

Multiglycan issues

# Batch Mode Issue

- The batch mode is not able to handle more than 15 raw files simultaneously. As you can see in the “MergeResult.csv”, we tried to process 18 raw files together, the last file shows “N/A” for all glycans. (Some times last two or three samples are all “N/A”. In other cases, Multiglycan crashed with >15 files loading.)
- The “pic” folders do not contain all the peak construction information, when batch mode is used. (Most of time, only several of the “pic” folders are empty. The ones we uploaded is the worst case, only “Cell\_Deter\_SP\_01” has 3 pictures.)

# Quantitation Issue

- There are two issues with the newest version of Multiglycan.
- 1. Some peaks are not picked.
- 2. Some quantitation results agreed with Xcalibur while some quantitation results did not.
- Examples are shown in the following slides.

## Issue Type 1

MergeResult.csv																																																		
	A				B				C				E				F				H				I																									
1	Glycan		Cell		Deter		SP		01		Cell		Deter		SP		02		Cell		Deter		SP		04		Cell		Deter		SP		05		Cell		Deter		SP		07		Cell		Deter		SP		08	
5	2-8-0-0-0				1.60L108				2.48L108				2.95L108				3.09L108				N/A				5.94L107																									

EICs of [28000+2H]<sup>2+</sup>

Clear Peak

Issue Type 2: quantitation of same glycan in different files (Multiglycan and Xcarlibur gives different ratio)

MerqzResult.csv							
	A	K	I	N	O	Q	R
1	Glycan	Cell_Deter_SP_10	Cell_Deter_SP_11	Cell_Deter_SP_13	Cell_Deter_SP_14	Cell_Deter_SP_16	Cell_Deter_SP_17
10	3-5-0-1-0	3.37E+05	1.38E+07	1.21E+07	8.58E+05	4.51E+05	3.38E+07

3.92 16.08 14.01 1 5.25 39.39

2.56

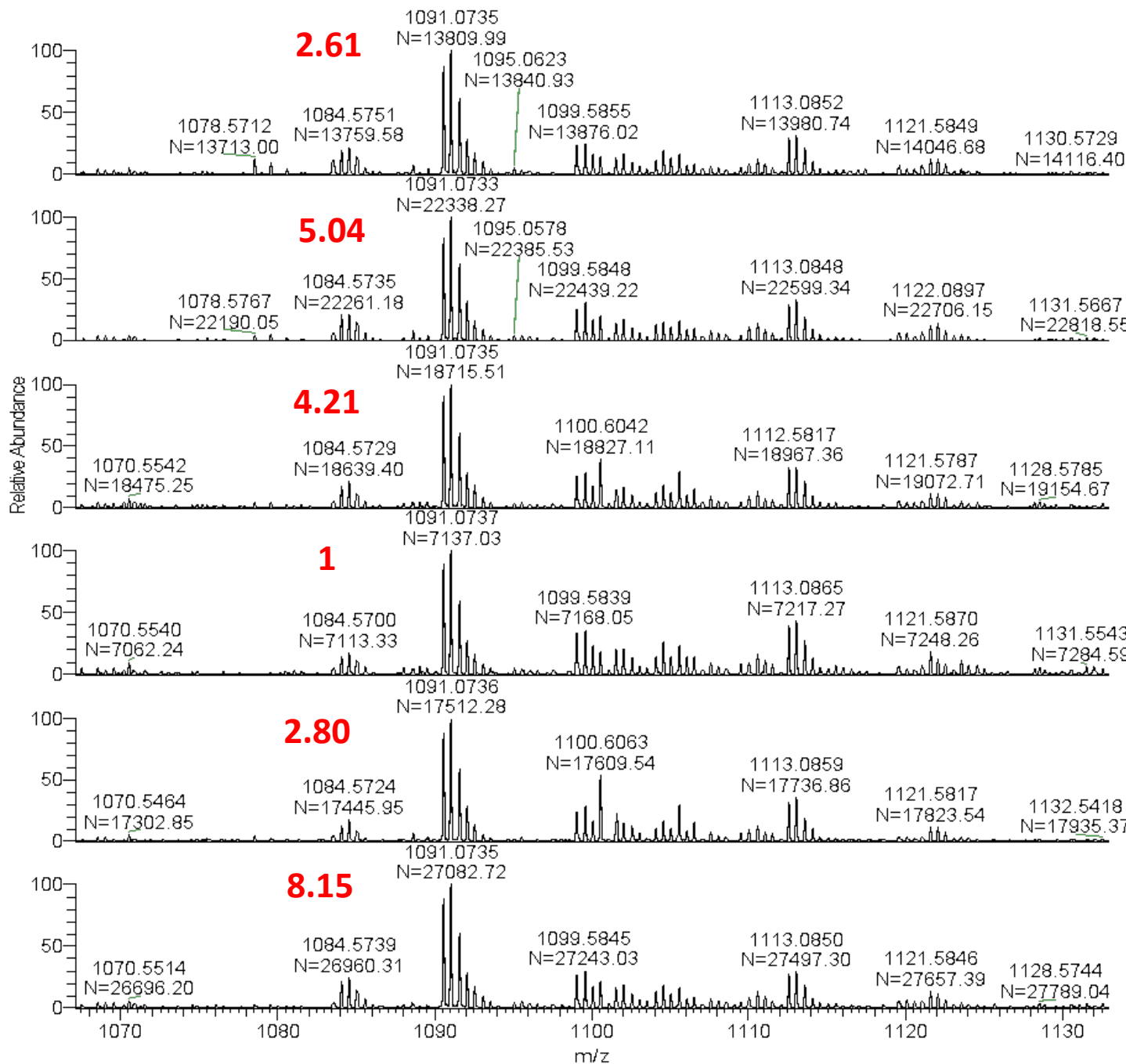
4.78

5.08

1

2.73

9.68



NL: 1.06E6  
cell\_deter\_sp\_10#2187-2218  
RT: 27.10-27.25 AV: 4 F:  
FTMS + p NSI Full ms  
[700.00-2000.00]

NL: 2.05E6  
cell\_deter\_sp\_11#2344-2371  
RT: 27.09-27.20 AV: 3 F:  
FTMS + p NSI Full ms  
[700.00-2000.00]

NL: 1.71E6  
cell\_deter\_sp\_13#2317-2355  
RT: 27.06-27.27 AV: 5 F:  
FTMS + p NSI Full ms  
[700.00-2000.00]

NL: 4.06E5  
cell\_deter\_sp\_14#1960-1996  
RT: 27.17-27.36 AV: 4 F:  
FTMS + p NSI Full ms  
[700.00-2000.00]

NL: 1.14E6  
cell\_deter\_sp\_16#2256-2288  
RT: 27.17-27.28 AV: 3 F:  
FTMS + p NSI Full ms  
[700.00-2000.00]

NL: 3.31E6  
cell\_deter\_sp\_17#2389-2431  
RT: 27.00-27.20 AV: 5 F:  
FTMS + p NSI Full ms  
[700.00-2000.00]

Issue Type 2: quantitation of same glycan in different files (Multiglycan and Xcarlibur gives similar ratio)

	A	K	L	N	O	Q	R
1	Glycan	Cell_Deter_SP_10	Cell_Deter_SP_11	Cell_Deter_SP_13	Cell_Deter_SP_14	Cell_Deter_SP_16	Cell_Deter_SP_17
2	2-5-0-0-0	1.35E+09	2.11E+09	1.03E+09	4.56E+08	9.50E+08	2.94E+09

2.96                      4.62                      3.57                      1                      2.08                      6.44

2.48

3.82

3.06

1

1.68

4.66