

MetaboQuant

A tool allowing accurate quantification from NMR spectra including outlier detection. The tool comes as executable file for Windows and as Matlab code.

MetaboQuant is a tool developed by Matthias S. Klein that allows reliable quantification from nuclear magnetic resonance (NMR) spectrum peak integrals by using individual calibration factors for each peak. Additionally, several outlier detection methods have been implemented to exclude overlapped and corrupted peaks from quantification. Detailed information about MetaboQuant can be found in the manual that is included in the file *MetaboQuant.zip* (to be found in the *Download* section).

System Requirements

MetaboQuant may be run as stand-alone application using the following operating systems:

- Windows (Windows 2000 or newer)

On other operating systems such as Linux or Mac OS, you may run MetaboQuant from within Matlab (The Mathworks, Natick, MA, USA). For this you need:

- Matlab version 7.1.0.246 (R14) Service Pack 3 or newer

Installation Instructions

To install MetaboQuant, download the following files from the *Download* section:

- MCRInstallerR2007b.exe
- MetaboQuant.zip.

Run the file *MCRInstallerR2007b.exe* to install the required Matlab run-time routines. Extract the file *MetaboQuant.zip* to a new folder. To run MetaboQuant, double-click on the file *MetaboQuant.exe*. Starting MetaboQuant may take some minutes, as the Matlab run-time environment takes some time to be loaded.

Running MetaboQuant from Within Matlab

Download the following file from the *Download* section:

- MetaboQuant.zip

Extract the file to a new folder.

Start Matlab and change the working directory to the MetaboQuant installation folder, *e.g.* using the command *cd*. To run MetaboQuant, type *MetaboQuant* in the Matlab command line.

Getting Help

For all fields of the main window, a help text is available that will pop up when you hold the mouse cursor over the field.

Additionally, you may want to read the user manual included in the program download file. The manual is also to be found separately in the *Download* section.

Download

The current version of MetaboQuant can be downloaded here:

http://genomics.uni-regensburg.de/software/NMR/MetaboQuant_1.3.zip

You will need to install the Matlab R2007b runtime environment to be able to use MetaboQuant:

<http://genomics.uni-regensburg.de/software/NMR/MCRInstallerR2007b.exe>

The manual can be downloaded here (is also part of the MetaboQuant .zip file):

<http://genomics.uni-regensburg.de/software/NMR/manual.pdf>

A urinary spike-in data set of eight 1D 1H and 1H-13C HSQC spectra was prepared for testing MetaboQuant quantification performance. It can be downloaded here in Bruker format. The .zip file also contains the parameters for repeating our measurements on a 600 MHz Avance III spectrometer. Also, peak integrals and MetaboQuant input and output files are included in the .zip file.

http://genomics.uni-regensburg.de/software/NMR/Latin_Square.zip

Archive

Older versions of MetaboQuant can be found below, although these versions may contain bugs. It is strongly recommended to only use the current version found above. Please note that until version 1.2, MetaboQuant was named QUANTIFY.

http://genomics.uni-regensburg.de/software/NMR/MetaboQuant_1.2.zip

http://genomics.uni-regensburg.de/software/NMR/QUANTIFY_1.1.1.zip

http://genomics.uni-regensburg.de/software/NMR/QUANTIFY_1.1.zip

http://genomics.uni-regensburg.de/software/NMR/QUANTIFY_1.0.zip

A urinary spike-in data set of eight HSQC spectra was prepared for testing quantification performance. It can be downloaded here in Bruker format. The .zip file also contains a parameter set for repeating our measurements on a 600 MHz Avance III spectrometer.

http://genomics.uni-regensburg.de/software/NMR/MetaboQuant_Latin_Square_2012.zip

The input and output files (peak integral and concentration values) of the above spike-in data set can be found in the following .zip file:

http://genomics.uni-regensburg.de/software/NMR/Input_and_Output_Files_Latin_Square.zip