MS Template Creator

Developer Documentation

Version 0.0.3

2018

# Version Control Table

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| --- | --- |
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| **Created By** | Jeremy John Selva |
| **Date Created** | 27 March 2018 |
| **Maintained By** | Jeremy John Selva |

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| 0.0.3 | Jeremy John | 14 Aug 2021 | Whole document as test dataset has changed | Draft |
| 0.0.2 | Jeremy John | 3 March 2021 | Added   * Part Four Testing “Dilution\_Annot” sheet | Draft |
| 0.0.1 | Jeremy John | 3 May 2018 | Initial commit and review | Approved |

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# Testing Checklist

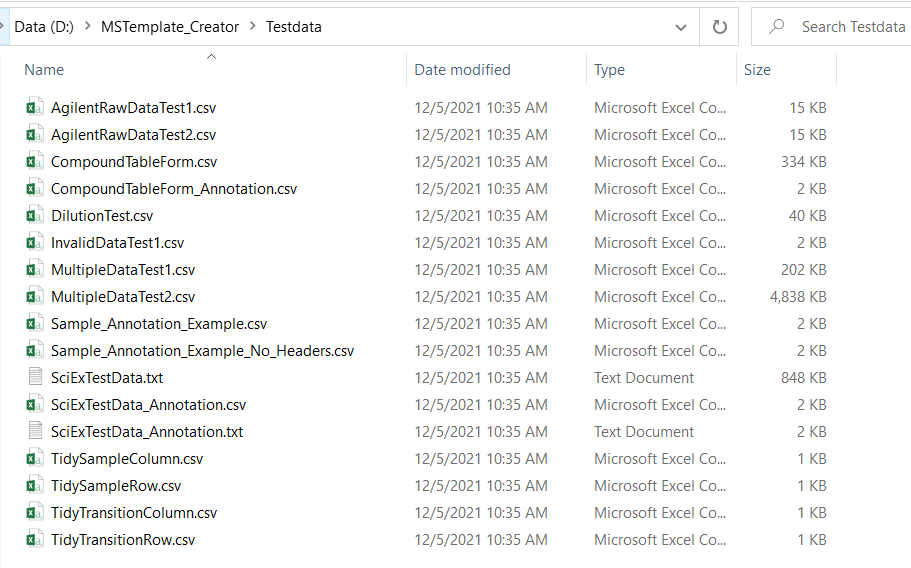
## Purpose

To check if the MS Template Creator Excel macro file is still in working condition when new codes has been added or old codes has been changed and updated.

Please update this book regularly so that we can create a program that works for everyone and in different situations.

## Test Datasets

The test files are as follows



# **Part One: Testing “Transition\_Name\_Annot” sheet**

## Loading of Transition Names from MRM transition names data

### Loading from Agilent csv file in WideTable form

#### Requirements

AgilentRawDataTest1.csv

#### Preconditions

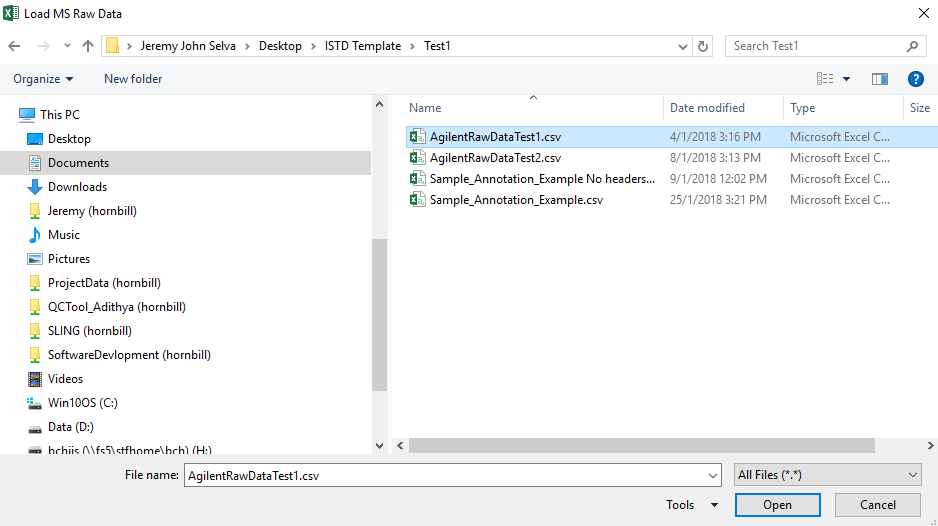
Users exported the csv file from MassHunter correctly.

#### Steps

Click on the button “Load Transition\_Name from Raw Data”



Browse for the file AgilentRawDataTest1.csv. Click Open



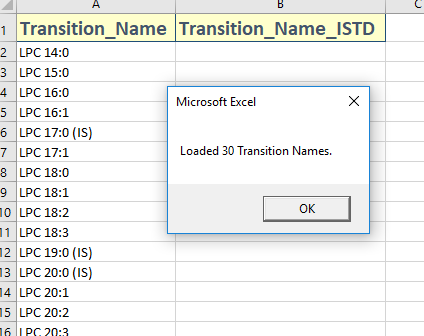
#### Expected Results

If there are existing entries in the “Transition\_Name” column. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten



Clicking on Cancel should cause the message box to leave and the original inputs are left alone

Clicking on Overwrite should cause the original inputs to be replaced with the Transition Names found in AgilentRawDataTest1.csv



Ensure that

* Transition\_Name are loaded unto the right column in the sheet
* 30 Transition\_Names should be found in AgilentRawDataTest1.csv
* Duplicates are removed
* Sorted in alphabetical order [A-Za-z]

### Loading from Agilent csv file in CompoundTable form

#### Requirements

CompoundTableForm.csv

#### Preconditions

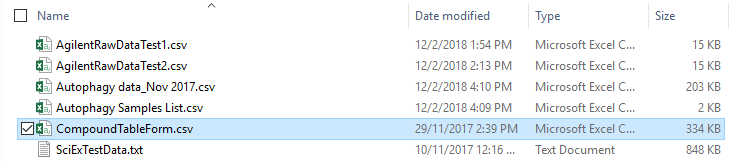
Users exported the csv file from MassHunter correctly.

#### Steps

Click on the button “Load Transition\_Name from Raw Data”



Browse for the file CompoundTableForm.csv. Click Open



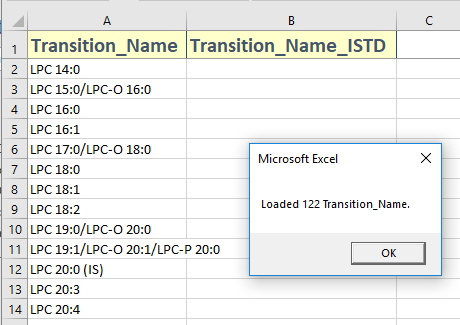
#### Expected Results

If there are existing entries in the “Transition\_Name” column. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten



Clicking on Cancel should cause the message box to leave and the original inputs are left alone

Clicking on Overwrite should cause the original inputs to be replaced with the Transition Names found in CompoundTableForm.csv



Ensure that

* Transition\_Name are loaded unto the right column in the sheet
* 122 Transition\_Names should be found in CompoundTableForm.csv
* Duplicates are removed
* Sorted in alphabetical order [A-Za-z]

### Loading from Sciex txt file

#### Requirements

SciExTestData.txt

#### Preconditions

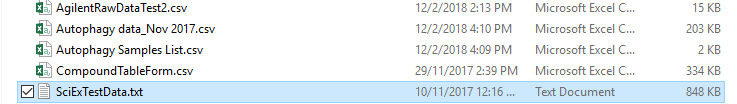
Users exported the txt file from MultiQuant correctly.

#### Steps

Click on the button “Load Transition\_Name from Raw Data”



Browse for the file SciExTestData.txt . Click Open



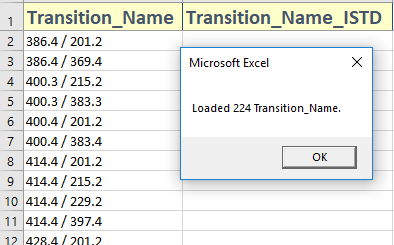
#### Expected Results

If there are existing entries in the “Transition\_Name” column. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten



Clicking on Cancel should cause the message box to leave and the original inputs are left alone

Clicking on Overwrite should cause the original inputs to be replaced with the Transition Names found in SciExTestData.txt



Ensure that

* Transition\_Name are loaded unto the right column in the sheet
* 224 Transition\_Names should be found in CompoundTableForm.csv
* Duplicates are removed
* Sorted in increasing order

### Loading multiple files both Agilent and Sciex

#### Requirements

MultipleDataTest1.csv

MultipleDataTest2.csv

SciExTestData.txt

#### Preconditions

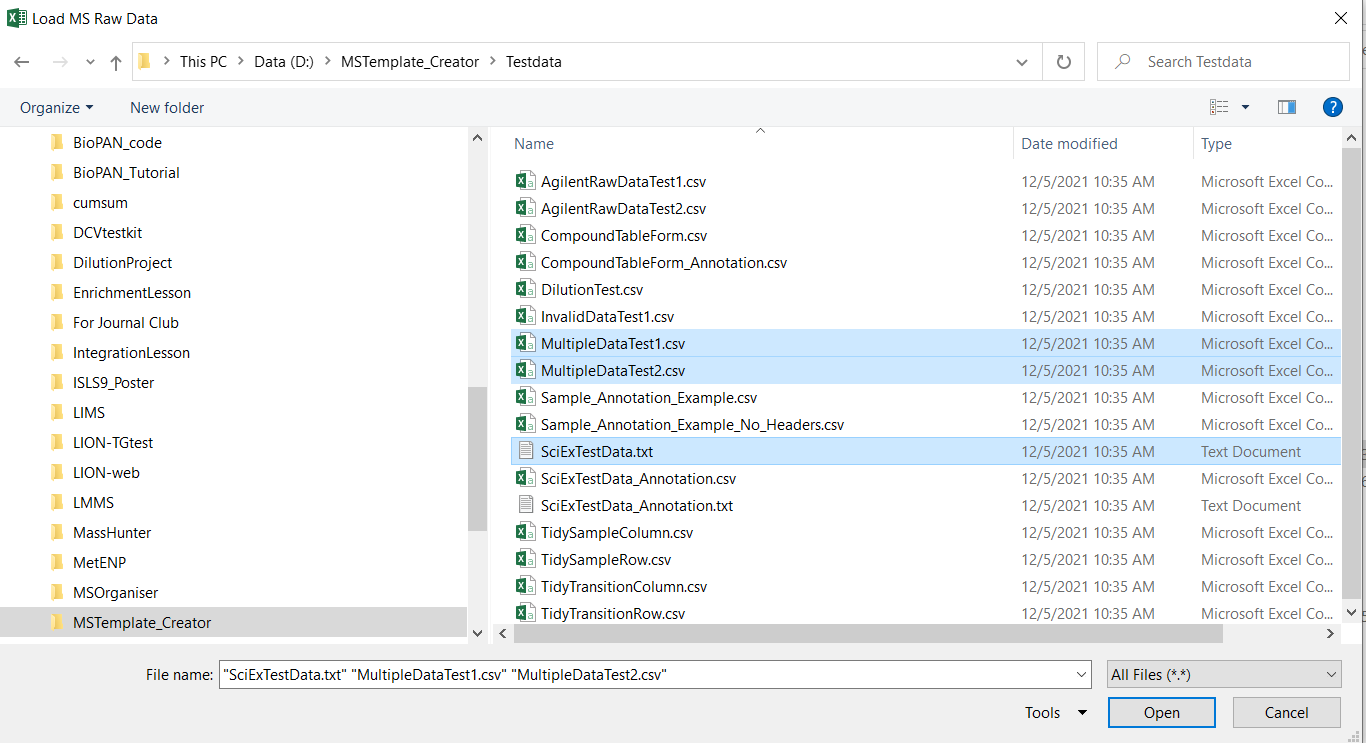
Users exported the csv file from MassHunter and the txt file from MultiQuant correctly.

#### Steps

Click on the button “Load Transition\_Name from Raw Data”



Browse for the three files. Click Open



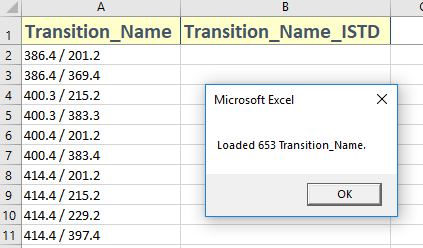
#### Expected Results

If there are existing entries in the “Transition\_Name” column. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten



Clicking on Cancel should cause the message box to leave and the original inputs are left alone

Clicking on Overwrite should cause the original inputs to be replaced with the Transition Names found in all three files



Ensure that

* Transition\_Name are loaded unto the right column in the sheet
* 653 Transition\_Names should be found in CompoundTableForm.csv
* Duplicates are removed
* Sorted in increasing order

#### Notes

You may wish to load both MultipleDataTest1.csv and sPerfect\_Index\_AllLipids\_raw.csv to double check that it is working.

MultipleDataTest1.csv has 419 Transition names.

sPerfect\_Index\_AllLipids\_raw.csv has 421 Transition names.

Their union gives 429 Transition names.

### Loading an invalid raw data file

#### Requirements

InvalidDataTest1.csv (that is a sample annotation file)

#### Preconditions

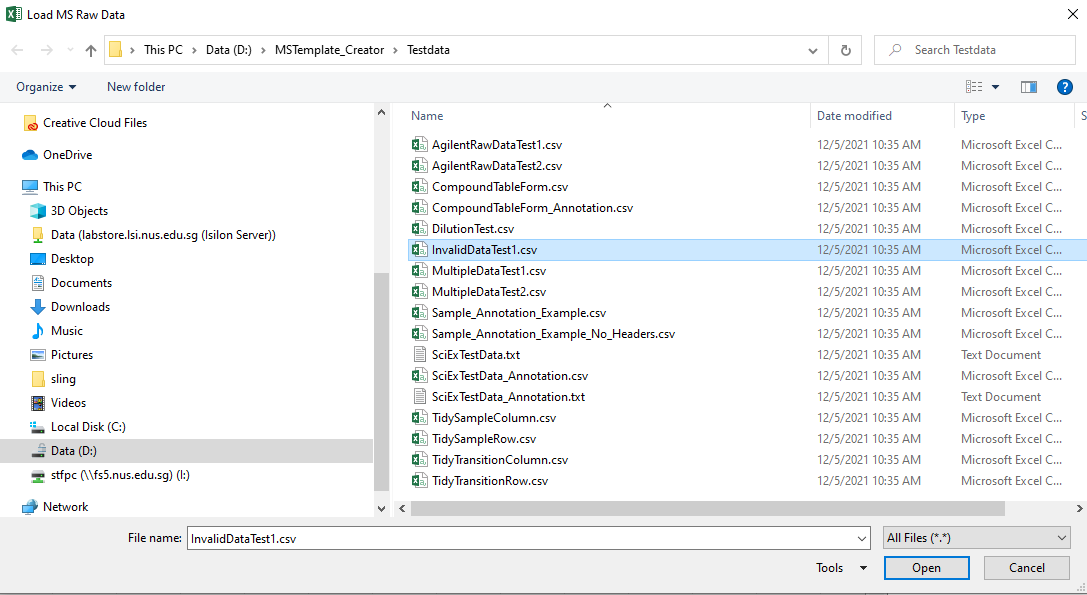
None

#### Steps

Click on the button “Load Transition\_Name from Raw Data”

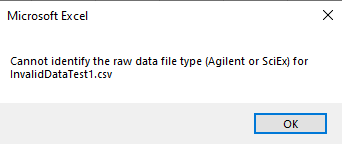


Browse for InvalidDataTest1.csv. Click Open



#### Expected Results

A message box will appear, telling the file is invalid.



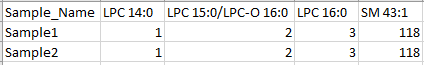
### Loading from a csv file in table form with transition as column variables

#### Requirements

TidyTransitionColumn.csv

#### Preconditions

Users imported the csv file in table form with transition as column variables.

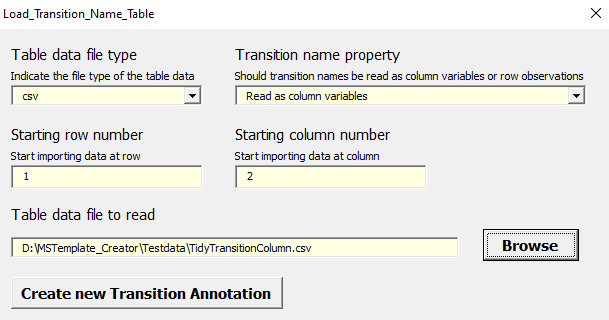


#### Steps

Click on the button “Load Transition\_Name from Table Data”



Fill in the entries as follows:



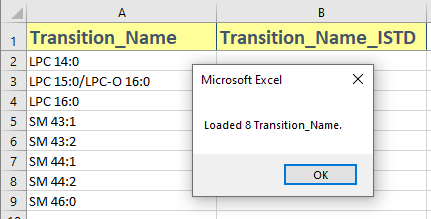
#### Expected Results

If there are existing entries in the “Transition\_Name” column. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten



Clicking on Cancel should cause the message box to leave and the original inputs are left alone

Clicking on Overwrite should cause the original inputs to be replaced with the Transition Names found in all three files



Ensure that

* Transition\_Name are loaded unto the right column in the sheet
* 8 Transition\_Names should be found in TidyTransitionColumn.csv
* Duplicates are removed
* Sorted in increasing order

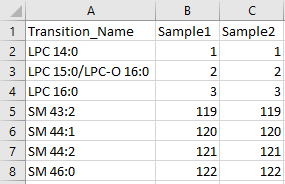
### Loading from a csv file in table form with transition as row observations

#### Requirements

TidyTransitionRow.csv

#### Preconditions

Users imported the csv file in table form with transition as row variables.

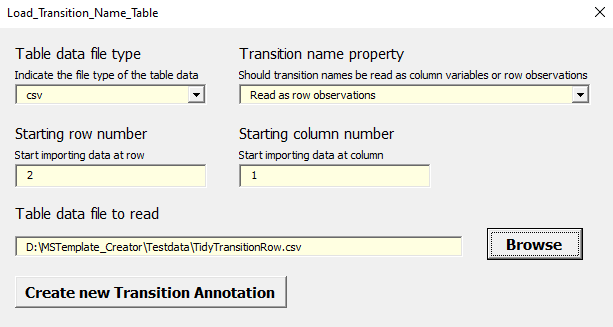


#### Steps

Click on the button “Load Transition\_Name from Table Data”



Fill in the entries as follows:



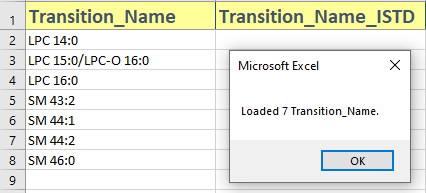
#### Expected Results

If there are existing entries in the “Transition\_Name” column. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten



Clicking on Cancel should cause the message box to leave and the original inputs are left alone

Clicking on Overwrite should cause the original inputs to be replaced with the Transition Names found in all three files



Ensure that

* Transition\_Name are loaded unto the right column in the sheet
* 7 Transition\_Names should be found in TidyTransitionRow.csv
* Duplicates are removed
* Sorted in increasing order

## Validating the ISTD

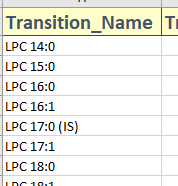
### Using the “Validate ISTD” button

#### Requirements

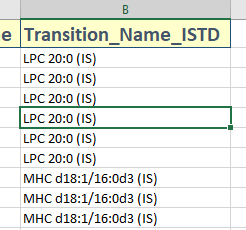
AgilentRawDataTest1.csv

#### Preconditions

Users must be able to successfully load some entries in the column “Transition Name”



Users key in some ISTD entries in the column “Transition\_Name\_ISTD”



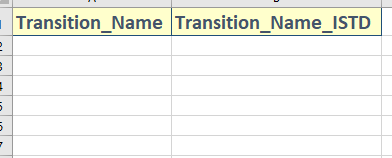
#### Steps

Click on the button “Validate ISTD”



#### Expected Results

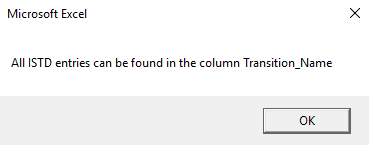
If either “Transition\_Name” or “Transition\_Name\_ISTD” is empty



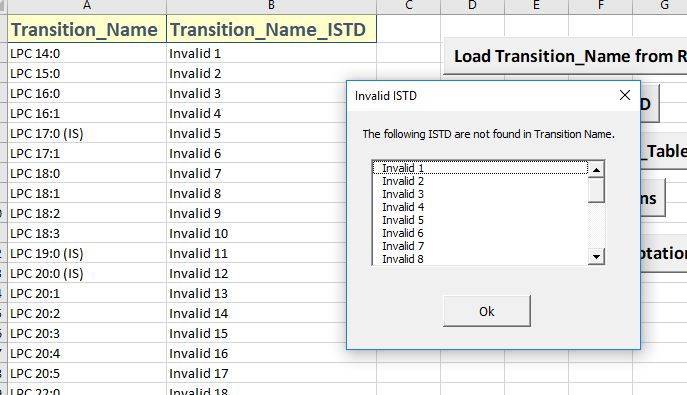
Clicking on the button **should not do anything**

If both entries are filled, the following will occur,

If there are no issues with the ISTD, this message box will appear.



Else, the program will show which ISTD are invalid



Ensure that

* Blank entries in Transition\_Name\_ISTD are ignored and should be treated as valid.
* Invalid ISTD are rightly indicated. (ISTD that are not found in the column “Transition\_Name”)

## Copying Transition Names from “Transition\_Name\_Annot” to “ISTD\_Annot”

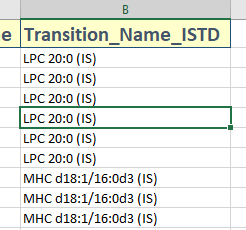
### Using the “Load ISTD to ISTD\_Table” button

#### Requirements

None

#### Preconditions

Users key in some ISTD entries in the column “Transition\_Name\_ISTD”



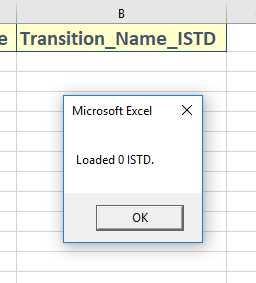
#### Steps

Click on the button “Load ISTD to ISTD\_Table”



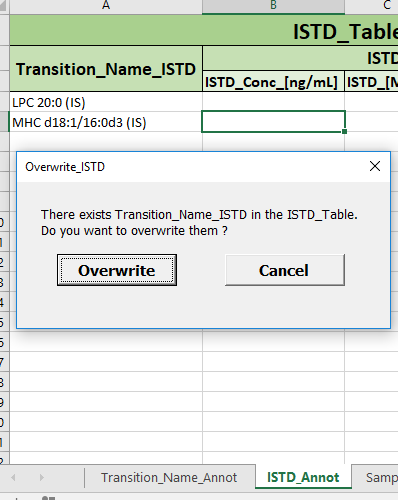
#### Expected Results

If there is no ISTD input, a message box will pop up saying



If there is at least one ISTD, users will be directed unto the “ISTD\_Annot” sheet.

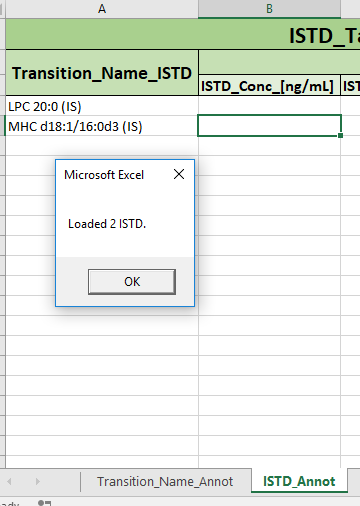
Following that, the program will check if there are existing entries in the ”ISTD\_Annot” sheet. If there is, an overwrite message box will appear



Clicking on Cancel should cause the message box to leave and the original inputs are left alone

Clicking on Overwrite should cause the original inputs to be replaced with the most recent ISTD entries in the “Transition\_Name\_Annot” sheet.

A message box will pop up saying the number of ISTD copied unto the “ISTD\_Annot” sheet



Ensure that

* Transition\_Name\_ISTD are loaded unto the right column in the sheet
* Correct amount of ISTD are copied
* Duplicate/Blank ISTD should be removed

## Clearing of columns in the “Transition\_Name\_Annot” sheet

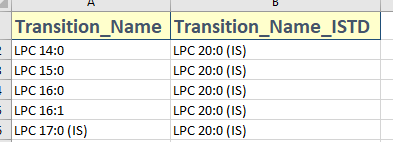
### Using the “Clear Columns” button

#### Requirements

None

#### Preconditions

Users key in some entries in the sheet

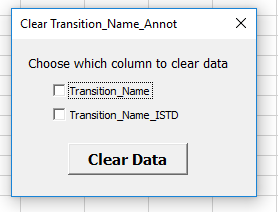


#### Steps

Click on the button “Clear Columns”



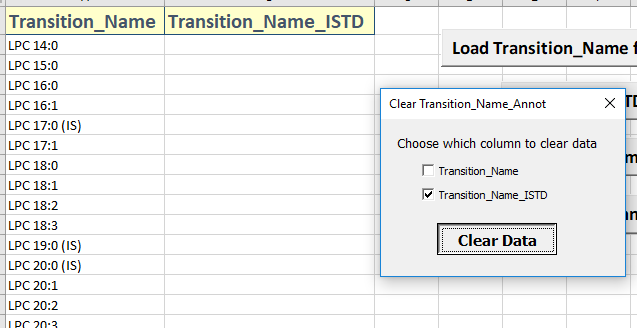
A message box will appear, asking which column to clear. Users can choose the columns by checking on the check box



When they have chosen their columns, click on “Clear Data

#### Expected Results

Data is cleared the data when the “Clear Data” button is pressed.



Ensure that

* The choices of which columns to clear are present and in the correct spelling.
* The correct columns are cleared.
* Only the contents are cleared, not the format. No cells should be deleted as well.

# **Part Two: Testing “ISTD\_Annot” sheet**

## Calculation of ISTD concentrations from ng/mL to nM

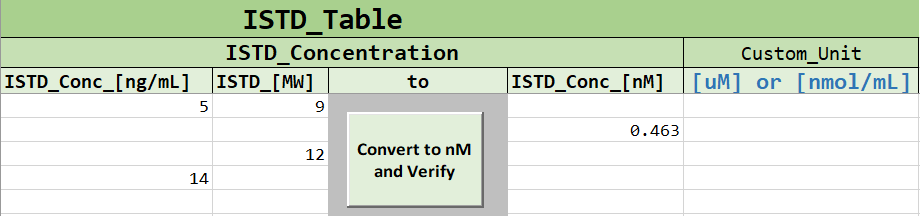
### Using the “Convert to nM and Verify” button

#### Requirements

None

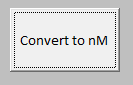
#### Preconditions

Users key in some entries in the “ISTD\_Conc\_[ng/mL]” and the “ISTD\_[MW] column”



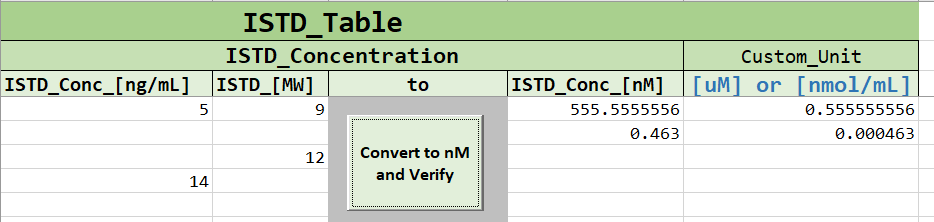
#### Steps

Click on the button “Convert to nM and verify”



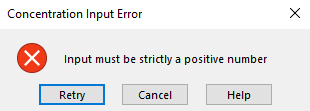
#### Expected Results

ISTD values will be calculated automatically



Ensure that

* Only positive numbers are accepted in “ISTD\_Conc\_[ng/mL]”, “ISTD\_[MW]” and “ISTD\_Conc\_[nM]”. Error should be given if an invalid values are given.



* Calculation is done only when both columns “ISTD\_Conc\_[ng/mL]”, “ISTD\_[MW]” are filled in a given row. Existing values of “ISTD\_Conc\_[nM]” are left alone
* Calculation is “ISTD\_Conc\_[ng/mL]” divided by “ISTD\_[MW]”
* Custom Unit values are correctly converted

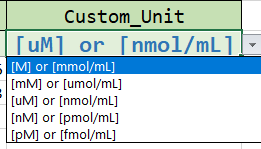
### Converting concentration from nM to other units

#### Requirement

First part is competed

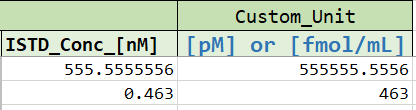
#### Steps

Change the custom unit



#### Expected Results

Values should be converted correctly.



## Clearing of columns in the “ISTD\_Annot” sheet

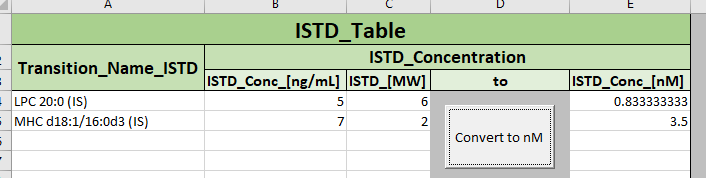
### Using the “Clear ISTD\_Table Columns” button

#### Requirement

None

#### Preconditions

Users key in some entries in the sheet

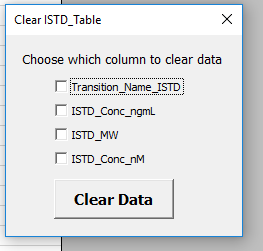


#### Steps

Click on the button “Clear ISTD\_Table Columns”



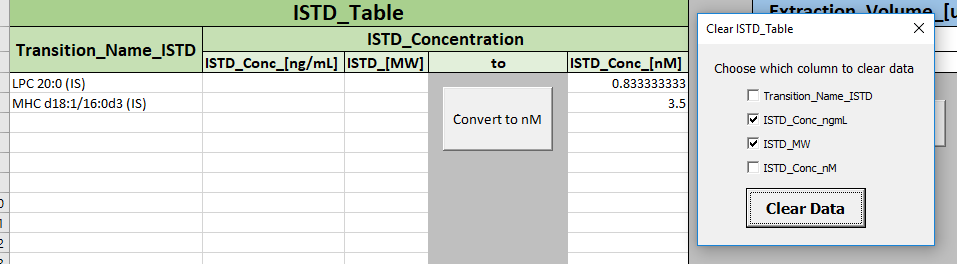
A message box will appear, asking which column to clear. Users can choose the columns by checking on the check box



When they have chosen their columns, click on “Clear Data”

#### Expected Results

Data is cleared the data when the “Clear Data” button is pressed.



Ensure that

* The choices of which columns to clear are present and in the correct spelling.
* The correct columns are cleared.
* Only the contents are cleared, not the format. No cells should be deleted as well.

# **Part Three: Testing “Sample\_Annot” sheet**

## Creating a new sample annotation template

### Creating from Agilent csv file in WideTable form

#### Requirements

MultipleDataTest2.csv

#### Preconditions

Users exported the csv file from MassHunter correctly.

#### Steps

Click on the button “Load Sample Annotation”



The following userform will appear.



Click on the top “Browse” button to upload the raw data file MultipleDataTest2.csv

Once done, you can see the file path of the raw data being recorded and the button “Create new Sample Annotation” being activated. Click on that button.



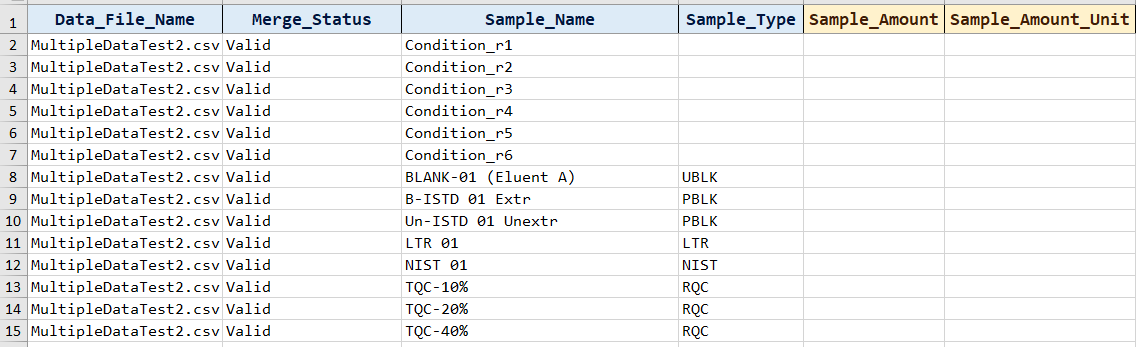
#### Expected Results

If there are existing entries in the sheet. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten



Clicking on Cancel should cause the message box to leave and the original inputs are left alone

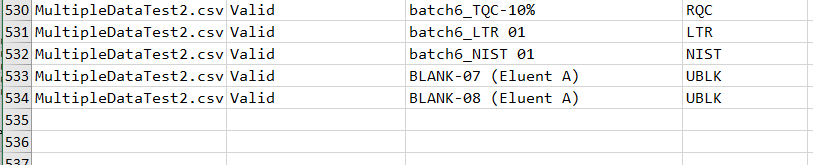
Clicking on Overwrite should cause some columns (Raw\_Data\_File\_Name, Merge\_Status, Sample\_Name and Sample\_Type) to be replaced with the data found in MultipleDataTest2.csv



The other columns should be left alone.

Ensure that

* Data file MultipleDataTest2.csv can be browse, selected and recorded
* The “Create new Sample Annotation” button is activated when there is a data file recorded
* Users are able to clear the data file path with a backspace. Users should not be able to edit the file path by keyboard.
* Make sure the “Create new Sample Annotation” gets deactivated when the data file entry is clear.
* When the “Create new Sample Annotation” button is clicked. The four columns (Data\_File\_Name, Merge\_Status, Sample\_Name and Sample\_Type) should be filled with some data
* Check that all the data has been loaded, especially the last row. There are a total of 534 lines used



* Check that the Data\_File\_Name is correct
* Check that the merge status is all set to Valid
* Check that there is an attempt by the macro file to guess if the sample is a “Blank, TQC, PQC, etc …”
* Ensure that it works even when the data has been filtered. The program should first unfiltered the data first before creating/overwrite a sample annotation template

### Creating from Agilent csv file in CompoundTable form

#### Requirements

CompoundTableForm.csv

#### Preconditions

Users exported the csv file from MassHunter correctly.

#### Steps

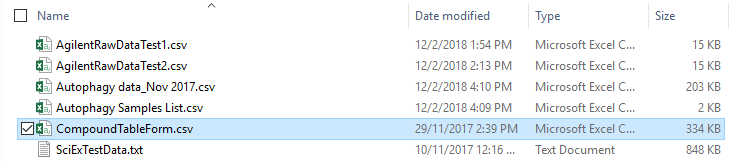
Click on the button “Load Sample Annotation”



The following userform will appear.



Click on the top “Browse” button to upload the raw data file CompoundTableForm.csv



Once done, you can see the file path of the raw data being recorded and the button “Create new Sample Annotation” being activated. Click on that button.



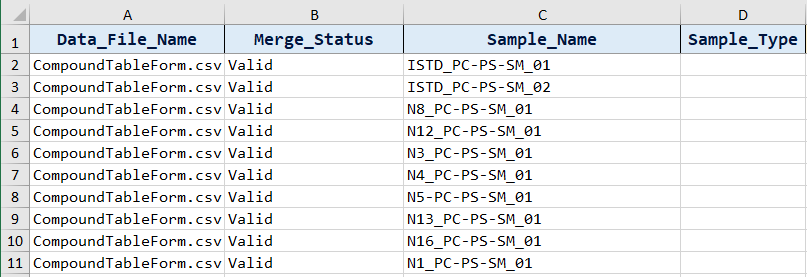
#### Expected Results

If there are existing entries in the sheet. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten



Clicking on Cancel should cause the message box to leave and the original inputs are left alone

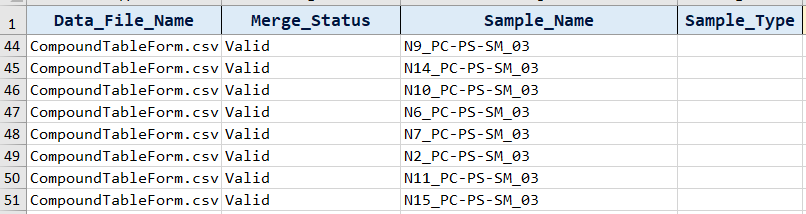
Clicking on Overwrite should cause some columns (Raw\_Data\_File\_Name, Merge\_Status, Sample\_Name and Sample\_Type) to be replaced with the data found in CompoundTableForm.csv



The other columns should be left alone.

Ensure that

* Data file CompoundTableForm.csv can be browse, selected and recorded
* The “Create new Sample Annotation” button is activated when there is a data file recorded
* Users are able to clear the data file path with a backspace. Users should not be able to edit the file path by keyboard.
* Make sure the “Create new Sample Annotation” gets deactivated when the data file entry is clear.
* When the “Create new Sample Annotation” button is clicked. The four columns (Data\_File\_Name, Merge\_Status, Sample\_Name and Sample\_Type) should be filled with some data
* Check that all the data has been loaded, especially the last row. There are a total of 51 lines are used



* Check that the Data\_File\_Name is correct
* Check that the merge status is all set to Valid
* Ensure that it works even when the data has been filtered. The program should first unfiltered the data first before creating/overwrite a sample annotation template

### Creating from Sciex txt file

#### Requirements

SciExTestData.txt

#### Preconditions

Users exported the txt file from MultiQuant correctly.

#### Steps

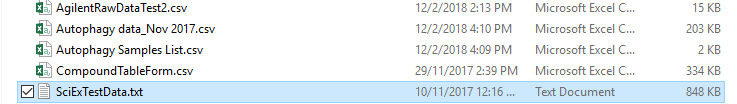
Click on the button “Load Sample Annotation”



The following userform will appear.



Click on the top “Browse” button to upload the raw data file SciExTestData.txt



Once done, you can see the file path of the raw data being recorded and the button “Create new Sample Annotation” being activated. Click on that button.



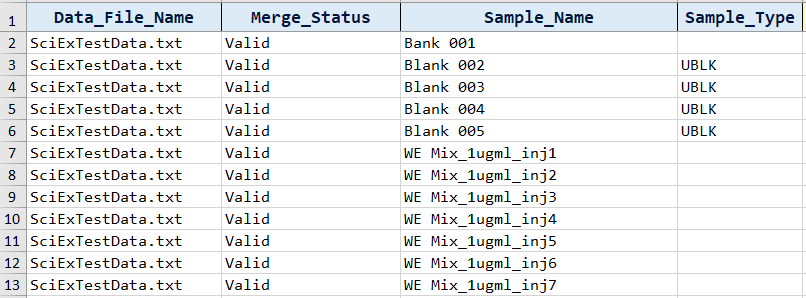
#### Expected Results

If there are existing entries in the sheet. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten



Clicking on Cancel should cause the message box to leave and the original inputs are left alone

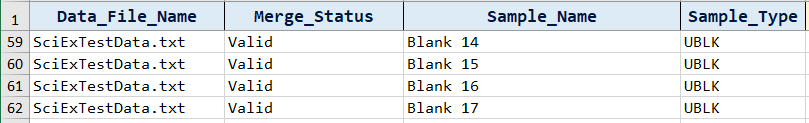
Clicking on Overwrite should cause some columns (Raw\_Data\_File\_Name, Merge\_Status, Sample\_Name and Sample\_Type) to be replaced with the data found in SciExTestData.txt



The other columns should be left alone.

Ensure that

* Data file SciExTestData.txt can be browse, selected and recorded
* The “Create new Sample Annotation” button is activated when there is a data file recorded
* Users are able to clear the data file path with a backspace. Users should not be able to edit the file path by keyboard.
* Make sure the “Create new Sample Annotation” gets deactivated when the data file entry is clear.
* When the “Create new Sample Annotation” button is clicked. The four columns (Data\_File\_Name, Merge\_Status, Sample\_Name and Sample\_Type) should be filled with some data
* Check that all the data has been loaded, especially the last row. There are a total of 62 lines are used



* Check that the Data\_File\_Name is correct
* Check that the merge status is all set to Valid
* Check that there is an attempt by the macro file to guess if the sample is a “Blank, TQC, PQC, etc …”
* Ensure that it works even when the data has been filtered. The program should first unfiltered the data first before creating/overwrite a sample annotation template

### Creating from multiple files both Agilent and Sciex

#### Requirements

MultipleDataTest1.csv

MultipleDataTest2.csv

SciExTestData.txt

#### Preconditions

Users exported the csv file from MassHunter and the txt file from MultiQuant correctly.

#### Steps

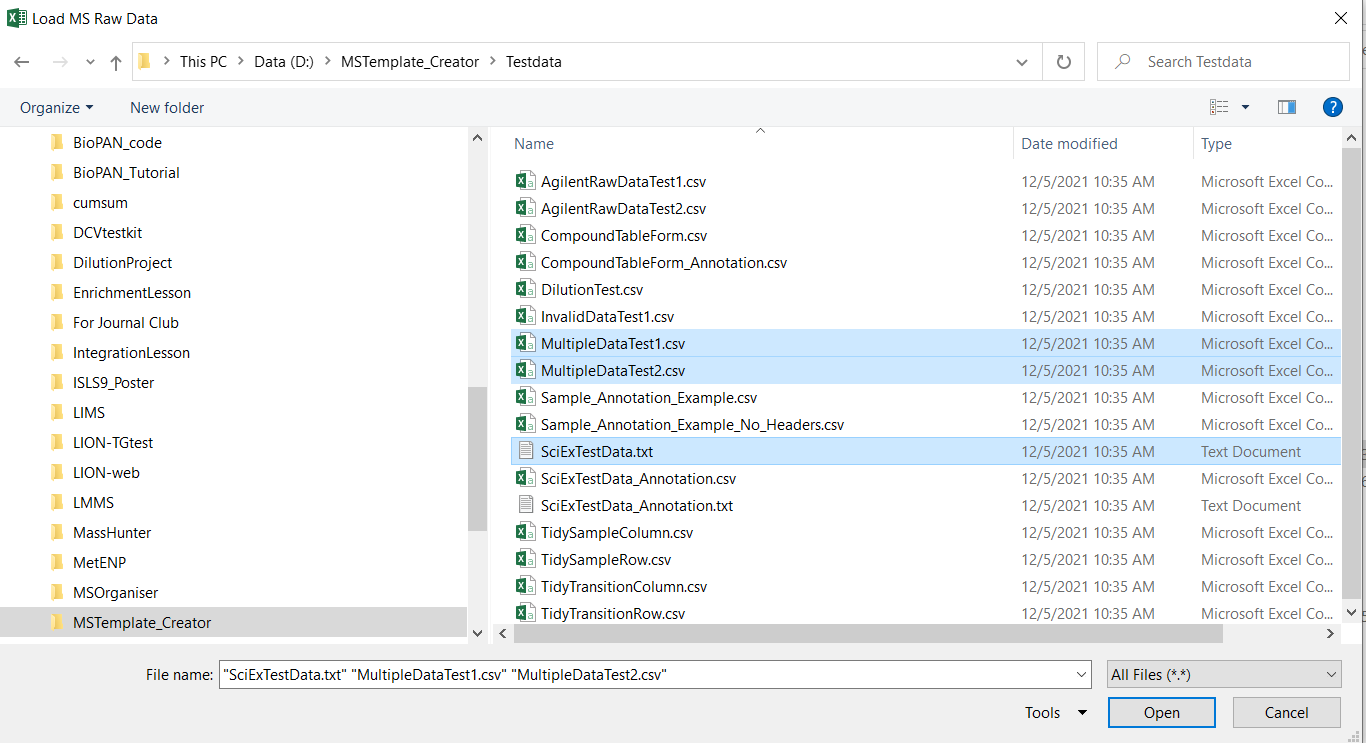
Click on the button “Load Sample Annotation”



The following userform will appear.



Click on the top “Browse” button to upload the three files



Once done, you can see the file path of the raw data being recorded and the button “Create new Sample Annotation” being activated. Click on that button.



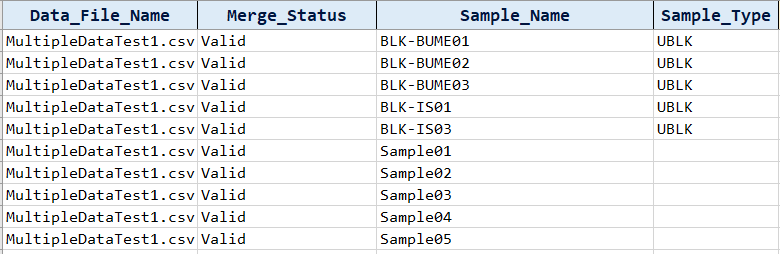
#### Expected Results

If there are existing entries in the sheet. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten



Clicking on Cancel should cause the message box to leave and the original inputs are left alone

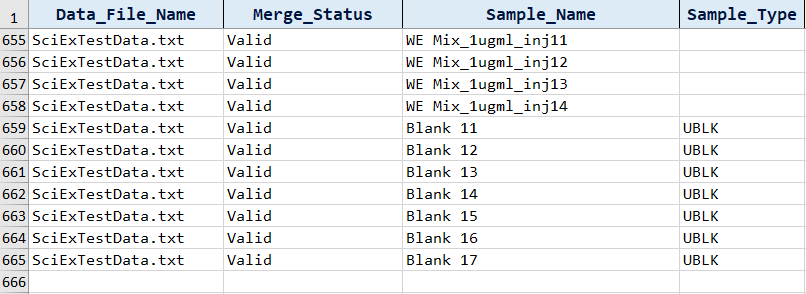
Clicking on Overwrite should cause some columns (Data\_File\_Name, Merge\_Status, Sample\_Name and Sample\_Type) to be replaced with the data found in the three files



The other columns should be left alone.

Ensure that

* Data file can be browse, selected and recorded
* The “Create new Sample Annotation” button is activated when there is a data file recorded
* Users are able to clear the data file path with a backspace. Users should not be able to edit the file path by keyboard.
* Make sure the “Create new Sample Annotation” gets deactivated when the data file entry is clear.
* When the “Create new Sample Annotation” button is clicked. The four columns (Data\_File\_Name, Merge\_Status, Sample\_Name and Sample\_Type) should be filled with some data
* Check that all the data has been loaded, especially the last row. There are a total of 665 lines are used



* Check that the Data\_File\_Name is correct
* Check that the merge status is all set to Valid
* Check that there is an attempt by the macro file to guess if the sample is a “Blank, TQC, PQC, etc …”
* Ensure that it works even when the data has been filtered. The program should first unfiltered the data first before creating/overwrite a sample annotation template

### Loading an invalid raw data file

#### Requirements

InvalidDataTest1.csv (that is a sample annotation file)

#### Preconditions

None

#### Steps

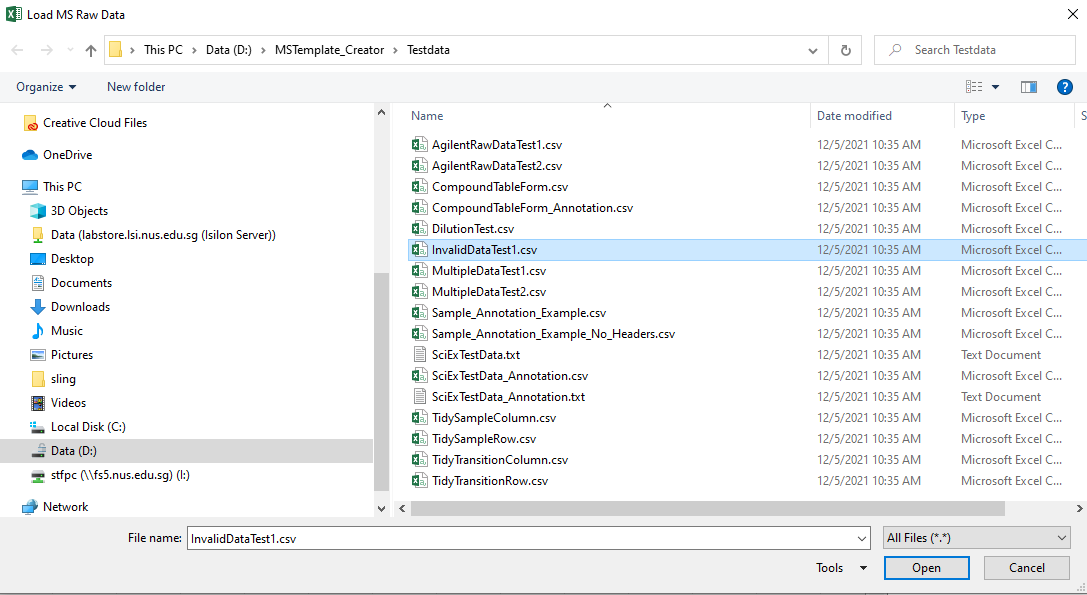
Click on the button “Load Sample Annotation”



The following userform will appear.



Click on the top “Browse” button to upload InvalidDataTest1.csv

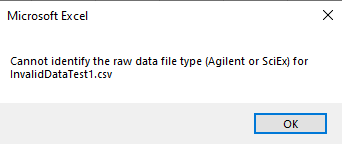


Once done, you can see the file path of the raw data being recorded and the button “Create new Sample Annotation” being activated. Click on that button.



#### Expected Results

A message box will appear, telling the file is invalid.



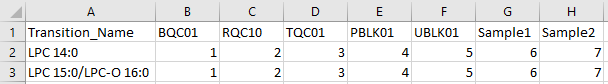
### Creating from a csv file in table form with sample name as column variable

#### Requirements

TidySampleColumn.csv

#### Preconditions

Users imported the csv file in table form with sample names as column variables.

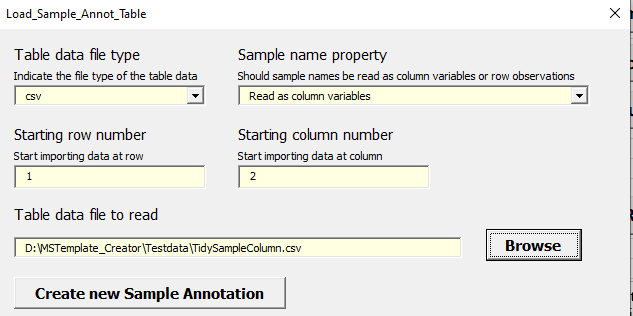


#### Steps

Click on the button “Load Sample Annotation from Table Data”



Fill in the entries as follows:



#### Expected Results

If there are existing entries in the sheet. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten



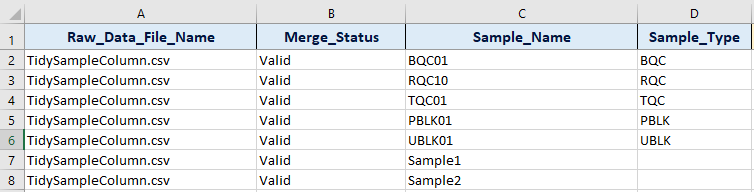
Clicking on Cancel should cause the message box to leave and the original inputs are left alone

Clicking on Overwrite should cause some columns (Data\_File\_Name, Merge\_Status, Sample\_Name and Sample\_Type) to be replaced with the data found in TidySampleColumn.csv.

The other columns should be left alone.

Ensure that

* Data file TidySampleColumn.csv can be browse, selected and recorded
* The “Create new Sample Annotation” button is activated when there is a data file recorded
* Users are able to clear the data file path with a backspace. Users should not be able to edit the file path by keyboard.
* Make sure the “Create new Sample Annotation” gets deactivated when the data file entry is clear.
* When the “Create new Sample Annotation” button is clicked. The four columns (Data\_File\_Name, Merge\_Status, Sample\_Name and Sample\_Type) should be filled with some data
* Check that all the data has been loaded, especially the last row. There are a total of 8 lines used



* Check that the Raw\_Data\_File\_Name is correct
* Check that the merge status is all set to Valid
* Check that there is an attempt by the macro file to guess if the sample is a “Blank, TQC, PQC, etc …”
* Ensure that it works even when the data has been filtered. The program should first unfiltered the data first before creating/overwrite a sample annotation template

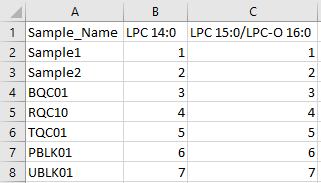
### Creating from a csv file in table form with sample name as row observations

#### Requirements

TidySampleRow.csv

#### Preconditions

Users imported the csv file in table form with sample names as column variables.

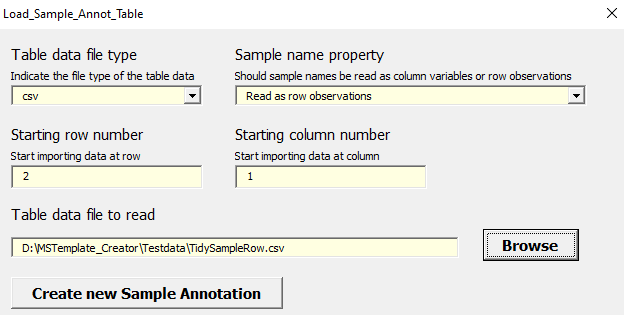


#### Steps

Click on the button “Load Sample Annotation from Table Data”



Fill in the entries as follows:



#### Expected Results

If there are existing entries in the sheet. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten



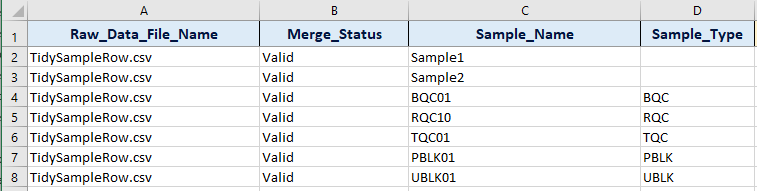
Clicking on Cancel should cause the message box to leave and the original inputs are left alone

Clicking on Overwrite should cause some columns (Data\_File\_Name, Merge\_Status, Sample\_Name and Sample\_Type) to be replaced with the data found in TidySampleColumn.csv.

The other columns should be left alone.

Ensure that

* Data file TidySampleRow.csv can be browse, selected and recorded
* The “Create new Sample Annotation” button is activated when there is a data file recorded
* Users are able to clear the data file path with a backspace. Users should not be able to edit the file path by keyboard.
* Make sure the “Create new Sample Annotation” gets deactivated when the data file entry is clear.
* When the “Create new Sample Annotation” button is clicked. The four columns (Data\_File\_Name, Merge\_Status, Sample\_Name and Sample\_Type) should be filled with some data
* Check that all the data has been loaded, especially the last row. There are a total of 8 lines used



* Check that the Data\_File\_Name is correct
* Check that the merge status is all set to Valid
* Check that there is an attempt by the macro file to guess if the sample is a “Blank, TQC, PQC, etc …”
* Ensure that it works even when the data has been filtered. The program should first unfiltered the data first before creating/overwrite a sample annotation template

## Autofill blank entries in the “Sample\_Type” column

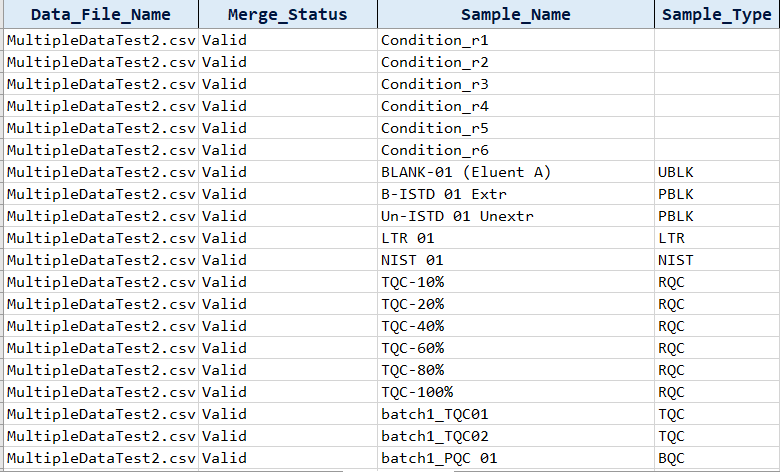
### Using the “Autofill ‘Sample’ in Sample\_Type” button

#### Requirements

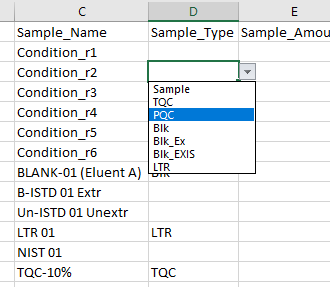
#### MultipleDataTest2.csv

#### Preconditions

Users should have created a new template from MultipleDataTest2.csv



And change the Sample\_Type to a relevant category that is not ‘SPL’



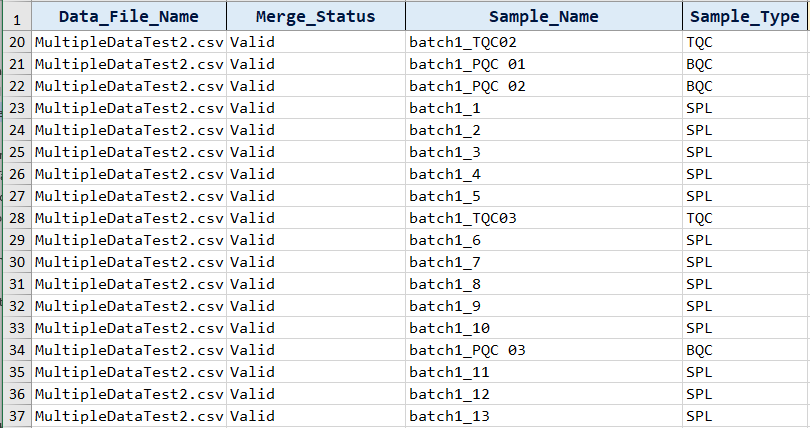
#### Steps

Click on the button “Autofill ‘Sample’ in Sample\_Type”



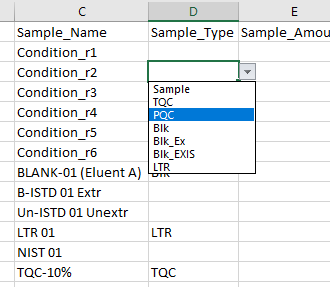
#### Expected Results

All empty cells in the column “Sample\_Type” should be filled with the word “SPL” till the end of the data

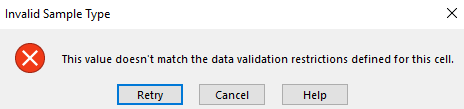


Ensure that

* In the “Sample\_Type” column, users can only choose a limited amount of options provided in the list box



* Users are not allowed to put in any input they want



* The program works even when the data has been filtered. The program should first unfiltered the data first before filling the entries.

## Merging an existing sample annotation file

### Merging an Agilent csv file in WideTable form with a sample annotation file

#### Requirements

AgilentRawDataTest1.csv

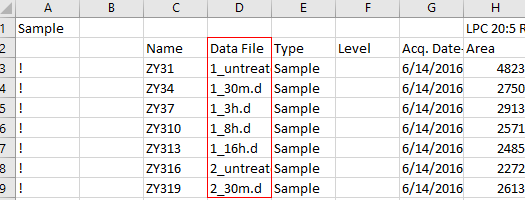
Sample\_Annotation\_Example.csv

#### Preconditions

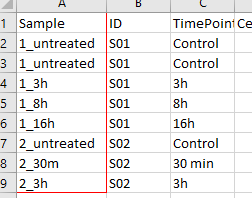
Users exported the csv file from MassHunter correctly and created their own annotation file in csv.

For Agilent Raw Data, users need to create a column in the sample annotation file that matches the Data File entries from MassHunter.

Data File entries in AgilentRawDataTest1.csv



Matching column from Sample\_Annotation\_Example.csv



#### Steps

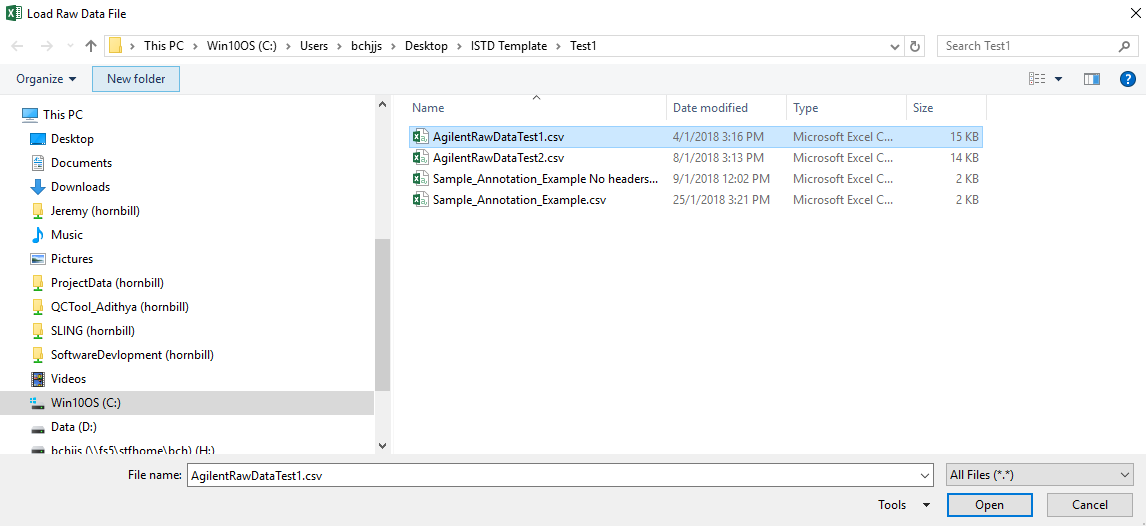
Click on the button “Load Sample Annotation”



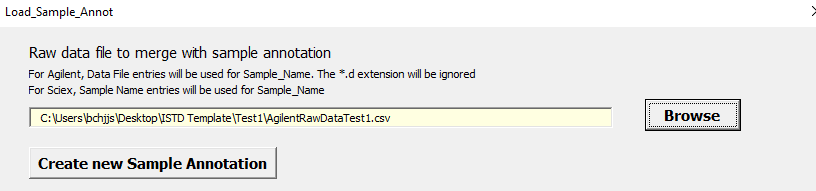
The following userform will appear.



Click on the top “Browse” button to upload the raw data file AgilentRawDataTest1.csv

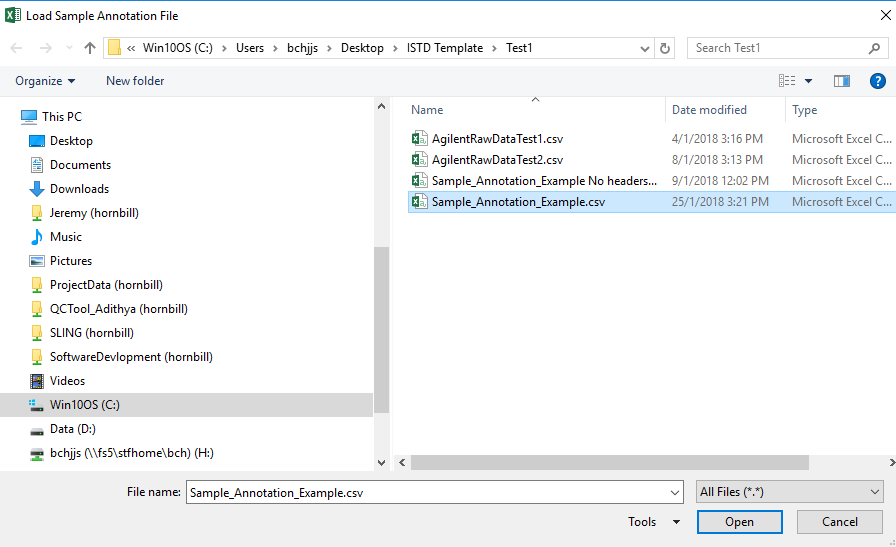


Once done, you can see the file path of the raw data being recorded.

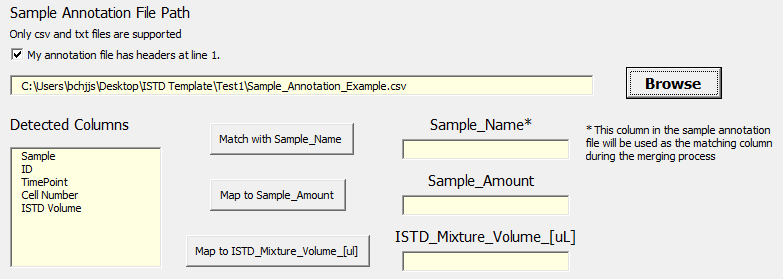


Click on the “Browse” button to upload the sample annotation file Sample\_Annotation\_Example.csv



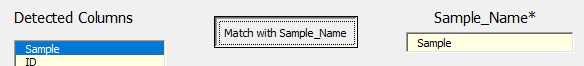


Once done, you can see the file path of the sample annotation being recorded.



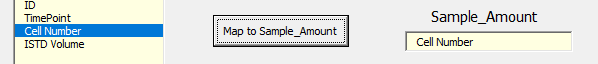
The program will list the column names found at the first line of the annotation file

Under the “Detected Columns” list box, choose “Sample” and then click on the button “Match with Sample\_Name”

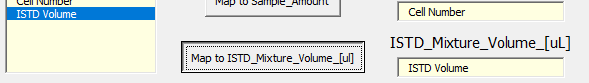


In doing so, the button “Merge with Sample Annotation” should be activated.

Under the “Detected Columns” list box, choose “Cell Number” and then click on the button “Map to Sample\_Amount”



Under the “Detected Columns” list box, choose “ISTD Volume” and then click on the button “Map to ISTD\_Mixture\_[uL]”



Click on the button “Merge with Sample Annotation”



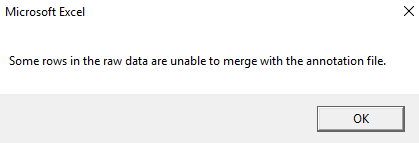
#### Expected Results

If there are existing entries in the sheet. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten



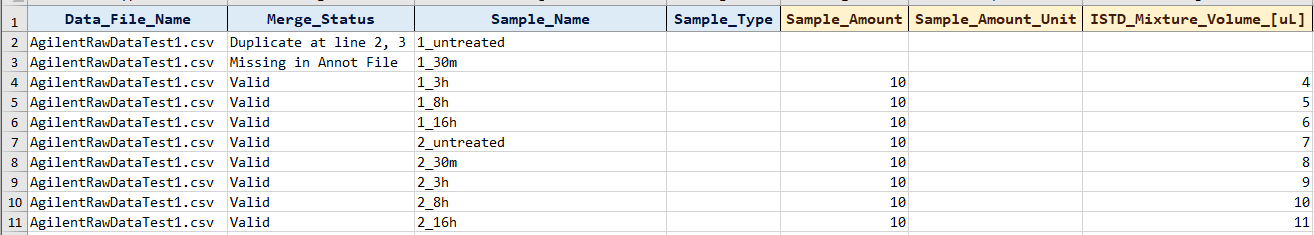
Clicking on Cancel should cause the message box to leave and the original inputs are left alone

Clicking on Overwrite, the following message box should appear

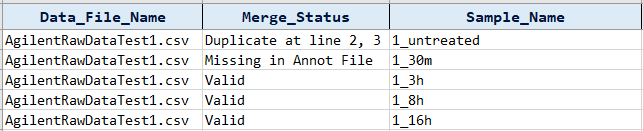


Some columns (Raw\_Data\_File\_Name, Merge\_Status, Sample\_Name, Sample\_Amount and ISTD\_Mixture\_Volume\_[uL]) will be replaced with the data found in AgilentRawDataTest1.csv and

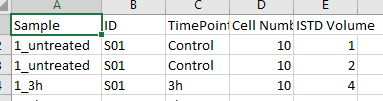
Sample\_Annotation\_Example.csv



The merge status for 1\_untreated and 1\_30m should be unsuccessful



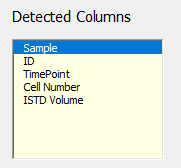
As 1\_untreated appeared twice in the sample annotation file



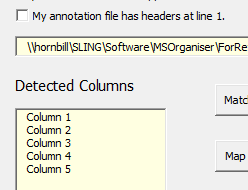
And 1\_30m is not presence in the sample annotation file

Ensure that

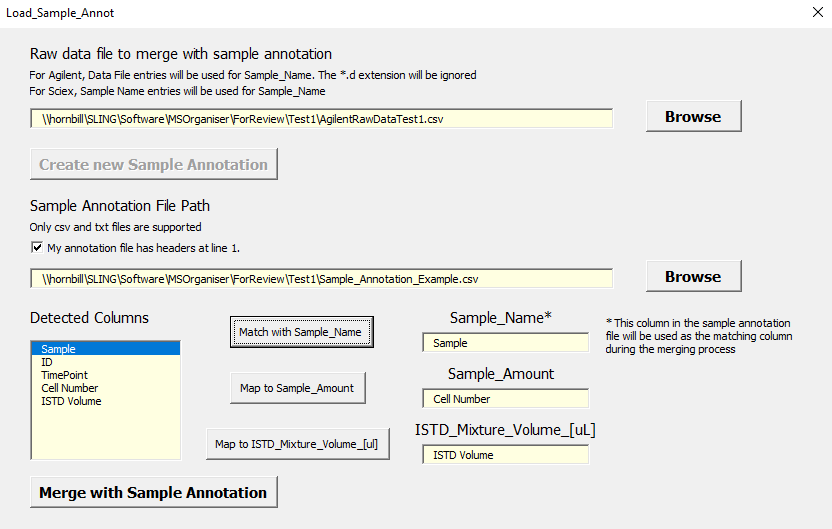
* Data file can be browse, selected and recorded
* Users are able to clear the data file path with a backspace. Users should not be able to edit the file path.
* Make sure the “Merge with Sample Annotation” button gets deactivated when the data file entry is cleared.
* Sample Annotation file can be browsed, selected and recorded.
* When the annotation file Sample\_Annotation\_Example.csv is recorded, the program should be able to display the headers found in the first row of the annotation file in the “Detected Columns” list box.



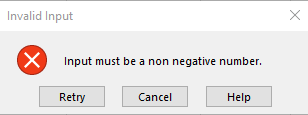
* In the case when the annotation file has no headers like Sample\_Annotation\_Example No headers.csv, the check box button beside “My annotation file has header at line 1” must be unchecked before loading the sample annotation file. When the annotation file is loaded, the “Detected Columns” list box will print out “Column 1”, “Column 2”, etc…



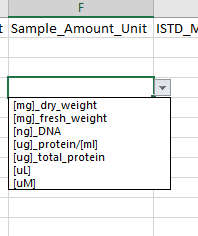
* Ensure that the three button “Match with Sample\_Name”, “Map to Sample\_Amount” and “Map to ISTD\_Mixture\_Volume\_[uL]” are working
* Ensure that the button “Merge with Sample Annotation” is activated only when the data file, sample annotation file and the Sample\_Name entries are filled



* Users are able to clear the sample annotation file path with a backspace. Users should not be able to edit the file path.
* Make sure the “Merge with Sample Annotation” button gets deactivated and all related entries (Detected Columns, Sample\_Name, Sample\_Amount, etc…) are also cleared.
* Users are able to clear the entries (Detected Columns, Sample\_Name, Sample\_Amount, etc…) with a backspace. Users should not be able to edit them.
* Make sure the “Merge with Sample Annotation” button gets deactivated when the entries in “Sample\_Name” removed.
* Columns “Sample\_Amount” and “ISTD\_Mixture\_Volume\_[uL]” accepts non negative values. Error should be given if an invalid values are given.



* Sample\_Amount\_Unit should have a drop down list available.



Users, however are still given a choice to type anything they want

Column names should be editable by the user

### Merging an Agilent csv file in CompoundTable form with a sample annotation file

#### Requirements

CompoundTableForm.csv

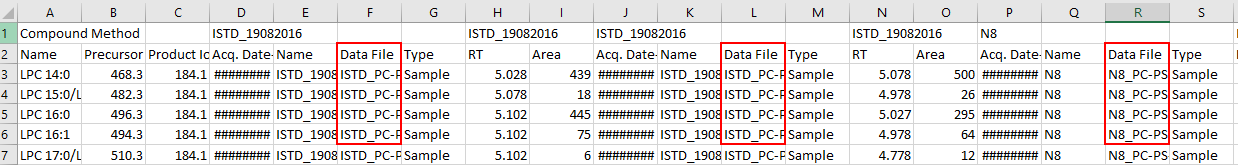
CompoundTableForm\_Annotation.csv

#### Preconditions

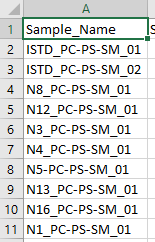
Users exported the csv file from MassHunter correctly and created their own annotation file in csv.

For Agilent Raw Data, users need to create a column in the sample annotation file that matches the Data File entries from MassHunter.

Data File entries in CompoundTableForm.csv



Matching column from CompoundTableForm\_Annotation.csv



#### Steps

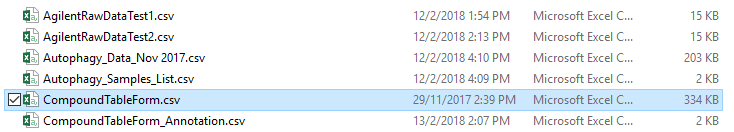
Click on the button “Load Sample Annotation”



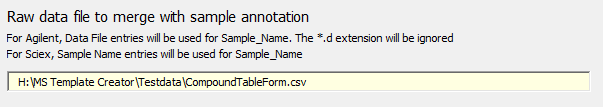
The following userform will appear.



Click on the top “Browse” button to upload the raw data file CompoundTableForm.csv



Once done, you can see the file path of the raw data being recorded.

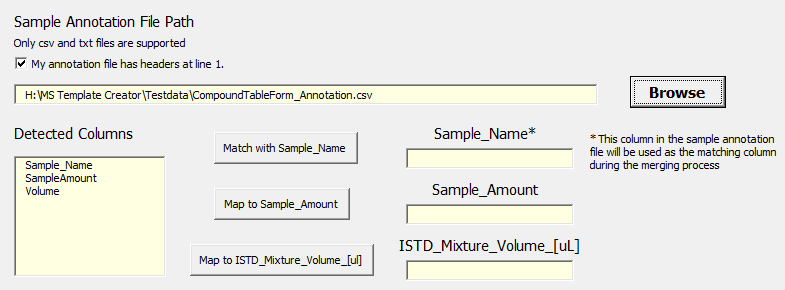


Click on the “Browse” button to upload the sample annotation file CompoundTableForm\_Annotation.csv



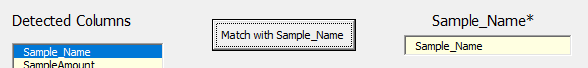


Once done, you can see the file path of the sample annotation being recorded.



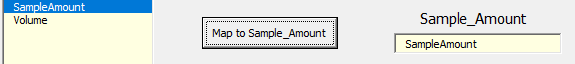
The program will list the column names found at the first line of the annotation file

Under the “Detected Columns” list box, choose “Sample\_Name” and then click on the button “Match with Sample\_Name”

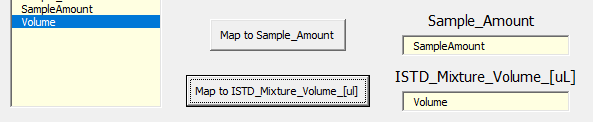


In doing so, the button “Merge with Sample Annotation” should be activated.

Under the “Detected Columns” list box, choose “SampleAmount” and then click on the button “Map to Sample\_Amount”



Under the “Detected Columns” list box, choose “Volume” and then click on the button “Map to ISTD\_Mixture\_[uL]”



Click on the button “Merge with Sample Annotation”



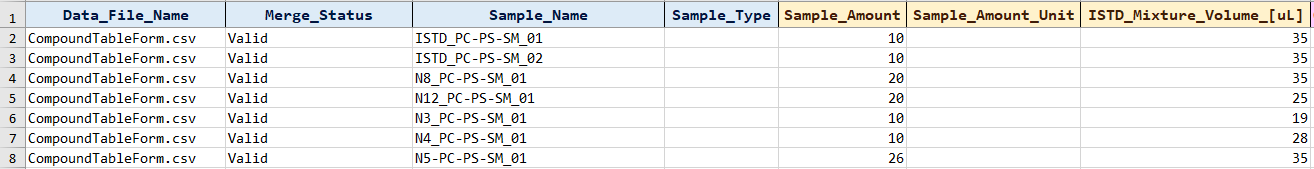
#### Expected Results

If there are existing entries in the sheet. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten



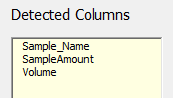
Clicking on Cancel should cause the message box to leave and the original inputs are left alone.

Clicking on Overwrite, the merged sample annotation template should be created.

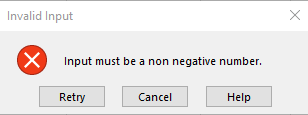


Ensure that

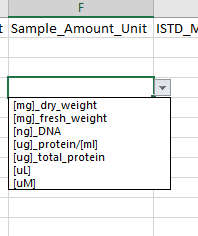
* Data file can be browse, selected and recorded
* Users are able to clear the data file path with a backspace. Users should not be able to edit the file path.
* Make sure the “Merge with Sample Annotation” button gets deactivated when the data file entry is cleared.
* Sample Annotation file can be browsed, selected and recorded.
* When the annotation file Sample\_Annotation\_Example.csv is recorded, the program should be able to display the headers found in the first row of the annotation file in the “Detected Columns” list box.



* Ensure that the three button “Match with Sample\_Name”, “Map to Sample\_Amount” and “Map to ISTD\_Mixture\_Volume\_[uL]” are working
* Ensure that the button “Merge with Sample Annotation” is activated only when the data file, sample annotation file and the Sample\_Name entries are filled
* Users are able to clear the sample annotation file path with a backspace. Users should not be able to edit the file path.
* Make sure the “Merge with Sample Annotation” button gets deactivated and all related entries (Detected Columns, Sample\_Name, Sample\_Amount, etc…) are also cleared.
* Users are able to clear the entries (Detected Columns, Sample\_Name, Sample\_Amount, etc…) with a backspace. Users should not be able to edit them.
* Make sure the “Merge with Sample Annotation” button gets deactivated when the entries in “Sample\_Name” removed.
* Columns “Sample\_Amount” and “ISTD\_Mixture\_Volume\_[uL]” accepts non negative values. Error should be given if an invalid values are given.



* Sample\_Amount\_Unit should have a drop down list available.



Users, however are still given a choice to type anything they want

Column names should be editable by the user

### Merging a Sciex txt file with a sample annotation file

#### Requirements

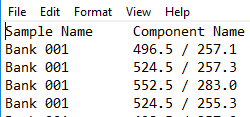
SciExTestData.txt

SciExTestData\_Annotation.txt

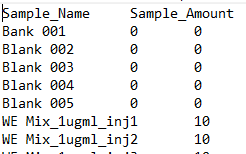
#### Preconditions

Users exported the txt file from MultiQuant correctly and created their own annotation file in txt.

For SciEx data, users need to create a column in the sample annotation file that matches the “Sample Name” entries from MultiQuant.



Matching column from SciExTestData\_Annotation.txt



#### Steps

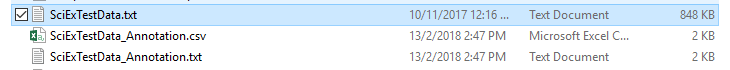
Click on the button “Load Sample Annotation”



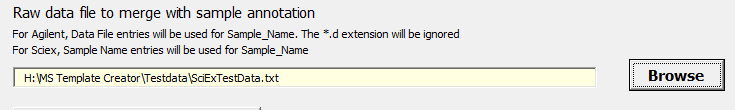
The following userform will appear.



Click on the top “Browse” button to upload the raw data file SciExTestData.txt

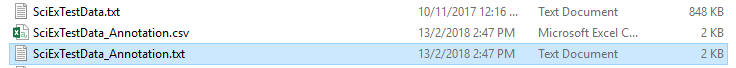


Once done, you can see the file path of the raw data being recorded.

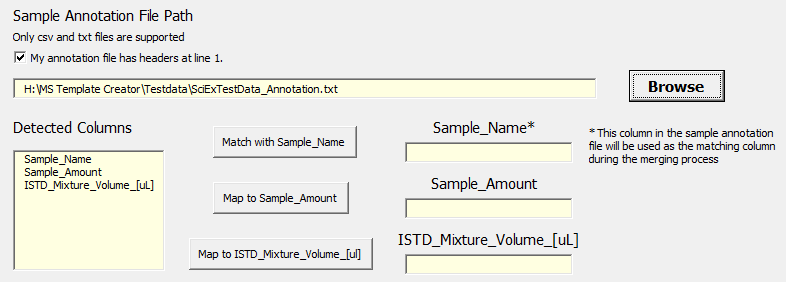


Click on the “Browse” button to upload the sample annotation file SciExTestData\_Annotation.txt



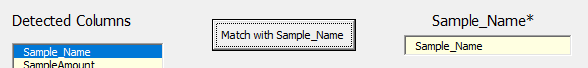


Once done, you can see the file path of the sample annotation being recorded.



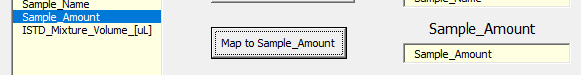
The program will list the column names found at the first line of the annotation file

Under the “Detected Columns” list box, choose “Sample\_Name” and then click on the button “Match with Sample\_Name”

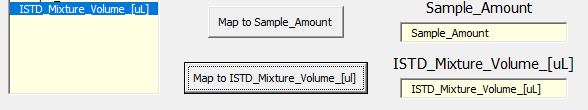


In doing so, the button “Merge with Sample Annotation” should be activated.

Under the “Detected Columns” list box, choose “Sample\_Amount” and then click on the button “Map to Sample\_Amount”



Under the “Detected Columns” list box, choose “ISTD\_Mixture\_Volume\_[uL]” and then click on the button “Map to ISTD\_Mixture\_[uL]”



Click on the button “Merge with Sample Annotation”



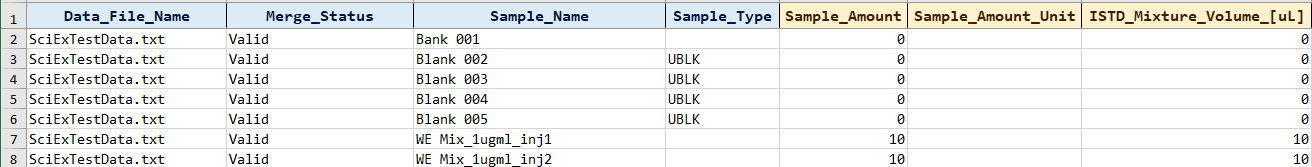
#### Expected Results

If there are existing entries in the sheet. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten



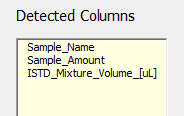
Clicking on Cancel should cause the message box to leave and the original inputs are left alone.

Clicking on Overwrite, the merged sample annotation template should be created.

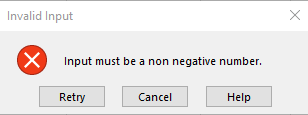


Ensure that

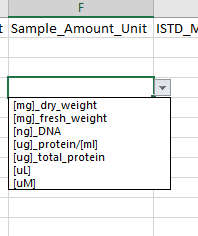
* Data file can be browse, selected and recorded
* Users are able to clear the data file path with a backspace. Users should not be able to edit the file path.
* Make sure the “Merge with Sample Annotation” button gets deactivated when the data file entry is cleared.
* Sample Annotation file can be browsed, selected and recorded.
* When the annotation file Sample\_Annotation\_Example.csv is recorded, the program should be able to display the headers found in the first row of the annotation file in the “Detected Columns” list box.



* Ensure that the three button “Match with Sample\_Name”, “Map to Sample\_Amount” and “Map to ISTD\_Mixture\_Volume\_[uL]” are working
* Ensure that the button “Merge with Sample Annotation” is activated only when the data file, sample annotation file and the Sample\_Name entries are filled
* Users are able to clear the sample annotation file path with a backspace. Users should not be able to edit the file path.
* Make sure the “Merge with Sample Annotation” button gets deactivated and all related entries (Detected Columns, Sample\_Name, Sample\_Amount, etc…) are also cleared.
* Users are able to clear the entries (Detected Columns, Sample\_Name, Sample\_Amount, etc…) with a backspace. Users should not be able to edit them.
* Make sure the “Merge with Sample Annotation” button gets deactivated when the entries in “Sample\_Name” removed.
* Columns “Sample\_Amount” and “ISTD\_Mixture\_Volume\_[uL]” accepts non negative values. Error should be given if an invalid values are given.



* Sample\_Amount\_Unit should have a drop down list available.



Users, however are still given a choice to type anything they want

Column names should be editable by the user

#### Notes

For this test, we use input the sample annotation file as a txt file. The program should still work if the file is in csv form.

### Merging multiple files with a sample annotation files

#### Requirements

AgilentRawDataTest1.csv

AgilentRawDataTest2.csv

Sample\_Annotation\_Example.csv

#### Preconditions

Users exported the csv file from MassHunter correctly and created their own annotation file in csv.

For Agilent Raw Data, users need to create a column in the sample annotation file that matches the Data File entries from MassHunter.

#### Steps

The same as part(i) except that we take in the two csv files.

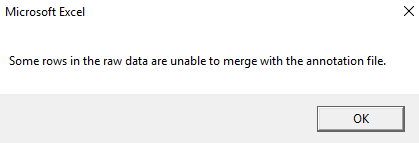
#### Expected Results

If there are existing entries in the sheet. A message box will pop up saying that there are existing entries and ask the user if the data should be overwritten

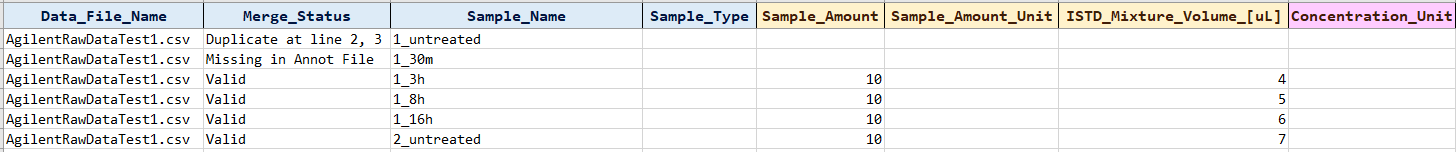


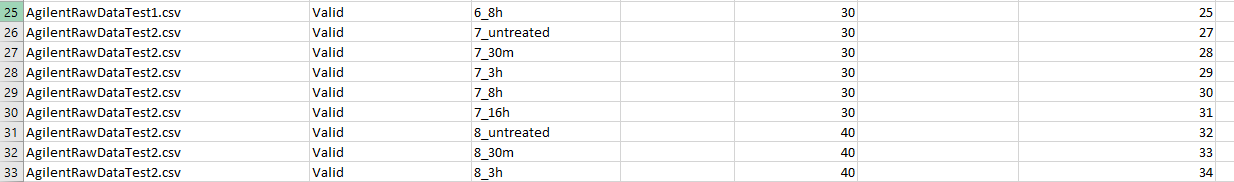
Clicking on Cancel should cause the message box to leave and the original inputs are left alone

Clicking on Overwrite, the following message box should appear

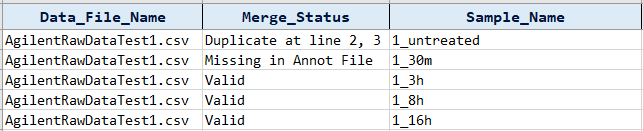


Some columns (Raw\_Data\_File\_Name, Merge\_Status, Sample\_Name, Sample\_Amount and ISTD\_Mixture\_Volume\_[uL]) will be replaced with the data found in AgilentRawDataTest1.csv and AgilentRawDataTest2.csv

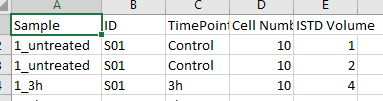




The merge status for 1\_untreated and 1\_30m should be unsuccessful



As 1\_untreated appeared twice in the sample annotation file



And 1\_30m is not presence in the sample annotation file

There should not be any merging issues with AgilentRawDataTest2.csv

Ensure that

* Same as i)

#### Notes

The above only test the case of two Agilent csv files WideTable form.

The program should also work in a mixture of Agilent CompoundTable form and Sciex txt files.

However, we only allow the input of one sample annotation files. Multiple annotation files will not be implemented as it will make the program more complicated and confusing for users

### Loading an invalid raw data file

#### Requirements

InvalidDataTest1.csv (that is a sample annotation file)

Sample\_Annotation\_Example.csv

#### Preconditions

None

#### Steps

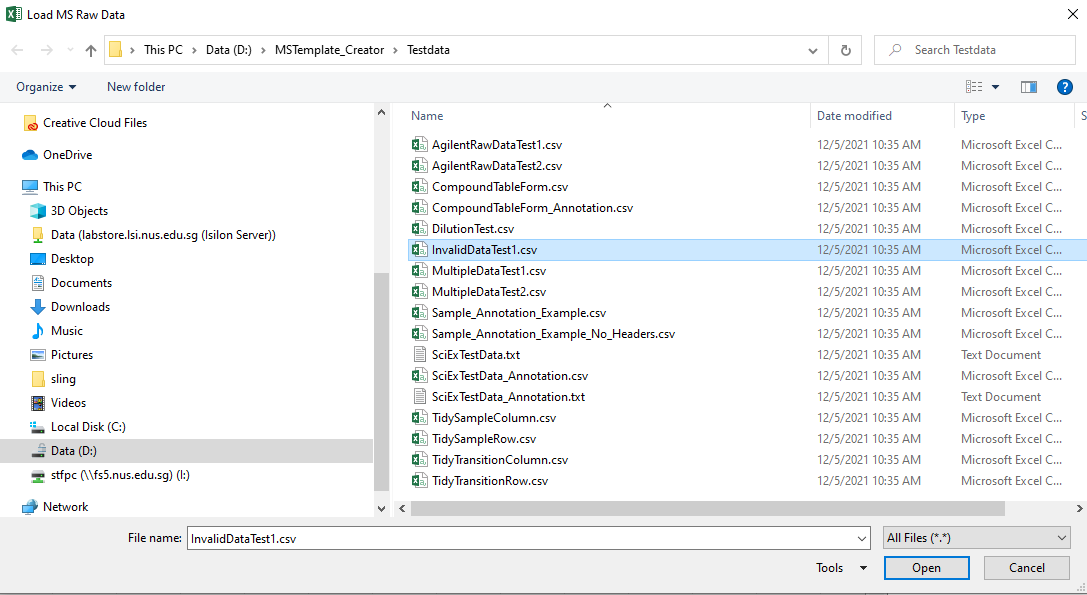
Click on the button “Load Sample Annotation”



The following userform will appear.



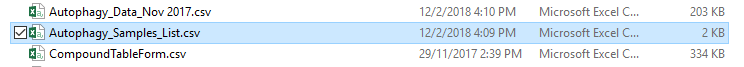
Click on the top “Browse” button to upload Sample\_Annotation\_Example



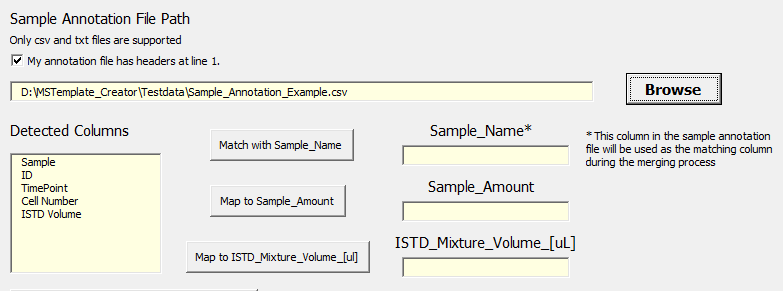
Once done, you can see the file path of the raw data being recorded.

Click on the “Browse” button to upload the sample annotation file Sample\_Annotation\_Example.csv



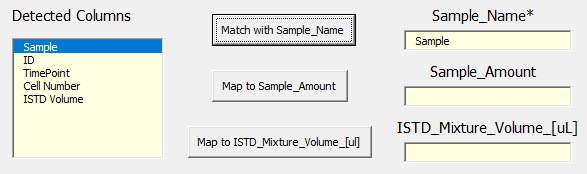


Once done, you can see the file path of the sample annotation being recorded.



The program will list the column names found at the first line of the annotation file

Under the “Detected Columns” list box, choose “Sample” and then click on the button “Match with Sample\_Name”

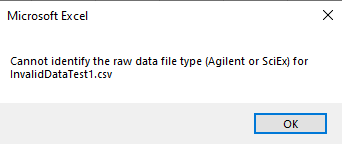


In doing so, the button “Merge with Sample Annotation” should be activated

Click on the button “Merge with Sample Annotation”

#### Expected Results

A message box will appear, telling the file is invalid.



## Autofill columns by “Sample\_Type”

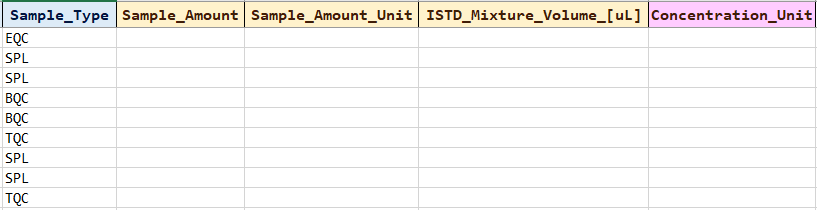
### Using the “Autofill by Sample\_type” button

#### Requirements

None

#### Preconditions

Users key in some entries in the sheet

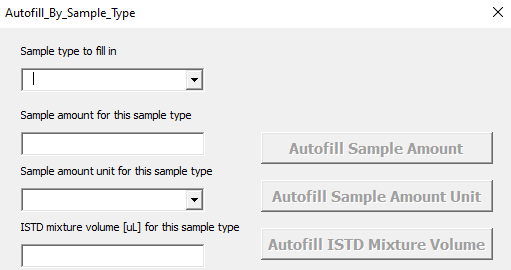


#### Steps

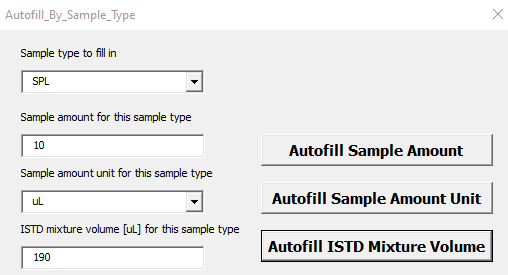
Click on the button “Autofill by Sample\_Type”



A message box will appear

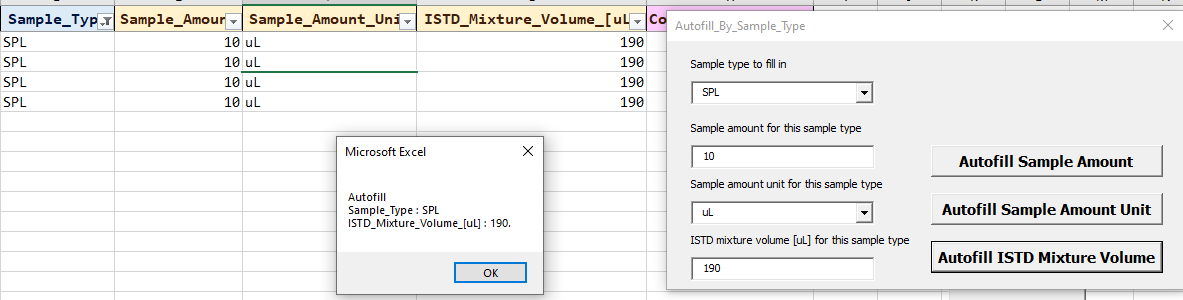


Choose the Sample type and key in the relevant values. The buttons will be unmasked. Click on the Autofill button



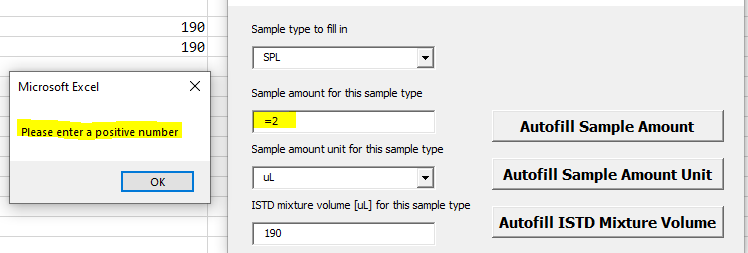
#### Expected Results

Sample\_Amount, Sample\_Amount\_Unit and ISTD\_Mixture\_Volume\_[uL] values are fill according to the input value



Ensure that

* The correct columns and Sample Type are filled with the user input values
* Invalid inputs are given a warning



## Autofill Concentration Unit

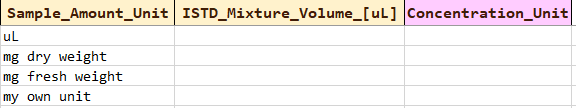
### Using the “Autofill Concentration\_Unit”

#### Requirement

None

#### Preconditions

Users key in some entries in the sheet



Users to choose an ISTD concentration unit (below case is nmol)



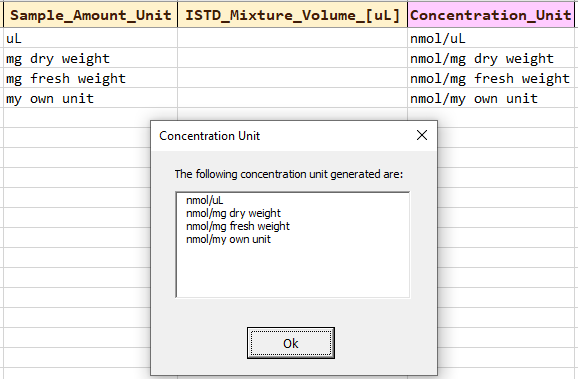
#### Steps

Click on the button “Autofill Concentration\_Unit”



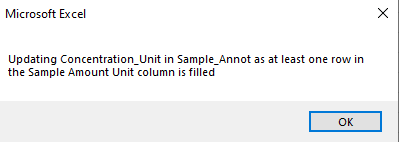
#### Expected Results

Concentration Unit is filled in



Ensure that

* Changing the ISTD concentration unit after this step with update the column. This is because the sample amount unit has been changed.



## Clearing of columns in the “Sample\_Annot” sheet

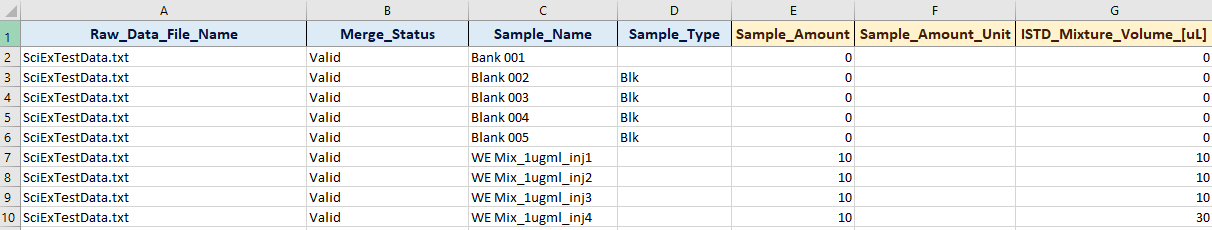
### Using the “Clear Columns” button

#### Requirements

None

#### Preconditions

Users key in some entries in the sheet

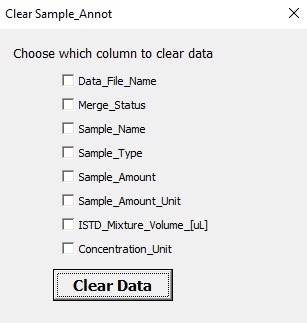


#### Steps

Click on the button “Clear Columns”



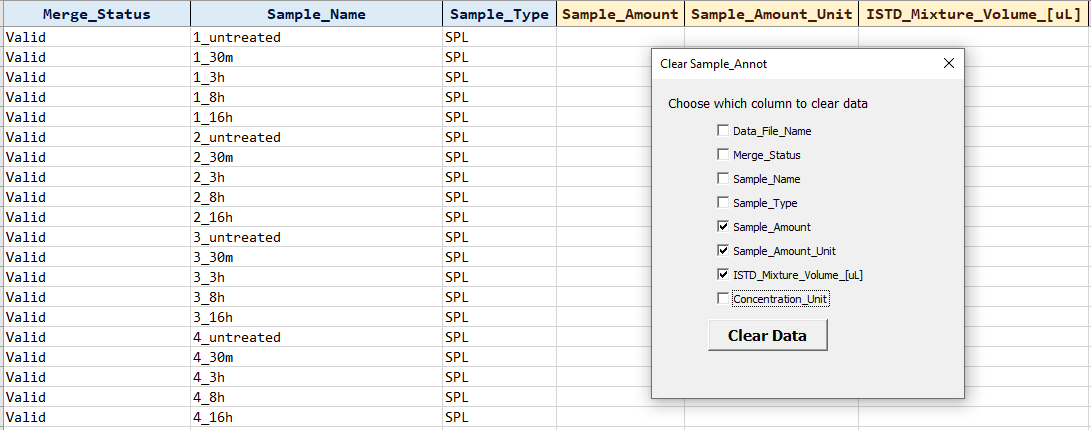
A message box will appear, asking which column to clear. Users can choose the columns by checking on the check box



When they have chosen their columns, click on “Clear Data

#### Expected Results

Data is cleared the data when the “Clear Data” button is pressed.



Ensure that

* The choices of which columns to clear are present and in the correct spelling.
* The correct columns are cleared.
* Only the contents are cleared, not the format. No cells should be deleted as well.

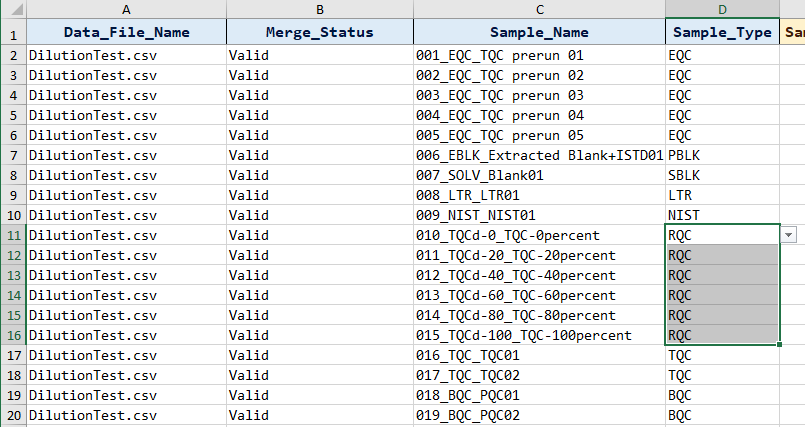
## Copying RQC Samples from “Sample\_Annot” to “Dilution\_Annot”

#### Requirements

None

#### Preconditions

Users key in some entries in the sheet. Ensure that there are some sample with Sample Type RQC



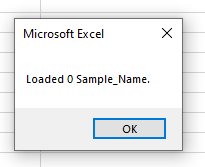
#### Steps

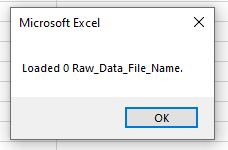
Click on the button “Load RQC Samples to Dilution\_Table”



#### Expected Results

If there is no RQC Samples, two message boxes will pop up saying

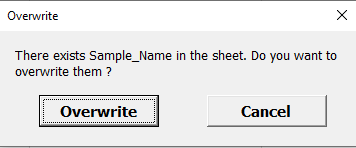
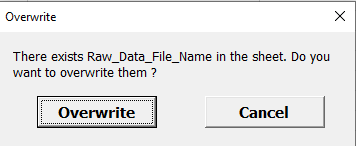




If there are RQC samples,

users will be directed unto the “Dilution\_Annot” sheet.

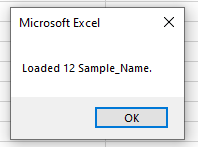
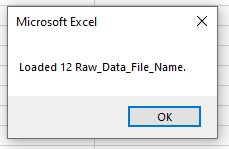
Following that, the program will check if there are existing entries in the ”Dilution\_Annot” sheet. If there is, overwrite message boxes will appear



Clicking on Cancel should cause the message box to leave and the original inputs are left alone

Clicking on Overwrite should cause the original inputs to be replaced with the most recent entries in the “Dilution\_Annot” sheet.

Message boxes will pop up saying the number of things copied unto the “Dilution\_Annot” sheet



Ensure that

* Data\_File\_Name and Sample\_Name are loaded unto the right column in the sheet
* Correction information (Only RQC samples) are copied
* Duplicate/Blank ISTD should be removed
* Replicated Sample\_Name is allowed for now.

# Part Four: Testing “Dilution\_Annot” sheet

## Clearing of columns in the “Dilution\_Annot” sheet

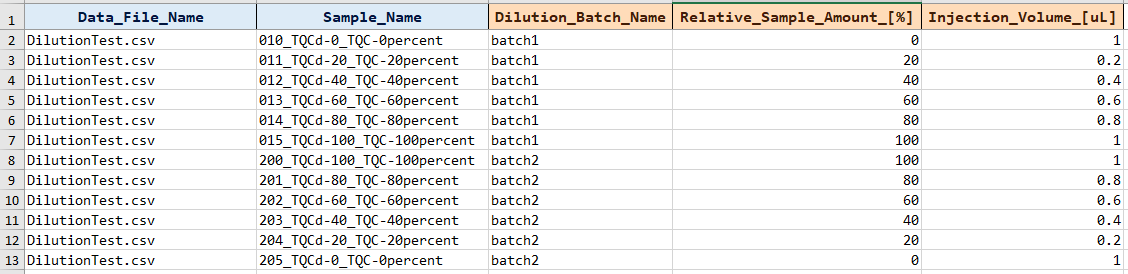
### Using the “Clear Columns” button

#### Requirements

None

#### Preconditions

Users key in some entries in the sheet

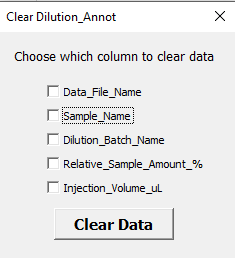


Steps

Click on the button “Clear Columns”



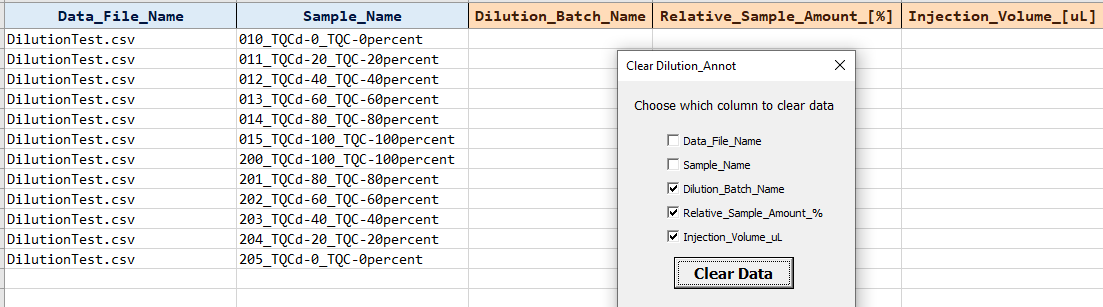
A message box will appear, asking which column to clear. Users can choose the columns by checking on the check box



When they have chosen their columns, click on “Clear Data

#### Expected Results

Data is cleared the data when the “Clear Data” button is pressed.



Ensure that

* The choices of which columns to clear are present and in the correct spelling.
* The correct columns are cleared.
* Only the contents are cleared, not the format. No cells should be deleted as well.