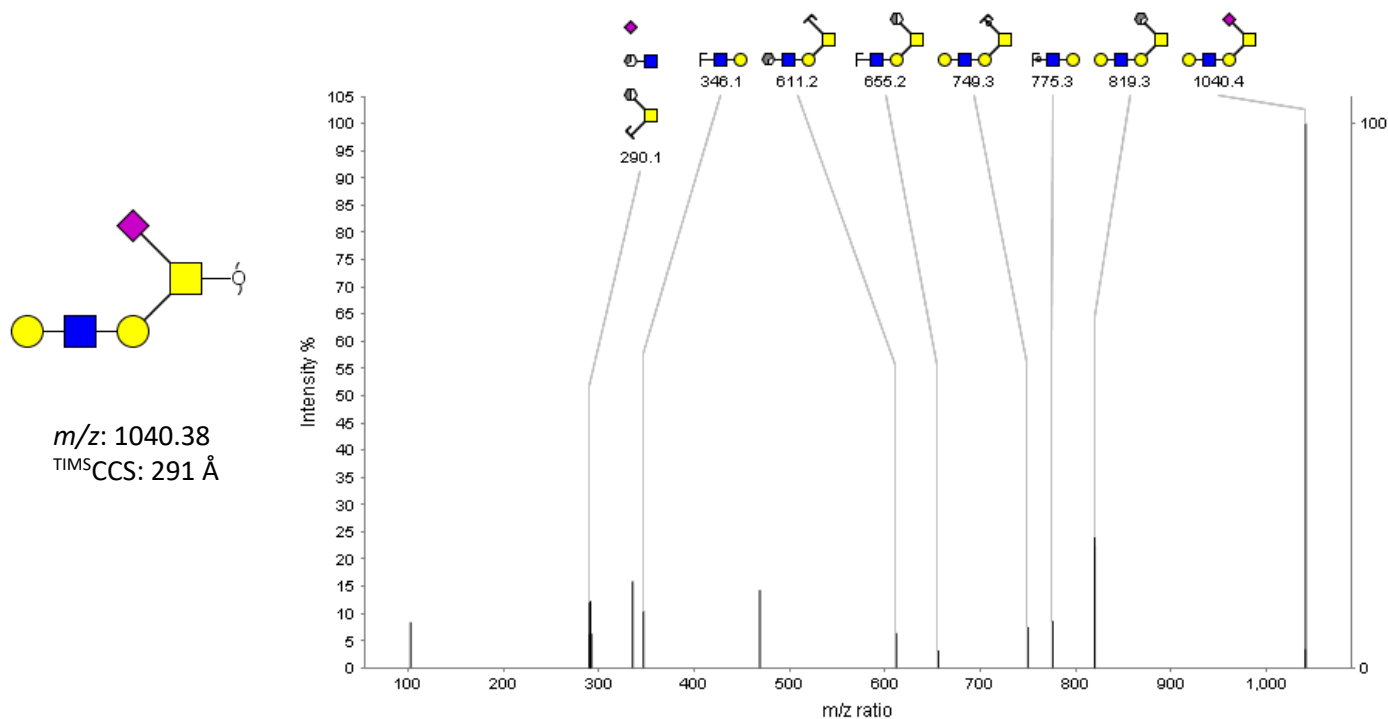
m/z : 966.34
TIMS⁺CCS: 288 Å



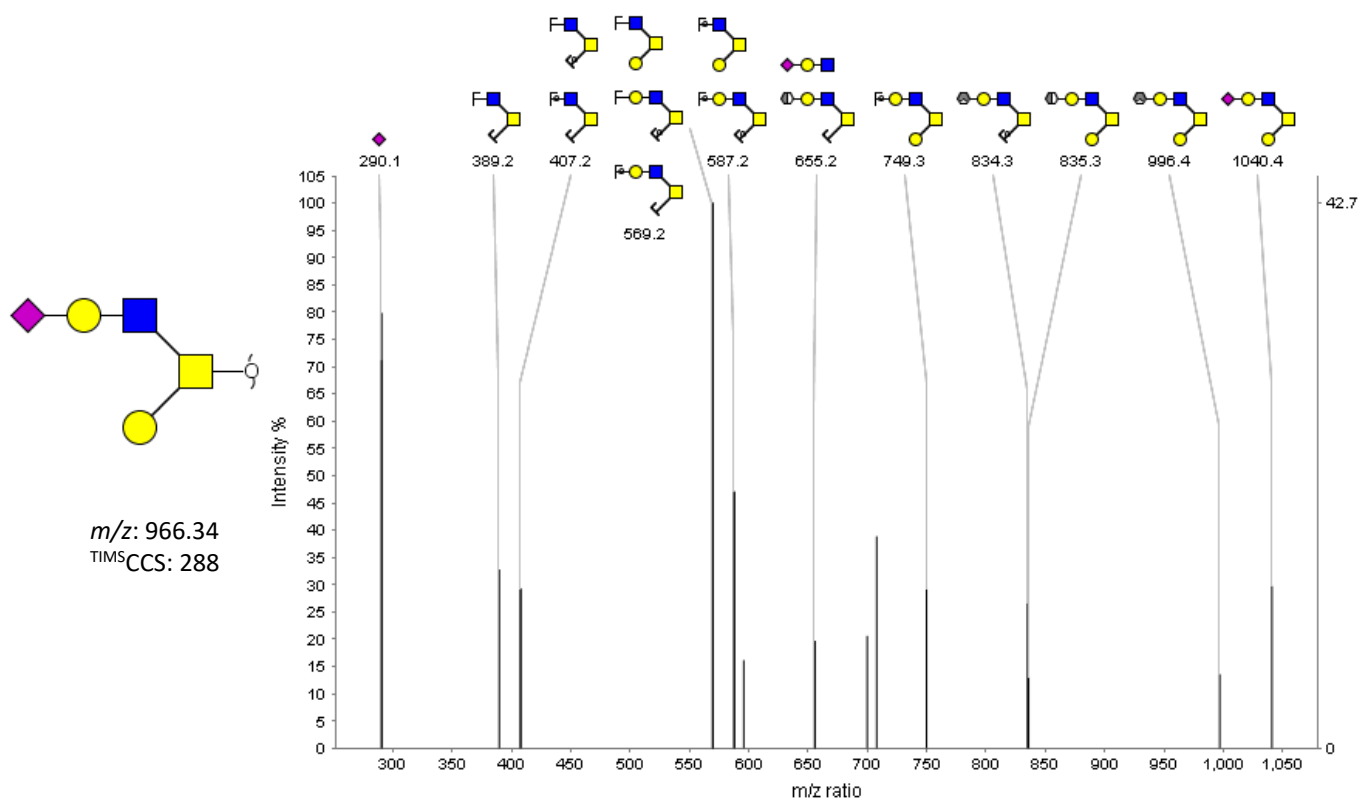
Glycan code: 966-2



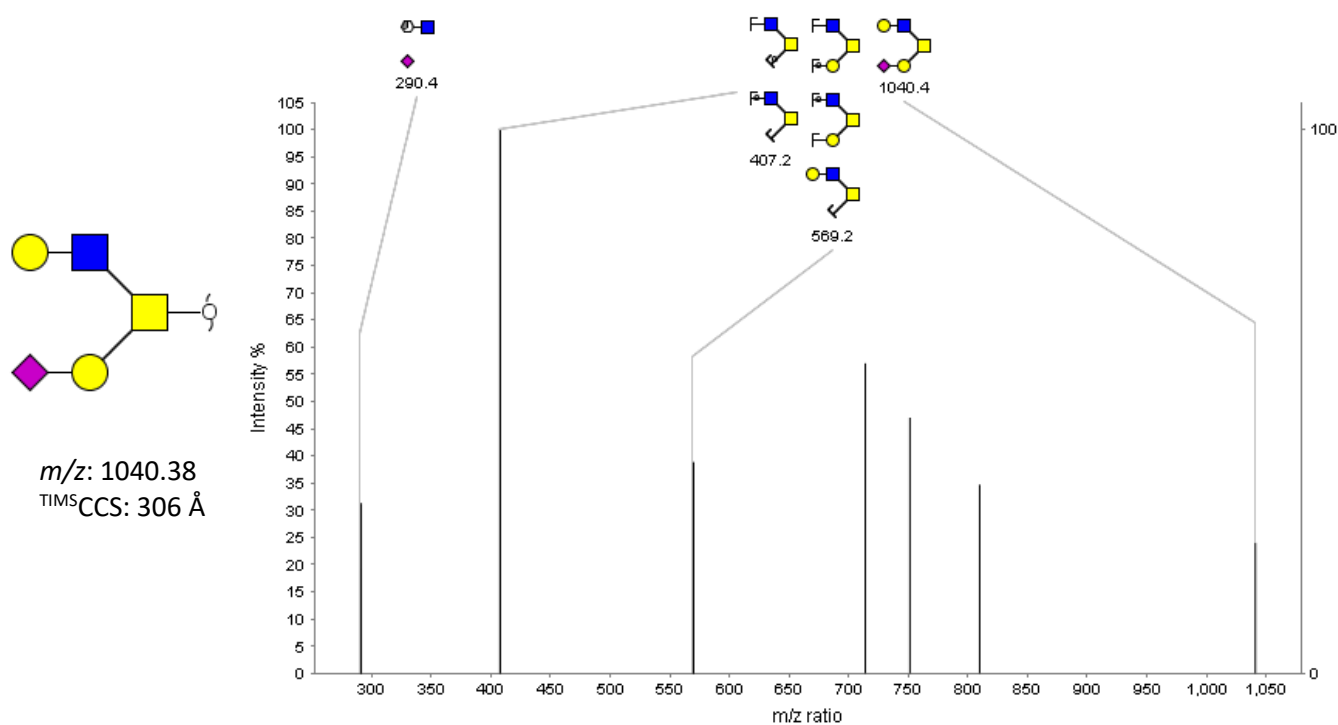
Glycan code: 1040-1



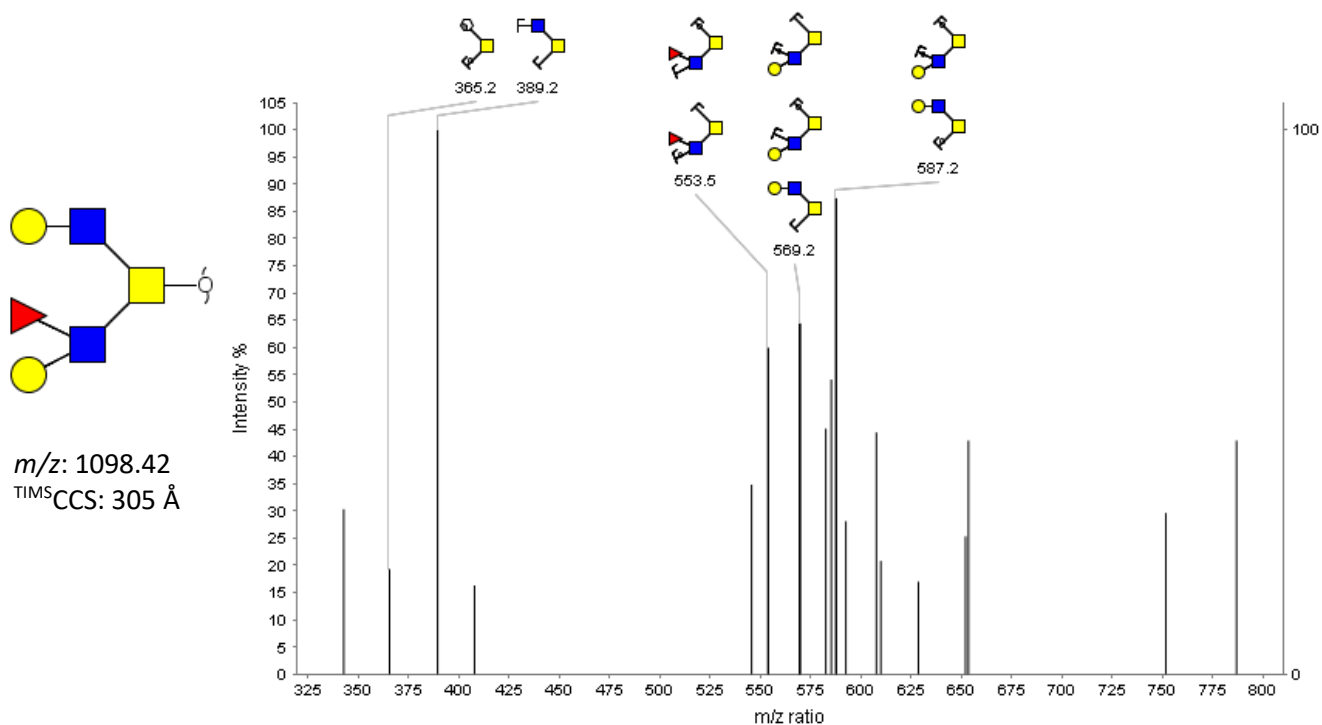
Glycan code: 1040-2



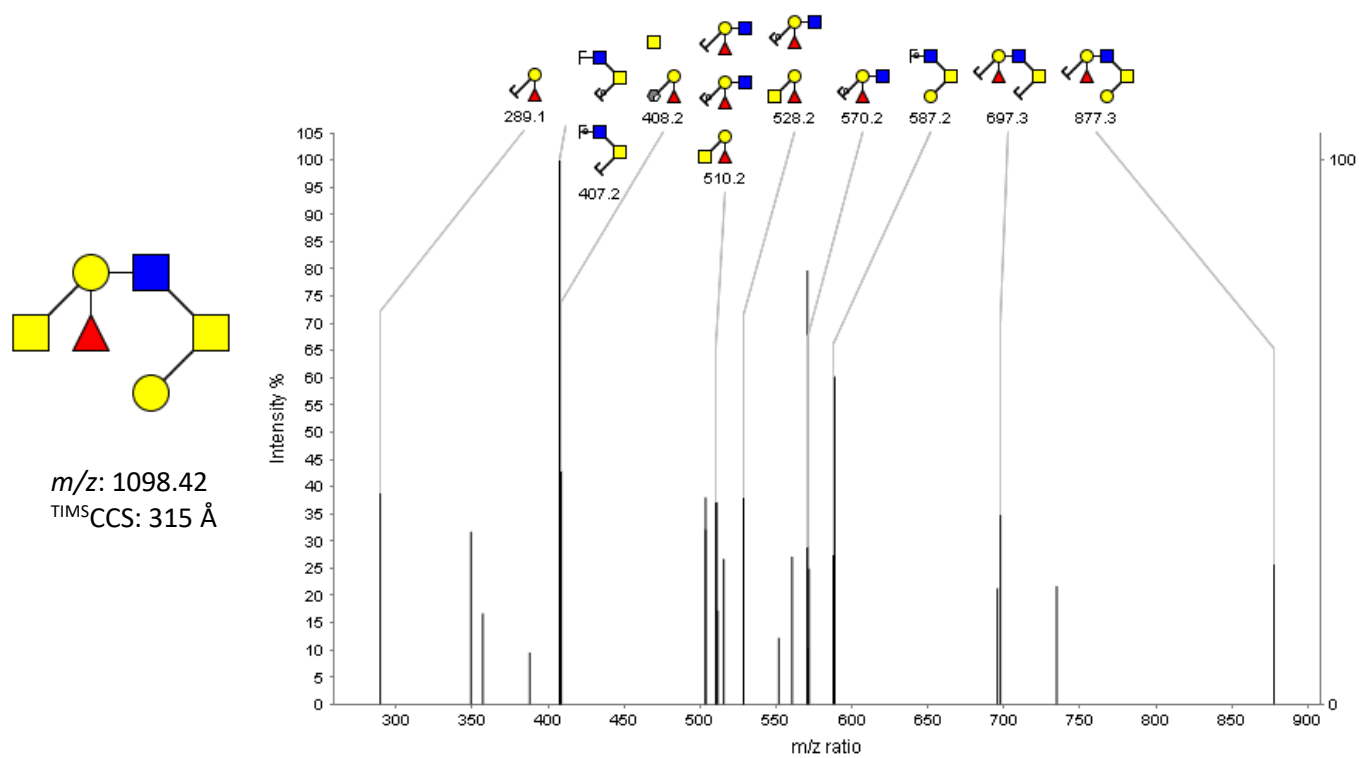
Glycan code: 1040-3



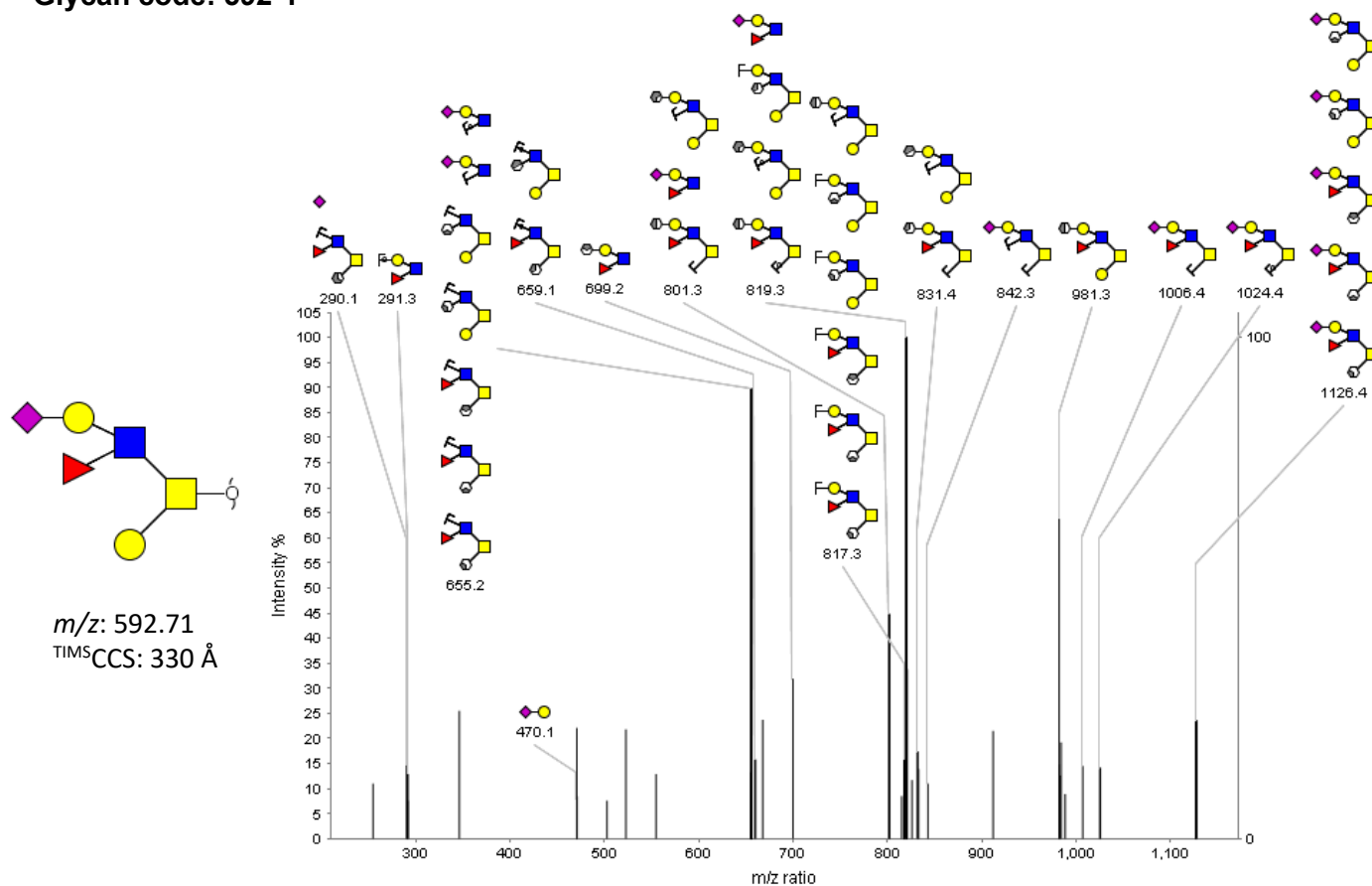
Glycan code: 1098-1



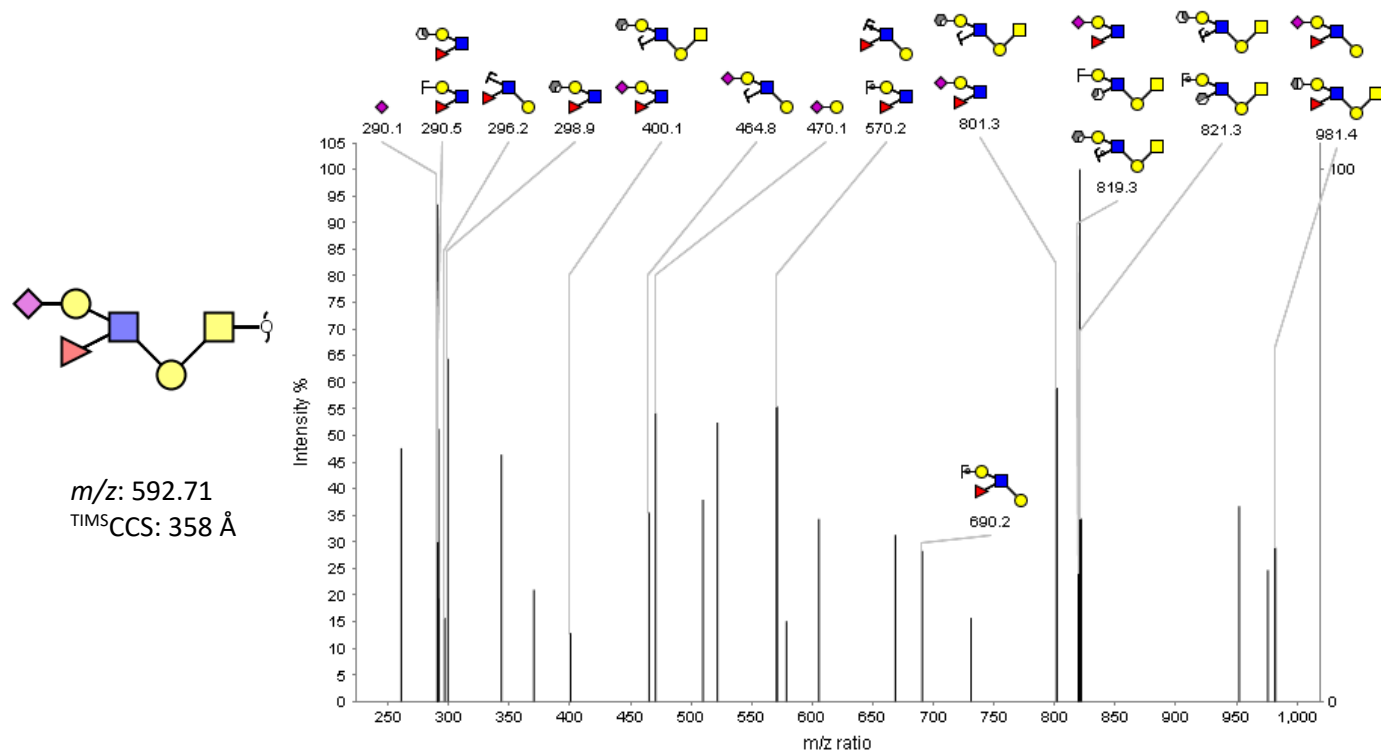
Glycan code: 1098-2



Glycan code: 592-1



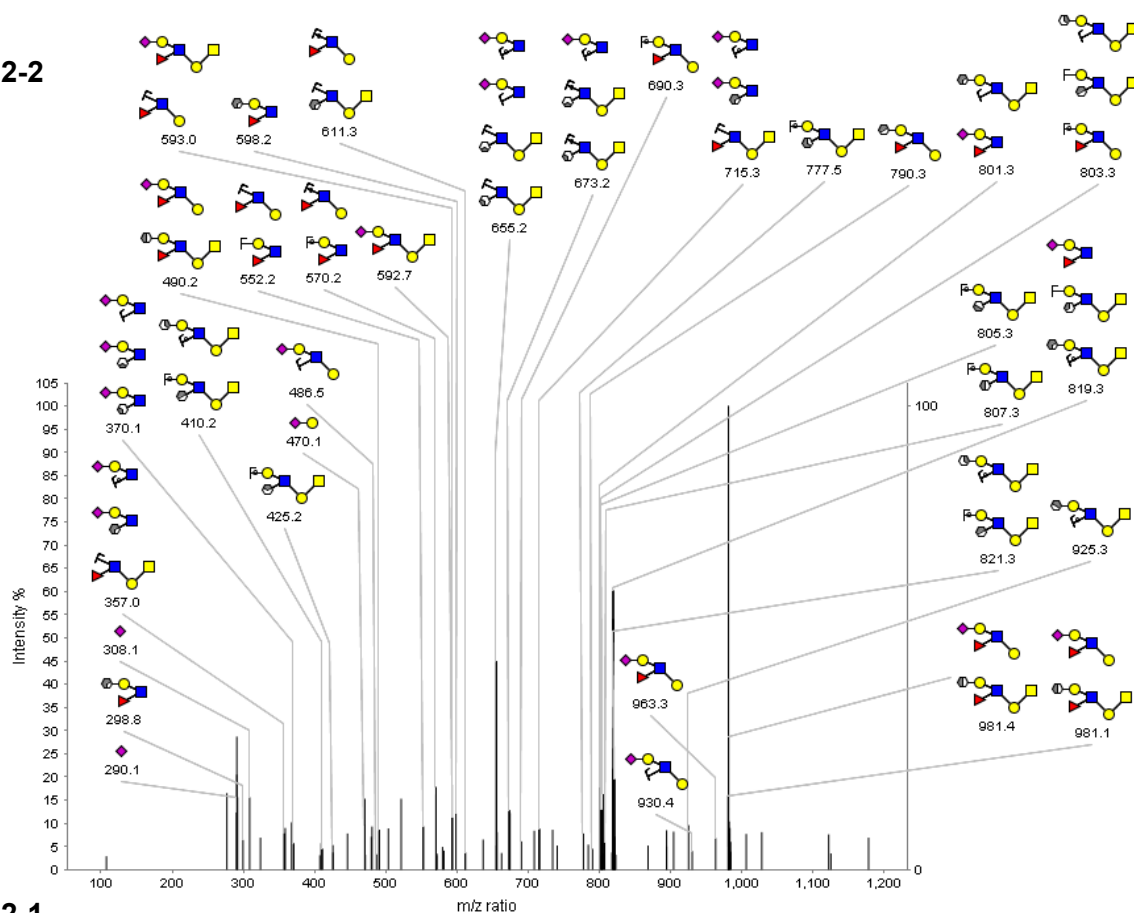
Glycan code: 592-3



Glycan code: 592-2

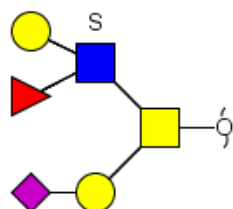


m/z : 592.71
TIMS^{CCS}: 345 Å

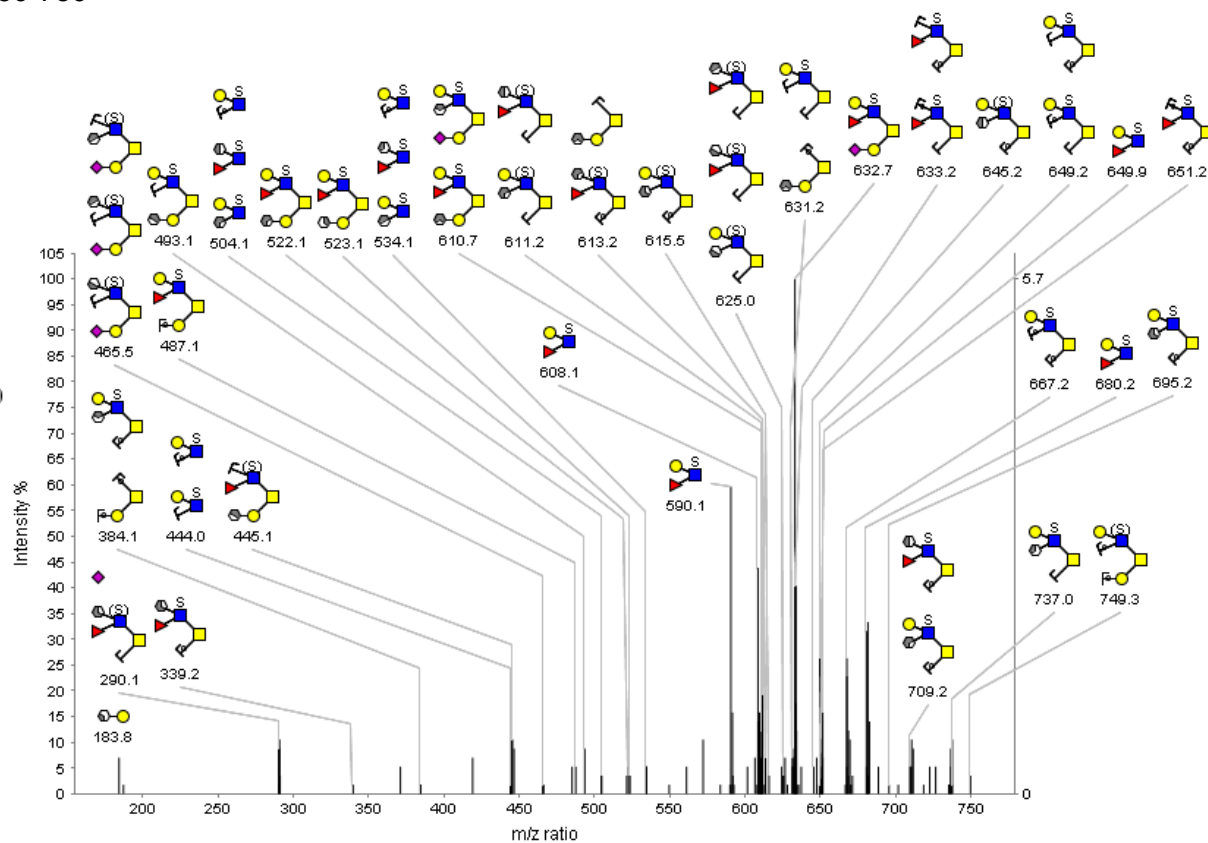


Glycan code: 632-1

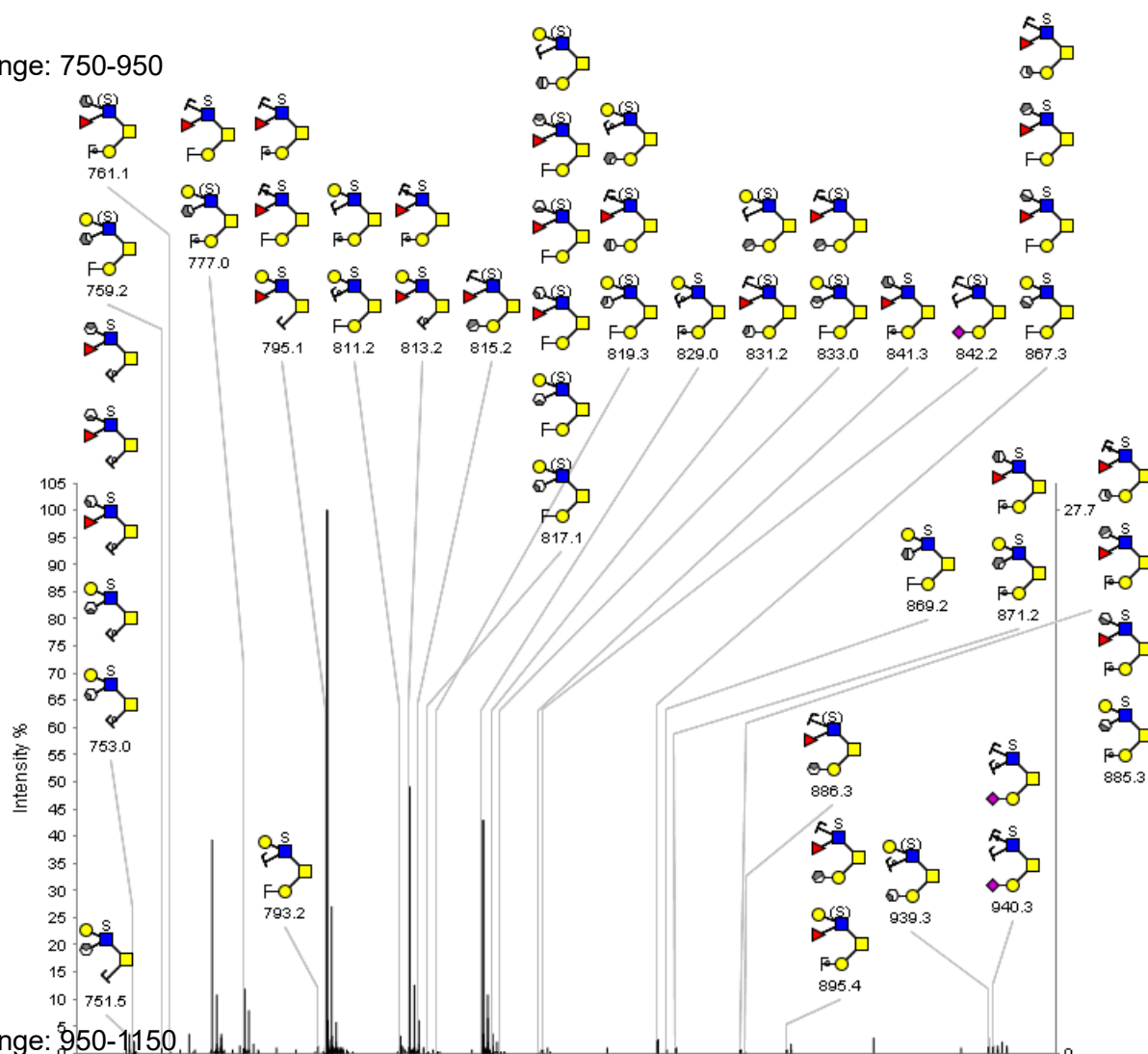
m/z range: 150-750



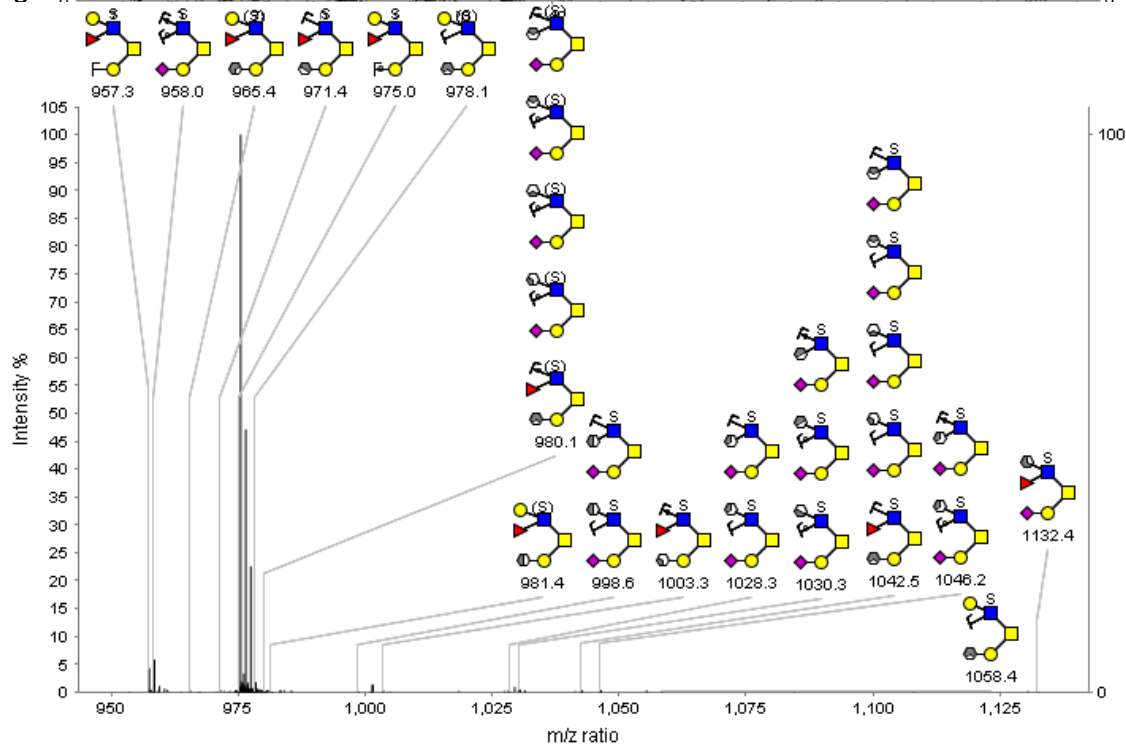
m/z : 632.69
TIMS^{CCS}: 338 Å



m/z range: 750-950

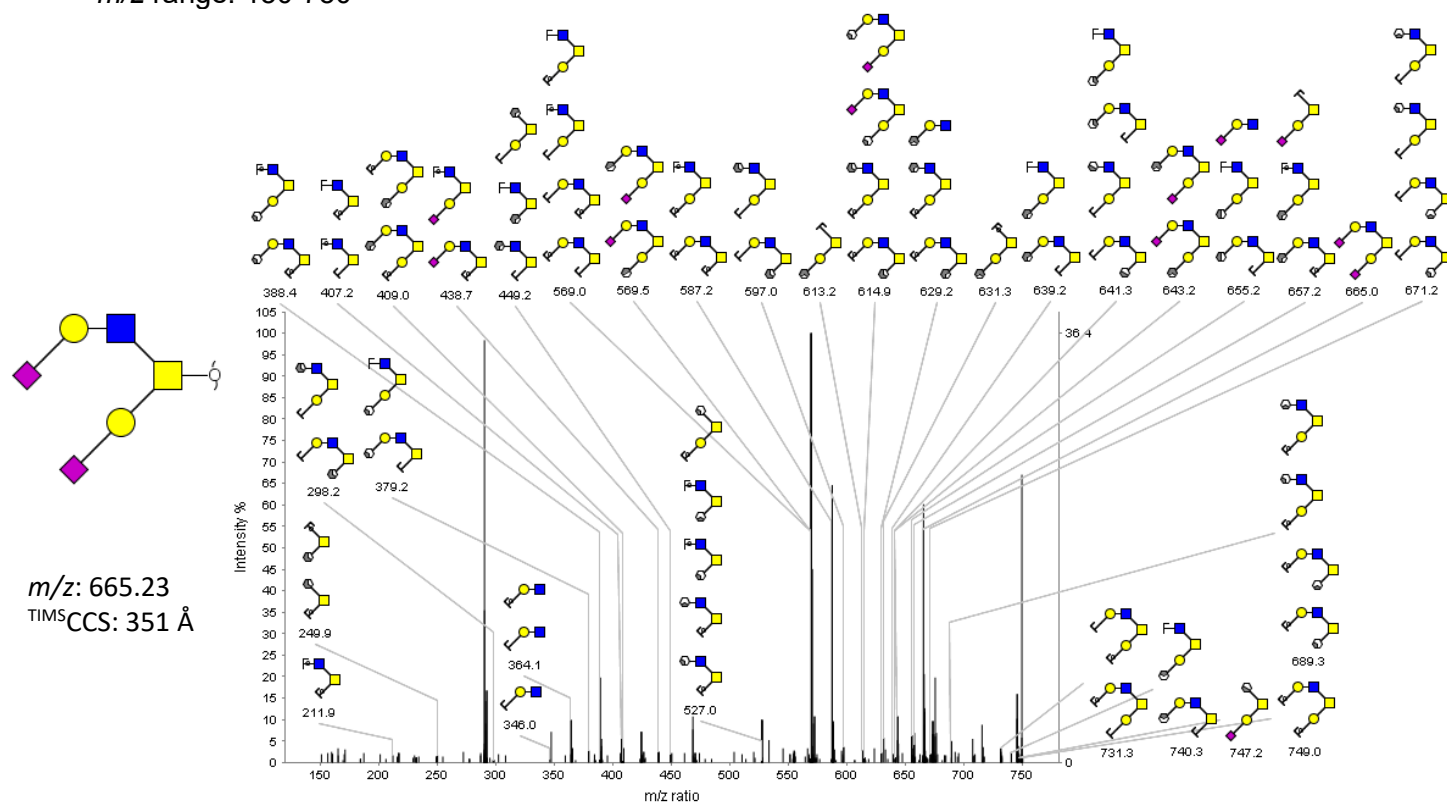


m/z range: 950-1150

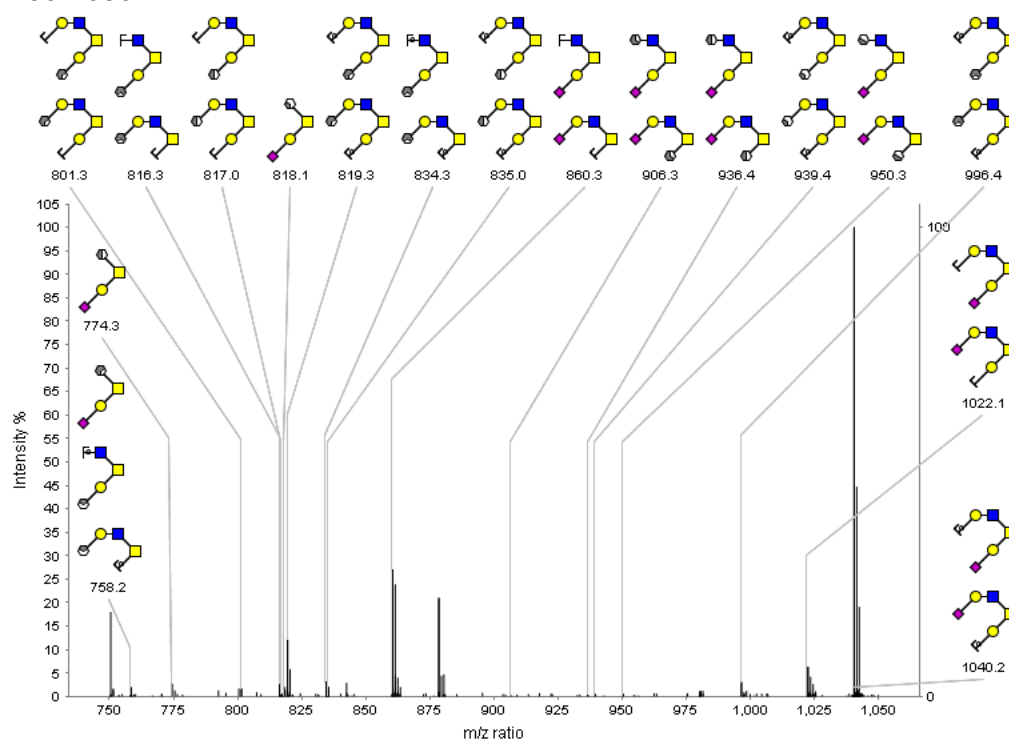


Glycan code: 665-1

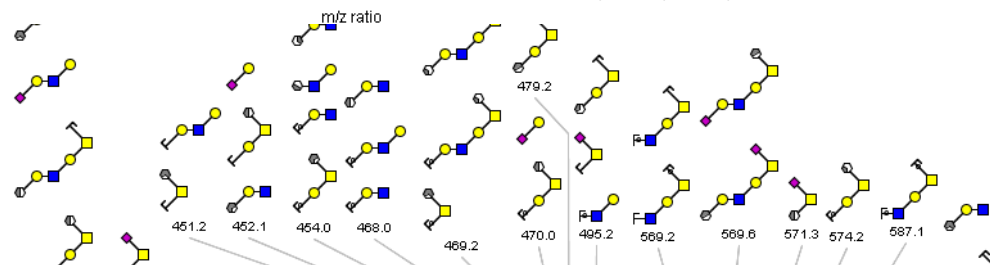
m/z range: 150-750



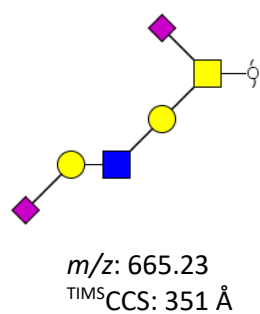
m/z range: 750-1050



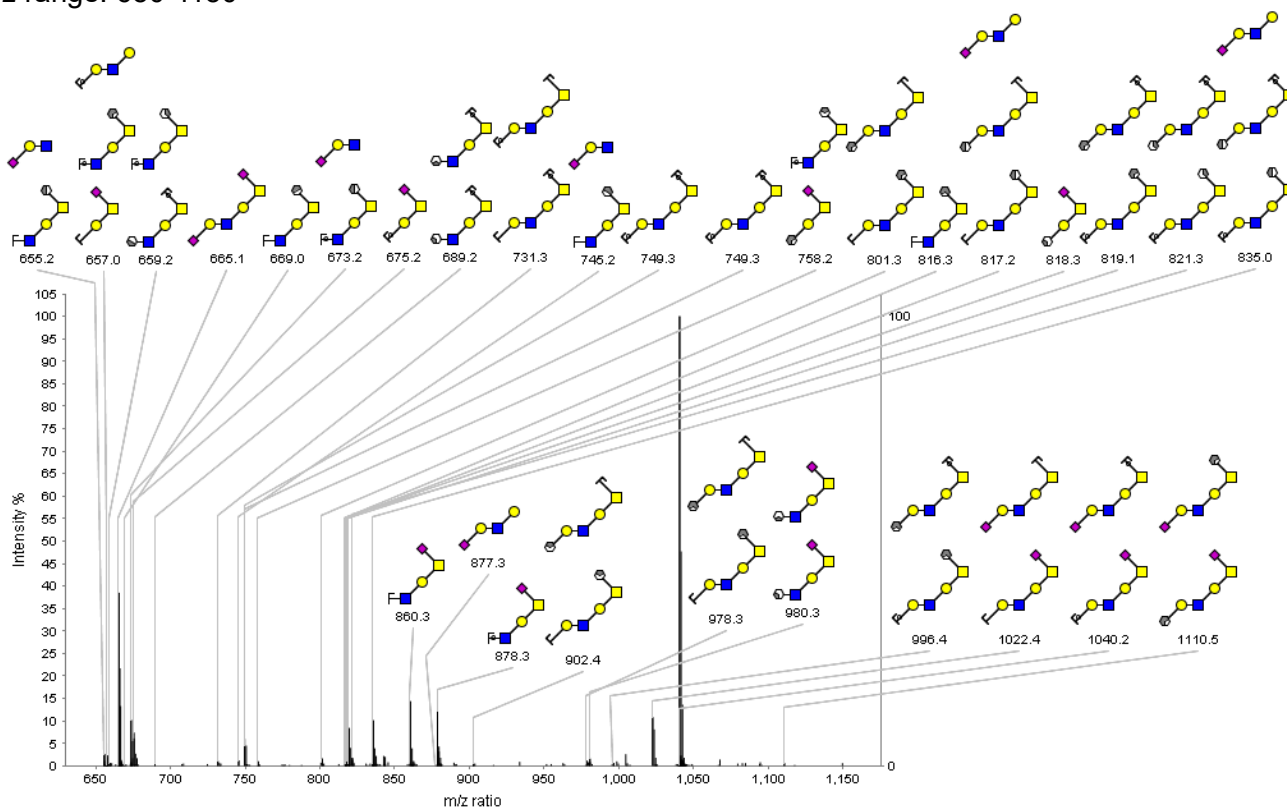
Glycan code: 665-2



m/z range: 150-650



m/z range: 650-1150



Glycan code: 738-1

m/z range: 150-750

