

This script calculates relative peak area for each isotopologue (already corrected for natural abundance) and writes it into an Excel spreadsheet.

If compounds are marked using the Checked column in the Compounds table, then only those checked compounds are exported. If no compounds are checked then the script will export all compounds.

1. Install R and some additional R libraries

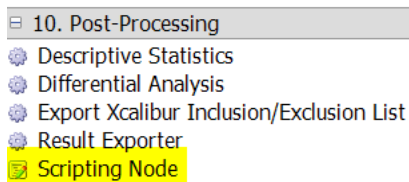
- a) If you don't have R installed on our PC already then you need to install R. Go to <https://cran.r-project.org/> . Select Download R for Windows -> Base
- b) After installing R, make sure the R package "rjson" is installed. To do that run R and type `install.packages('rjson')`
- c) Also install the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

2. Copy the R script

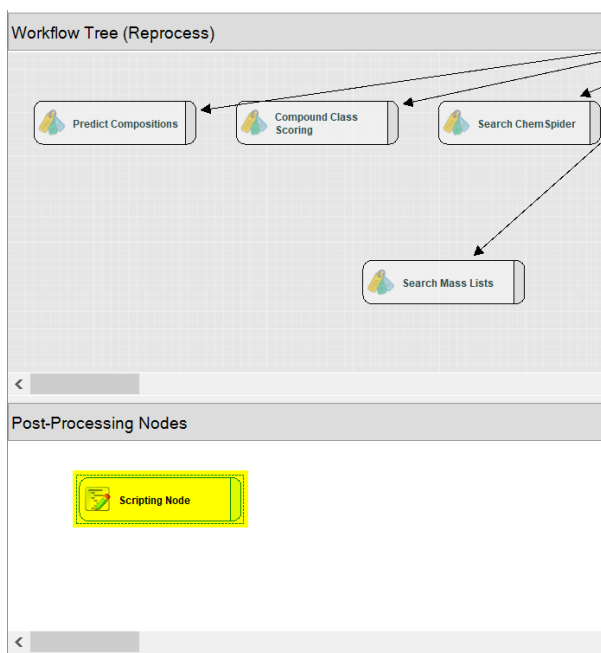
- a) Create a folder C:\Rscripts
- b) Navigate to this folder and create a new subfolder "SIL_Area"
- d) Copy the file *SIL_Area.R* into this folder

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.



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



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-4.3.1\bin\Rscript.exe
Command Line Arguments	C:\Rscripts\SIL_Area\SIL_Area.R %NODEARGS%
Requested Tables and Columns	Compounds: Checked, Calc MW, Name, Formula, RT in min; Labeled Compounds per File; Input Files ...
Use R-Friendly Columns	True
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\SIL_Area\SIL_Area.R

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

Compounds: Checked, Calc MW, Name, Formula, RT in min; Labeled Compounds per File; Input Files

Use R-friendly Columns: True.

Archive Datafiles : False.

c) Run the analysis.

4. Expected result

You should see 6 additional files in the same folder where your cdresult file is located.

- [cdresult file name] + _SIL_Relative_Area_NA.csv (result table as .csv file)
- [cdresult file name] + _SIL_Relative_Area.xlsx (result table as .xlsx file)
- [cdresult file name] + _SIL_Relative_Area_OFill.xlsx (result table as .xlsx file, NA's filled in with zeroes)
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- [cdresult file name] + _SIL_Exchange_Rate_NA.csv (result table as .csv file)
- [cdresult file name] + _SIL_Exchange_Rate.xlsx (result table as .xlsx file)
- [cdresult file name] + _SIL_Exchange_Rate_OFill.xlsx (result table as .xlsx file, NA's filled in with zeroes)

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	Name	Formula	Molecular Weight	RT in min	Area	Status	Study File ID	Filename	Relative Area 0	Relative Area 1	Relative Area 2	Relative Area 3	Relative Area 4	Relative Area 5	Relative Area 6	Relative Area 7	Relative Area 8	Relative Area 9	Relative Area 10
2	L-Glutamic acid	C5 H9 N O	147.05291	1.288	2.05E+09	NoWarninF3	Ecoli_12C_02.raw	2050244998	1980002	0	74787	0	0	0	0	0	0	0	0
3	L-Glutamic acid	C5 H9 N O	147.05291	1.287	2.04E+09	NoWarninF4	Ecoli_12C_03.raw	2033548833	3278886	0	63493	0	0	0	0	0	0	0	0
4	L-Glutamic acid	C5 H9 N O	147.05291	1.286	1.93E+09	NoWarninF9	Ecoli_13C_01.raw	1057314	51	1061581	8701115	141092548	1.775E+09	0	0	0	0	0	0
5	L-Glutamic acid	C5 H9 N O	147.05291	1.288	1.96E+09	NoWarninF10	Ecoli_13C_02.raw	2991080	71	1031743	8954270	145401935	1.805E+09	0	0	0	0	0	0
6	L-Glutamic acid	C5 H9 N O	147.05291	1.289	1.99E+09	NoWarninF11	Ecoli_13C_03.raw	2729361	80	1121040	8721715	147077791	1.833E+09	0	0	0	0	0	0
7	L-Glutamic acid	C5 H9 N O	147.05291	1.378	176615.1	ContamininF1	Blank_01.raw	164073	0	0	12393	0	149	0	0	0	0	0	0
8	L-Glutamic acid	C5 H9 N O	147.05291	1.286	2.08E+09	NoWarninF2	Ecoli_12C_01.raw	2073956140	1318335	0	1065018	361639	0	0	0	0	0	0	0
9	L-Glutathione (reduced)	C10 H17 N	307.08328	2.085	1.65E+09	NoWarninF3	Ecoli_12C_02.raw	1631802733	15611601	0	0	0	1881	0	0	0	0	0	0
10	L-Glutathione (reduced)	C10 H17 N	307.08328	2.087	1.61E+09	NoWarninF4	Ecoli_12C_03.raw	1601334507	5347603	0	0	0	1651	0	0	0	0	0	0
11	L-Glutathione (reduced)	C10 H17 N	307.08328	2.089	2.31E+09	NoWarninF9	Ecoli_13C_01.raw	4001739	0	1332596	341476	838876	4179009	1549369	11299534	42670853	2.95E+08	1.94E+09	
12	L-Glutathione (reduced)	C10 H17 N	307.08328	2.092	2.8E+09	NoWarninF10	Ecoli_13C_02.raw	5619268	0	1725119	416988	996852	4661344	2008388	14863752	53813947	3.82E+08	2.34E+09	
13	L-Glutathione (reduced)	C10 H17 N	307.08328	2.094	2.41E+09	NoWarninF11	Ecoli_13C_03.raw	4297721	17430	1342103	454198	742282	3830718	1617183	12045261	43554458	3.08E+08	2.03E+09	
14	L-Glutathione (reduced)	C10 H17 N	307.08328	2.087	1.59E+09	NoWarninF2	Ecoli_12C_01.raw	1578013975	7833502	0	0	0	929	0	0	0	0	0	0
15	L-Glutathione oxidized	C20 H32 N	612.15127	2.771	7.13E+08	NoWarninF3	Ecoli_12C_02.raw	710908510	245425	575207	0	2000	0	846367	0	0	0	0	0
16	L-Glutathione oxidized	C20 H32 N	612.15127	2.767	8.03E+08	NoWarninF4	Ecoli_12C_03.raw	801215569	0	626503	0	2211	0	1031862	0	0	0	0	9355
17	L-Glutathione oxidized	C20 H32 N	612.15127	2.765	7.21E+08	NoWarninF9	Ecoli_13C_01.raw	270582	0	0	0	0	0	0	2	1	265235	2075850	
18	L-Glutathione oxidized	C20 H32 N	612.15127	2.77	7.42E+08	NoWarninF10	Ecoli_13C_02.raw	2361076	0	0	0	0	0	0	2	0	377459	2376646	
19	L-Glutathione oxidized	C20 H32 N	612.15127	2.766	9.11E+08	NoWarninF11	Ecoli_13C_03.raw	2287504	0	0	0	0	0	0	2	8	341598	2517622	
20	L-Glutathione oxidized	C20 H32 N	612.15127	2.772	7.41E+08	NoWarninF2	Ecoli_12C_01.raw	739266798	0	573420	0	1505	0	1137586	0	0	0	0	0

Note: If you prefer many individual result tables (one per compound) instead of one large result table for all compounds, then you can set this option to TRUE (line number 15 in the R script).

ONE_FILE_PER_COMPOUND = TRUE