

SMolESY_platform

INSTALLATION GUIDE

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1. Installing/Running NMRpQuant

i) Installing/running NMRpQuant by MATLAB

After downloading the Github repo folder from <https://github.com/pantakis/NMRpQuant>, open the “Set Path” dialog window from MATLAB (Fig. 1):

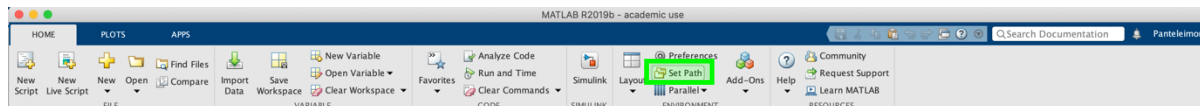


Figure 1.

and in the popped-up window choose the option “Add with Subfolders...” (Fig. 2) and select the parent folder, which contains all the MATLAB code of the GUI, and click “save”.

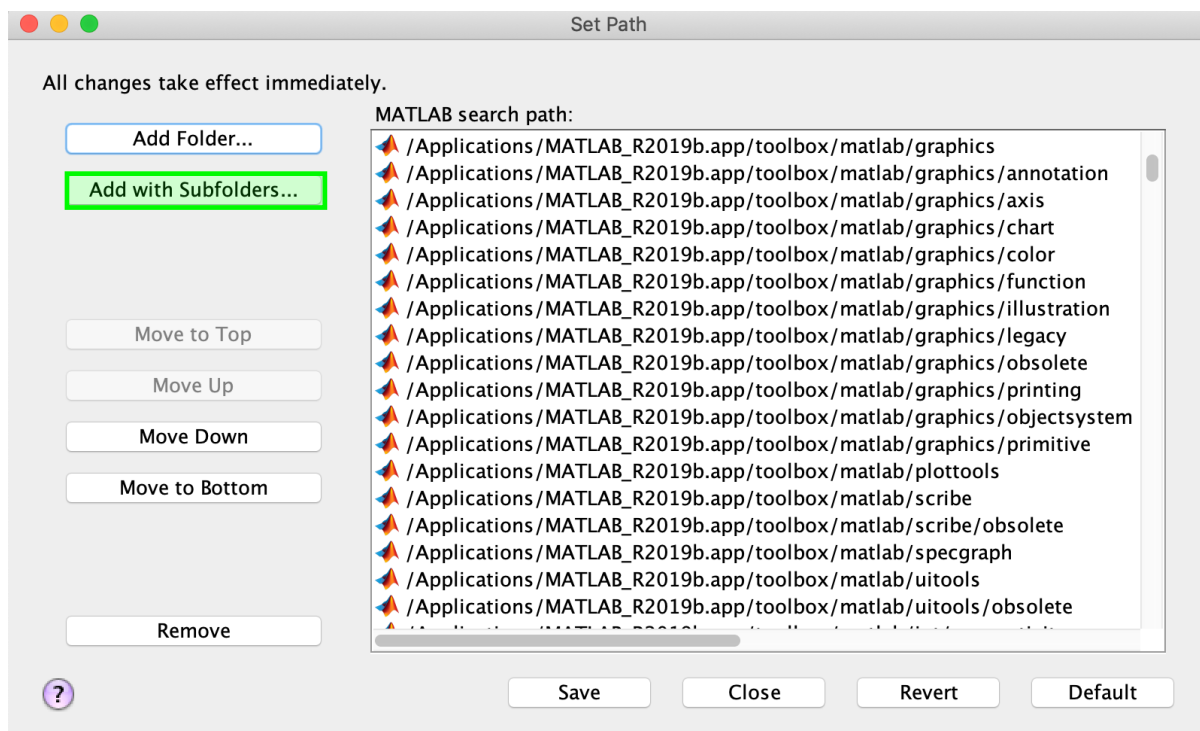


Figure 2.

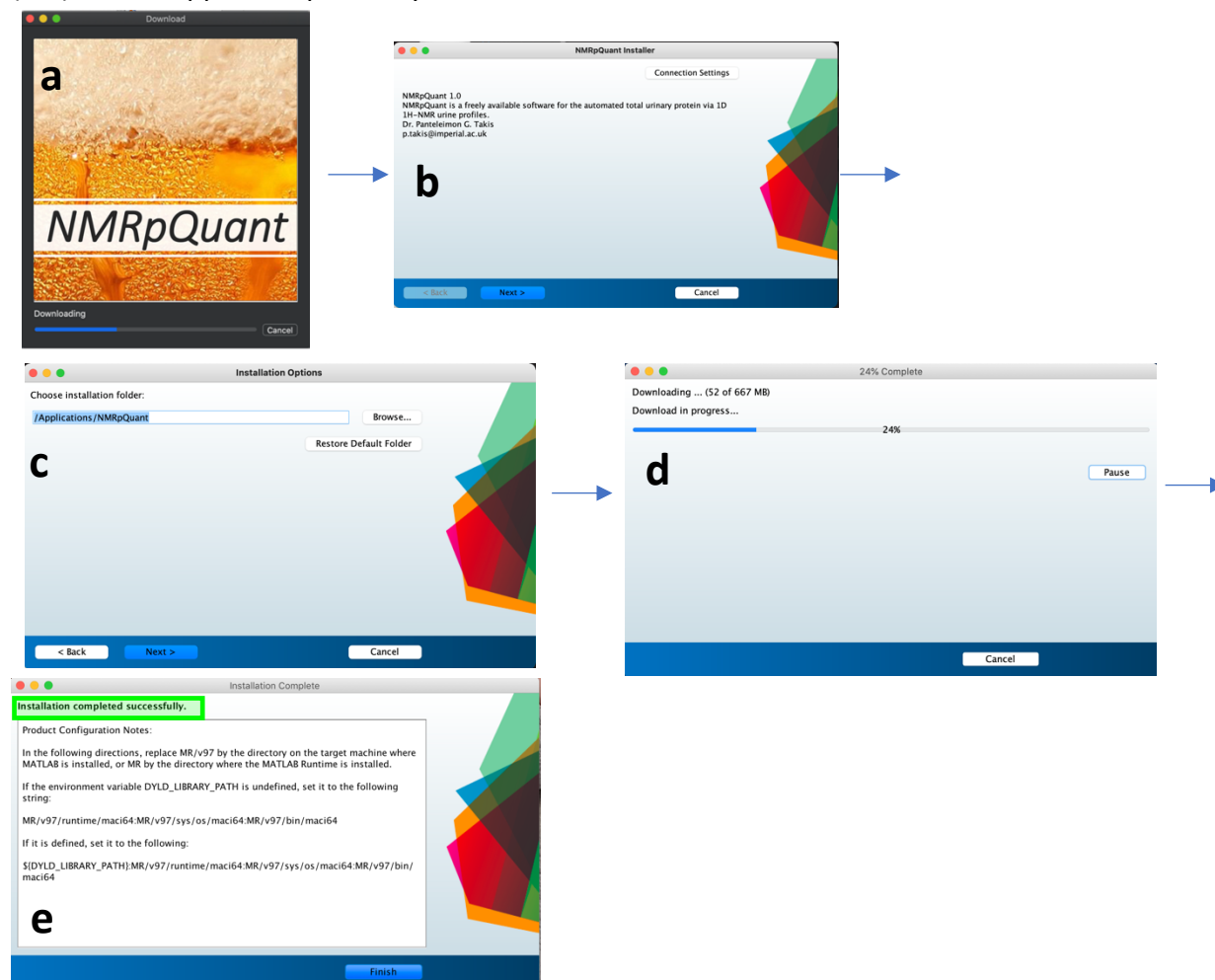
Finally, from the MATLAB command window type: “NMRpQuant” and press “Enter” to launch the GUI (Fig. 3).



Figure 3.

ii) Installing/running NMRpQuant by the compiled file for macOS

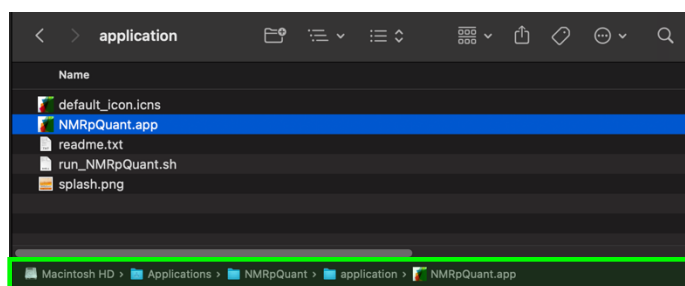
After downloading the Github repo folder from <https://github.com/pantakis/NMRpQuant>, in the folder “**Compiled_for_MAC_OS**”, double click the file “**NMRpQuant_installer.app**”. Then follow the on-screen instructions (internet connection is required) for downloading/installing the MATLAB RUNTIME modules in order to run the software. The following dialog windows (**a-e**) should appear sequentially on screen:



→ In panel **c**, please ensure that the installation folder is: **/Applications/NMRpQuant**

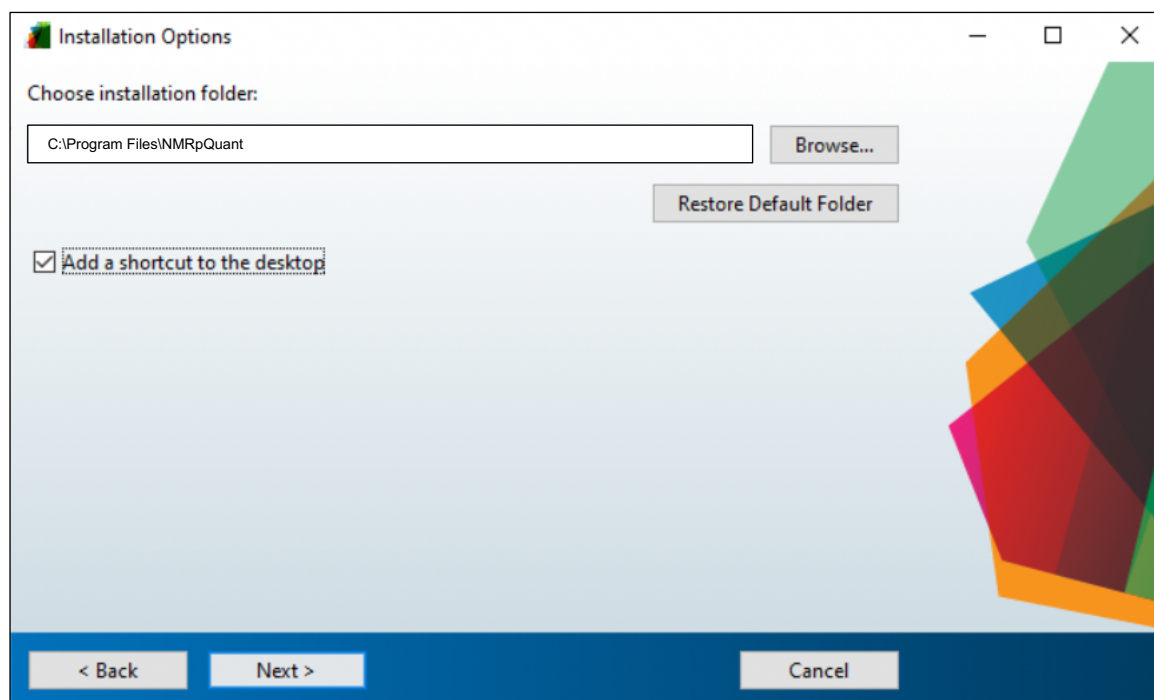
→ In panel **e**, ignore the Product Configuration Notes, once the installation is completed successfully.

→ **To launch** the application please double-click the “**NMRpQuant.app**”, which should be located in the folder: “**./Applications/ NMRpQuant /application**”, as you could see below:



iii) Installing/running NMRpQuant by the compiled file for Windows

After downloading the Github repo folder from <https://github.com/pantakis/NMRpQuant>, in the folder "Compiled_for_Windows", double click the file "NMRpQuant_installer.exe". Then follow the on-screen instructions (internet connection is required) for downloading/installing the MATLAB RUNTIME modules in order to run the toolbox as indicated above (i.e. for macOS). Please ensure that you create a desktop shortcut of the toolbox in order to launch it as shown below:



2. User Guide NMRpQuant

For extra details about how to operate the software please look at the Supplementary Material of the corresponding published research.