

This script calculates the O/C ratio and the H/C ratio for each compound and returns the result as two new columns.

1. Install node dependencies

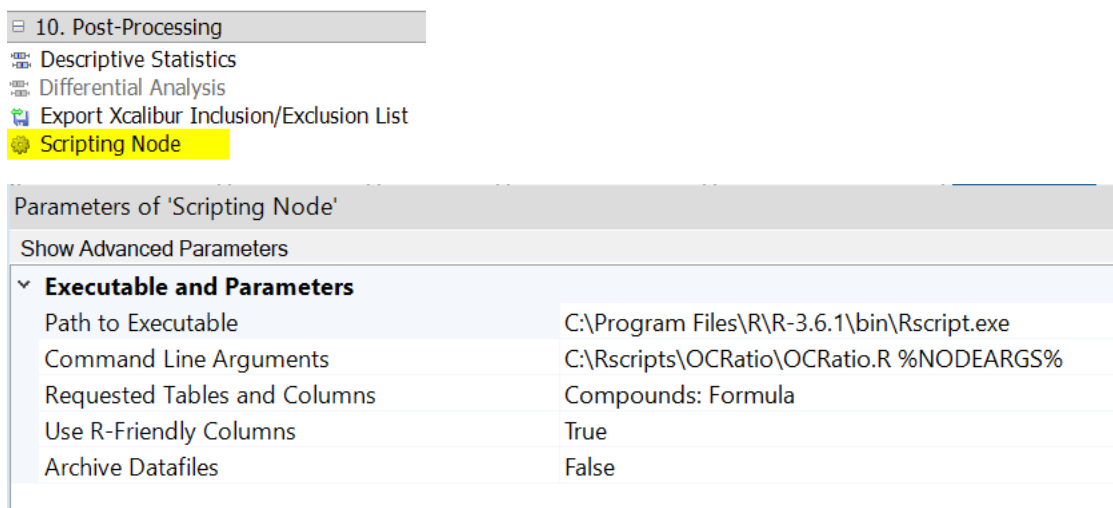
- If you don't have R installed on our PC already then you need to install R. Go to <https://cran.r-project.org/> . Select Download R for Windows -> Base
- After installing R, make sure the R package "rjson" is installed. To do that run R and type `install.packages("rjson")`. Please also install package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

2. Copy the R script

- Create a folder C:\Rscripts
- Navigate to this folder and create a new subfolder "OCRatio"
- Copy the file *OCRatio.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 *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\OCRatio\OCRatio.R %NODEARGS%

Compounds: Formula

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

Run the analysis.

4. Expected result

Name	Formula	Molecular Weight	RT [min]	Area (Max.)	O/C	H/C
Ethylenediaminetetraacetic acid (EDTA)	C10 H16 N2 O8	292.09008	0.932	85836478826	0.80	1.60
DA9185000	C12 H10 O S	202.04498	0.834	20360836859	0.08	0.83
L-Norleucine	C6 H13 N O2	131.09453	2.009	17671595759	0.33	2.17
Betaine	C5 H11 N O2	117.07877	0.862	17227484266	0.40	2.20
D-(+)-Tryptophan	C11 H12 N2 O2	204.08974	3.113	14935877741	0.18	1.09
Creatine	C4 H9 N3 O2	131.06929	0.895	13731682864	0.50	2.25
L-Phenylalanine	C9 H11 N O2	165.07892	2.573	13086972275	0.22	1.22
L-Tyrosine	C9 H11 N O3	181.07382	1.620	12173763807	0.33	1.22
Creatinine	C4 H7 N3 O	113.05880	0.921	11284215174	0.25	1.75
L-Valine	C5 H11 N O2	117.07877	1.181	10762788065	0.40	2.20
Acetyl-L-carnitine	C9 H17 N O4	203.11558	1.329	10080578865	0.44	1.89
Benzene	C6 H6	78.04684	2.572	8828044750	0.00	1.00
L-Isoleucine	C6 H13 N O2	131.09453	1.921	8746385312	0.33	2.17
3-Methylsulfolene	C5 H8 O2 S	132.02440	1.356	8055302245	0.40	1.60
DL-Carnitine	C7 H15 N O3	161.10499	0.855	7950007130	0.43	2.14
L-(-)-Methionine	C5 H11 N O2 S	149.05093	1.531	6231613732	0.40	2.20

5. Visualization using Result Charts

