4: MS Experiment

4.1: New MS Experiment

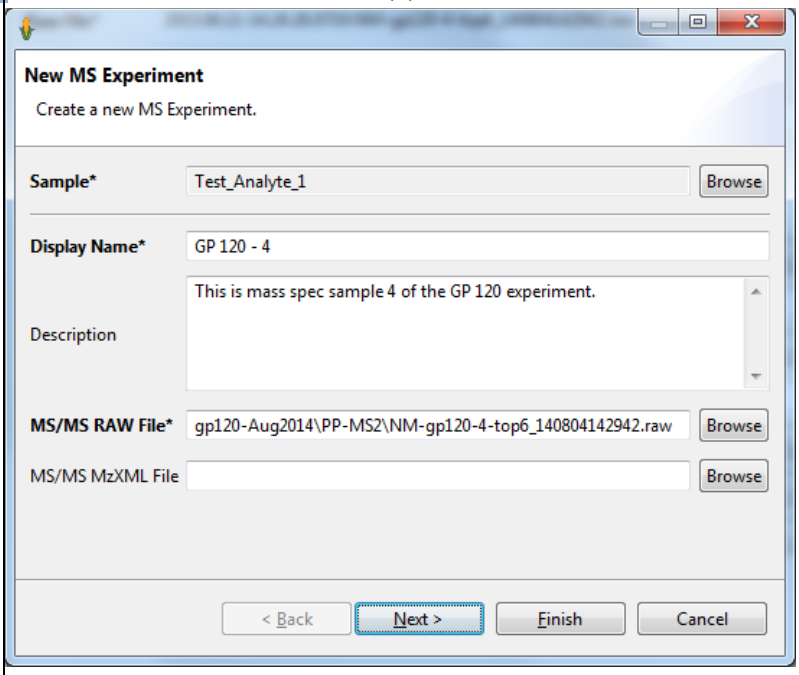
Note: If a RAW file is selected without a corresponding MzXML file, Grits will prompt you with the option to automatically convert the MS RAW file into a usable MzXML file. However, this only works for RAW files of 20 mb or less. For files larger than 20 mb, please convert the file to XML in advance.

Creating a MS Experiment:
1. Right-click on a project
2. Select “New MS Experiment”

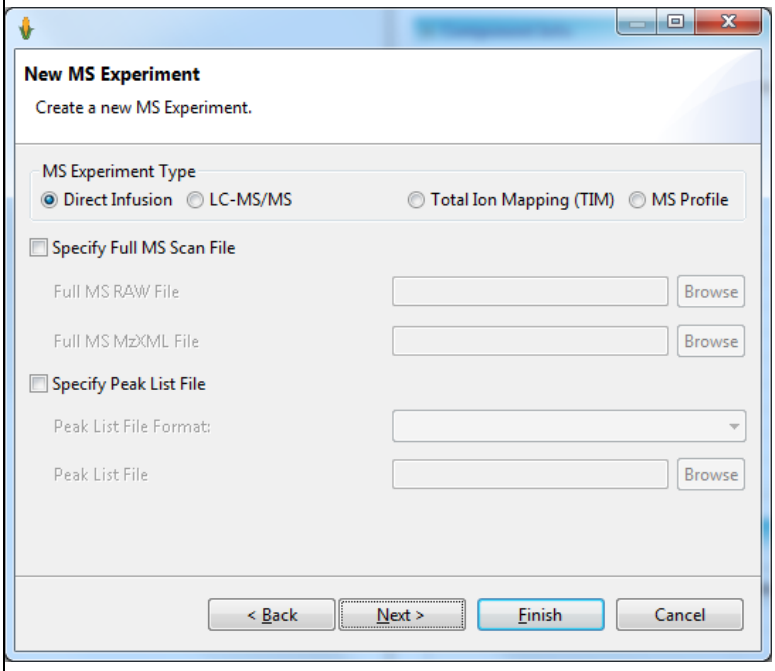
Part 1:
1. Display Name
2. Description
3. MS/MS RAW File
4. MS/MS MzXML File

Part 2:
1. MS Experiment Type
2. Specify Full MS Scan File
3. Specify Peak List File

4.1(a):



4.1(b):



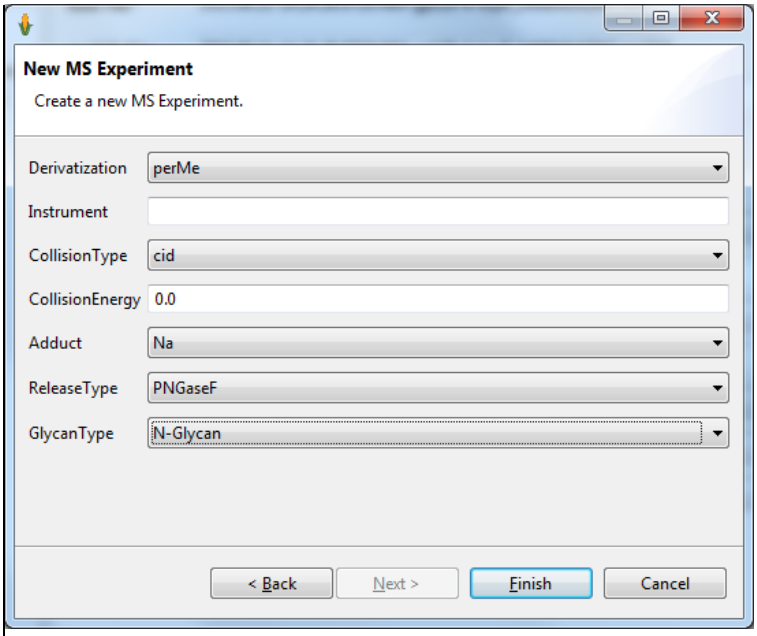
Note: Most categories have an “other” option. When selected, a new widow appears that enables one to specify a new variable from text.

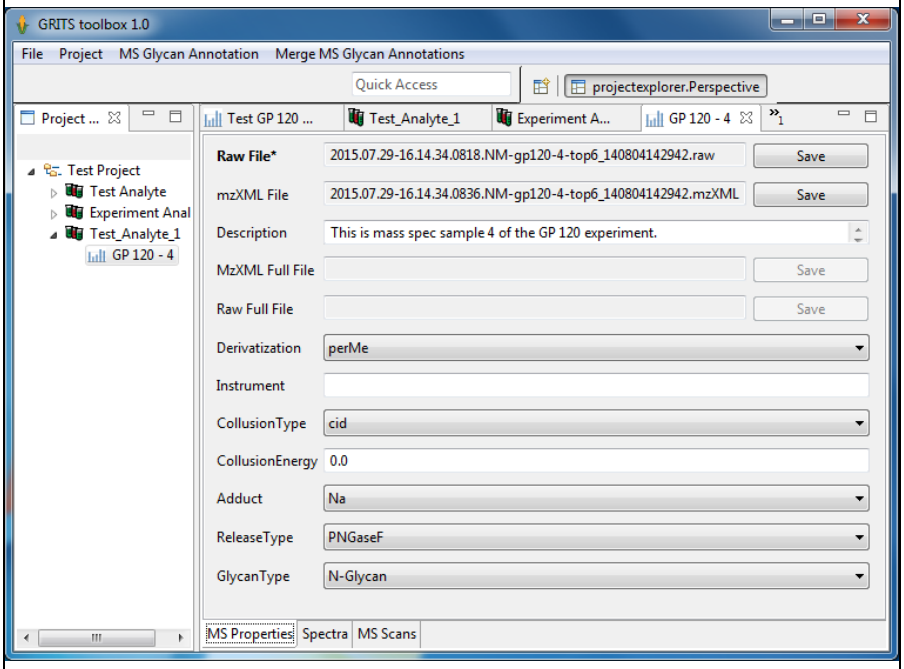
Part 3:

1. Derivatization
2. Instrument
3. Collision Type
4. Adduct
5. Release Type:
6. Glycan Type

MS Properties

This page displays all the experiment specifications designated in creation of a new MS Experiment. If necessary, these values can be altered later.





4.2: Scans, Sub-scans and Peak List

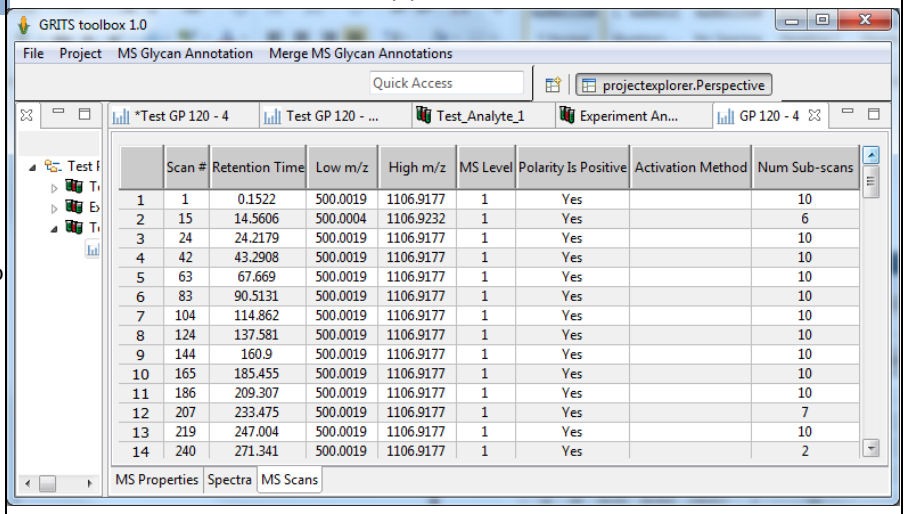
Sort: clicking on a column heading orders the data according to that column's value.

- Single-click: ascending order
- Double-click: descending order
- Triple-click: default order

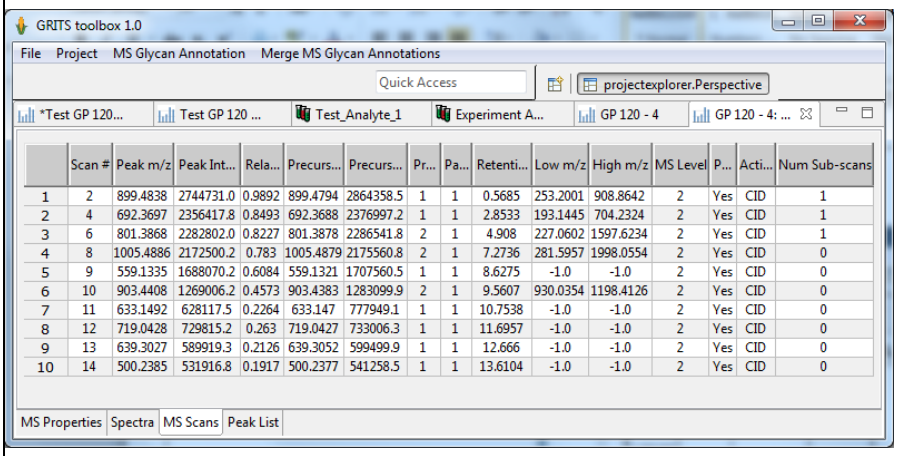
Right-clicking on a column provides the option to hide certain columns or display previously hidden columns.

Left-clicking on a column's boundaries lets you resize the column.

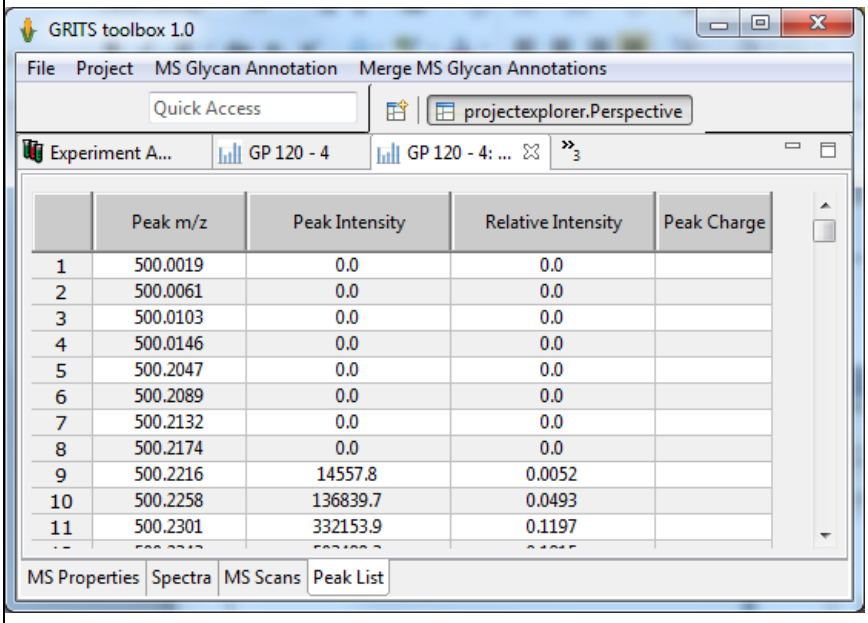
4.2(a):



	Scan #	Retention Time	Low m/z	High m/z	MS Level	Polarity Is Positive	Activation Method	Num Sub-scans
1	1	0.1522	500.0019	1106.9177	1	Yes		10
2	15	14.5606	500.0004	1106.9232	1	Yes		6
3	24	24.2179	500.0019	1106.9177	1	Yes		10
4	42	43.2908	500.0019	1106.9177	1	Yes		10
5	63	67.669	500.0019	1106.9177	1	Yes		10
6	83	90.5131	500.0019	1106.9177	1	Yes		10
7	104	114.862	500.0019	1106.9177	1	Yes		10
8	124	137.581	500.0019	1106.9177	1	Yes		10
9	144	160.9	500.0019	1106.9177	1	Yes		10
10	165	185.455	500.0019	1106.9177	1	Yes		10
11	186	209.307	500.0019	1106.9177	1	Yes		10
12	207	233.475	500.0019	1106.9177	1	Yes		7
13	219	247.004	500.0019	1106.9177	1	Yes		10
14	240	271.341	500.0019	1106.9177	1	Yes		2



	Scan #	Peak m/z	Peak Int...	Rela...	Precurs...	Precurs...	Pr...	Pa...	Retenti...	Low m/z	High m/z	MS Level	P...	Acti...	Num Sub-scans
1	2	899.4838	2744731.0	0.9892	899.4794	2864358.5	1	1	0.5685	253.2001	908.8642	2	Yes	CID	1
2	4	692.3697	2356417.8	0.8493	692.3688	2376997.2	1	1	2.8533	193.1445	704.2324	2	Yes	CID	1
3	6	801.3868	2282802.0	0.8227	801.3878	2286541.8	2	1	4.908	227.0602	1597.6234	2	Yes	CID	1
4	8	1005.4886	2172500.2	0.783	1005.4879	2175560.8	2	1	7.2736	281.5957	1998.0554	2	Yes	CID	0
5	9	559.1335	1688070.2	0.6084	559.1321	1707560.5	1	1	8.6275	-1.0	-1.0	2	Yes	CID	0
6	10	903.4408	1269006.2	0.4573	903.4383	1283099.9	2	1	9.5607	930.0354	1198.4126	2	Yes	CID	0
7	11	633.1492	628117.5	0.2264	633.147	777949.1	1	1	10.7538	-1.0	-1.0	2	Yes	CID	0
8	12	719.0428	729815.2	0.263	719.0427	733006.3	1	1	11.6957	-1.0	-1.0	2	Yes	CID	0
9	13	639.3027	589919.3	0.2126	639.3052	599499.9	1	1	12.666	-1.0	-1.0	2	Yes	CID	0
10	14	500.2385	531916.8	0.1917	500.2377	541258.5	1	1	13.6104	-1.0	-1.0	2	Yes	CID	0



	Peak m/z	Peak Intensity	Relative Intensity	Peak Charge
1	500.0019	0.0	0.0	
2	500.0061	0.0	0.0	
3	500.0103	0.0	0.0	
4	500.0146	0.0	0.0	
5	500.2047	0.0	0.0	
6	500.2089	0.0	0.0	
7	500.2132	0.0	0.0	
8	500.2174	0.0	0.0	
9	500.2216	14557.8	0.0052	
10	500.2258	136839.7	0.0493	
11	500.2301	332153.9	0.1197	

4.3: Spectra

Click and Drag:

- Creates a box on the spectra
- Top-left to bottom-right zooms in on the selected area
- Any other drag direction zooms out all the way

Right-click:

- Properties: alter how the spectra is displayed
- Save-as: exports the spectra to an image file
- Print: prints the spectra
- Zoom-in
- Zoom-out
- Auto-range: goes to the default view