

origin Supplemental Material 2. Demo of macro script for multiple data process.txt

```
Attribute VB_Name = "Module1"
Sub Multiple_Samples_Same_Weight()

' Statistic_Summary_Report_Results Macro
' Macro recorded 6/24/2005 by Wei Yin Zhou

' row range
Dim rRange As Range
Dim Rng As Range
Dim Cng As Range

Dim myCol As String
Dim varAnswer As String
Dim myCol_C As String
Dim myCol_D As String
Dim myCol_A As String
Dim myCol_E As String
Dim myCol_H As String
Dim myCol_I As String
Dim myCol_J As String
Dim myCol_G As String

Dim myCol_Begin As Integer
Dim myRow_Begin As Integer
Dim myOldCol As Integer
Dim myRow_Next As Integer

Dim total rows As Integer
Dim total columns As Integer
Dim Row As Integer
Dim Column As Integer
Dim ISTD As Double
Dim totalRowsAfter As Integer
Dim lastVial As Integer
Dim StartCol As Integer
Dim CurrentVial As Integer
Dim NumCompounds As Integer
Dim NumSamples As Integer
Dim NumVials As Integer
Dim CurrentCompound As Integer
Dim CountRows As Integer
Dim Vol As Double
Dim CountNoBlankRows As Integer
Dim Ceiling As Integer
Dim Floor As Integer
Dim MeanRangeBegin As Integer
Dim MeanRangeEnd As Integer

myCol_G = "G"
myCol_C = "C"
myCol_D = "D"
myCol_A = "A"
myCol_E = "E"
myCol_H = "H"
myCol_I = "I"
myCol_J = "J"
```

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```
NumCompounds = 0
LastVial = 1
StartCol = 5
CurrentVial = 2
CurrentCompound = 2
CountRows = 0
CountNoBlankRows = 0
MeanRangeBegin = 4
MeanRangeEnd = 4
```

```
ActiveSheet.Name = "Original_Report"
```

```
' Add Sheet2, and Sheet2 is active now
ActiveSheet.Worksheets.Add
```

```
Sheet1.Range("A1:IV65536").Copy Destination:=ActiveSheet.Cells(1, 1)
```

```
ActiveSheet.Name = "Summary_Report"
```

```
' How many total rows are actually used in the worksheet
total rows = ActiveSheet.UsedRange.Rows.Count
```

```
' if column 4's value is b, f, ... then delete these values and put next column's
value into this column. This happens when do column separation, in type column,
some type is VV b, VV f, which separate to two column, and shift rest column's
values into wrong columns
```

```
For Row = 1 To total rows Step 1
    If Cells(Row, 4).Value = "b" Or Cells(Row, 4).Value = "f" Or Cells(Row, 4).Value
= "B" Or Cells(Row, 4).Value = "F" Then
        Cells(Row, 4).Value = Cells(Row, 5).Value
        Cells(Row, 5).Value = Cells(Row, 6).Value
        Cells(Row, 6).Value = Cells(Row, 7).Value
        Cells(Row, 7).Value = Cells(Row, 8).Value
        Cells(Row, 8).Value = Cells(Row, 9).Value
        Cells(Row, 9).Value = Cells(Row, 10).Value
    End If
Next Row
```

```
' Find out how many rows in Statistic Report
For Row = 1 To total rows Step 1
    If Cells(Row, 9).Value = "Height" Then
        CountRows = CountRows + 3
    Exit For
    Else
        CountRows = CountRows + 1
    End If
Next Row
```

```
' Add Sheet3, and Sheet3 will be copied for Statistic report.
ActiveSheet.Worksheets.Add
```

```
' Copy data from Summary_Report to Sheet3.
```

```
For Row = 1 To CountRows Step 1
    ActiveSheet.Cells(Row, 1) = Worksheets("Summary_Report").Cells(Row, 1).Value
    ActiveSheet.Cells(Row, 2) = Worksheets("Summary_Report").Cells(Row, 2).Value
    ActiveSheet.Cells(Row, 3) = Worksheets("Summary_Report").Cells(Row, 3).Value
    ActiveSheet.Cells(Row, 4) = Worksheets("Summary_Report").Cells(Row, 4).Value
    ActiveSheet.Cells(Row, 5) = Worksheets("Summary_Report").Cells(Row, 5).Value
    ActiveSheet.Cells(Row, 6) = Worksheets("Summary_Report").Cells(Row, 6).Value
```

```
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ActiveSheet.Cells(Row, 7) = Worksheets("Summary_Report").Cells(Row, 7).Value
ActiveSheet.Cells(Row, 8) = Worksheets("Summary_Report").Cells(Row, 8).Value
ActiveSheet.Cells(Row, 9) = Worksheets("Summary_Report").Cells(Row, 9).Value
Next Row
```

```
ActiveSheet.Name = "Statistic_Report"
```

```
' Delete peak width, type and index columns
```

```
Cells(1, myCol_J).EntireColumn.Delete
```

```
Cells(1, myCol_I).EntireColumn.Delete
```

```
Cells(1, myCol_H).EntireColumn.Delete
```

```
Cells(1, myCol_G).EntireColumn.Delete
```

```
Cells(1, myCol_E).EntireColumn.Delete
```

```
Cells(1, myCol_D).EntireColumn.Delete
```

```
Cells(1, myCol_C).EntireColumn.Delete
```

```
Cells(1, myCol_A).EntireColumn.Delete
```

```
' How many total rows are actually used in the worksheet
```

```
total rows = ActiveSheet.UsedRange.Rows.Count
```

```
' Counting backwards in For loop
```

```
For Row = total rows To 1 Step -1
```

```
    ' If in column contains blanks and ? then delete entire rows
```

```
    If Cells(Row, 2).Value = 0 Or Cells(Row, 1).Value = "Type" Or Cells(Row, 1).Value = "#"  
    Or Cells(Row, 2).Value = "File" Or Cells(Row, 2).Value = "not" Or Cells(Row, 2).Value = "S"  
    Or Cells(Row, 2).Value = "FileName" Or Cells(Row, 2).Value = "[min]"  
    Then
```

```
        Cells(Row, 1).EntireRow.Delete
```

```
    End If
```

```
Next Row
```

```
' How many samples in the sequence
```

```
NumSamples = InputBox("Please enter total number of samples in the sequence:")
```

```
' Delete first number of rows, which are just names of vials
```

```
For Row = NumSamples + 1 To 1 Step -1
```

```
    Cells(Row, 1).EntireRow.Delete
```

```
Next Row
```

```
' How many total rows are after another deletion
```

```
total rows = ActiveSheet.UsedRange.Rows.Count
```

```
' Find total number of compounds in one sample
```

```
For Row = total rows To 1 Step -1
```

```
    If Cells(Row, 2).Value = "" Or Cells(Row, 2).Value = "A" Then
```

```
        NumCompounds = NumCompounds + 1
```

```
    End If
```

```
Next Row
```

```
' If some rows are missing, then insert blank and copy to column5 for compound name  
and column6 for areas
```

```
For Row = 1 To NumCompounds Step 1
```

```
    If Cells(CurrentVial - 1, 2).Value = "" Or Cells(CurrentVial - 1, 2).Value = "A"  
    Then
```

```
        Cells(CurrentVial - 1, 5).Value = Cells(CurrentVial - 1, 1).Value
```

```
        Cells(CurrentVial - 1, 6).Value = Cells(CurrentVial - 1, 1).Value
```

```
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```

```

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For NumVials = 2 To NumSamples + 1 Step 1
  If Cells(CurrentVial, 1).Value <> NumVials - 1 Then
    Cells(CurrentVial, 1).EntireRow.Insert
    Cells(CurrentVial, 1).Value = NumVials - 1
    Cells(CurrentVial, 5).Value = Cells(CurrentVial - NumVials + 1, 1).Value
    ' Cells(CurrentVial, 6).Value = Cells(CurrentVial, 2).Value
  End If
  Cells(CurrentVial, 5).Value = Cells(CurrentVial - NumVials + 1, 1).Value
  Cells(CurrentVial, 6).Value = Cells(CurrentVial, 2).Value
  CurrentVial = CurrentVial + 1

Next NumVials

CurrentVial = CurrentVial + 5

' If compound only exist in one sample of sequence, therefore, mean and sd are 0,
and columns not exist
Else
  CurrentVial = CurrentVial - 4

  Cells(CurrentVial - 1, 5).Value = Cells(CurrentVial - 1, 1).Value
  Cells(CurrentVial - 1, 6).Value = Cells(CurrentVial - 1, 1).Value
  For NumVials = 2 To NumSamples + 1 Step 1
    If Cells(CurrentVial, 1).Value <> NumVials - 1 Then
      Cells(CurrentVial, 1).EntireRow.Insert
      Cells(CurrentVial, 1).Value = NumVials - 1
      Cells(CurrentVial, 5).Value = Cells(CurrentVial - NumVials + 1, 1).Value

    End If
    Cells(CurrentVial, 5).Value = Cells(CurrentVial - NumVials + 1, 1).Value
    Cells(CurrentVial, 6).Value = Cells(CurrentVial, 2).Value
    CurrentVial = CurrentVial + 1

  Next NumVials

  CurrentVial = CurrentVial + 5
End If

Next Row

' Add Sheet3, and Sheet3 is active now
ActiveWorkbook.Worksheets.Add

' Copy data from Processed_Report to Sheet3.
Worksheets("Stati stic_Report").Range("E1:IV65536").Copy
Destination: =ActiveSheet.Cells(1, 1)
ActiveSheet.Name = "Report"

' How many total rows are actually used in the worksheet
total rows = ActiveSheet.UsedRange.Rows.Count

' Delete mean, sd..rows, only leave Area rows
For Row = total rows To 1 Step -1

  ' If in column contains blanks and ? then delete entire rows
  If Cells(Row, 1).Value = 0 Then
    Cells(Row, 1).EntireRow.Delete
  End If
Next Row

```

origin Supplemental Material 2. Demo of macro script for multiple data process.txt  
' Sort the compound names according to column A1

```
Columns("A:C").Select  
Selection.Sort Key1:=Range("A1"), Order1:=xlAscending, Header:=xlGuess, _  
OrderCustom:=1, MatchCase:=False, Orientation:=xlTopToBottom
```

```
' Reset CurrentVial  
CurrentVial = 1  
CurrentRow = 1
```

```
' Copy to row  
For Row = 1 To NumCompounds + 1 Step 1  
    For NumVials = 1 To NumSamples + 1 Step 1  
        Cells(CurrentVial, StartCol).Value = Cells(CurrentRow, 2).Value  
        CurrentRow = CurrentRow + 1  
        CurrentVial = CurrentVial + 1  
    Next NumVials  
    StartCol = StartCol + 1  
    CurrentVial = 1  
Next Row
```

```
' delete first three columns  
Cells(1, 3).EntireColumn.Delete  
Cells(1, 2).EntireColumn.Delete  
Cells(1, 1).EntireColumn.Delete
```

```
' Concentration of internal startard  
ISTD = InputBox("Please enter the amount of internal standard (mg):")  
Vol = InputBox("Please enter the amount of your sample (ml or g):")
```

```
' Add row name, which is Area  
Cells(1, 1).Value = "Area"  
Cells(1, 1).Font.Bold = True
```

```
' Add index to first column  
For Row = 1 To NumSamples Step 1  
    Cells(Row + 1, 1).Value = Row  
Next Row
```

```
' How mant total columns are actually used in the worksheet  
total columns = ActiveSheet.UsedRange.Columns.Count
```

```
' Add columns for concentration  
Cells(1, total columns + 2).Value = "Concentration"  
Cells(1, total columns + 2).Font.Bold = True
```

```
' If blank cell or if concentraion of ISTD is 0, then concentration of compound is  
blank
```

```
For Column = total columns + 3 To 2 * total columns + 1 Step 1  
    Cells(1, Column).Value = Cells(1, CurrentCompound).Value  
    For Row = 2 To NumSamples + 1 Step 1  
        If Cells(Row, CurrentCompound).Value = "" Then  
            Cells(Row, Column).Value = ""  
        ElseIf Cells(Row, total columns).Value <> 0 Then  
            Cells(Row, Column).Value = Cells(Row, CurrentCompound).Value * ISTD /  
Cells(Row, total columns).Value / Vol  
        Else  
            Cells(Row, Column).Value = ""  
        End If  
    Next Row
```

```
CurrentCompound = CurrentCompound + 1
```

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Next Column

' Go to the Processed\_Report to process Summary Report  
Worksheets("Summary\_Report").Activate

' How many total rows are actually used in the worksheet  
total rows = ActiveSheet.UsedRange.Rows.Count

For Row = CountRows To 1 Step -1  
Cells(Row, 1).EntireRow.Delete  
Next Row

' How many total rows are actually used in the worksheet  
total rows = ActiveSheet.UsedRange.Rows.Count

' Counting backwards in For loop  
For Row = total rows To 1 Step -1  
    ' If in column contains blanks and ? then delete entire rows  
    If Cells(Row, 2).Value = "" Then  
        Cells(Row, 2).EntireRow.Delete  
    End If  
Next Row

' Set initial values to column G and H  
Cells(1, 8).Value = "Total Area"  
For NumVials = 2 To NumSamples + 1 Step 1  
    Cells(NumVials, 7).Value = NumVials  
    Cells(NumVials, 8).Value = 0  
Next NumVials

NumVials = 1

' Calculate total areas for each sample then put to column G and H  
For Row = 1 To total rows Step 1  
    If Cells(Row, 2).Value = 0 Then  
        NumVials = NumVials + 1  
        Elseif Cells(Row, 4).Value = "-" Then  
    Else  
        Cells(NumVials, 8).Value = Cells(NumVials, 8).Value + Cells(Row, 4).Value  
    End If

Next Row

' Copy total areas for each sample to Final Report sheets  
For Row = 1 To NumSamples + 1 Step 1  
    Worksheets("Report").Cells(Row, 2 \* total columns + 3).Value =  
ActiveSheet.Cells(Row, 8)  
Next Row

' Activate Final\_Report and calculate real total areas for each samples, which should  
subtract 1STD  
Worksheets("Report").Activate

Cells(1, 2 \* total columns + 4).Value = "Real TArea"

For Row = 2 To NumSamples + 1 Step 1  
    Cells(Row, 2 \* total columns + 4).Value = Cells(Row, 2 \* total columns + 3).Value  
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- Cells(Row, total columns). Value  
Next Row

```
' Add columns for concentration  
Cells(1, 2 * total columns + 6). Value = "% Area"  
Cells(1, 2 * total columns + 6). Font.Bold = True
```

```
CurrentCompound = 2
```

```
For Column = 2 * total columns + 7 To 3 * total columns + 5 Step 1  
  Cells(1, Column). Value = Cells(1, CurrentCompound). Value  
  For Row = 2 To NumSamples + 1 Step 1  
    If (Cells(Row, CurrentCompound). Value) = "" Then  
      Cells(Row, Column). Value = ""  
    Else  
      Cells(Row, Column). Value = 100 * Cells(Row, CurrentCompound). Value /  
Cells(Row, 2 * total columns + 4). Value  
    End If  
  Next Row
```

```
  CurrentCompound = CurrentCompound + 1  
Next Column
```

```
' Now do the error checking.
```

```
' First ask user to input the range of the rows he/she wants to average. It should  
exclude hexane and 462 from mean
```

```
MeanRangeBegin = InputBox("Now we want to computer average area value for a  
particular compound. Please enter start row number you want to average:")  
MeanRangeEnd = InputBox("Please enter end row number you want to average:")
```

```
' Set initial values for mean row to zero
```

```
For Column = 2 To total columns Step 1  
  Cells(NumSamples + 2, Column). Value = 0  
Next Column
```

```
Cells(NumSamples + 2, 1). Value = "Mean"
```

```
' Calculate mean for area
```

```
For Column = 2 To total columns Step 1
```

```
  ' Total for each column, if blank, not count in total and mean  
  For Row = MeanRangeBegin To MeanRangeEnd
```

```
    If Cells(Row, Column). Value = "" Then
```

```
    Else
```

```
      Cells(NumSamples + 2, Column). Value = Cells(NumSamples + 2, Column). Value  
+ Cells(Row, Column). Value  
      CountNoBlankRows = CountNoBlankRows + 1
```

```
    End If
```

```
  Next Row
```

```
  ' Check if CountNoBlankRows is 0. If is, it means that this kind of compound in  
the sequence are all zeros.
```

```
  If CountNoBlankRows = 0 Then  
    Cells(NumSamples + 2, Column). Value = 0
```

```
  Else
```

```
    ' Mean for each column
```

```

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Cells(NumSamples + 2, Column).Value = Cells(NumSamples + 2, Column).Value /
CountNoBlankRows

```

```

' Reset CountNoBlankRows to zero
CountNoBlankRows = 0

```

```
End If
```

```
Next Column
```

```
' Compare area of each column's value with its average, if it below average, then put
yellow marker as flag
```

```
Ceiling = InputBox("Compare area of each cell's value with its compound average, if
it above or below the product of threshold and average, then put blue marker as
flag. Please enter high threshold, if enter 3, it means 3 times of average value
for a compound in sequence samples:")
```

```
Floor = InputBox("Please enter low threshold, if enter 0.2, it means 20% of average
value for a compound in sequence samples:")
```

```
For Column = 2 To total columns Step 1
```

```
For Row = MeanRangeBegin To MeanRangeEnd
```

```
If Cells(Row, Column).Value < 0.3 * Cells(NumSamples + 2, Column).Value Or
Cells(Row, Column).Value > 3 * Cells(NumSamples + 2, Column).Value Then
```

```
Cells(Row, Column).Interior.ColorIndex = 34
```

```
End If
```

```
Next Row
```

```
Next Column
```

```
' Compare B1: 18: 1n9 and B2: 18: 1n7, 18: 1n9 should always bigger than 18: 1n7. If not,
then either both peaks are exchange the identification or 18: 1n7 did not identified.
If that happend, put yellow marks as flag on these cells
```

```
' For Column = 2 To total columns Step 1
```

```
' If Cells(1, Column).Value = "B1: 18: 1n9" Then
```

```
' Find right column, ready to compare two columns
```

```
' For Row = 2 To NumSamples + 1
```

```
' If Cells(Row, Column).Value < Cells(Row, Column + 1).Value Then
```

```
Cells(Row, Column).Interior.ColorIndex = 36
```

```
Cells(Row, Column + 1).Interior.ColorIndex = 36
```

```
' End If
```

```
' Next Row
```

```
' Exit For
```

```
' End If
```

```
' Next Column
```

```
' Add Sheet5, and Sheet5 is active now
```

```
ActiveWorkbook.Worksheets.Add
```

```
Worksheets("Report").Range("A1:IV65536").Copy Destination:=ActiveSheet.Cells(1, 1)
```

```
ActiveSheet.Name = "Final_Report"
```

```
End Sub
```