Manual for the

Package 'MSeasyTkGUI'
May, 2012

Type Package

Title MSeasy Tcl/Tk Graphical User Interface

Version 5.3

Date 2012-05-04
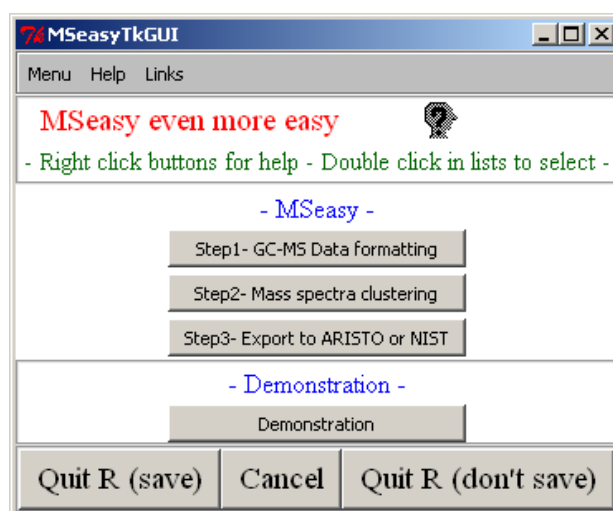
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Depends R (>= 2.13.0), MSeasy (>= 5.3), tcltk

Description A Tcl/Tk GUI for some basic functions in the MSeasy package

License GPL-2

Table of Contents

Installation

Download the MSeasyTkGUI package from here (URL)
Install the package with the R GUI Packages menu or with install.packages() R function

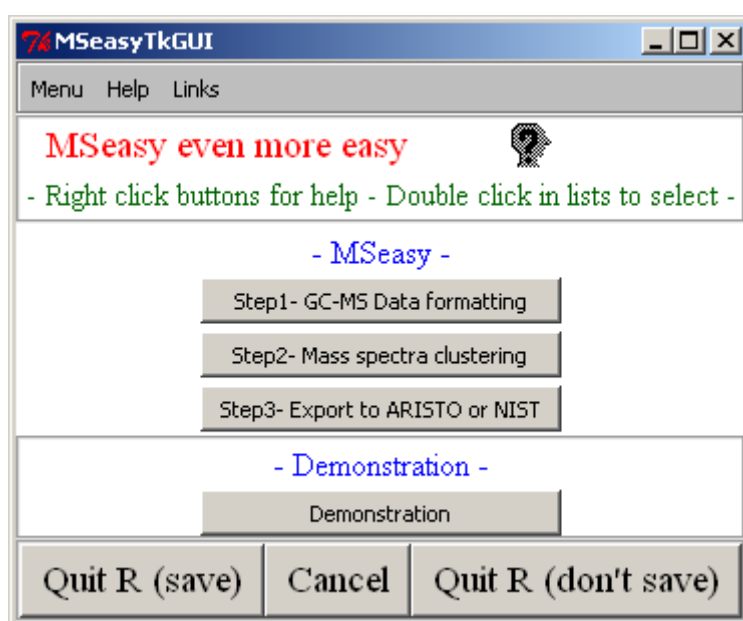*Note: MSeasy package must be installed first (download MSeasy here (URL))*

Starting MSeasyTkGUI

Open R
Copy/paste the command line and press Enter:

Library("MSeasyTkGUI");MSeasyTkGUI()

Now the first window pops up.

List of MSeasy functions available in MSeasyTkGUI

MS.DataCreation
trans.ASCII
MS.test.clust
MS.clust
MSeasyToMSP
MSeasyToARISTO
SearchNIST

MSeasyTkGUI Menu & buttons

All MSeasy functions can be started either from the menu bar or a button (Figure 1). Several windows pops up (see example in Figure 2), fill up the parameters and click on "Submit" button.
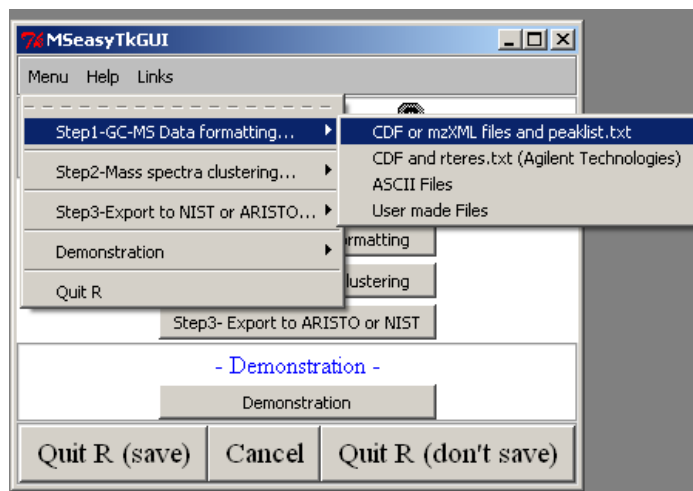
- From the Menu:

FIGURE1: MSEASYTKGUI MENU

Data path or Data frame: allows the selection of folders or files if necessary

Output name: put the name of the R object created by the function (or leave blank)

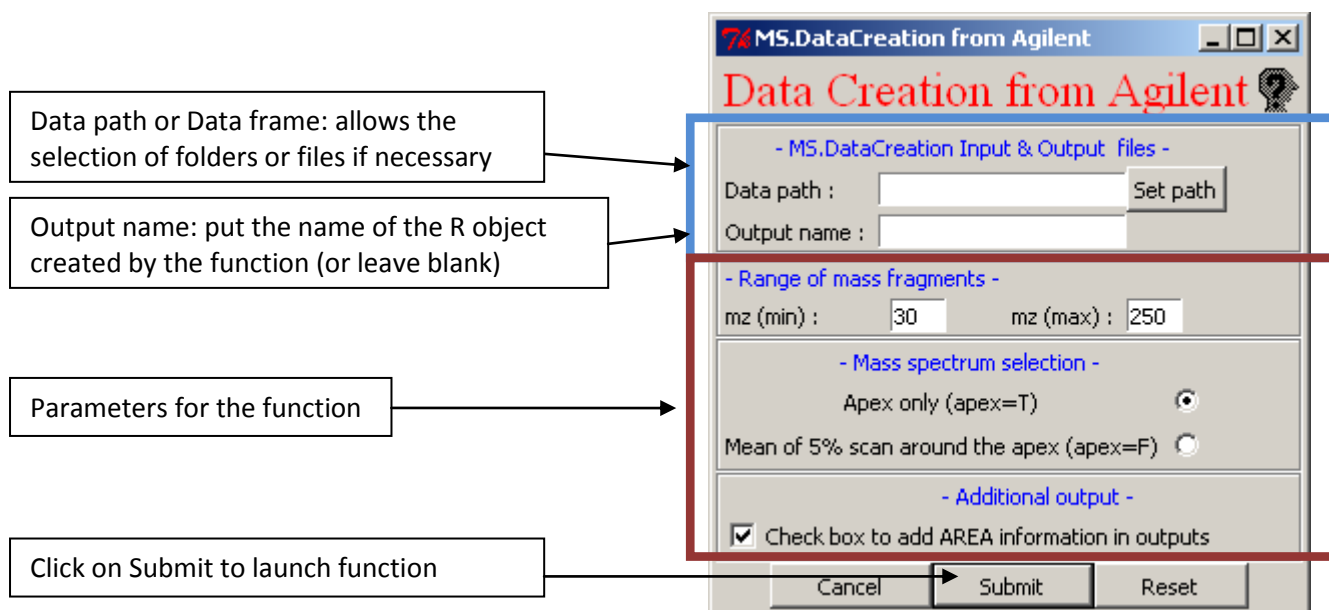Parameters for the function

Click on Submit to launch function

FIGURE2: EXAMPLE OF WINDOW

- From the buttons

All the buttons gives you access to the same functions and windows described above

Menu details:

➔ Step1-Data formatting
   o CDF or mzXML and peaklist.txt: creates a MSeasy data file from CDF(or mzXML) GC-MS files if there are peaklist.txt files containing peakpicking information
   o CDF and rteres.txt (Agilent Technologies): creates a MSeasy data file from CDF GC-MS files created by your chemstation (Export to AIA/ANDi) if rteres.txt files created also by your chemstation are presents
   o ASCII Files: creates a MSeasy data file from GC-MS files in ASCII format
   o User made files (.txt, .csv…): open a data file made by user (*.*txt or *.* csv) in the specified MSeasy data file format (see MS.DataCreation help file for format details)

NOTE for all function using CDF or mzXML files you need R XCMS package
Copy/paste that code in R console:

source("http://bioconductor.org/biocLite.R")
biocLite("xcms", dep=T)

➔ Step2-Data clustering
   o MS.clust : open a window
   o MS.test.clust

➔ Step3-Export to ARISTO or NIST
   o MSeasyToARISTO : open a window
   o MSeasyToMSP
   o SearchNIST

➔ Demonstration
   See below

Button details:

Submit buttons: launch MSeasy functions
Cancel buttons: close pop up
Reset buttons: reset parameters to default values

Quit buttons:
   To quit MseasyTkGUI without leaving R press the "Cancel" button.

   To quit R AND save your session information press "Quit R (save)" button.

   To quit R without saving your session information click on "Quit R (don't save)" button.

How to use "Demonstration"

By clicking on the "Demonstration" button (or via the Menu➔ Demonstration…) you can test the MSeasy functions on reduced Data sets ("Data_testclust","Agilent_quantF_MSclust","Agilent_quantT_MSclust","ASCII_MSclust") or on example files (raw Agilent files (Agilent_MSDataCreation) or raw ASCII files (ASCII_transASCII)).For details see MSeasy help files.

On the pop up windows the mains parameters are already filled and the only thing to do is to click on the submit button (except for MS.clust). For MS.clust you have to fill up the drop down lists (Figure 3).

All demonstration data sets are loaded automatically when you press the "Demonstration" button. So, you can easily access them by using the "Set" button generally situated on the top of the prompt windows.

FIGURE3: MS.CLUST DEMONSTRATION WINDOW

Help files

An easy way to access to the help files (for MSeasy and for MSeasyTkGUI) is to *Right-click* on the button to get help.

Example: A right-click on the "Step1- Ms Data formatting" button opens the help file for the MSeasy function MS.DataCreation.

On several windows help files can be accessed by clicking on the "*Question Head*".

or CDF or mzXML files exemple see MSeasy web site http://sites.google.com/site/rpackagemseasy/