Protocol of Sirius batch processing in R (windows)

1. Download the newest 64bit version SIRIUS+CSI:FingerID GUI and CLI from https://bio.informatik.uni-jena.de/software/sirius/.

2.

3.

variables → Path → Edit → New → Browse folder of Sirius →OK

4. Under the folder User/.sirius open the file "sirius.properties" in a text editor. Set the line "de.unijena.bioinf.sirius.treebuilder=glpk"

Change the file name "sirius-console-64.exe" to "sirius.exe".

Unzip the folder and move it to the desired location of your pc.

Set path for sirius: Edit the environment variable → System

for all targeted scans) for MS2 and another for MS1 (optional). Following meta data are necessary in the MS2 file for each scan.

For MS1 file only PEPMASS and ID are required. ID should be the same as

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 http://www.oracle.com/technetwork/java/javase/downloads/jdk10-downloads-4416644.html

 Data preparation: single mgf file (combined meta + spectra data)
- However, user may add any other metadata.
 PEPMASS Precursor m/z
 ADDUCT Must be one of "M+H", "M-H", "M+Na" or "M+Cl"
 IONMODE Positive or Negative
 FORMULA Precursor formula. If unknown, please set to "N/A"
- the corresponding MS2 scan.

 7. Copy MS2.mgf, (MS1.mgf), "main.R" and "process_sirius.R" in the

ID Unique ID for each scan, SIRIUS output is saved as "dotfiles/ID.dot".

same folder.
8. Make sure the path of your working directory does NOT contain white space or special characters. Underscores are allowed.
9. Open "main.R" in Rstudio and check:

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