Supporting information

Characterization of glycan isomers using magnetic carbon nanoparticles as a MALDI co-matrix

Alireza Banazadeh[1], Reed Nieman[1], Mona Goli[1], Wenjing Peng[1], Ahmed Hussein[1,2], Ercan Bursal[3], Hans Lischka[1,4], Yehia Mechref[1,5]

[1]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, TX, 79409.

[2]Department of Biotechnology, Institute of Graduate Studies and Research, University of Alexandria, Alexandria, 21526, Egypt.

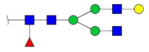
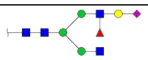
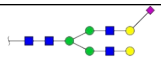
[3]Department of Nursing, School of Health, Mus Alparslan University, Mus, Turkey.

[4]School of Pharmaceutical Sciences and Technology, Tianjin University, Tianjin, 300072, P.R. China.

[5]Center for Biotechnology and Genomics, Texas Tech University, Lubbock, TX, 79409.

Table of Contents

Table 1S. Structures of standard N-glycans that were used in this study.

Glycan	Structure
$N_4H_4F_1$	
$F_1N_4H_4$	
$N_4H_4F_1S_1$	
$F_1N_4H_4S_1$	
$N_4H_4F_1S_1(2,3)$	
$N_4H_4F_1S_1(2,6)$	

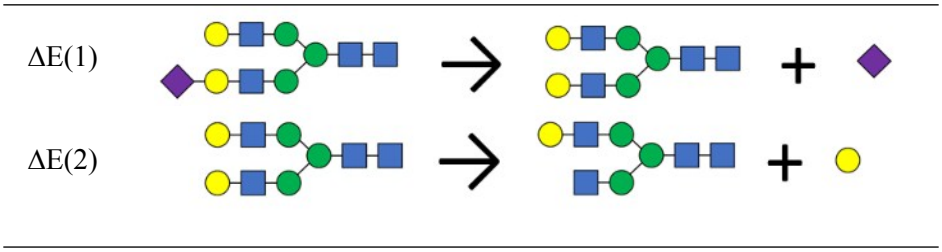
Note: Nomenclature of glycans: N: N-acetylhexosamine, H: hexose, F: fucose, and S: sialic acid; numbers denote the number of relative sugars. When F is before N, it is core fucosylation; when F is after N, it is branch fucosylation. 2,3 and 2,6 represent sialic acid linkage.

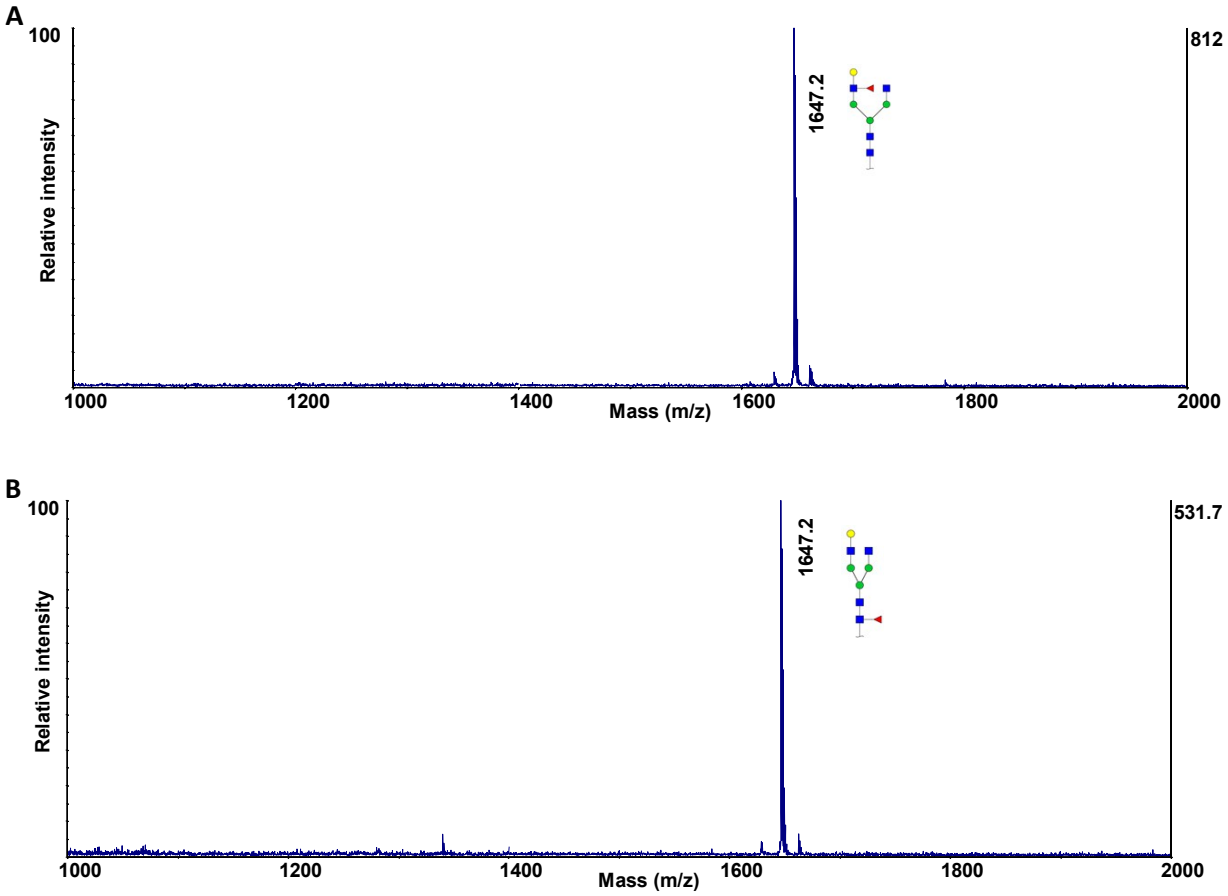
Table 2S. Calculated relative intensity ratios for the five selected fragment ions originated by each pair of the isomer.

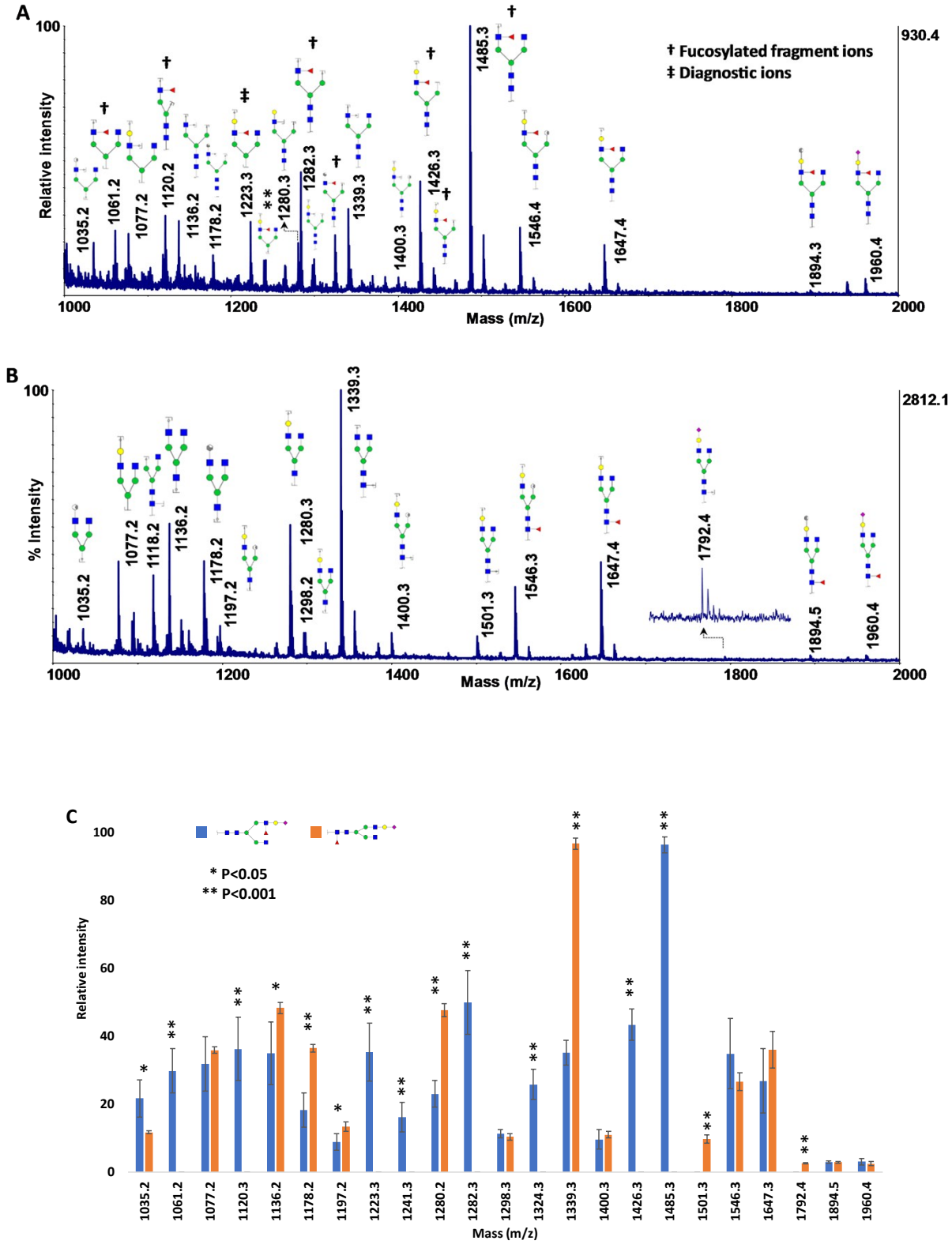
m/z	Relative intensity ratio	S.D. (n=9)
$N_4H_4F_1/F_1N_4H_4$		
1647.4	0.592	0.082
1546.3	1.624	0.134
1340.3	0.379	0.043
1280.3	0.538	0.071
915.2	1.423	0.115
$N_4H_4F_1S_1/F_1N_4H_4S_1$		
1035.2	2.135	0.097
1136.2	0.656	0.075
1178.2	0.438	0.036
1280.2	0.523	0.022
1339.3	0.371	0.031
$N_4H_5S_1(2,3)/N_4H_5S_1(2,6)$		
1136.2	1.291	0.045
1442.2	1.545	0.067
1501.2	1.800	0.105
1663.3	0.546	0.018
1976.3	0.320	0.037

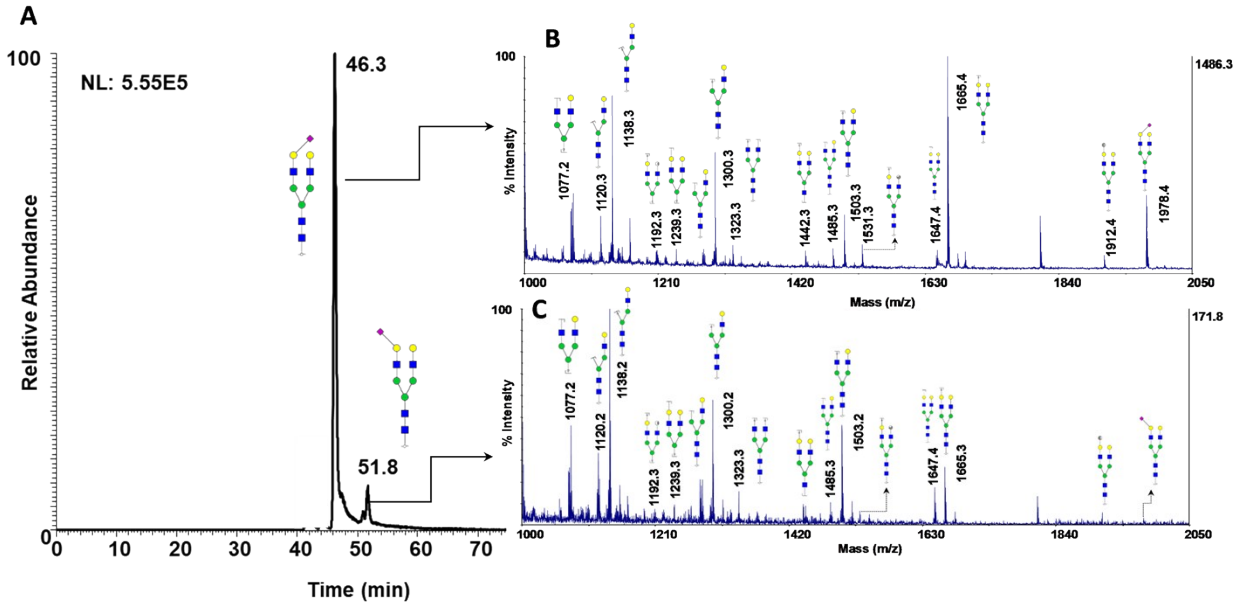
Table 3S. Calculated bond dissociation energies for α2,3- and α2,6-linked sialic acid isomers

Bond dissociation energy (ΔE, kcal/mol)	α2,3-linkage sialic acid	α2,6-linkage sialic acid
ΔE(1)	129.43	138.91
ΔE(2)	109.00	119.82




A
100
Relative intensity
1647.2
812
1000
1200
1400
Mass (m/z)
1600
1800
2000
B
100
Relative intensity
1647.2
531.7
1000
1200
1400
Mass (m/z)
1600
1800
2000


A
100
Relative Intensity
930.4
† Fucosylated fragment ions
‡ Diagnostic ions
1035.2
1061.2
1077.2
1120.2
1136.2
1178.2
1223.3
1280.3
1282.3
1339.3
1400.3
1426.3
1485.3
1546.4
1647.4
1894.3
1960.4
1000
1200
1400
1600
1800
2000
Mass (m/z)
B
100
% Intensity
2812.1
1035.2
1077.2
1118.2
1136.2
1178.2
1197.2
1280.3
1298.2
1339.3
1400.3
1501.3
1546.3
1647.4
1792.4
1894.5
1960.4
1000
1200
1400
1600
1800
2000
Mass (m/z)
C
100
80
60
40
20
0
Relative intensity
* P<0.05
** P<0.001
1035.2
1061.2
1077.2
1120.3
1136.2
1178.2
1197.2
1223.3
1241.3
1280.2
1282.3
1298.3
1324.3
1339.3
1400.3
1426.3
1485.3
1501.3
1546.3
1647.3
1792.4
1894.5
1960.4
Mass (m/z)


A
100
NL: 5.55E5
46.3
51.8
Relative Abundance
0
0 10 20 30 40 50 60 70
Time (min)
B
100
% Intensity
1077.2
1120.3
1138.3
1192.3
1239.3
1300.3
1323.3
1442.3
1485.3
1503.3
1531.3
1647.4
1665.4
1912.4
1978.4
1486.3
1000 1210 1420 1630 1840 2050
Mass (m/z)
C
100
% Intensity
1077.2
1120.2
1138.2
1192.3
1239.3
1300.2
1323.3
1485.3
1503.2
1647.4
1665.3
171.8
1000 1210 1420 1630 1840 2050
Mass (m/z)