

Manual for the



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Type Package

Title MSeasy Tcl/Tk Graphical User Interface

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Depends R (>= 2.13.0), MSeasy, tcltk

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

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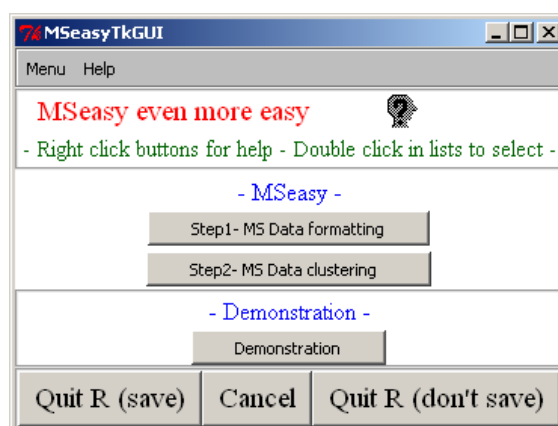


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Installation

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))

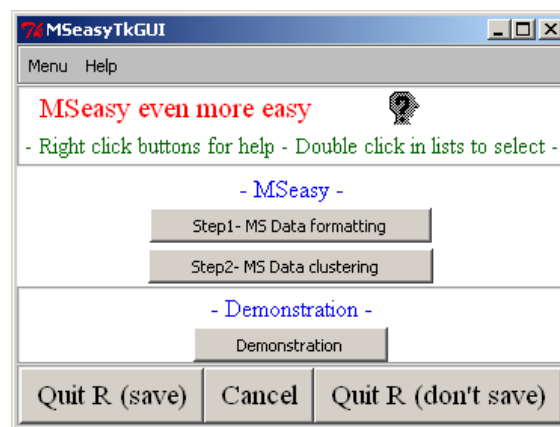
Starting MSeasyTkGUI

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
MS.DataCreationCDF
trans.ASCII
MS.test.clust
MS.clust

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:

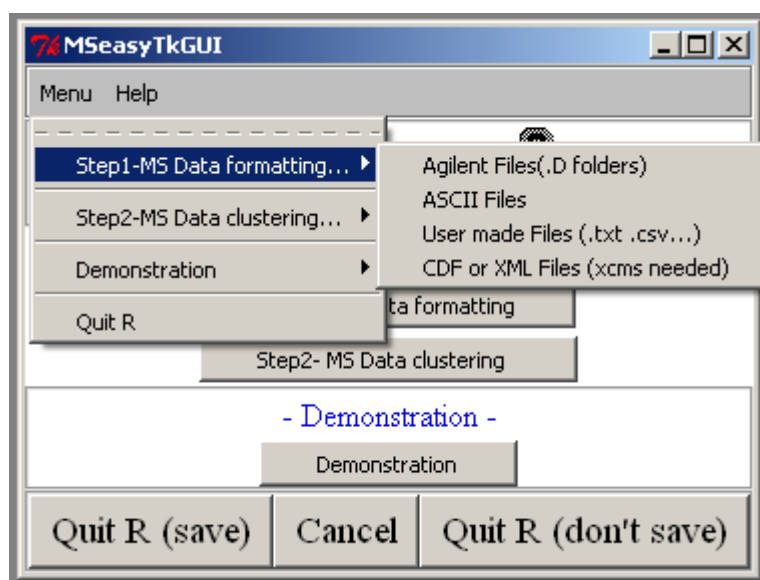


FIGURE1: MSeasyTkGUI MENU

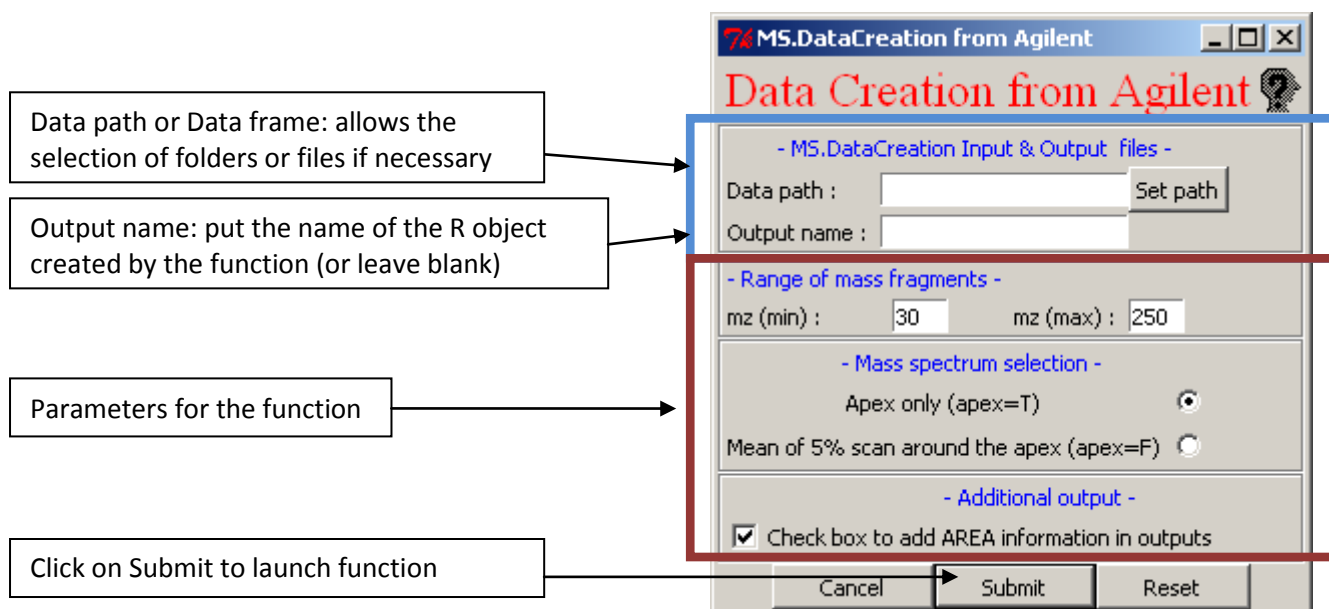


FIGURE2: EXAMPLE OF WINDOW

- From the buttons

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

Menu details:**→ Step1-Data formatting**

- Agilent Files (.D folders) : creates a MSeasy data file from Agilent GC-MS files
- ASCII Files: creates a MSeasy data file from GC-MS files in ASCII format
- 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)
- CDF or XML Files (xcms needed): creates a MSeasy data file from Agilent GC-MS files With raw data in CDF or XML format rather than export3D.CSV. You need XCMS package.

→ Step2-Data clustering

- MS.clust : open a form window with all the MS.clust function parameters/options. Once the form completed press OK and the MSeasy MS.clust function is launched. For details on MS.clust function see MSeasy help files (or click on Menu/Help/MS.clust)
- MS.test.clust: open a form window with all the MS.test.clust function parameters/options. Once the form completed press OK and the MSeasy MS.test.clust function is launched. For details on MS.test.clust function see MSeasy help files (or click on Menu/Help/MS.test.clust)

→ 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.

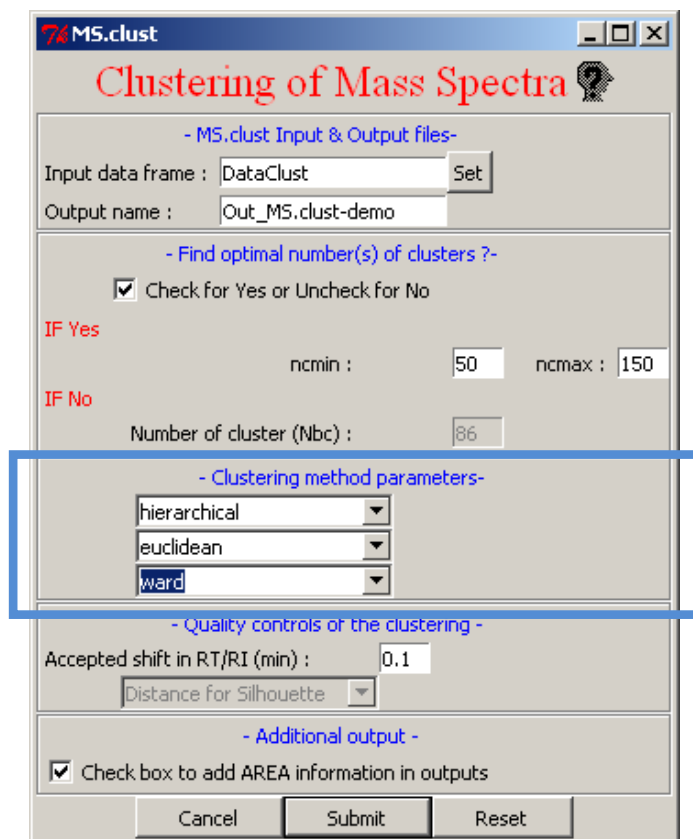


FIGURE3: MS.CLUST DEMONSTRATION WINDOW

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”.



For CDF or mzXML files exemple see MSeasy web site