

Software: excel as the vision of 2016

Funktion: this macro links the m/z values of MALDI-IMS with m/z values of LC-MS/MS and present identified peptides for MALDI-IMS data.

Sub MH()

Application.ScreenUpdating = False

Application.AskToUpdateLinks = False

Application.EnableEvents = False

Application.DisplayAlerts = False

Dim crr

Dim drr

Dim dic(1 To 3)

For i = 1 To UBound(dic)

Set dic(i) =

CreateObject("scripting.dictionary")

Next

With ThisWorkbook.Worksheets("MH")

lr = .Range("A"

& .Rows.Count).End(xlUp).Row

lc

= .Cells(1, .Columns.Count).End(xlToLeft).Column

.[a1].Resize(lr, 1).Value = .[a1].Resize(lr, 1).Value

.[a1].Resize(lr, lc).Sort key1:=.[a1], order1:=1, Header:=xlYes

arr = .[a1].Resize(lr, lc)

For i = 2 To lr

arr(i, 2) = Val(Split(arr(i, 2), " ")(0))

temp_k = "A" & (arr(i, 1) * 10 ^ 12)

temp_v = .Cells(i, 1).Resize(1, 7)

If i = 52 Then

Debug.Print i

End If

If dic(1).exists(temp_k) = False Then

dic(1)(temp_k) = arr(i, 2)

dic(2)(temp_k) = temp_v

dic(3)(temp_k) = 1

Else

If dic(1)(temp_k) < arr(i, 2) Then

dic(1)(temp_k) = arr(i, 2)

dic(2)(temp_k) = temp_v

dic(3)(temp_k) = 1

ElseIf dic(1)(temp_k) = arr(i, 2) Then

dic(3)(temp_k) = dic(3)(temp_k) + 1

ReDim drr(1 To dic(3)(temp_k), 1 To

7)

For m = 1 To 7

drr(UBound(drr), m) = temp_v(1,

m)

Next

temp_v = dic(2)(temp_k)

For m = 1 To UBound(drr) - 1

For n = 1 To UBound(drr, 2)

drr(m, n) = temp_v(m, n)

Next

Next

dic(2)(temp_k) = drr

Erase drr

End If

End If

Next

End With

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With ThisWorkbook.Worksheets("MZ")

    lr = .Range("A"
& .Rows.Count).End(xlUp).Row

    lc
= .Cells(1, .Columns.Count).End(xlToLeft).Colu
mn

    brr = .[a1].Resize(lr, lc + 1)

    brr(1, lc + 1) = "FZ"

    For i = 2 To lr

        brr(i, lc + 1) = Split(brr(i, 1), " ")(0)

    Next

    .[a1].Resize(lr, lc).NumberFormatLocal = "@"

    .[a1].Resize(lr, lc + 1) = brr

    .[a1].Resize(lr, lc + 1).Sort key1:=.Cells(1, lc +
1), order1:=1, Header:=xlYes

    .Range("A:A").Offset(, lc).Clear

    brr = .[a1].Resize(lr, lc)

    For i = 2 To lr

        brr(i, 1) = Val(Split(brr(i, 1), " ")(0))

    Next

End With

ReDim crr(1 To UBound(brr) * 100, 1 To
UBound(arr, 2) + UBound(brr, 2))

k2 = dic(2).keys

For i = 0 To UBound(k2)

    k2(i) = --Replace(k2(i), "A", "")

Next

t = 1

For i = 1 To UBound(brr, 2)

    crr(t, i) = brr(1, i)

Next

For i = UBound(brr, 2) + 1 To UBound(crr, 2)

    crr(t, i) = arr(1, i - UBound(brr, 2))

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Next

For j = 1 To dic(2).Count

    If Abs(arr(2, 1) - k2(j - 1) / 10 ^ 12) < 1 Then

        flag = j

    Exit For

End If

Next

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For i = 2 To UBound(brr)

    t1 = t

    For j = flag To 1 Step -1

        If brr(i, 1) - k2(j - 1) / 10 ^ 12 < 1 Then

            If Abs(brr(i, 1) - k2(j - 1) / 10 ^ 12) < 1
Then

                For m = 1 To dic(3)("A" & k2(j - 1))

                    t = t + 1

                    For l = 1 To UBound(brr, 2)

                        crr(t, l) = brr(i, l)

                    Next

                    temp_v = dic(2)("A" & k2(j - 1))

                    For l = UBound(brr, 2) + 1 To
UBound(crr, 2)

                        crr(t, l) = temp_v(m, l -
UBound(brr, 2))

                    Next

                Next

            End If

        Else

            Exit For

        End If

    Next

Next

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For j = flag + 1 To dic(2).Count
    If k2(j - 1) / 10 ^ 12 - brr(i, 1) < 1 Then
        If Abs(brr(i, 1) - k2(j - 1) / 10 ^ 12) < 1
Then
            t = t + 1
            For l = 1 To UBound(brr, 2)
                crr(t, l) = brr(i, l)
            Next
            temp_v = dic(2)("A" & k2(j - 1))
            For l = UBound(brr, 2) + 1 To
UBound(crr, 2)
                crr(t, l) = temp_v(1, l - UBound(brr,
2))
            Next
        End If
    Else
        flag = j
    Exit For

    End If
Next
If t1 = t Then
    t = t + 1
    For l = 1 To UBound(brr, 2)
        crr(t, l) = brr(i, l)
    Next
End If

Next

With ThisWorkbook.Worksheets("RS")
    .UsedRange.Clear
    .[a1].Resize(t, UBound(crr, 2)) = crr

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End With
MsgBox "Done"
Application.ScreenUpdating = True
Application.AskToUpdateLinks = True
Application.EnableEvents = True
Application.DisplayAlerts = True 'Zhiyang
Wu, zhiyang.wu@charite.de'
End Sub

Sub test()
    Set dic = CreateObject("scripting.dictionary")
    With ThisWorkbook.Worksheets("MH")
        lr = .Range("A"
& .Rows.Count).End(xlUp).Row
        lc
= .Cells(1, .Columns.Count).End(xlToLeft).Colu
mn
        .[a1].Resize(lr, 1).Value = .[a1].Resize(lr,
1).Value
        .[a1].Resize(lr, lc).Sort key1:=.[a1], order1:=1,
Header:=xlYes
        arr = .[a1].Resize(lr, lc)
        For i = 2 To lr
            dic(arr(i, 1)) = dic(arr(i, 1)) + 1
            .Cells(i, lc + 1) = dic(arr(i, 1))
        Next
    End With

End Sub

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