

How to download and setup DrugBank database

Description:

DrugBank is a database that provides bioinformatic and chemical information that is associated to all drug proprieties. For more information please refer to: <https://www.drugbank.ca/>

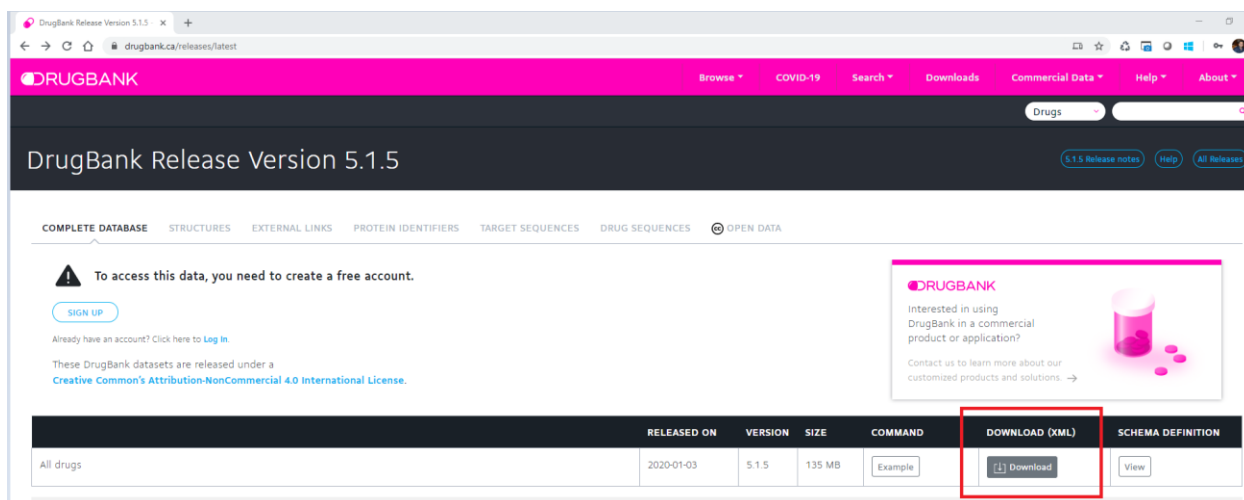
Import R script description:

The provided R script leverages the out of the box DrugBank Database XML Parser R Library to parse the entire extracted DrugBank.xml and restore and persists the entire drugbank database into the targeted central PostgreSQL. For detailed information about the library, please refer to following article.

<https://cran.r-project.org/web/packages/dbparser/dbparser.pdf>

Where and How to Download DrugBank database:

1. Please follow the instruction below to ensure you have an existing account registered with drugbank.ca
 - https://www.drugbank.ca/public_users/sign_up
2. Once the registration is complete please navigate to:
 - <https://www.drugbank.ca/releases/latest>and click on “download” as shown in the picture below



3. Once the registered account information is provided, please download and unzip the following zip file into your desired folder “drugbank_all_full_database.xml.zip”

Pre-installation requirement:

Please ensure R is installed on your system.

- For windows please follow the steps here:
 - <https://cran.r-project.org/bin/windows/base/>
- For Mac please follow the steps here:
 - <http://lib.stat.cmu.edu/R/CRAN/>

How to run the code:

1. Open “drug_bank_import.R” file using your preferred editor and provide:

- path to downloaded .xml file
 - where you have un-zipped the .xml file as following:
 - `read_drugbank_xml_db("FULL PATH TO DRUG BANK.xml")`

Example:

```
#the following line read the entire xml database and store it into memory
read_drugbank_xml_db("C:/Development/School/CSCI-E 599/data/drugbank_all_full_database.xml/full database.xml")
```

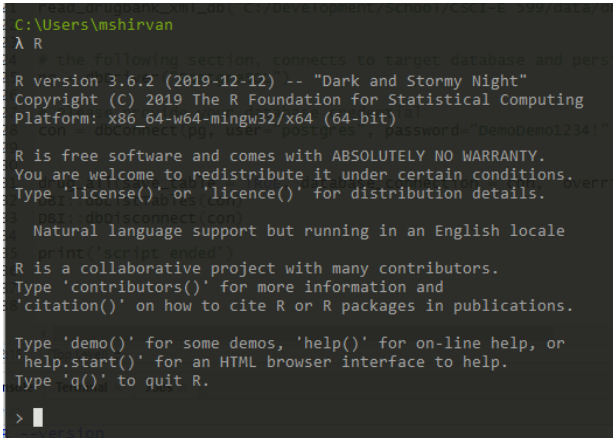
- Provide the targeted database information:

Example:

```
# Please provide your database credential
con = dbConnect(pg, user="YOUR_USER", password="YOUR_PASS!", host="localhost", port=5432, dbname="drugbank")
```

4. Open a terminal window or command prompt as an administrator

- Type R and press Enter/return

A screenshot of an R console window. The title bar shows the path 'C:\Users\mshirvan'. The prompt is 'λ R'. The output includes the R version (3.6.2), copyright notice, platform information (x86_64-w64-mingw32/x64), and a message about connecting to a PostgreSQL database. It also displays the R license and a list of contributors. The prompt is now '>'.

```
C:\Users\mshirvan
λ R
R version 3.6.2 (2019-12-12) -- "Dark and Stormy Night"
Copyright (C) 2019 The R Foundation for Statistical Computing
Platform: x86_64-w64-mingw32/x64 (64-bit)
con = dbConnect(pg, user="YOUR_USER", password="YOUR_PASS!", host="localhost", port=5432, dbname="drugbank")

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

> dbConnect(con)
Natural language support but running in an English locale
print("script ended")

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

>
```

- Type: `source('PATH_TO/drug_bank_import.R',echo=TRUE)` and Press enter

```
> source('C:/Development/drug_bank_import.R',echo=TRUE)
```

- You are done!!
 - i. Please note this script is going to take couple hours to complete, so please be patient.