

A very basic example for a Scripting Node in Thermo Scientific™ Compound Discoverer™ software. All it does is adding a fixed value (1.007276) to the Calc. MW in the Compounds table to create a new "M+H" column.

1. Install node dependencies

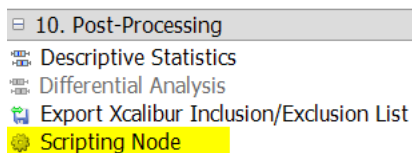
- If you don't have R installed on our PC already then you need to install R. Go to <https://cran.r-project.org/> . Select Download R for Windows -> Base
- After installing R, make sure the R package "rjson" is installed. To do that run R and type `install.packages("rjson")`.

2. Copy the R script

- Create a folder C:\Rscripts
- Navigate to this folder and create a new subfolder "SimpleTest"
- Copy the file *SimpleTest.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, so make sure you have the *Detect Compounds* node in your workflow.



Parameters of 'Scripting Node'	
Hide Advanced Parameters	
▼ Executable and Parameters	
Path to Executable	C:\Program Files\R\R-4.2.1\bin\Rscript.exe
Command Line Arguments	C:\Rscripts\SimpleTest\SimpleTest.R %NODEARGS%
Requested Tables and Columns	Compounds
Use R-Friendly Columns	True
Archive Datafiles	False

Set the parameters of the Scripting node so that the file path in the Command Line Arguments matches the folder where you copied the script in step 2. For this basic example, we are only exporting the column Molecular Weight from the Compounds table.

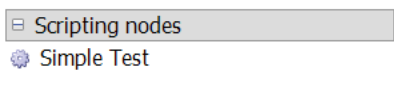
C:\Rscripts\SimpleTest\SimpleTest.R %NODEARGS%

Compounds

Run the analysis. Go to step 5 to verify that you get the expected result.

4. Optional (alternative to step 3.) : register the node as a *standalone* Scripting node

Scripting nodes can be registered as *standalone* scripting nodes, so that they appear in the list of nodes and can be used without utilizing the general “Scripting node” UI. That way multiple scripting nodes can be installed and additional options like parameters for the node can be defined. Below is an example for a custom node section “Scripting nodes” that contains this example node.



Installing the node as a standalone scripting node requires a JSON file which defines the node and its parameters.

a) Copy the node description file

- Use Windows Explorer to navigate to the folder
C:\Program Files\Thermo\Compound Discoverer 3.3\Tools\Scripts\
- Create a new subfolder with the name “SimpleTest”
- Copy the **node.rjson** file into this folder

b) Check the file paths in the node description file

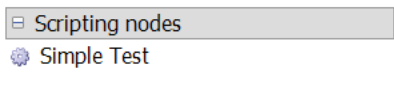
- Open the node description file that you just copied (C:\Program Files\Thermo\Compound Discoverer 3.3\Tools\Scripts\node.rjson) in a text editor like Microsoft Notepad or notepad++ or Microsoft Code Writer. Do not use Microsoft Word.
- Check the file path to the R executable (line 20) to make sure it matches your R installation.

d) Register the node in CD

- Open Compound Discoverer
- Close all open studies and result files
- Select Help -> License Manager
- Click “Scan for Missing Features”
- Optional: Open C:\ProgramData\Thermo\Compound Discoverer 3.3\Logs\CompoundDiscovererServer.log and navigate to the bottom of the log file. It should say something like *ProcessingNodeManager - Node: Simple Test registered*
If there were any errors parsing the JSON file they will show up in this log file, like *DEBUG [xx] ScriptingNodeFactory - Error while reading node data from ...*

e) Test the standalone scripting node

Create a new workflow that contains the node or reprocess an existing result and add the new post-processing node (“Simple Test”) which you should now see in the list of nodes.



5. Expected result

There should be a new column in the Compounds table “MH” that contains the Calc. MW + 1.007276. For this basic example this new column is not inserted at a specific position. Scroll to the right to located the new column. Using drag and drop, move it next to the Calc. MW column so you can better see the result.

Calc. MW	MH	RT [min]
292.09007	293.09735	0.926
292.09014	293.09742	1.258
131.09454	132.10182	2.006
202.04497	203.05225	0.827
117.07877	118.08605	0.856
131.06930	132.07658	0.888
165.07892	166.08620	2.570
115.06313	116.07041	0.915
117.07879	118.08607	1.174
203.11559	204.12287	1.324

Note: If you modify the R-script you do not have to repeat any of the steps above. Just reprocess the Scripting node (or your standalone scripting node).