Installation guide for Java environment and CDK to OSX (9.5 or later) & rJava, rcdk to R environment

Statistical recipe for quantifying microbial functional diversity from EcoPlate metabolic profiling

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This box implies the command line of terminal window

This box implies the command line of R

This box implies the content of text file opened by emacs

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1) Install X11 (XQuartz 2.7.11 or later)

Just visit https://www.xquartz.org, download "XQuartz-2.7.11.dmg" and follow the installation guidance.

2) Check the version of java and java compiler (javac)

Open terminal window and conduct the following two commands, one by one:

```
$java -version
$javac -version
```

If the installed version < 1.8, the update of Java SE Development Kit is needed. Visit http://www.oracle.com/technetwork/java/javase/downloads/jdk8-downloads-2133151.html

, download "jdk-8u111-macosx-x64.dmg" and follow the installation guide.

3) Install Java Chemistry Development Kit (CDK) to your Java environment

Visit https://sourceforge.net/projects/cdk/files/latest/download?source=files, and download the library file "cdk-1.5.13.jar" or newer version.

Copy (with superuser password) the library file above (CDK) into another directory via terminal:

```
$sudo cp cdk-1.5.13.jar /Library/Java/JavaVirtualMachines/jdk1.
8.0_111.jdk/Contents/Home/jre/lib/ext
```

4) Install the latest R (R-3.3.2.pkg) & Rstudio Desktop

Visit the official website

5) Set up proxy for Rstudio via terminal and emacs (if necessary)

At your home directory, you need to make a new setting file (".Rprofile") via the following command with terminal:

```
$emacs .Rprofile
```

At the editing window of emacs (can be the same as the terminal window), add the following two lines and save the file.

```
Sys.setenv(http_proxy="http://XXXXX:nnnn")
Sys.setenv(https_proxy="http://XXXXX:nnnn")
```

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5) Install the libraries "rJava" and "rcdk" via Rstudio

First, it is necessary to make R environment recognize the installed version of R in OSX via terminal:

```
$sudo R CMD javareconf
```

Then, install the following two libraries to R in R command line (or via R script)

```
>install.packages("rJava")
>install.packages("rcdk")
```

Then, load rJava

```
>library("rJava")
```

This may return some error messages. Then, try again the following command in terminal and then load rJava again.

```
$sudo R CMD javareconf
```

If it does not change the condition, edit ".bash_profile" at your home directory by adding the following two lines at the end of file via emacs:

```
$emacs .bash_profile
```

```
export
JAVA_HOME="/Library/Java/JavaVirtualMachines/jdk1.8.0_111.jdk/
Contents/Home/jre"
export LD_LIBRARY_PATH="$JAVA_HOME/lib:$JAVA_HOME/lib/server"
```

Thereafter, try to install again rJava and rcdk from source:

```
>install.packages("rJava", type='source')
>install.packages("rcdk", type='source')
```

5) Install the libraries "rJava" and "rcdk" via Rstudio (continued)

Load library again

```
>library("rJava")
```

If it returns the error message with the keyword "Library not loaded: @rpath/libjvm.dylib" such as:

```
Error: .onLoad failed in loadNamespace() for 'rJava', details: call: dyn.load(file, DLLpath = DLLpath, ...) error: unable to load shared object '/Library/Frameworks/R.framework/Versions/3.2/Resources/library/rJava/libs/rJava.s o': dlopen(/Library/Frameworks/R.framework/Versions/3.2/Resources/library/rJava/libs/rJava.so, 6): Library not loaded: @rpath/libjvm.dylib Referenced from: /Library/Frameworks/R.framework/Versions/3.2/Resources/library/rJava/libs/rJava.s o Reason: image not found Error: package or namespace load failed for 'rJava'
```

This means that the rJava cannot find the part of java libraries that should be already installed in your system. To resolve this, you can make a symbolic link for the library "libjvm.dylib" via terminal:

```
$sudo ln -f -s
/Library/Java/JavaVirtualMachines/jdk1.8.0_111.jdk/
Contents/Home/jre/lib/server/libjvm.dylib /usr/local/lib
```

Then, load libraries and they should work well.

```
>library("rJava")
>library("rcdk")
```

If it doesn't work, go to the step 6.

6) Start analysis with pre-calculated chemical dissimilarity information, without using Java libraries

```
>#When rJava and/or rcdk installation were failed
>fp.dist_a<-read.csv("./fp.dist_a.csv")
>fp.dist_b<-read.csv("./fp.dist_b.csv")</pre>
```