

Export the Compounds table with *d//\** ions for each compound, instead of using the reference ion.

\*Ions to export are based on the sample with the highest peak area for each compound.

### 1. Install node dependencies

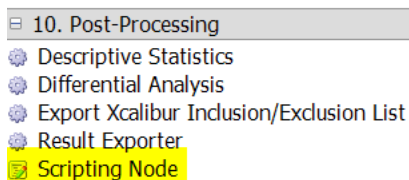
- a) If you don't have R installed on our PC already then you need to install R. Go to <https://cran.r-project.org/> . Select Download R for Windows -> Base
- b) After installing R, make sure the R package "rjson" is installed. To do that run R and type `install.packages("rjson")`

### 2. Copy the R script

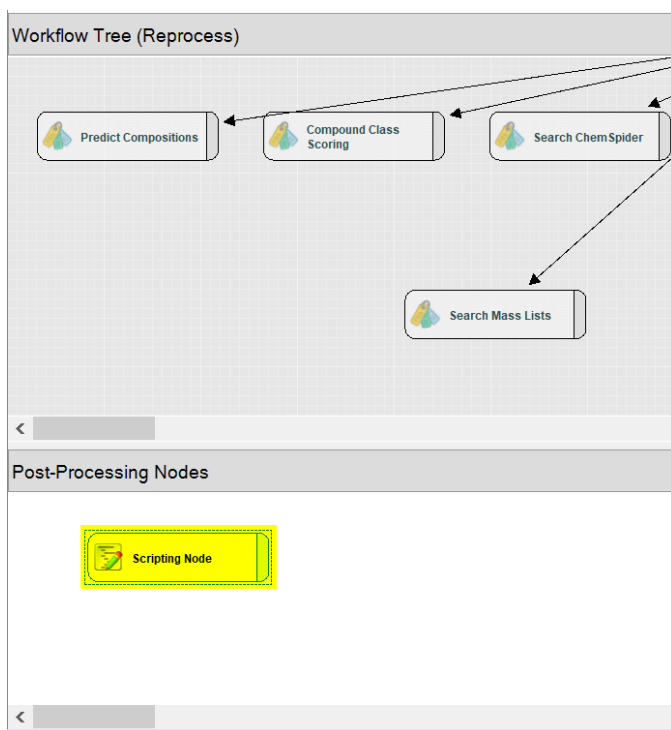
- a) Create a folder C:\Rscripts
- b) Navigate to this folder and create a new subfolder "ExportCpdsAllIons"
- c) Copy the file *ExportCpdsAllIons.R* into this folder

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

- a) Create a new workflow that contains the Scripting node **or** reprocess an existing result and add the Scripting node.



The Scripting node is a post-processing node. Drag it into the Post-Processing Node area. Post-processing nodes are not connected.



b) enter parameters

Click on the Scripting node to enter the parameters for this node.

Parameters of 'Scripting Node'	
Show Advanced Parameters	
▼ Executable and Parameters	
Path to Executable	C:\Program Files\R\R-4.5.0\bin\Rscript.exe
Command Line Arguments	C:\Rscripts\ExportCpdsAllIons\ExportCpdsAllIons.R %NODEARGS%
Requested Tables and Columns	Compounds: Name, Formula, Calc. MW, RT [min], Area (Max.); Features: Ion, m/z, Area (Max.), Intensity (Max.)
Use R-Friendly Columns	False
Archive Datafiles	False

**Path to R executable.** Your R version might be different. Make sure to select Rscript.exe.

**Command Line Arguments:** The path to your R script. You can [copy & paste](#) from below. Do not modify %NODEARGS% i.e., insert right path before %NODEARGS%, leave one space in between.

*C:\Rscripts\ExportCpdsAllIons\ExportCpdsAllIons.R*

**Requested Tables and Columns:** Tables and columns to export for use within the script. You can [copy & paste](#) from below.

*Compounds: Name, Formula, Calc. MW, RT [min], Area (Max.); Features: Ion, m/z, Area (Max.), Intensity (Max.)*

**Use R-friendly Columns:** False.

**Archive Datafiles :** False.

c) Run the analysis.

#### 4. Expected result

You should see an additional file with the extension “.Export\_All\_Ions.csv” in the same folder where your .cdresult file is located. This table has the following format.

	A	B	C	D	E	F	G
1	Name	Formula	Calc. MW	RT [min]	Ion	m/z	Intensity (Max.)
4740	EDTA	C10 H16 N	292.0901	0.94	[M+H] <sup>+</sup> 1	293.0974	9471281152
4741	EDTA	C10 H16 N	292.0901	0.94	[M+Na] <sup>+</sup> 1	315.079	580941760
4742	EDTA	C10 H16 N	292.0901	0.94	[M+Na] <sup>+</sup> 1	315.0789	321410048
4743	EDTA	C10 H16 N	292.0901	0.94	[X-e] <sup>+</sup> 1	70.06513	266997504
4744	EDTA	C10 H16 N	292.0901	0.94	[X-e] <sup>+</sup> 1	160.0603	163104064
4745	EDTA	C10 H16 N	292.0901	0.94	[X-e] <sup>+</sup> 1	132.0654	63901904
4746	EDTA	C10 H16 N	292.0901	0.94	[X-e] <sup>+</sup> 1	247.092	48485620
4747	EDTA	C10 H16 N	292.0901	0.94	[X-e] <sup>+</sup> 1	104.0704	43320708
4748	EDTA	C10 H16 N	292.0901	0.94	[2M+K] <sup>+</sup> 1	623.1409	24505694
4749	EDTA	C10 H16 N	292.0901	0.94	[M+K] <sup>+</sup> 1	331.053	18571934
4750	EDTA	C10 H16 N	292.0901	0.94	[X-e] <sup>+</sup> 1	129.0544	6700538

#### Options:

Features can be ordered by and exported using either the **Area (Max.)** or **Intensity (Max.)** values. The default setting is Area (Max.). If you want to change this setting, please edit line 19 of the R script accordingly.

```
18
19 # Option: export Area (Max.) or Intensity (Max.) for each feature
20 ExportValue = "Area (Max.)" # or use ExportValue = "Intensity (Max.)"
21
```