

This script creates a column with m/z values for each expected compound, based on features detected in the sample with highest abundance for this compound. It also copies the delta mass in ppm for this feature to the Expected Compounds table.

### 1. Install node dependencies

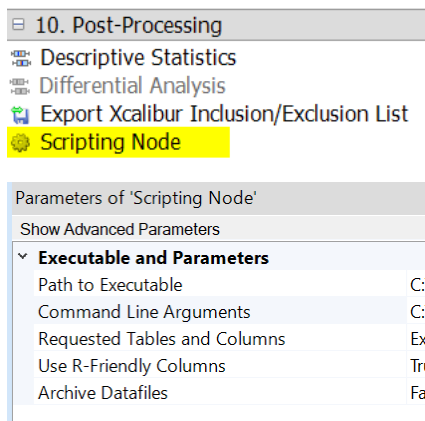
- If you don't have R installed on our PC already then you need to install R. Go to <https://cran.r-project.org/> . Select Download R for Windows -> Base
- After installing R, make sure the R package "rjson" is installed. To do that run R and type `install.packages("rjson")`.

### 2. Copy the R script

- Create a folder C:\Rscripts
- Navigate to this folder and create a new subfolder "ExpectedCompoundsMZDeltaPPM"
- Copy the file ExpectedCompoundsMZDeltaPPM.R into this folder

### 3. Execute the Script using the Scripting node

- Create a new workflow that contains the Scripting node or reprocess an existing result and add the Scripting node. This example modifies the *Expected Compounds* table.



First parameter: Your R version might be different. Make sure to select Rscript.exe.

Second and third parameter: copy & paste for from below

`C:\Rscripts\ExpectedCompoundsMZDeltaPPM\ExpectedCompoundsMZDeltaPPM.R %NODEARGS%`  
*Expected Compounds: Molecular Weight; Expected Compounds per File: Area; Expected Features*

Note: If you did not copy the script to C:\Rscripts\ ExpectedCompoundsMZDeltaPPM \ but elsewhere make sure to enter the correct path.

Run the analysis.

#### 4. Expected result

<div> <div>Compounds</div> <div>Compounds per File</div> <div>Expected Compounds</div> <div>Expected Compounds per File</div> <div>Expected Formulas</div> <div>Merged Features</div> <div>Feat</div> </div>								
	Checked	Name	Parent Compound	Formula	Molecular Weight	m/z	Delta Mass [ppm]	Dealkylated
1	<input type="checkbox"/>		Omeprazole	C17 H19 N3 O4 S	361.10963	362.11642	-1.32	X
2	<input checked="" type="checkbox"/>	5-Hydroxyomeprazole	Omeprazole	C17 H19 N3 O4 S	361.10963	362.11642	-1.32	
3	<input checked="" type="checkbox"/>		Omeprazole	C17 H17 N3 O3 S	343.09906	344.10593	-1.20	
4	<input type="checkbox"/>		Omeprazole	C17 H17 N3 O3 S	343.09906	344.10593	-1.20	X
5	<input checked="" type="checkbox"/>		Omeprazole	C17 H19 N3 O5 S	377.10454	378.11130	-1.38	
6	<input type="checkbox"/>		Omeprazole	C17 H19 N3 O5 S	377.10454	378.11130	-1.38	X
7	<input type="checkbox"/>		Omeprazole	C17 H17 N3 O4 S	359.09398	360.10083	-1.18	X
8	<input checked="" type="checkbox"/>		Omeprazole	C17 H17 N3 O4 S	359.09398	360.10083	-1.18	
9	<input checked="" type="checkbox"/>	Parent	Omeprazole	C17 H19 N3 O3 S	345.11471	346.12158	-1.17	
10	<input checked="" type="checkbox"/>		Omeprazole	C17 H19 N3 O6 S2	425.07153	426.07825	-1.31	
11	<input checked="" type="checkbox"/>		Omeprazole	C16 H17 N3 O2 S	315.10415	316.11099	-1.37	X
12	<input checked="" type="checkbox"/>		Omeprazole	C23 H27 N3 O9 S	521.14680	522.15363	-0.86	
13	<input checked="" type="checkbox"/>		Omeprazole	C17 H19 N3 O3	313.14264	314.14929	-1.99	