

Based on Kaufmann et al., **Simplifying Nontargeted Analysis of PFAS in Complex Food Matrixes**,
<https://doi.org/10.1093/jaoacint/qsac071>

This script creates the columns related to <https://doi.org/10.1093/jaoacint/qsac071>

- "eC" (estimated number of carbons based on A1/A0 ratio),
- "m/C" (molecular mass / eC),
- "md/C" (mass defect / eC), and

For each compound, this script will extract the MS1 scan and calculate eC based on the ratio of A1 and A0 peak for the reference ion.

The script also creates some additional columns that can be helpful in the context of PFAS analysis

- "F", the number of fluorine atoms in assigned Formula
- "maxF(EC)": the maximum number of fluorine atoms out of all predicted compositions for this compound
- "maxF(CS)": maximum number of fluorine atoms out of all ChemSpider Hits for this compound
- "maxF(ML)": maximum number of fluorine atoms out of all Mass List Hits for this compound

Installation

- 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. Download R and run the installer.
- b) After installing R, make sure the R packages rjson, stringr, XML and RSQLite are installed. To do that run R and use the command

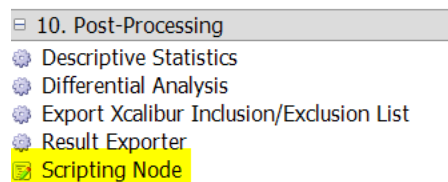
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install.packages(c("rjson", "stringr", "XML", "RSQLite"))
```

Close the R application after package installation is complete.

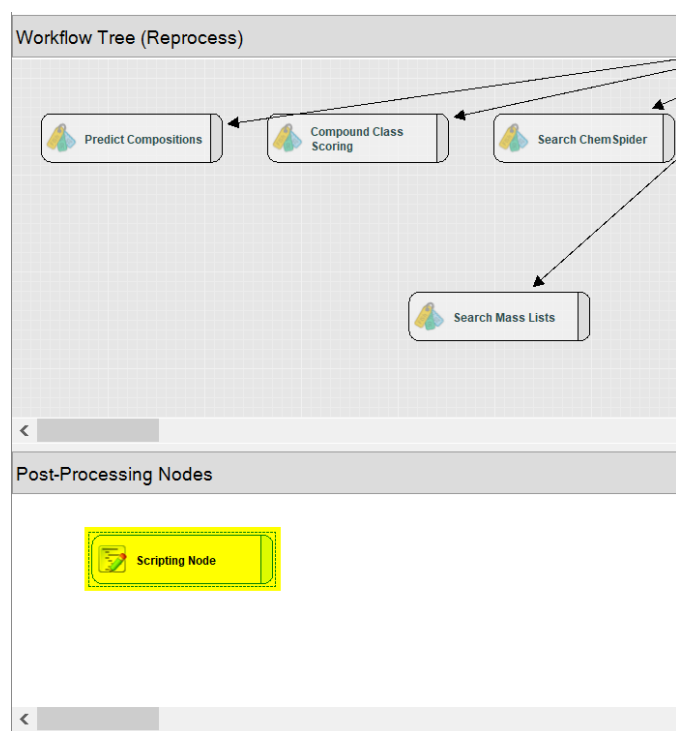
- c) Create a folder C:\Rscripts
- d) Navigate to this folder and create a new subfolder "PFAS"
- e) Copy the file *PFAS.R* into this folder

Using the Scripting node in your workflow

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

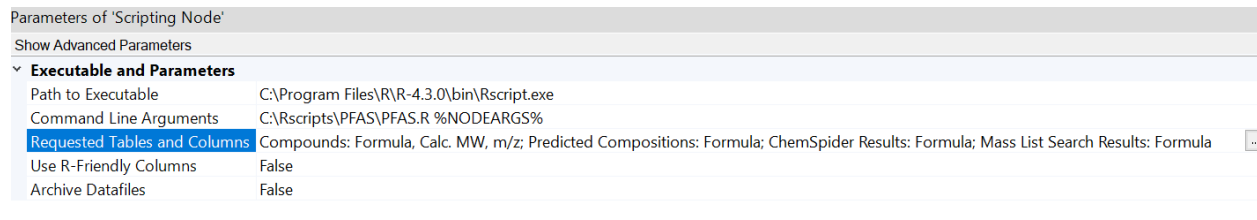


The Scripting node is a post-processing node. Drag it into the Post-Processing Node area. Post-processing nodes are not connected to other nodes.



- b) Enter parameters for the Scripting node

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



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\PFAS\PFAS.R

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

Compounds: Formula, Calc. MW, m/z; Predicted Compositions: Formula; ChemSpider Results: Formula; Mass List Search Results: Formula

Use R-friendly Columns: False.

Archive Datafiles : False.

c) Run the analysis.

Expected result (Compounds Table)

Name	Formula	Annot. Source	eC	m/C	md/C	F	maxF(EC)	maxF(CS)	maxF(ML)	Annot. ΔMass [ppm]	Calc. MW
Perfluoro-1-hexanesulfonic acid (PFHxS)	C6 H F13 O3 S		4.59117	87.11149	-0.01226	13	13	13	13	-0.48	399.94369
Perfluoro-1-pentanesulfonate	C5 H F11 O3 S		3.88535	90.06819	-0.01370	11	11	11	11	-0.81	349.94679
Perfluoro-1-butanesulfonic acid (PFBS)	C4 H F9 O3 S		4.25633	70.47163	-0.01168	9	9	9	9	0.10	299.95030
1H-Perfluorohexane	C6 H F13		5.89150	54.31336	-0.00218	13	13	13	13	0.23	319.98714
Perfluorooctane sulfonamidoacetic acid	C10 H4 F17 N O4 S		10.27206	54.22076	-0.00400	17	17	17	17	-0.10	556.95890
Perfluoro-1-dodecanesulfonate	C12 H F25 O3 S		11.06175	63.27430	-0.00684	25	20	25	25	-0.60	699.92430
Perfluoro-1-nonanesulfonate	C9 H F19 O3 S		9.46546	58.09905	-0.00696	19	19	19	19	-0.27	549.93415
Perfluoro-1-pentanesulfonate	C5 H F11 O3 S		4.05628	86.27292	-0.01313	11	11	11	11	-0.90	349.94676
Perfluorooctylsulfonamide (PFOSA)	C8 H2 F17 N O2 S		8.88342	56.16684	-0.00524	17	17	17	17	-0.04	498.95346
Perfluoro-1-decanesulfonic acid (PFDS)	C10 H F21 O3 S		9.88395	60.69750	-0.00698	21	21	21	21	-0.15	599.93101
Perfluoro-1-heptanesulfonate	C7 H F15 O3 S		7.05431	63.78240	-0.00843	15	15	15	15	-0.30	449.94055
Perfluoro-1-octanesulfonic acid (PFOS)	C8 H F17 O3 S		7.01604	71.25635	-0.00892	17	17	17	17	-0.12	499.93743
1,2,2,3,3,4,5,5,6,6-Decafluoro-4-(pentafluoroethyl)cyclo	C8 H F15 O3 S		7.75829	59.54153	-0.00766	15	15	15	15	-0.20	461.94060
Perfluoro-1-hexanesulfonamide	C6 H2 F13 N O2 S		6.13026	65.08035	-0.00658	13	13	13	13	-0.49	398.95967
11-Chlorohexadecafluoro-3-oxanonane-1-sulfonate	C10 H Cl F20 O4 S		11.29280	55.95570	-0.00918	20	20	0	20	-0.15	631.89638

The additional columns eC, m/C, md/C, F, maxF(EC), maxF(CS) and maxF(ML) are shown in the Compounds table.

Visualize result using Result Charts in CD

Click on View – Result Charts.

Select:

- Data Source: *Compounds*
- X Data: *m/C*
- Y Data: *md/C*

Click Refresh.

