

## 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):

The screenshot shows the 'New MS Experiment' dialog box with the following fields and values:

- Sample\***: Test\_Analyte\_1
- Display Name\***: GP 120 - 4
- Description**: This is mass spec sample 4 of the GP 120 experiment.
- MS/MS RAW File\***: gp120-Aug2014\PP-MS2\NM-gp120-4-top6\_140804142942.raw
- MS/MS MzXML File**: (empty)

Navigation buttons at the bottom: < Back, Next >, Finish, Cancel.

4.1(b):

The screenshot shows the 'New MS Experiment' dialog box with the following options and fields:

- MS Experiment Type**:
  - Direct Infusion
  - LC-MS/MS
  - Total Ion Mapping (TIM)
  - MS Profile
- Specify Full MS Scan File**:
  - Full MS RAW File: (empty) Browse
  - Full MS MzXML File: (empty) Browse
- Specify Peak List File**:
  - Peak List File Format: (empty) dropdown
  - Peak List File: (empty) Browse

Navigation buttons at the bottom: < Back, Next >, Finish, Cancel.

Note: Most categories have an "other" option.  
When selected, a new window 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.

The screenshot shows a dialog box titled "New MS Experiment" with the subtitle "Create a new MS Experiment." The dialog contains several fields for configuring an experiment:

- Derivatization: perMe
- Instrument: (empty)
- CollisionType: cid
- CollisionEnergy: 0.0
- Adduct: Na
- ReleaseType: PNGaseF
- GlycanType: N-Glycan

At the bottom of the dialog are four buttons: "< Back", "Next >", "Finish", and "Cancel".

The screenshot shows the main interface of the "GRITS toolbox 1.0" software. The "MS Properties" tab is active, displaying the same configuration as the "New MS Experiment" dialog box. The interface includes a menu bar (File, Project, MS Glycan Annotation, Merge MS Glycan Annotations), a toolbar with "Quick Access" and "projectexplorer.Perspective", and a project explorer on the left showing a tree view of the current project. The main panel displays the following fields:

- Raw File\*: 2015.07.29-16.14.34.0818.NM-gp120-4-top6\_140804142942.raw (Save)
- mzXML File: 2015.07.29-16.14.34.0836.NM-gp120-4-top6\_140804142942.mzXML (Save)
- Description: This is mass spec sample 4 of the GP 120 experiment.
- MzXML Full File: (Save)
- Raw Full File: (Save)
- Derivatization: perMe
- Instrument: (empty)
- CollisionType: cid
- CollisionEnergy: 0.0
- Adduct: Na
- ReleaseType: PNGaseF
- GlycanType: N-Glycan

At the bottom of the window are tabs for "MS Properties", "Spectra", and "MS Scans".

## 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...	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

