

2: Sample Editor

2.1(a): Create Analyte in Project

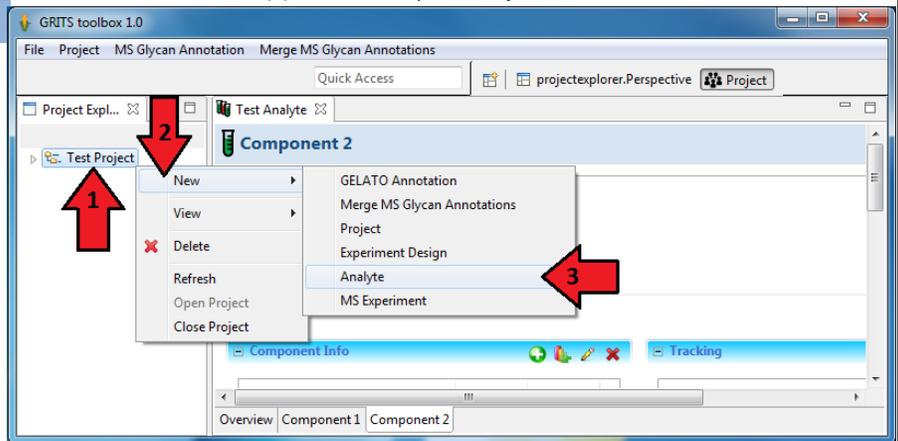
2.1: Create an Analyte

Steps:

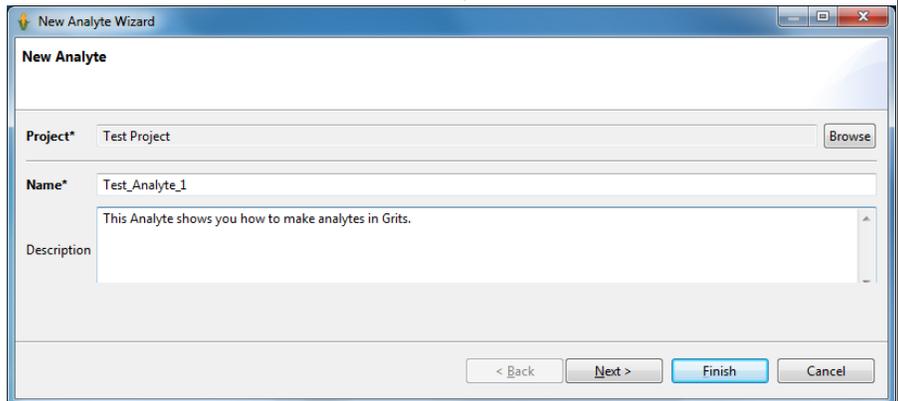
1. Right-Click on a Project
2. Select "New"
3. Select "Analyte"
4. Give the Analyte a name
5. Give the Analyte a description
6. Select "Next"
7. Name your first component
 - The default name is the name of the Analyte
8. Select the base for the component
 - "Completely New": uses default settings
 - "Copy of Previous Component": uses the settings of a selected component
 - "From a Template": uses a template to format the component, useful if you have a pre-existing format
9. Select "Finish" to finish
10. Save by pressing "Ctrl+S" or selecting "File" and then selecting "Save," this will save all work in Grits.

Save frequently:

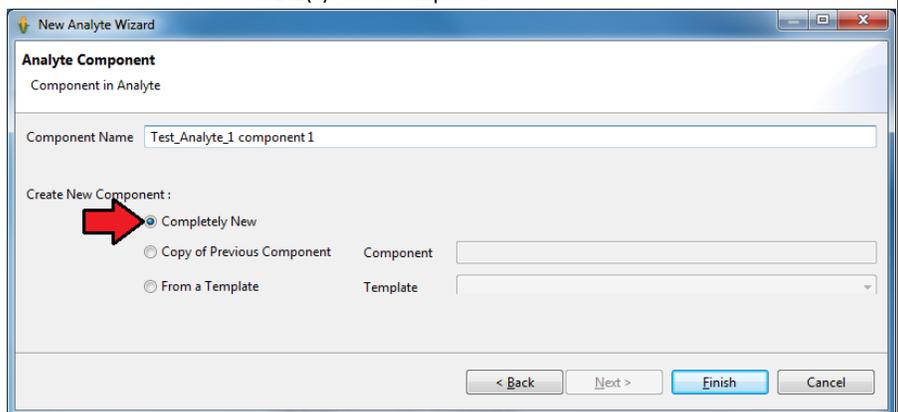
- Press "Ctrl + S"
- Go to "File" and click "Save"
- This will save everything
- Parts of Grits will only work with saved data



2.1(b): Name Analyte



2.1(c): First Component



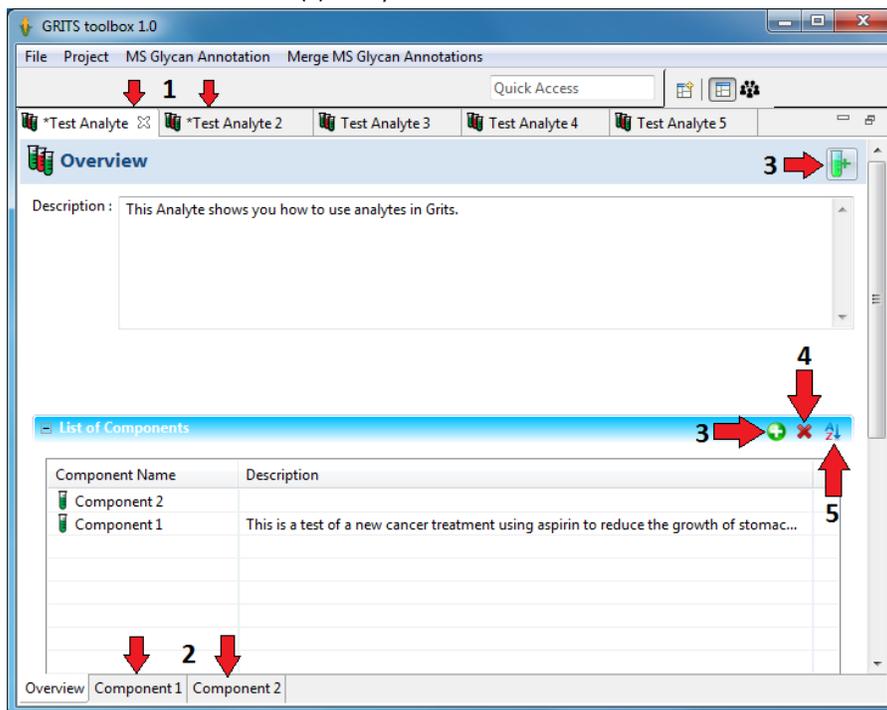
2:2 Analyte Overview

In Grits, analytes serve as sub-folders for projects. Each analyte represents a single experiment. An analyte must contain at least one component or sample. Additionally, analytes may store other types of data, such as MS data or Gelato annotations. All data within an analyte is associated together for other Grits programs to utilize.

Buttons:

1. Cycling through Analytes
 2. Cycling through components
 3. Adding new components
 4. Delete a component
 5. Sort components
- Useful for complex analytes

2.2(a): Analyte Overview



2.3: Components

Analytes are composed of components, which contain information about a single sample. An analyte can have any number of components.

Buttons:

1. Add a descriptor
2. Add a descriptor group
3. Edit
4. Delete
5. Add a new component
6. Edit the name of the component
7. Create a template using this component
8. Close Analyte

Overview

- A. An "*" indicates that a file is not saved
 - Only Saved files can be used by Grits
 - Save by pressing "Ctrl+S"
- B. Component Information
 - Describes the contents of the sample
- C. Tracking
- D. Amount
- E. Purity

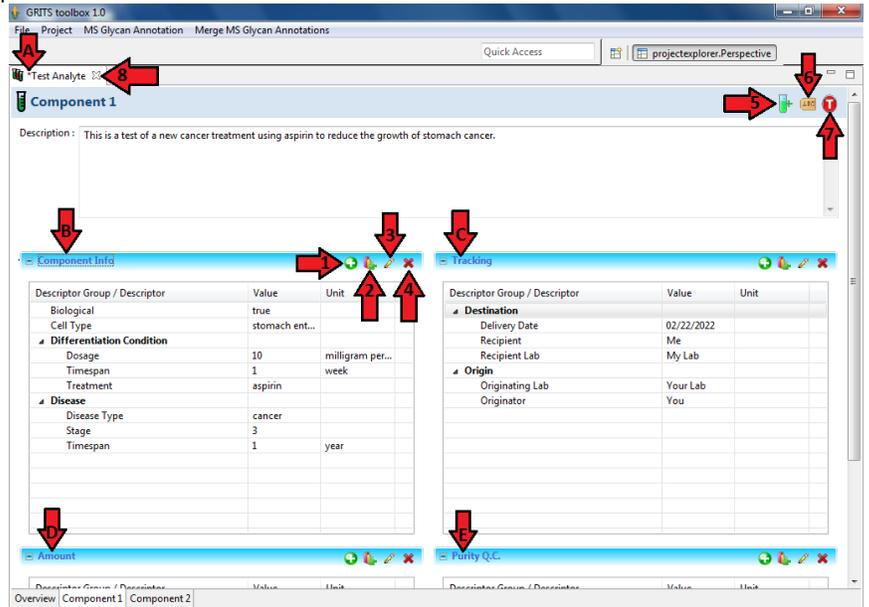
Descriptors

- Descriptors store information about a given sample
- Descriptors are predefined and draw from an extensive database in order to maintain internal consistency while still providing enough options

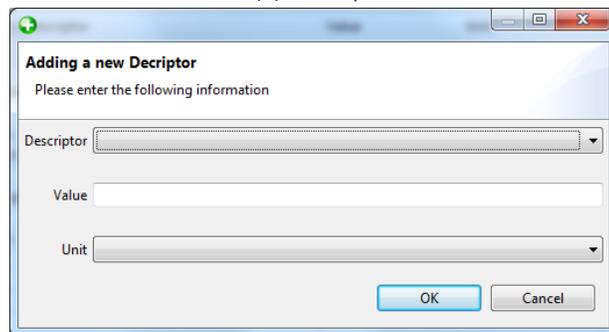
Descriptor Groups

- Work like descriptors
- More general than descriptors.

2.3(a): Component Overview



2.3(b): Descriptors



2.3(c): Descriptor Groups

