

Plotting PSD histograms in R: Shell implementation

Marielle Pinheiro

Version 1.0, March 6, 2013

Note: Tutorial written for Linux shell implementation. It is possible to run in Windows and Mac as well, with or without GUI interface, but there might be some minor differences in the file syntax.

Required:

R installed on system

R scripts, all contained in same working directory

-noninteractive_graph.R

-noninteractive_graph_functions.R

-parameters.R

1. Navigate to correct directory

This script will only work if all of the scripts are contained in the same directory. The input files may be contained in a separate directory

2. Customize parameters (optional)

By default, the script calculates the extent of the X and Y axes within the function and generates a plot optimized to the PSD's dimensions. If you wish to change plot titles or maintain a consistent axis scale, open parameters.R and change the variable inputs to the desired values before running the script.

3. Run script

This will only work if R is installed. The command line syntax is as follows:

R --slave --args dir_path input output customize

The parameters that should be changed are the ones that follow **--args**:

- **dir_path**: The complete path to the directory that contains your input files (this sets your working directory)
Example: **/home/mpinheiro/structures/**
- **input**: The file name (only put the file name, not the complete path)
Example: **ABW.distr**
- **output**: The output file name (if you wish to save the file in a different directory, include the directory path as well). The plot is saved as a PostScript (.ps) file.
Examples: **ABW.ps**, **/home/mpinheiro/plots/ABW.ps**

- **customize:** If you wish to keep the default parameters (optimized to file's parameters) type **N**. Otherwise, type **Y** (you should have already edited the parameters file).

Hit <ENTER> to run script.

If you get message “Cannot plot function; distribution is 0.” this means that your structure does not have any peaks.