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

- Download and install Java (jdk10 64 bin for windows):
   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:

# **Pointclickcare User Manual**

**Arturo Cuomo** 

**Pointclickcare User Manual:** 

Pointclickcare User Manual: Bestsellers in 2023 The year 2023 has witnessed a noteworthy surge in literary brilliance, with numerous captivating novels captivating the hearts of readers worldwide. Lets delve into the realm of top-selling books, exploring the fascinating narratives that have charmed audiences this year. Pointclickcare User Manual: Colleen Hoovers "It Ends with Us" This touching tale of love, loss, and resilience has captivated readers with its raw and emotional exploration of domestic abuse. Hoover masterfully weaves a story of hope and healing, reminding us that even in the darkest of times, the human spirit can prevail. Pointclickcare User Manual: Taylor Jenkins Reids "The Seven Husbands of Evelyn Hugo" This captivating historical fiction novel unravels the life of Evelyn Hugo, a Hollywood icon who defies expectations and societal norms to pursue her dreams. Reids absorbing storytelling and compelling characters transport readers to a bygone era, immersing them in a world of glamour, ambition, and self-discovery. Pointclickcare User Manual: Delia Owens "Where the Crawdads Sing" This captivating coming-of-age story follows Kya Clark, a young woman who grows up alone in the marshes of North Carolina. Owens crafts a tale of resilience, survival, and the transformative power of nature, entrancing readers with its evocative prose and mesmerizing setting. These popular novels represent just a fraction of the literary treasures that have emerged in 2023. Whether you seek tales of romance, adventure, or personal growth, the world of literature offers an abundance of compelling stories waiting to be discovered. The novel begins with Richard Papen, a bright but troubled young man, arriving at Hampden College. Richard is immediately drawn to the group of students who call themselves the Classics Club. The club is led by Henry Winter, a brilliant and charismatic young man. Henry is obsessed with Greek mythology and philosophy, and he quickly draws Richard into his world. The other members of the Classics Club are equally as fascinating. Bunny Corcoran is a wealthy and spoiled young man who is always looking for a good time. Charles Tavis is a quiet and reserved young man who is deeply in love with Henry. Camilla Macaulay is a beautiful and intelligent young woman who is drawn to the power and danger of the Classics Club. The students are all deeply in love with Morrow, and they are willing to do anything to please him. Morrow is a complex and mysterious figure, and he seems to be manipulating the students for his own purposes. As the students become more involved with Morrow, they begin to commit increasingly dangerous acts. The Secret History is a exceptional and suspenseful novel that will keep you speculating until the very end. The novel is a cautionary tale about the dangers of obsession and the power of evil.

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