MSOrganiser

User Documentation

Version 0.0.2

2021

# Version Control Table

|  |  |
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| **Title** | MSOrganiser User Documentation |
| **Created By** | Jeremy John Selva |
| **Date Created** | 10 October 2018 |
| **Maintained By** | Jeremy John Selva |

|  |  |  |  |  |
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| 0.0.1 | Jeremy John | 10 October 2018 | Initial commit and review | Draft |

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# Introduction

This document highlights the functionalities of MSOrganiser

## Purpose

MSOrganiser is created to provide users a convenient way to extract and organise MRM output files from MassHunter and Quant into an Excel file in a few button clicks.

With the addition of the MS Annotation Template Creator, the software is also able to normalized the peak area with respect to the internal standard’s peak area as well as calculating the concentration of the analytes.

## Scope

This guide will assist users to use the MSOrganiser properly in SLING. The guide does not cover how to use the MS Annotation Template Creator and assumes that it was used correctly.

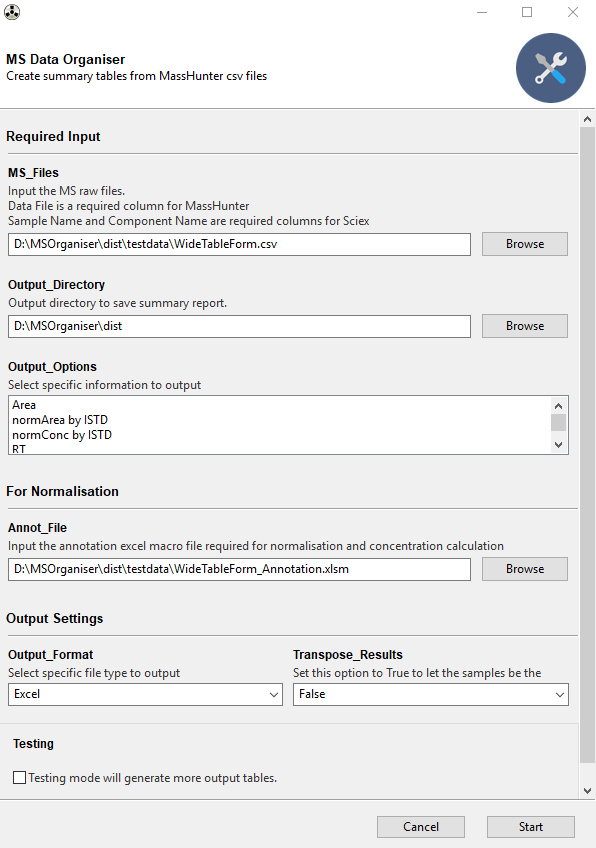
# Starting the MSOrganiser

## Starting the system

Go to the folder called MSOrganiser. Double click on MSOrganiser.exe



A successful startup will look like this



# Exporting MRM transition names data

MSOrganiser currently supports certain MRM transition names data format.

We define them as WideTable and CompoundTable form from Agilent and LongTable form from SciEx

## Compulsory Features.

Before showing how to export the MRM transition names data correctly for the program to work, we shall show the compulsory column names that the program use. You may use the below tables as a checklist.

Please note that there are also restricted column names that we advise having them removed before outputting them as text file of csv

|  |  |  |  |
| --- | --- | --- | --- |
| **MRM transition names data form** | **Compulsory column names** | | **Restricted column names** |
| **Without Qualifiers** | **With Qualifier** |
| Agilent’s WideTable form | Sample   * Data File   Compound Results   * Area | Qualifier Results   * Area | Sample   * Quantitation Message   Columns from   * ISTD Compound Methods * ISTD Compound Results |
| Agilent’s CompoundTable form | Sample   * Data File   Compound Method   * Name   Compound Results   * Area | Qualifer Method   * Transition   Qualifier Results   * Area |
| Sciex’s LongTable form | Sample Name  Component Name | Not Applicable |  |

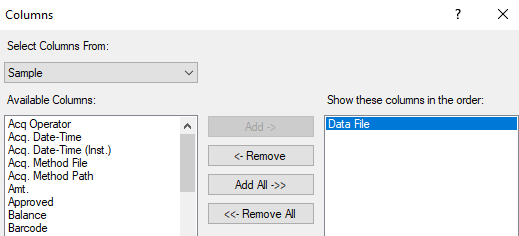
## Exporting MRM transition names data from MassHunter by Agilent

### WideTable Form

Ensure that you are viewing the MRM transition names data under “Flat Table” and “Display Multiple Compounds/Sample in Batch Table”

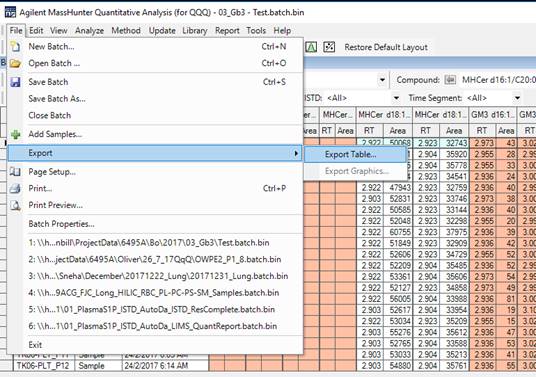
|  |  |
| --- | --- |
|  |  |

Ensure that “Data File” is present under the Sample Column.

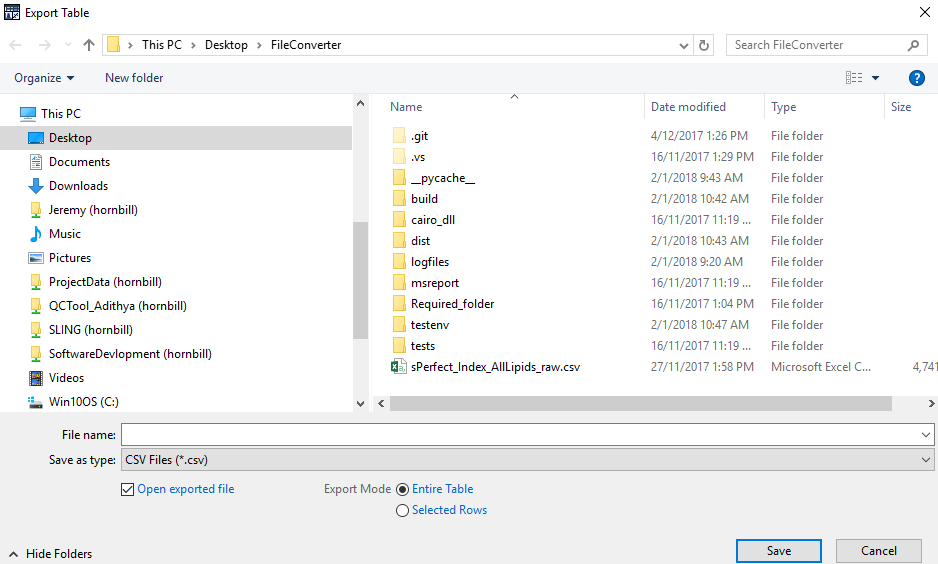




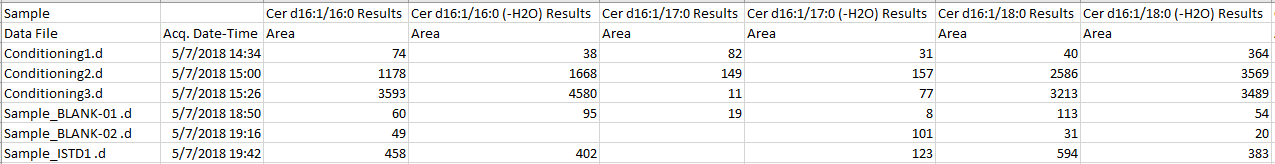
Click on File -> Export -> Export Table



Choose File type as csv



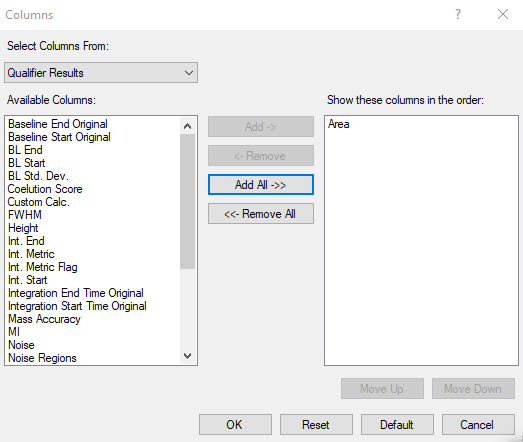
The exported raw data should look like this



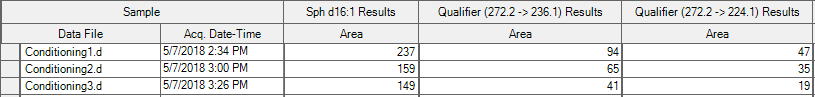
### WideTable Form with Qualifier

In addition to the conditions mentioned in the previous section,

Ensure that relevant columns from the Qualifier Results Column are selected.



To give

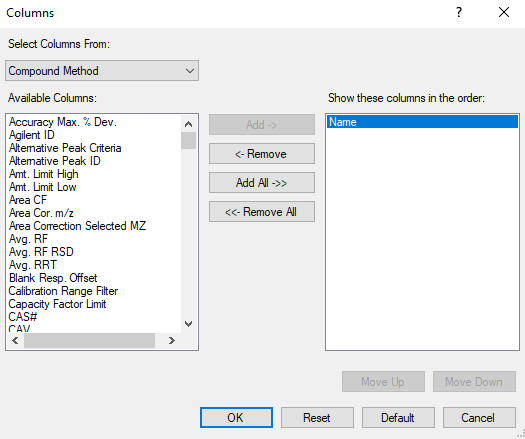


### CompoundTable Form

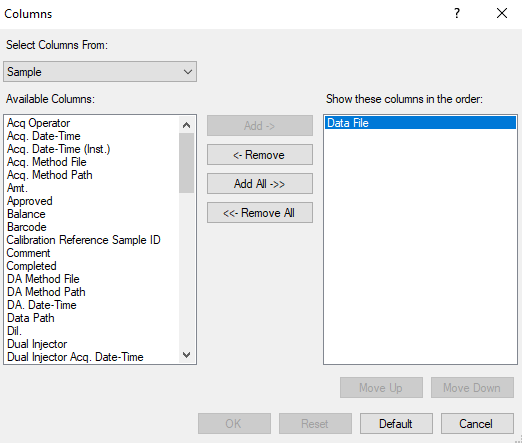
Ensure that you are viewing the MRM transition names data under “Compound Table” and “Display Multiple Compounds/Sample in Batch Table”

|  |  |
| --- | --- |
|  |  |

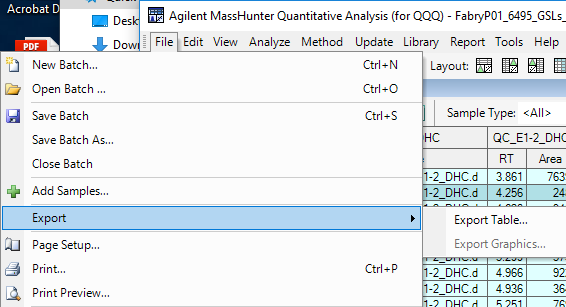
Ensure that “Name” is present under the Compound Method Column.

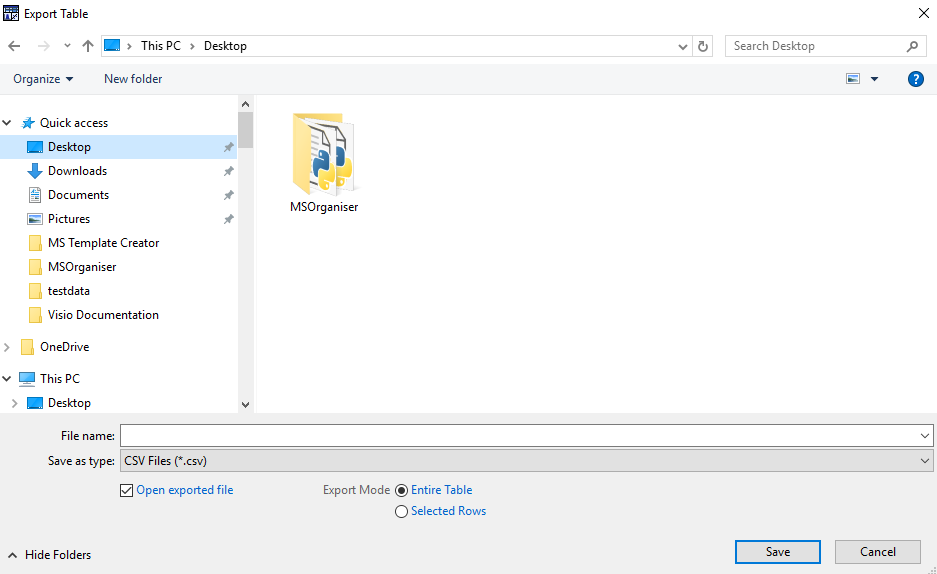
Ensure that “Data File” is present under the Sample Column.

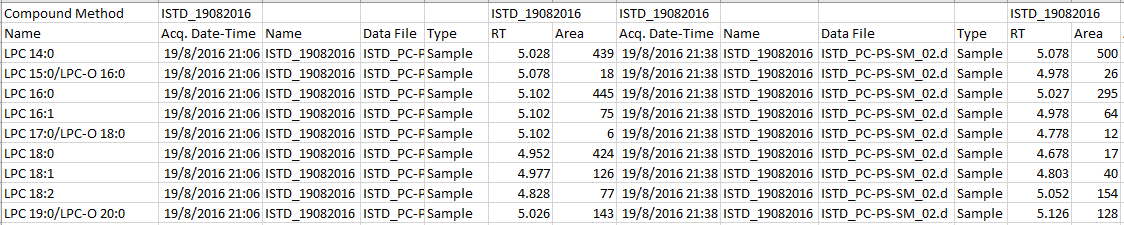
Click on File -> Export -> Export Table



Choose File type as csv



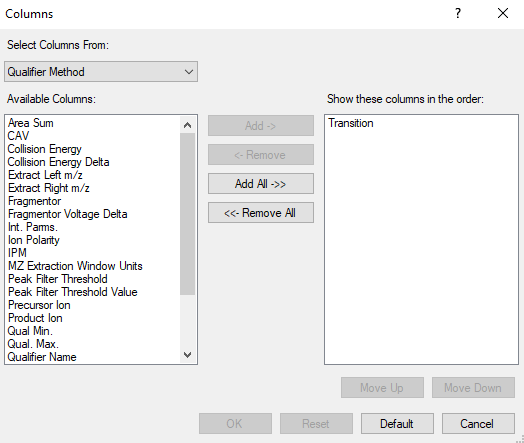
The exported raw data should look like this



### CompoundTable Form with Qualifier

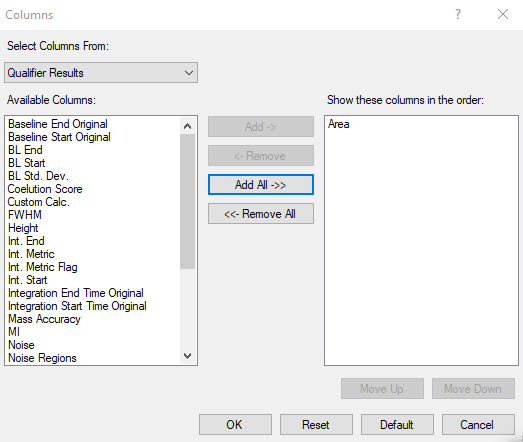
In addition to the conditions mentioned in the previous section,

Ensure that relevant “Transition” from the Qualifier Method Column is selected

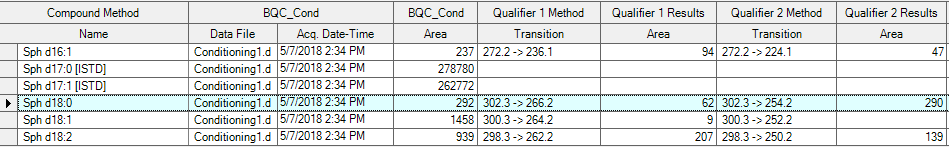
.



Ensure that relevant columns from the Qualifier Results Column are selected.



To give

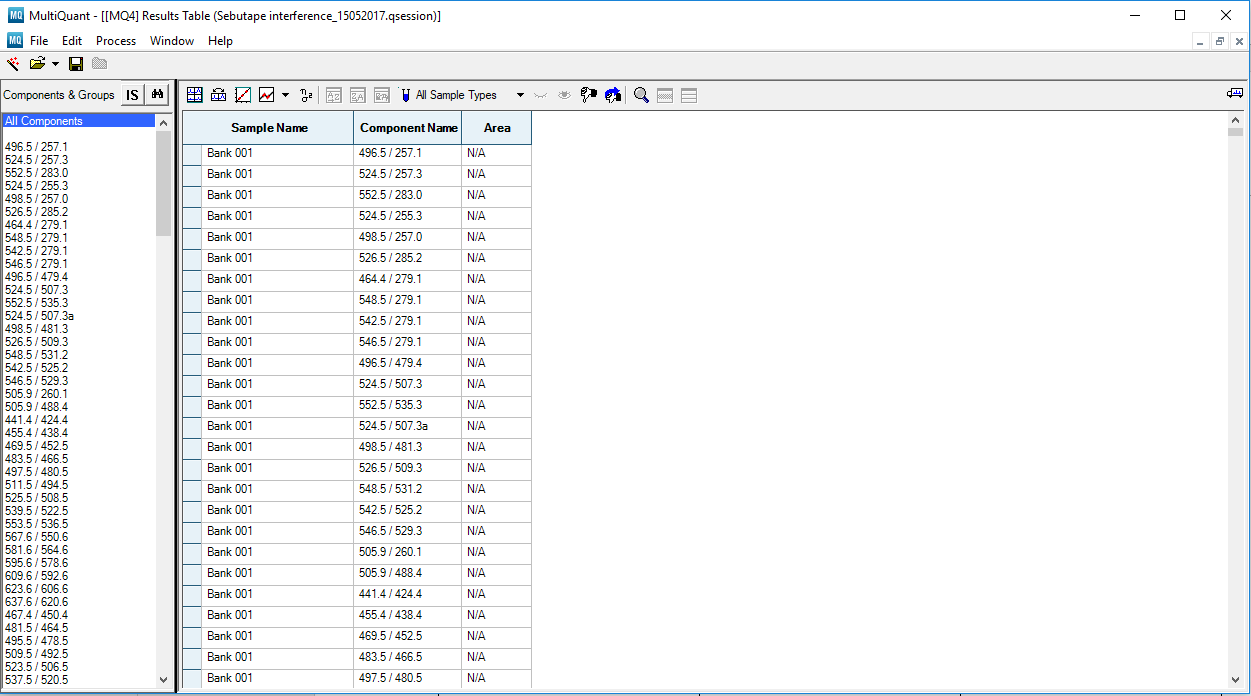


## Exporting MRM transition names data from MultiQuant by SciEx

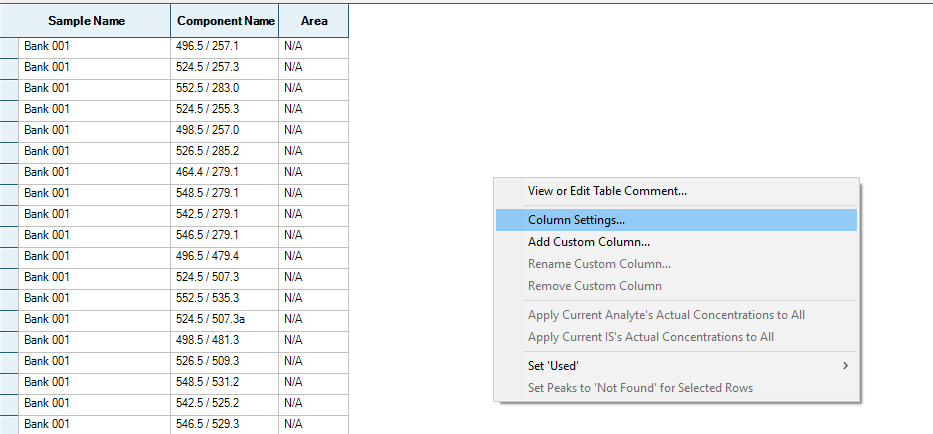
Open your MultiQuant session file, in MultiQuant



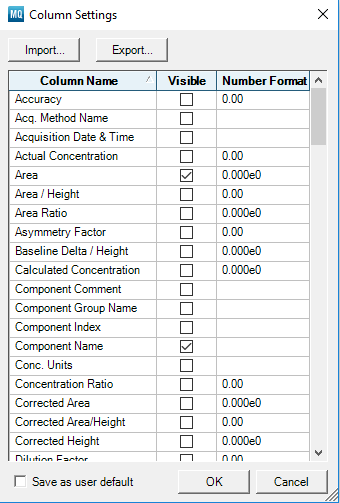
You will see this



Right click on the “Results Table”. Click on “Column Settings”



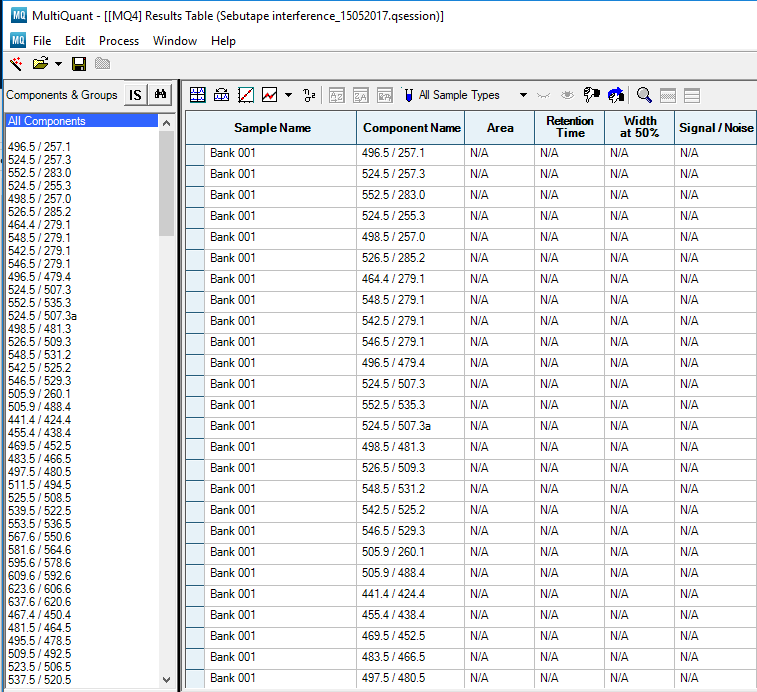
Choose your relevant columns that you wish to display in the “Results Table” and click Ok.



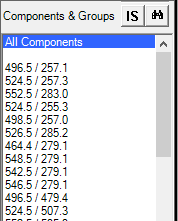
The relevant columns are as follows:

|  |
| --- |
| Compulsory Columns |
|  |
|  |
| Output Options |
|  |
|  |
|  |
|  |

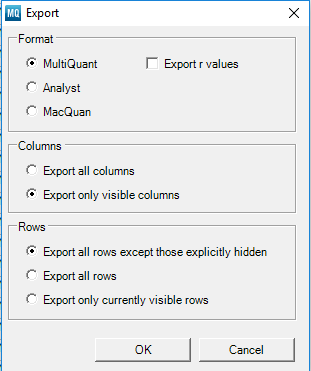
The output will look like this



To export the file correctly, make sure “All Components” is selected

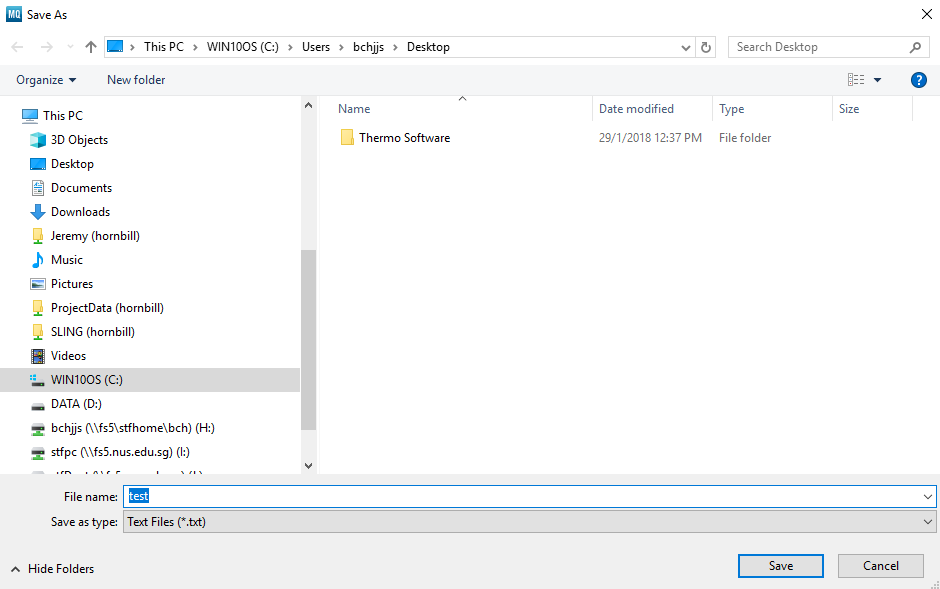


Click on File -> Export -> Results Table… You will see

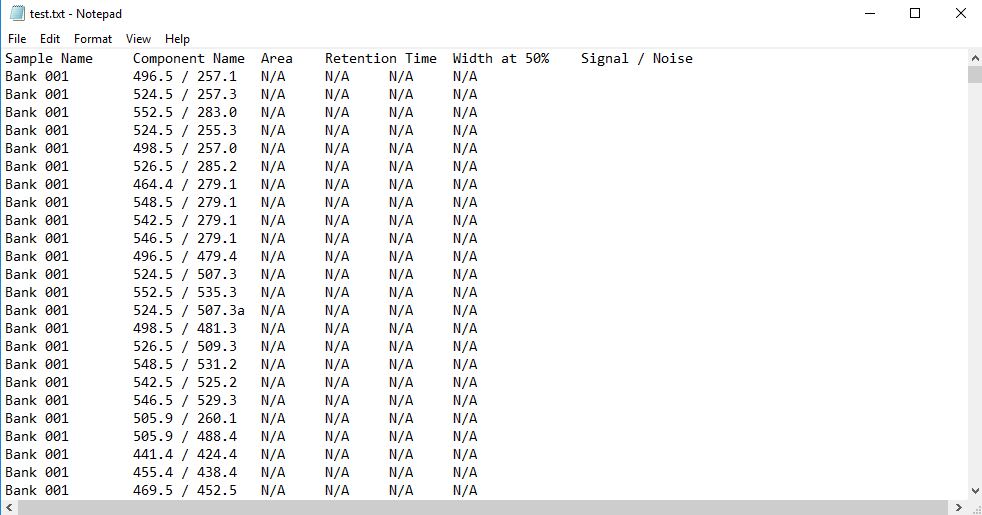


Just keep the settings the same as the above figure and click Ok.

You will now need to select the folder to output the text file. Click Save



MultiQuant will save a text file which looks like this



# Data extraction/calculation from MRM transition names data

MSOrganiser is able to extract the following information from the MRM transition name data and output as an Excel or csv file.

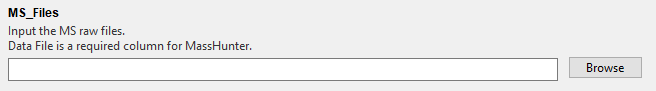
Table 4‑1: Things you can extract out from MRM transition name data

|  |  |  |
| --- | --- | --- |
| MSOrganiser Output Options | MassHunter from Agilent | Quant from SciEx |
| Area | Area | Area |
| RT | RT | Retention Time |
| FWHM | FWHM | Width at 50% |
| S/N | S/N | Signal / Noise |

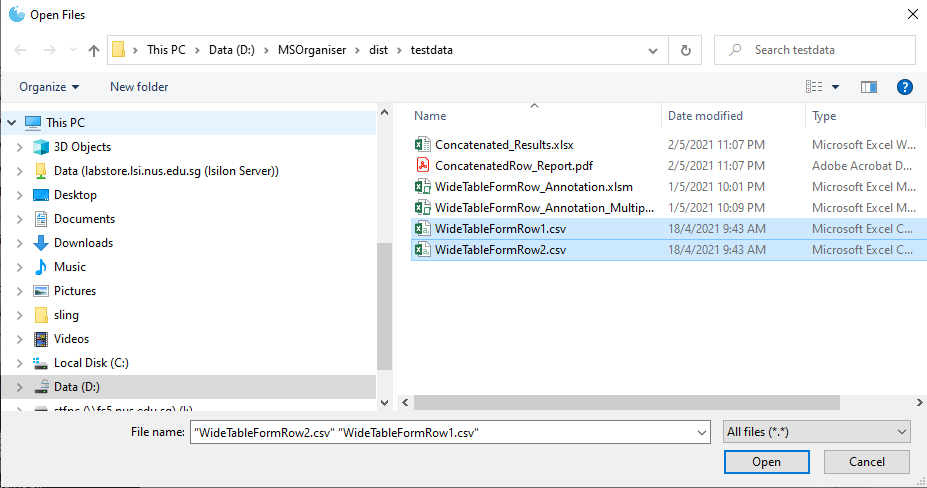
## Data Extraction Steps

Ensure that the MRM transition name data are exported properly as described in 3.

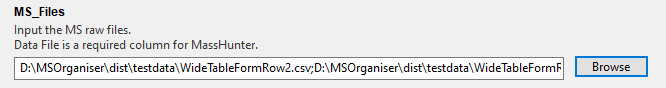
Under the MS\_Files section, click on Browse to select your input file



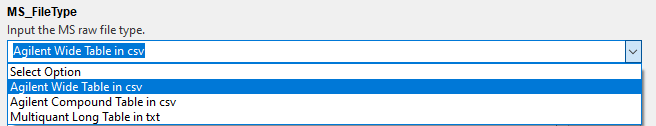
And choose the files. You may pick more than one.



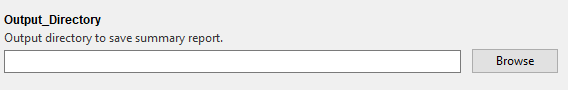
The files that you have chosen will be recorded.



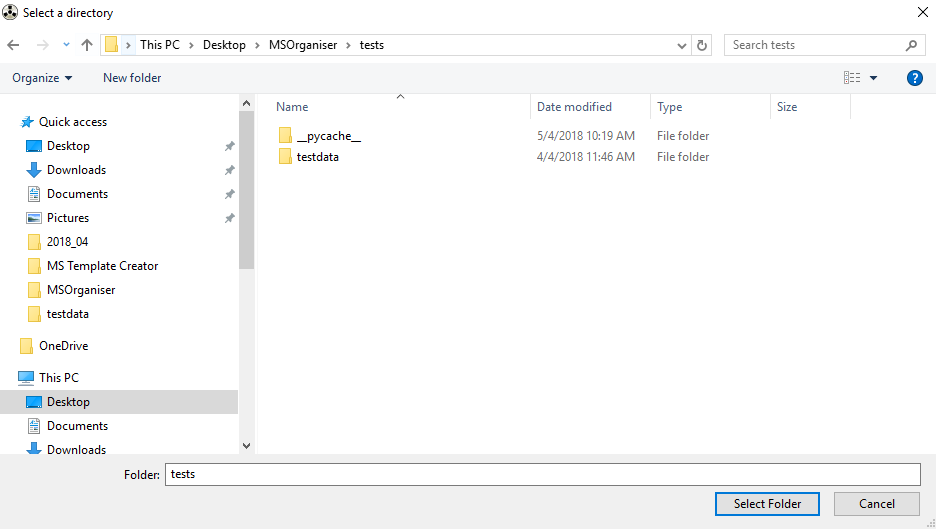
Under the MS\_FileType section, choose the input MS file type, for the above example, it is “Agilent Wide Table in csv”



Under the Output\_Directory section, click on Browse to select the folder where you wish to output your data.



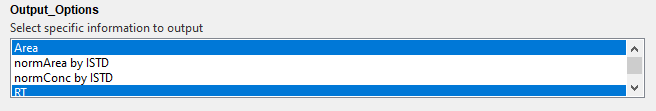
You can only select one directory

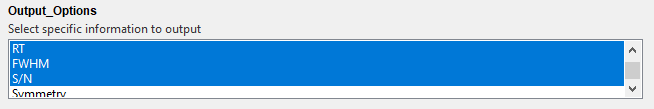


The output folder that you have chosen will be recorded.



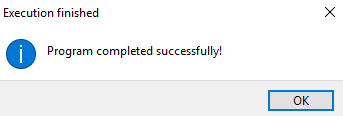
Under the Output\_Options section, click on the information that you wish to extract from your data. For the list of what kind of info can be extracted, refer to Table 4.1



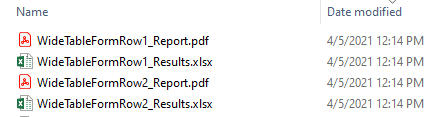


When you are done click Start.

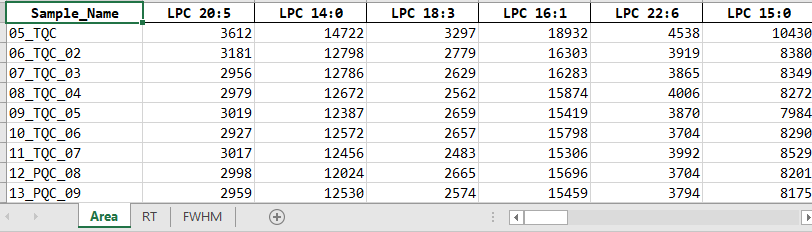
The machine will pop out this message box below when it has finished the data extraction successfully.



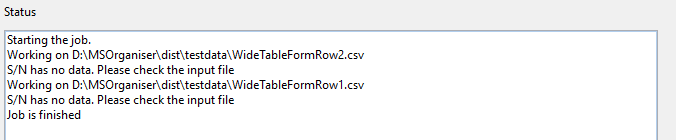
In the output folder, you will be a able to see an excel file containing the extracted data as well as a pdf file containing a report for each data set chosen earlier.



Extracted data will look like this



The machine also indicate the status of its extraction process.



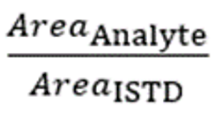
Warnings will be given out when there is something is not right with the input file.

## Data Calculation Steps

With the addition of the MS Annotation Template Creator, we are able to create additional annotation information that will allows us to do additional calculation with the MSOrganiser.

To this date, MSOrganiser can do the following calculations

Equation 4‑1: Equation for normArea by ISTD



Equation 4‑2: Equation for normConc by ISTD

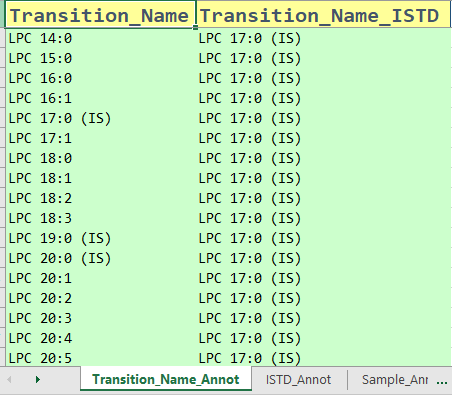


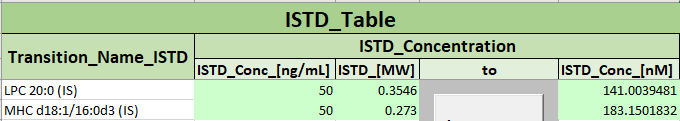
The requirements to perform these calculations are as follows:

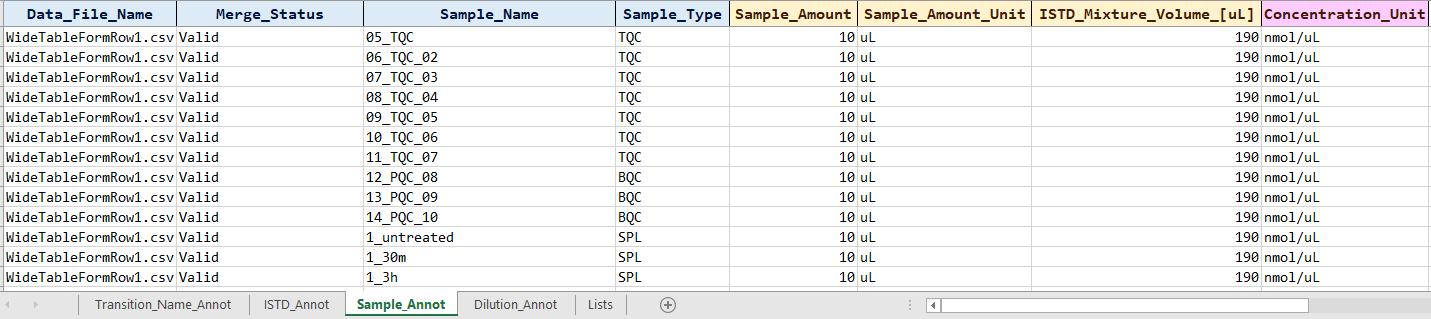
Table 4‑2: Calculation requirements

|  |  |  |
| --- | --- | --- |
| MSOrganiser Output Options | MRM transition name data requirements | MS Annotation Template Creator requirements |
| normArea by ISTD | Peak Area | Transition\_Name\_Annot sheet filled correctly |
| normConc by ISTD | Peak Area | Transition\_Name\_Annot, ISTD\_Annot and Sample\_Annot sheet filled in correctly |

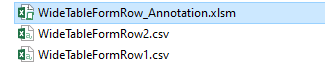
Samples of the completed sheets are as follows:





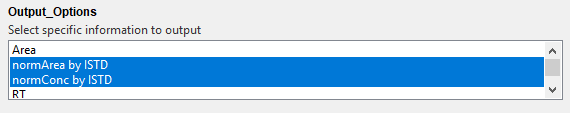


The procedures on how to fill in the sheet correctly in MS Annotation Template are not discussed here. Users can refer to the \*.xlsm file in test data set for example

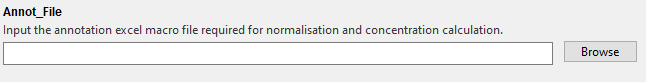


The steps are similar to 4.1 except for these additional changes

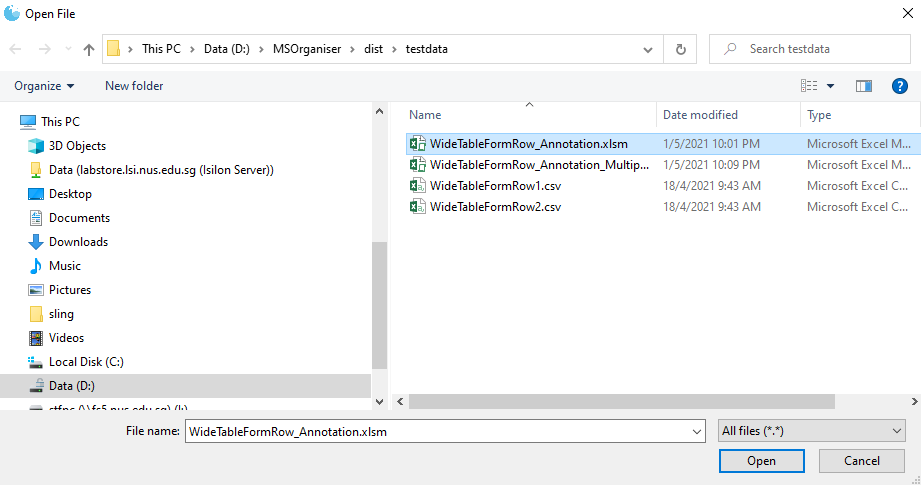
Firstly, you will need to select the output options listed in Table 4-2



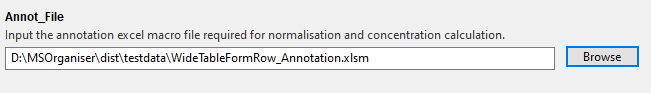
Secondly, you will need to input the MS Template Creator Excel Macro file under the Annot\_File section. Click on Browse



You can only select one Excel Macro file

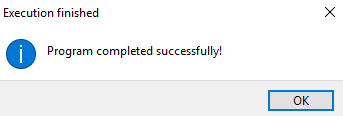


The file that you have chosen will be recorded.

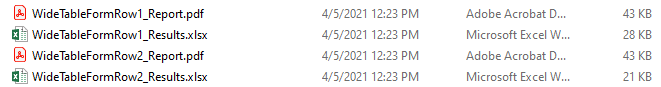


Click on Start.

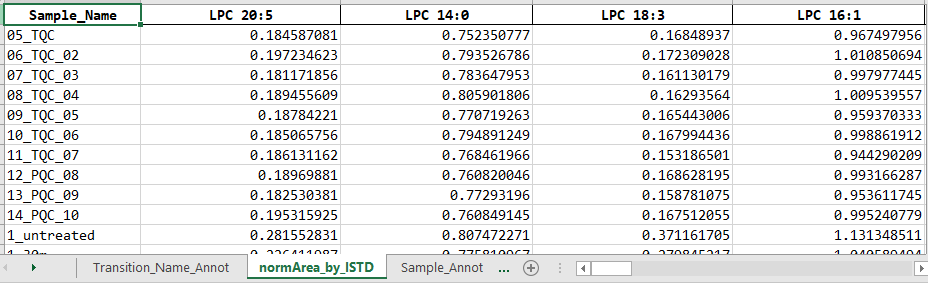
The machine will pop out this message box below when it has finished the data extraction successfully.



In the output folder, you will be a able to see an excel file containing the extracted data as well as a pdf file containing a report for each data set chosen earlier.

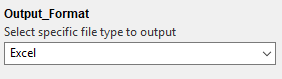


Extracted data will look like this



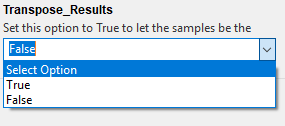
# Other Features in MSOrganiser

## Output\_Format



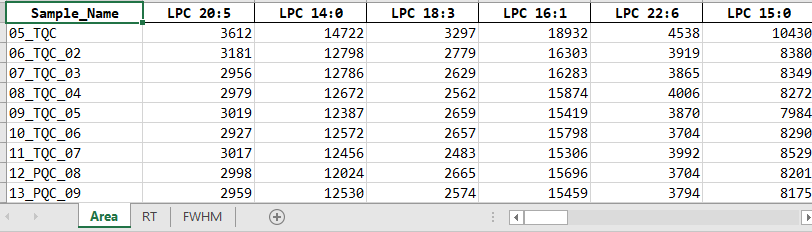
We only have two ways to output the file which is in Excel and csv.

## Transpose\_Results

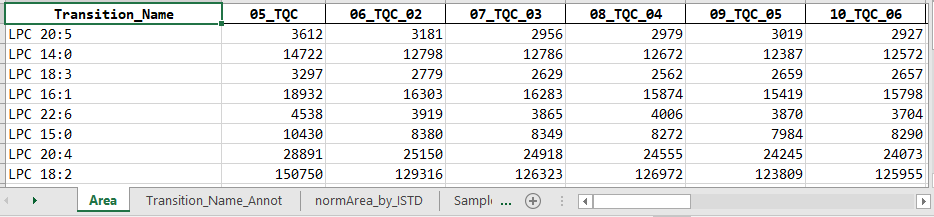


By default, this is set to False. Setting it to True will transpose your output data.

No Transpose Output

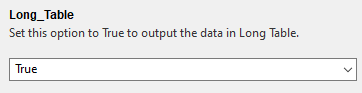


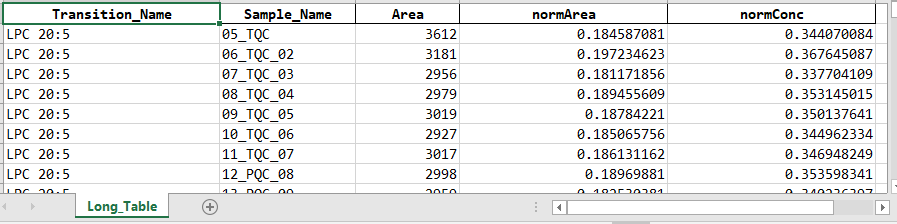
Transposed Output



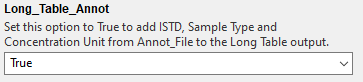
## Long Table Output

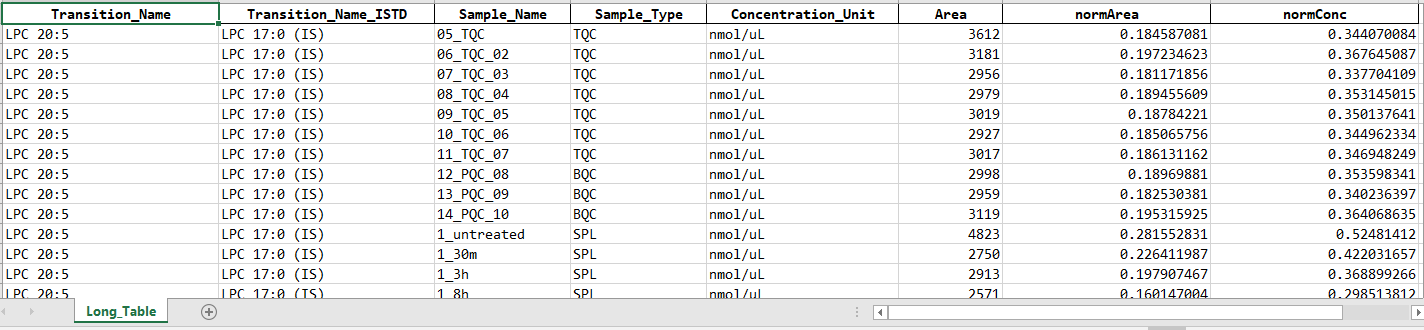
By default, results are presented in a wide table form, MSOrganiser offers the option to output the results in a long table form. Simply set “Long\_Table” to True





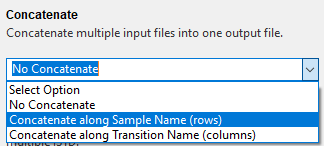
Set “Long\_Table\_Annot” to True to show some additional information



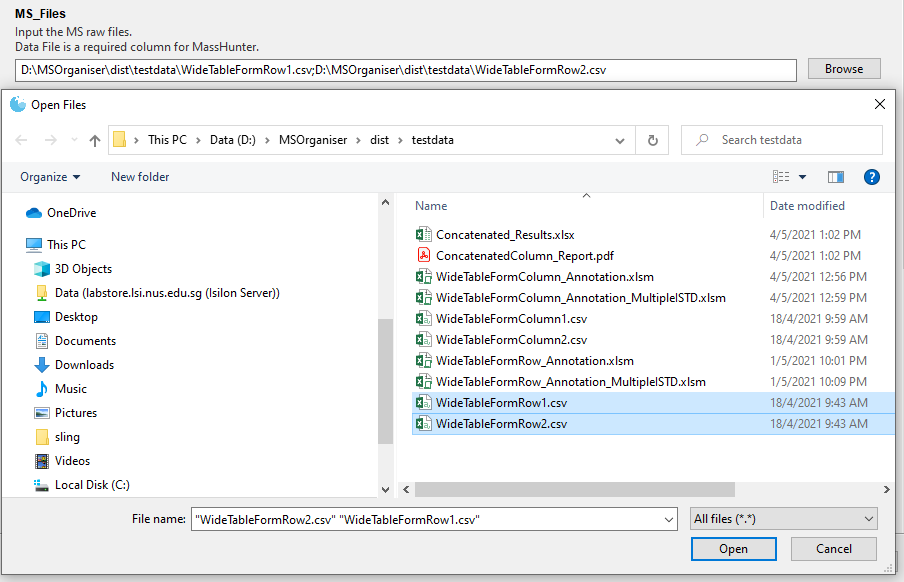


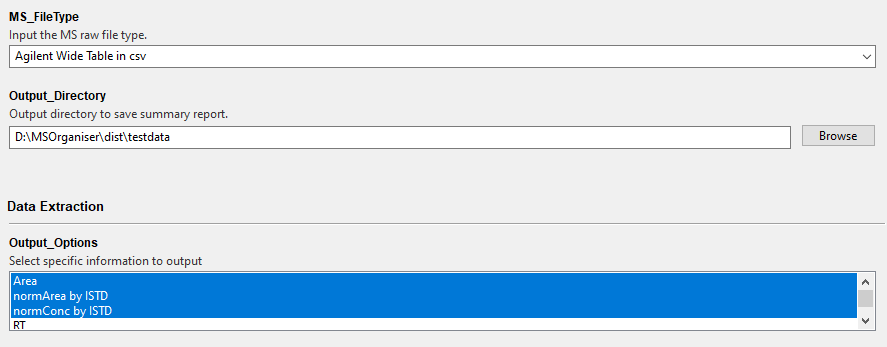
## Concatenation

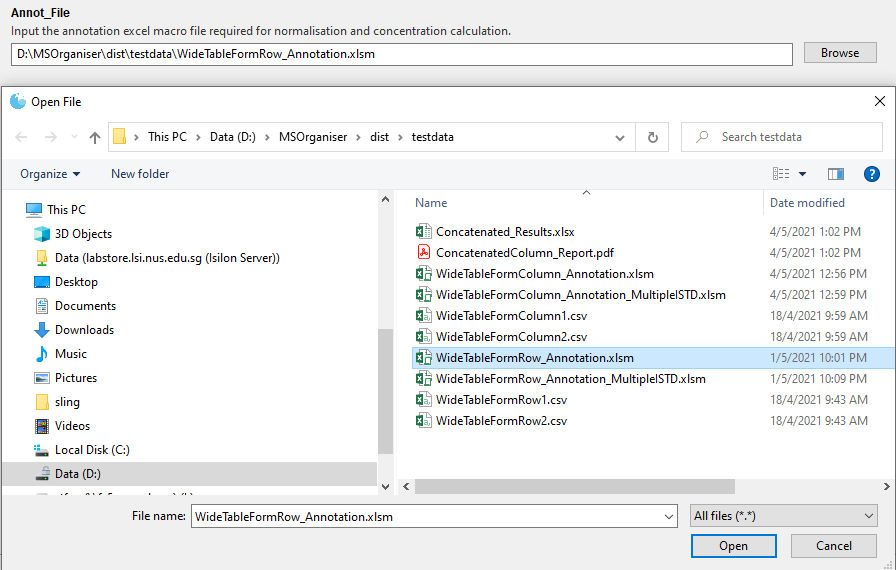
When there are several input data file with the same transitions but different sample names in each file, the results can be concatenated by setting the Concatenate settings to Concatenate along Sample Name (rows)

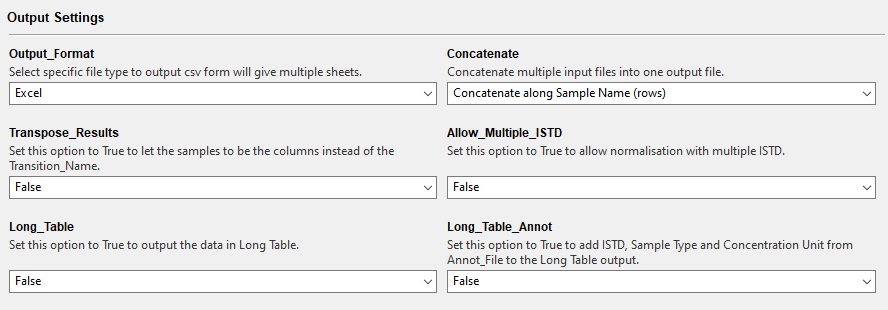


Example Input are as follows:







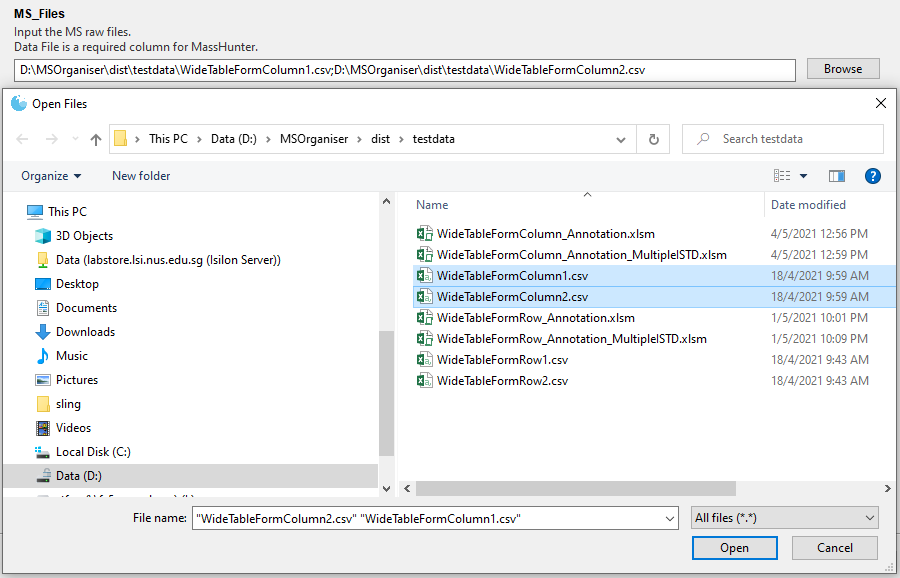


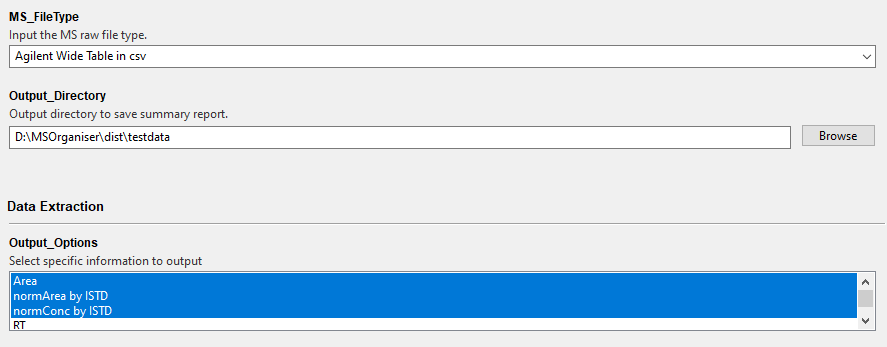
Results are as follows:

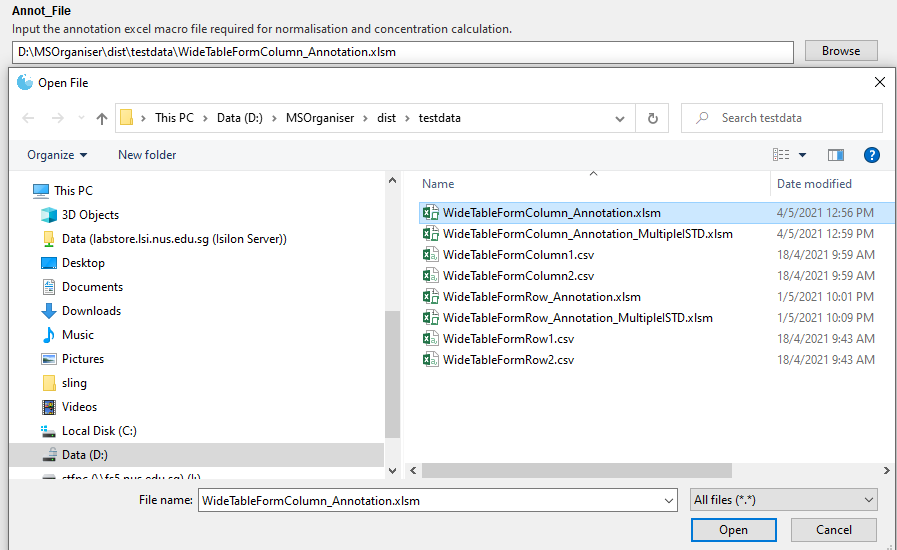


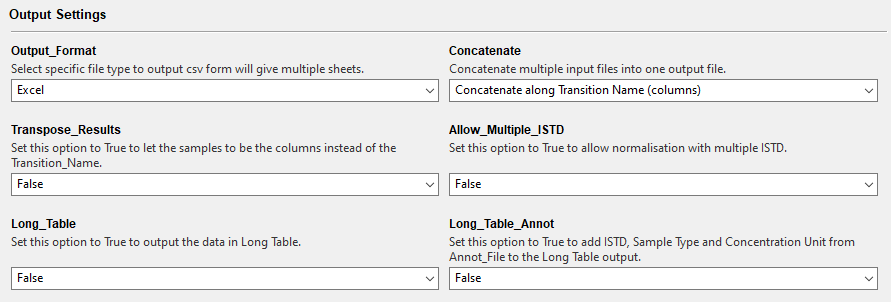
When there are several input data file with the same sample name but different transitions in each file, the results can be concatenated by setting the Concatenate settings to Concatenate along Transition Name (columns)

Example Input are as follows:







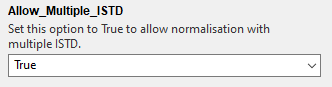


Results are as follows:

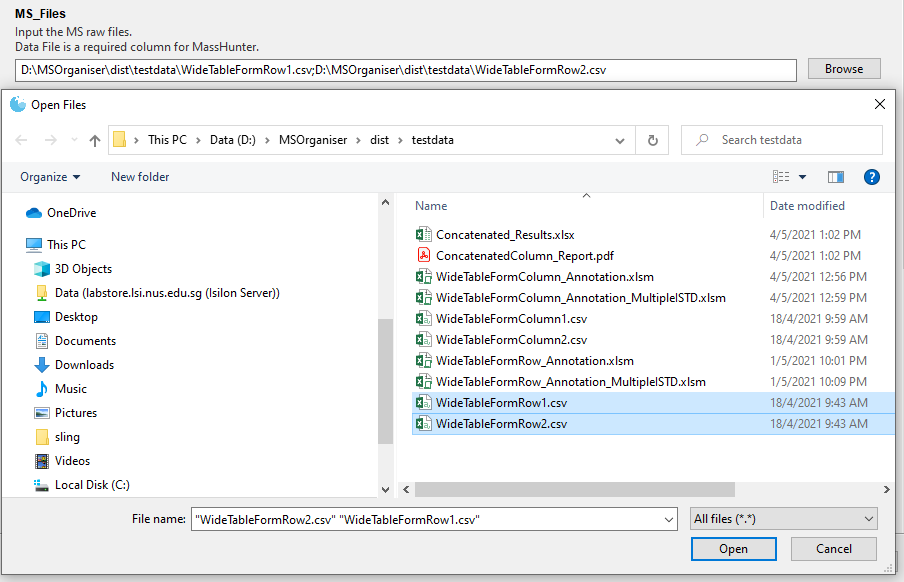


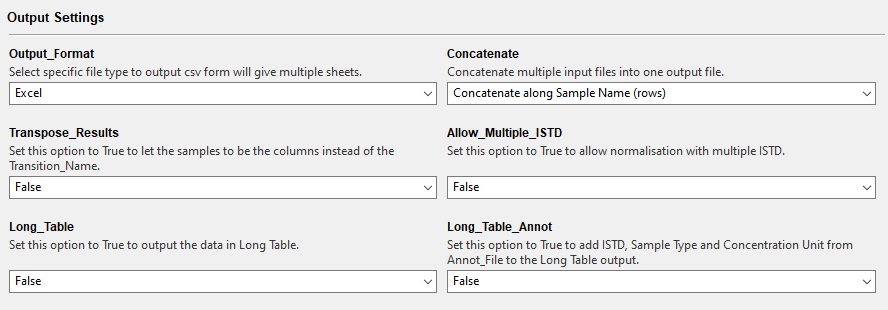
## Allow Normalisation With Multiple ISTD

By default, the software will only allow one transition to be normalised by one ISTD. However, during method development, there may be a need for one transition to be normalised by multiple ISTD to see which one is the best one to use. To relax this restriction, ensure that Allow\_Multiple\_ISTD is set to True

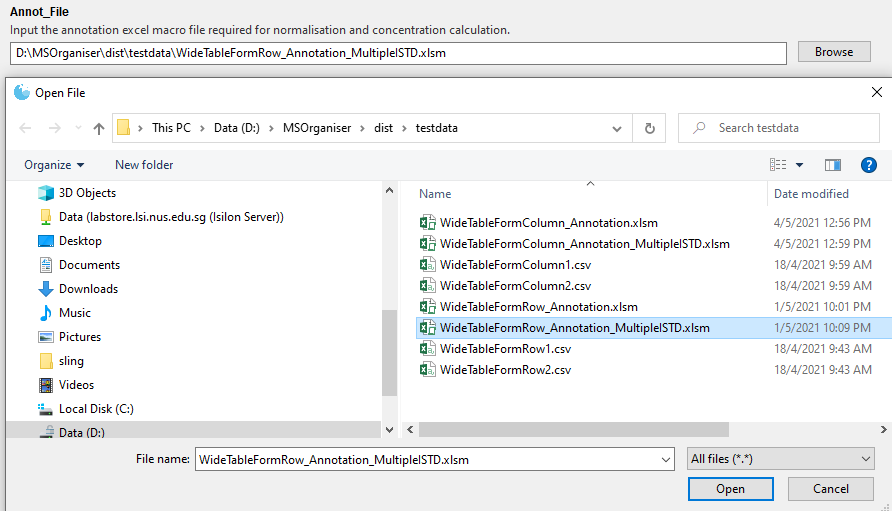


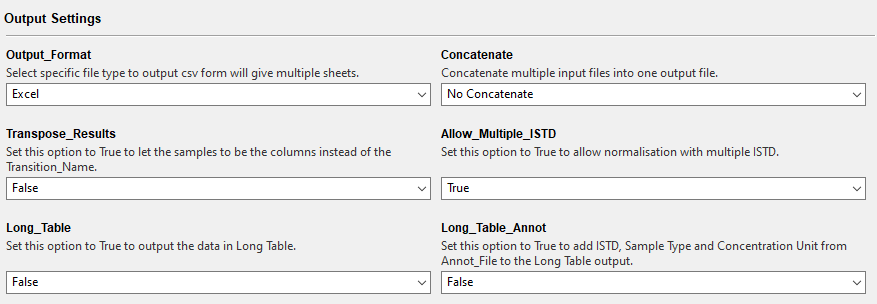
Example Input are as follows:



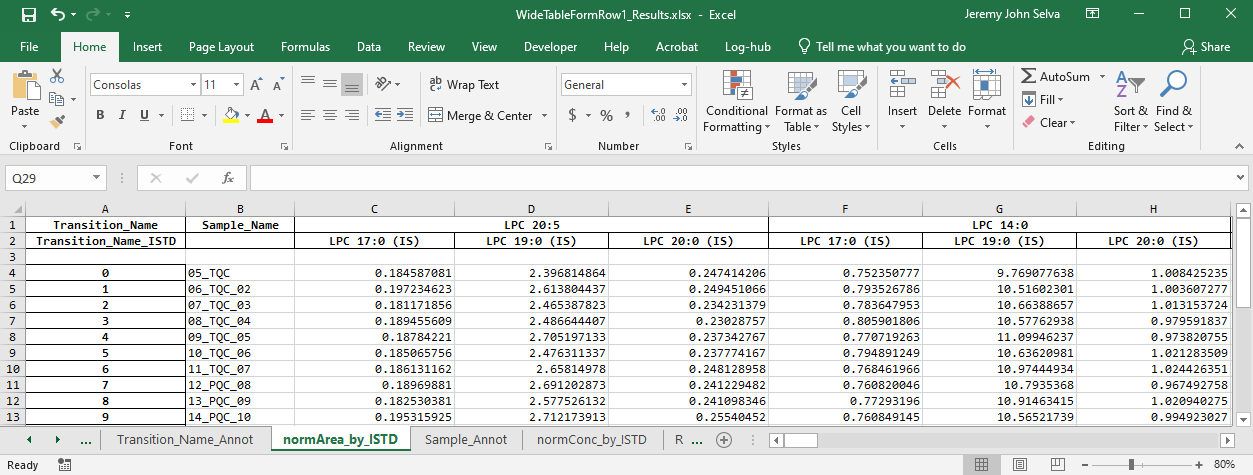


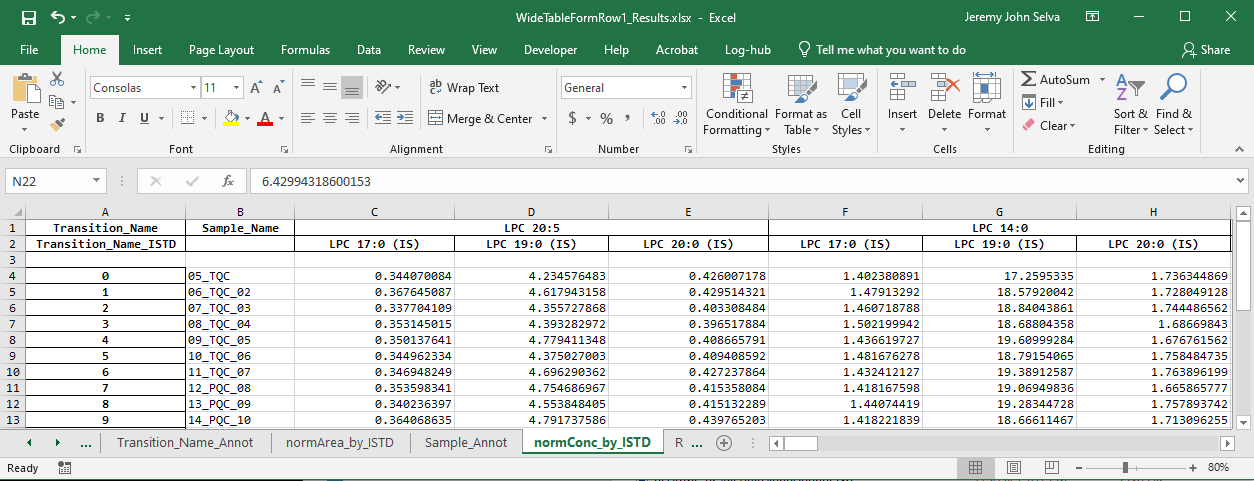
For the Annotation File, choose



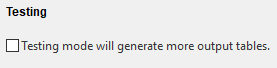


Results are as follows:





## Testing Mode



You may check this box if you wish to run the program on testing mode.

The purpose of the testing mode is to generate more output sheets to check for logical errors

By default, this is set to False and will not be saved.

## Saving your settings with a Json file

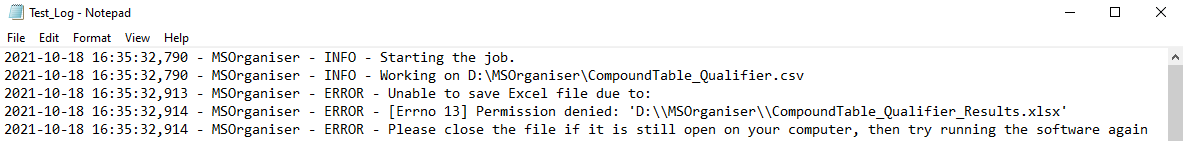
When you open MSOrganiser for a second time, you will realise that MSOrganiser is able to remember your previous settings. This is due to the presence of a json file created when the software starts to run



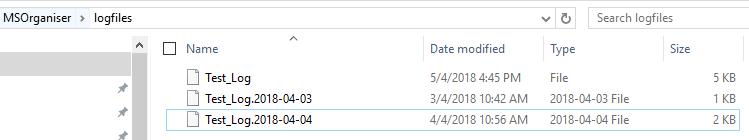
To clear your settings, just delete the json file.

## Log files

MSOrganiser also keep some log files to keep track of its work status and save any warnings that you have missed.



Currently MS Organiser is able to keep track of log files for three days.



# Errors, Warnings and Troubleshooting

MSOrganiser is able to issue some warnings and error messages when there is something wrong with the data set.

We provide the following known warnings and errors and ways to troubleshoot them.

## Parsing problems from MSOrganiser

|  |  |
| --- | --- |
| Warning/Error Messages | Troubleshooting procedures |
| Please key in at least one input MS file | Ensure that this is filled |
| Please key in at least one output directory | Ensure that this is filled |
| Please key in at least one result to output | Ensure that this is filled |
| Please key in an annotation file when ‘normArea by ISTD’ or ‘normConc by ISTD’ are selected in Output\_Options | Ensure that this is filled    when the following Output Options are selected. |
| Warning: Unable to save input settings in {file\_path} due to this error message. {error\_message} | MSOrganiser has problems trying to output the json file. Ensure that MSOrganiser is in a folder with read and write permissions. |
| Unable to create log directory in {file\_path} due to this error message. {error\_message} | MSOrganiser has problems trying to create a log directory to output its log files. Ensure that MSOrganiser is in a folder with read and write permissions. |

## Reading MRM transition names data related problems

### In General

|  |  |
| --- | --- |
| Warning/Error Messages | Troubleshooting procedures |
| Input file path {file\_path} must have a csv/txt extention | Ensure that the input file extension is csv if the MS\_FileType is Agilent Wide Table in csv or Agilent Compound Table in csv    Ensure that the input file extension is txt if the MS\_FileType is Multipquant Long Table in txt |
| Input file path {file\_path} could not be found. Please check the input file. | While the MS\_Files entry is filled with at least one file path, the software could not find the file based on the file path. Ensure that the file path is correct. |
| Input file path {file\_path} does not lead to a system file. Please check if the input file path is a system file and not a folder | While the MS\_Files entry is filled with at least one file path, the software thinks it is not a file but something else, example a directory. Ensure that the file path is correct. |
| {file\_path} is an empty file. Please check the input file | The MS\_Files has no data. Please output the MS file correctly |

### MassHunter from Agilent

|  |  |
| --- | --- |
| Output option {output\_option} is not a valid column in MassHunter or not available as a valid output for this program. | Please ensure that the Output Options are properly selected. |
| {file\_path} is missing “Sample” at first row and column in Wide Table form or missing "Compound Method" at first row and column in Compound Table form. Please check the input file | The software could not identify if the MassHunter MRM transition name data file is in the WideTable or CompoundTable form. Please output the file from MassHunter correctly. |
| {file\_path} has no column “Data File”. Please check the input file | There are two possible reasons why this can happen  The software recognises that it is a MassHunter’s MRM transition name data in the WideTable form. However, it does not have the column “Data File” containing the sample names    The software recognises that it is a MassHunter’s MRM transition name data in the CompoundTable form. However, it does not have the column “Data File” containing the sample names |
| {file\_path} has no column containing “Name” in Compound Method Table. Please check the input file | The software recognises that it is a MassHunter’s MRM transition name data in the CompoundTable form. However, it does not have the column “Name” containing the transition names |
| Unable to read csv file with the available encoders. (Or any errors related to pd.read\_csv ) | Currently, MSOrganiser uses the following encoders in order to read the csv file.  ["ANSI","ISO-8859-1","utf-8"].  This implies that Agilent Masshunter may use a different encoder to create the csv file. By right a csv file should be encoded in UTF-8…  Please send your data to the developers for testing |

### Quant from SciEx

|  |  |
| --- | --- |
| Warning/Error Messages | Troubleshooting procedures |
| {file\_path} must have Sample Name and Component Name present in the Sciex file. | The Sciex Text file is missing the “Sample Name” and the “Component Name” column. |
| {Output\_option} is not a valid column in Sciex or not available as a valid output for this program | The software finds an invalid output option. Current accepted output options are |

## Reading MS Annotation Template Creator related problems

### In General

|  |  |
| --- | --- |
| Warning/Error Messages | Troubleshooting procedures |
| Input annotation {file\_name} could not be found. Please check the input file. | The software could not find the file based on the file path provided for the Annotation file. Ensure that the file path is correct. |
| This program no longer accepts csv file as input for the annotation file. Please use the excel template file given | We do not accept csv file as an input for the Annotation File. Please use the MS Annotation Template Creator Excel Macro file. |
| Unable to read excel file {file\_path} | The input seems to be an invalid excel file which could not be read by the software. Ensure that the Annotation file is uncorrupted. |

### Transition\_Name\_Annot Sheet

|  |  |
| --- | --- |
| Sheet name {sheet\_name} does not exists. Please check the input excel file. | The MS Annotation Template Creator is missing some important sheets. Please do not modify the sheet names. |
| The input {sheet\_name} has no data. | While the sheet exists, the software realise there is no data in the excel sheet. Please check that the excel sheet template is not modified. |
| There are transition name annotations that are not associated with a transition name at row(s) {Some number}. Ensure that every annotation is associated with a Transition\_Name. | Please fill in the missing Transition Name |
| The Transition\_Name\_Annot sheet is missing the column {Some column name} | Please ensure that columns Transition\_Name and Transition\_Name\_ISTD are present in the sheet. |
| The {col\_name} in the {sheet\_name} has duplicate transition names at row {some\_number} | In the “Transition\_Name\_Annot” sheet, “Transition\_Name” column has duplicated transition name which is not allowed. Please correct the Excel sheet. |
| There are Transition\_Name\_ISTD in Transition\_Name\_Annot not mentioned in ISTD\_Annot  {List of Transition ISTD}  Check that these ISTD are in the ISTD\_Annot sheet. | The software is unable to calculate concentration correctly because though the ISTD is mentioned in the Transition\_Name\_Annot sheet, it is not highlighted in the ISTD\_Annot sheet |
| There are Transition\_Names mentioned in the Transition\_Name\_Annot sheet but have a blank Transition\_Name\_ISTD.  {List of Transition Names} | Please fill in the missing Transition Name ISTD |
| There are transitions in the input data set not mentioned in the Transition\_Name column of the Transition\_Name\_Annot sheet.  {List of Transition Names} | Ensure that all transitions are fill in the Transition\_Name\_Annot sheet. |
| There are Transition\_Names mentioned in the Transition\_Name\_Annot sheet whose Transition\_Names\_ISTD does not exists in the input dataset.  {List of Transition Names} | Ensure that all transition ISTDs are fill in the Transition\_Name\_Annot sheet can also be found in your input dataset.. |

### ISTD\_Annot Sheet

|  |  |
| --- | --- |
| Sheet name {sheet\_name} does not exists. Please check the input excel file. | The MS Annotation Template Creator is missing some important sheets. Please do not modify the sheet names. |
| Sheet ISTD\_Annot is missing the column Transition\_Name\_ISTD at position A2  Sheet ISTD\_Annot is missing the column ISTD\_Conc\_nM at position E3 | In the ISTD\_Annot sheet, the important column names could be modified or it has shifted to another cell. Please do not change the column name or shift it around. |
| Sheet ISTD\_Annot's column Custom\_Unit option  {Custom Unit Option}  is no longer accepted in MSOrganiser. Please use a later version of MSTemplate\_Creator (above 1.0.1). | An old version of MSTemplate\_Creator is used. Please use a new version. |
| Sheet ISTD\_Annot's column Custom\_Unit option { Custom Unit Option } is invalid | Please do not change the units given in the Custom Unit column. |
| Data at Transition\_Name\_ISTD column(s) in the ISTD\_Annot sheet has duplicates at row  {some\_number} | Ensure that the column Transition\_Name\_ISTD has no duplicate entries. |

### Sample\_Annot Sheet

|  |  |
| --- | --- |
| Sheet name {sheet\_name} does not exists. Please check the input excel file. | The MS Annotation Template Creator is missing some important sheets. Please do not modify the sheet names. |
| The Sample\_Annot sheet contains the column "Raw\_Data\_File\_Name". This column name is no longer accepted in MSOrganiser. Please use a later version of MSTemplate\_Creator (above 0.0.1) that uses “Data\_File\_Name" instead. | Use a later version of the MS\_Template\_creator file such that the column name “Data\_File\_Name” is used. |
| The Sample\_Annot sheet is missing the column {Some column name} | Please ensure that the relevant column names are present. |
| There are sample names that are not associated with a data file name at row(s)  {some\_number}  They will not be used during analysis.  Ensure that both columns Data\_File\_Name and Sample\_Name are filled for each sample. | Ensure that both columns Data\_File\_Name and Sample\_Name are filled for each sample. |
| There are data file names that are not associated with a sample name at row(s)  {some\_number}  They will not be used during analysis.  Ensure that both columns Data\_File\_Name and Sample\_Name are filled for each sample. | Ensure that both columns Data\_File\_Name and Sample\_Name are filled for each sample. |

## Output to Excel/csv problems

|  |  |
| --- | --- |
| Warning/Error Messages | Troubleshooting procedures |
| {Some Output\_option} has no data. Please check the input file | The software is unable to extract this output option info as it is not presence in the MRM transition name file in the first place. Please check the file and export the file correctly if this information is truly missing. |
| Unable to save Excel file due to {error\_message}  Unable to save Excel file due to {error\_message}. Please close the file if it is still open on your computer, then try running the software again | MSOrganiser has problems trying to create an excel file to output its results. Ensure that MSOrganiser is in a folder with read and write permissions. Ensure that the excel is sheet is not opened before overwriting it. |
| Unable to save Excel file due to {error\_message}. Ensure that output options give at least one non-empty data set to output into one sheet in excel | MSOrganiser has problems trying to create an excel file to output its results because the results is empty and excel cannot be creted without a worksheet. |
| Unable to write df to csv due to {error\_message} | MSOrganiser has problems trying to create a csv file to output its results. Ensure that MSOrganiser is in a folder with read and write permissions. Ensure that the excel is sheet is not opened before overwriting it. |

## Report creation problems

|  |  |
| --- | --- |
| Warning/Error Messages | Troubleshooting procedures |
| Parameters\_df is empty | This implies that there are no parameters input for the MSOrganiser to report. Ensure that these are filled |
| Cannot locate MSreport resources. It seems that the program was frozen, but resource files were not copied into directory of the executable file. Please copy `msreport` folders from gooey module directory into {resource\_dir\_path} directory. Using PyInstaller, a.datas in .spec file must be specified | This error message is copied and pasted from the Gooey package. Please ensure that all resource files are copied into resource directory path indicated. See the Developers documentation for more info on what needs to be in the resource directory. |