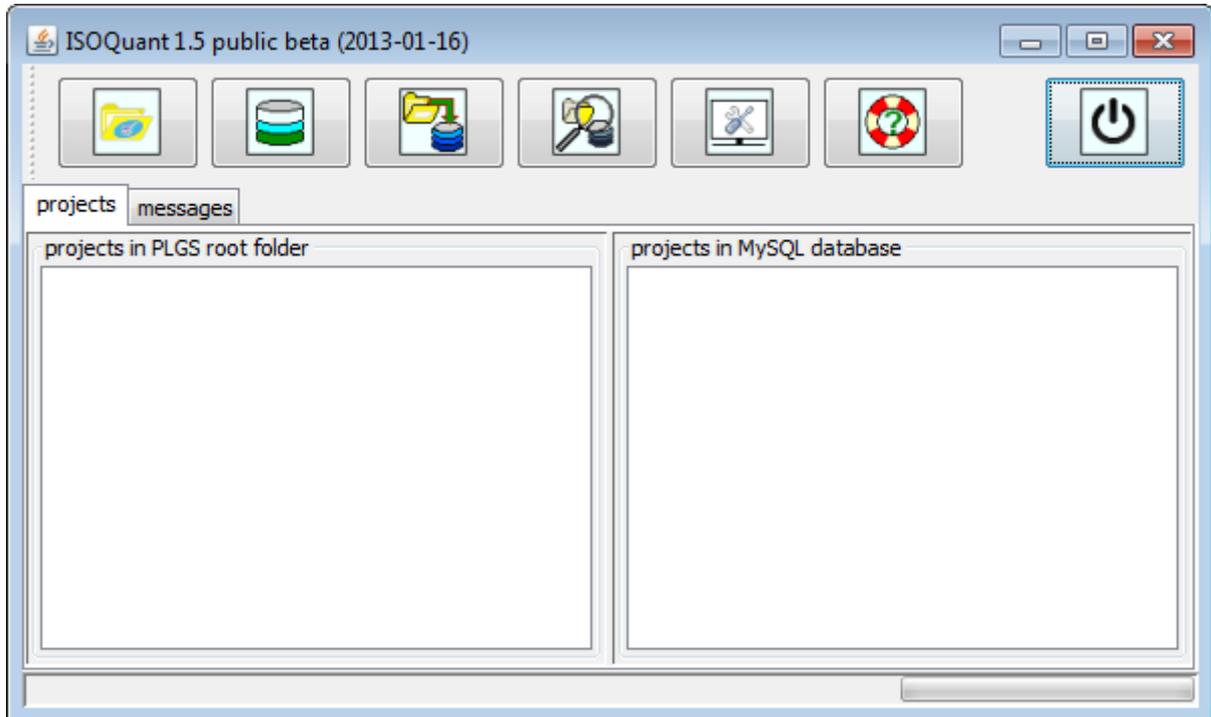


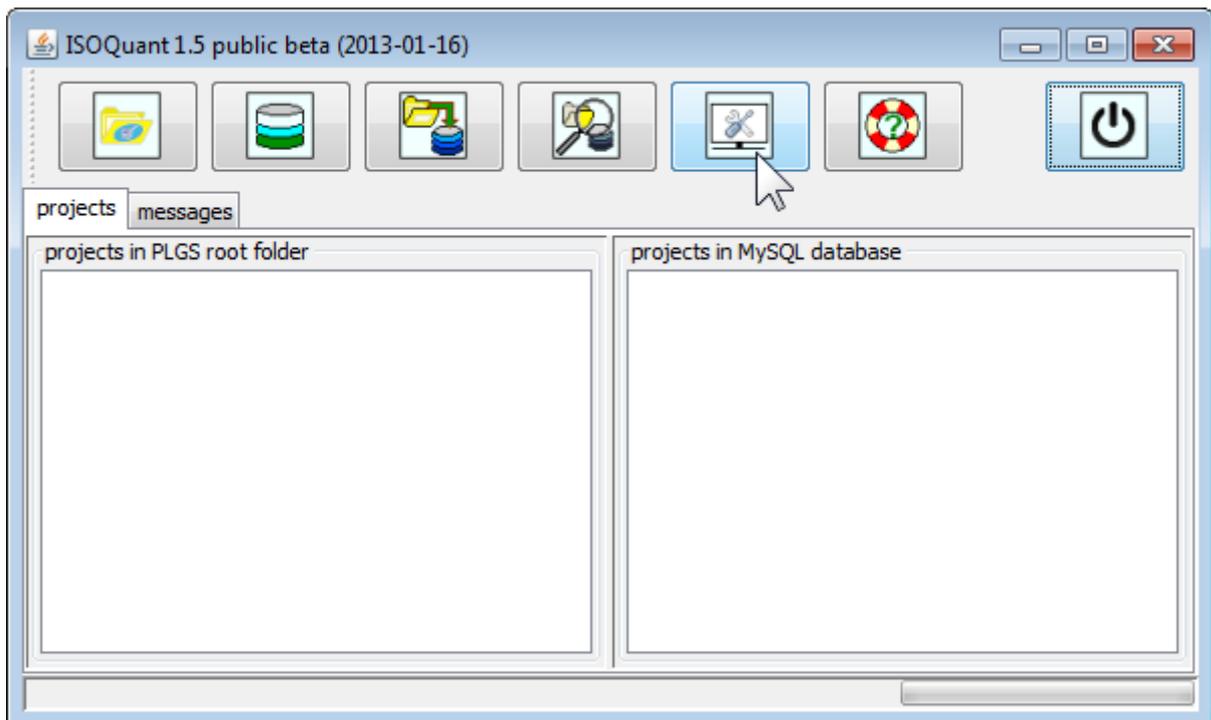
ISOQuant application basic usage instructions

Start ISOQuant application e.g. by double-clicking ISOQuant program icon.

Main window will appear.

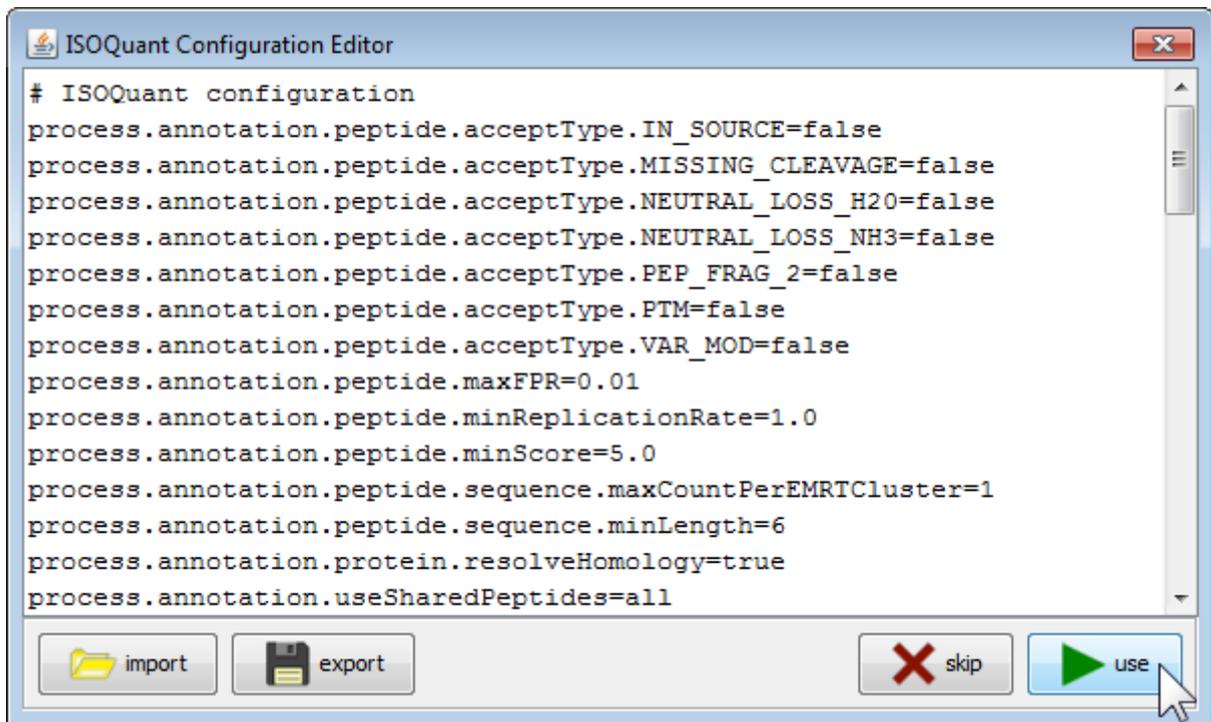


click „configuration“ button (with screwdriver and wrench icon) to start configuration editing.



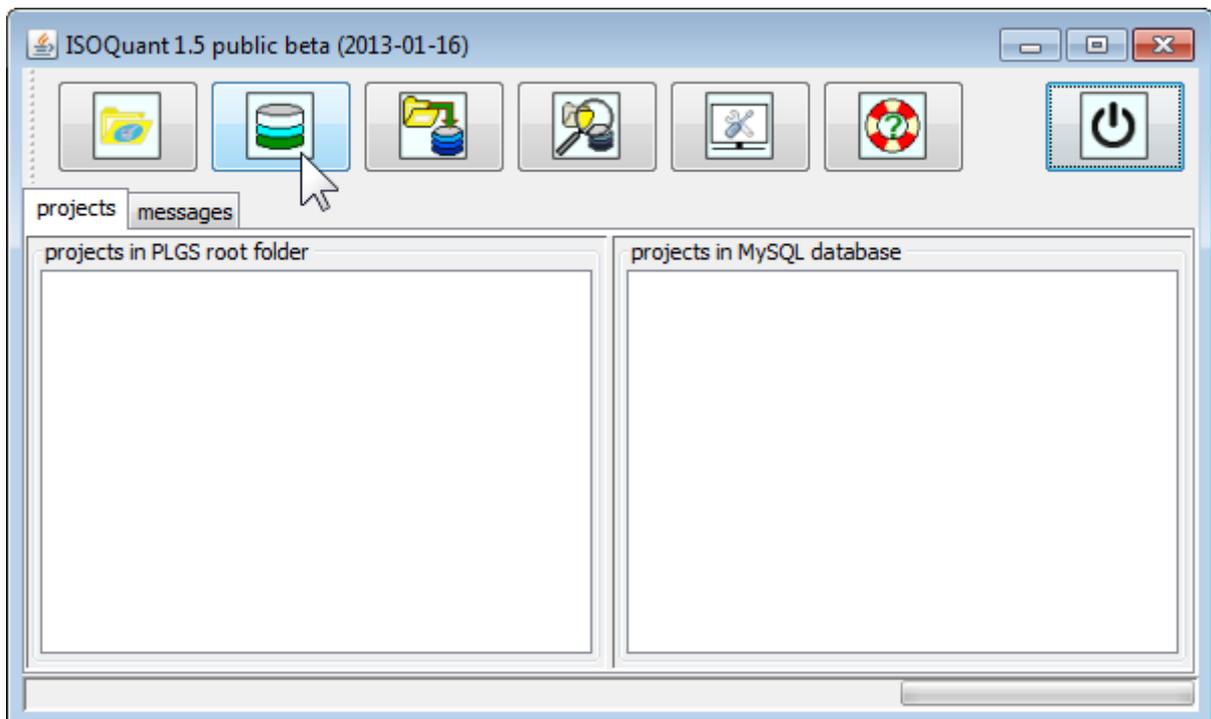
Configuration Editor window will appear.

Adapt configuration parameters on your needs and finish editing by clicking „use“ button.



Main window will appear.

To connect to a MySQL database click on „database“ button.



type your MySQL connection data into proper fields and click „ok“.

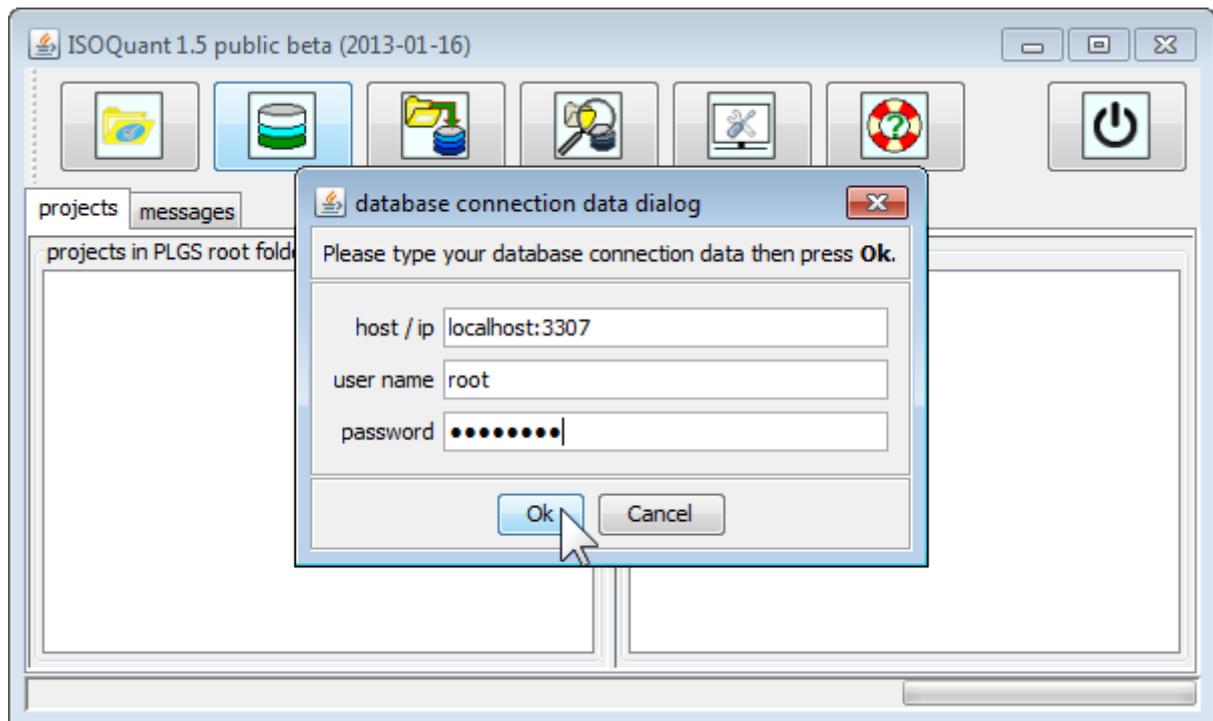
Please refer to connection data defined during MySQL installation. In case of default XAMPP Installation on a local PC, the proper connection data is:

Host: localhost

User name: root

Password:

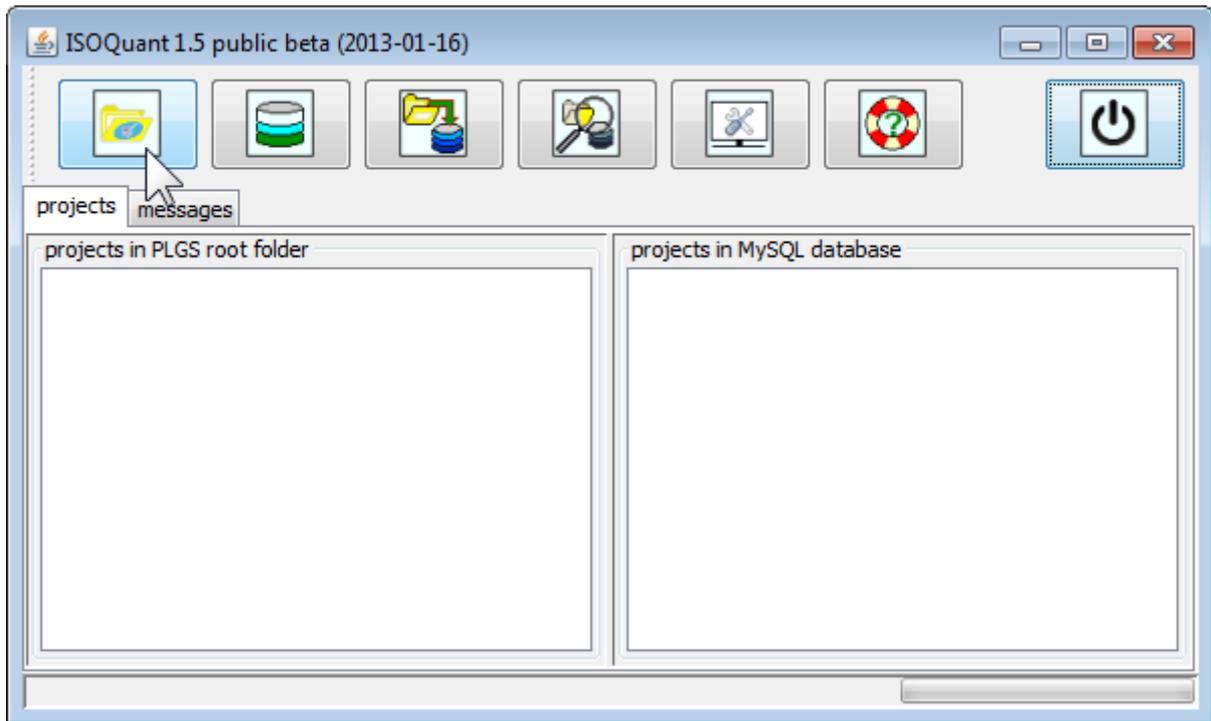
(that means, the password field remains empty)



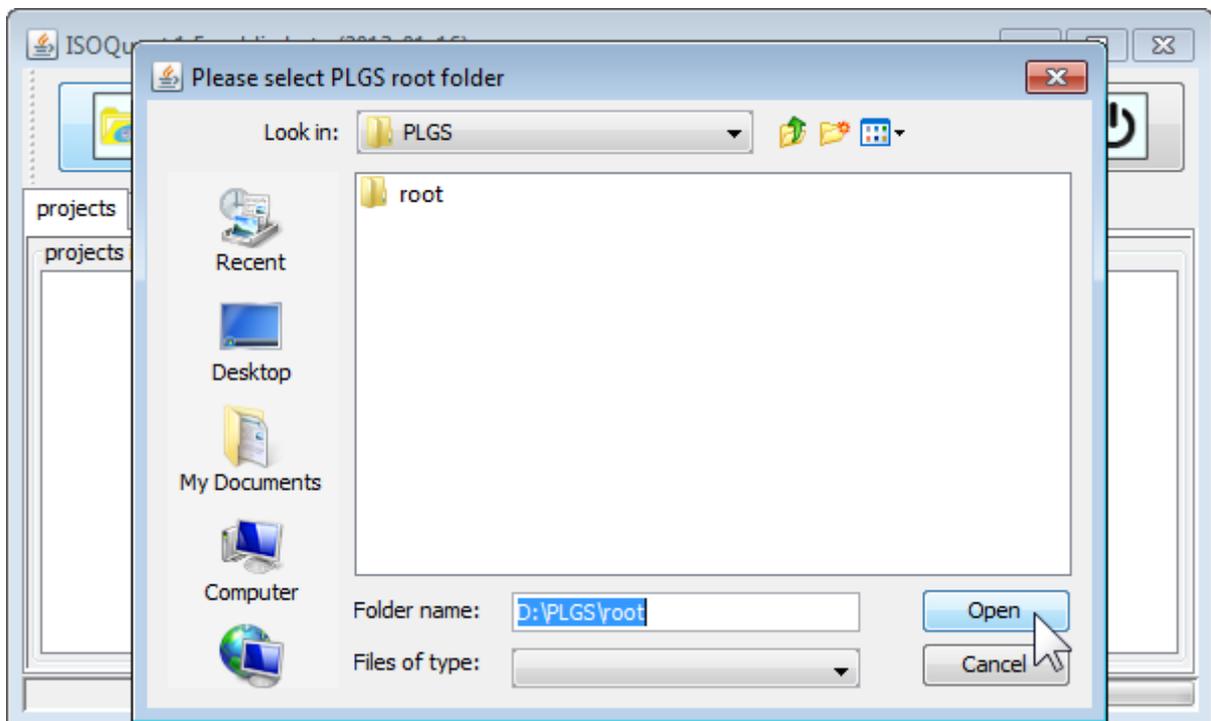
After first time successfully connecting a MySQL database ISOQuant will create the required database structures and store connection data for future usage.

In case the database already contains processed ISOQuant projects, they will be listed inside of “projects in MySQL database” pane of main window.

To start PLGS root folder selection, click on „PLGS root folder“ button



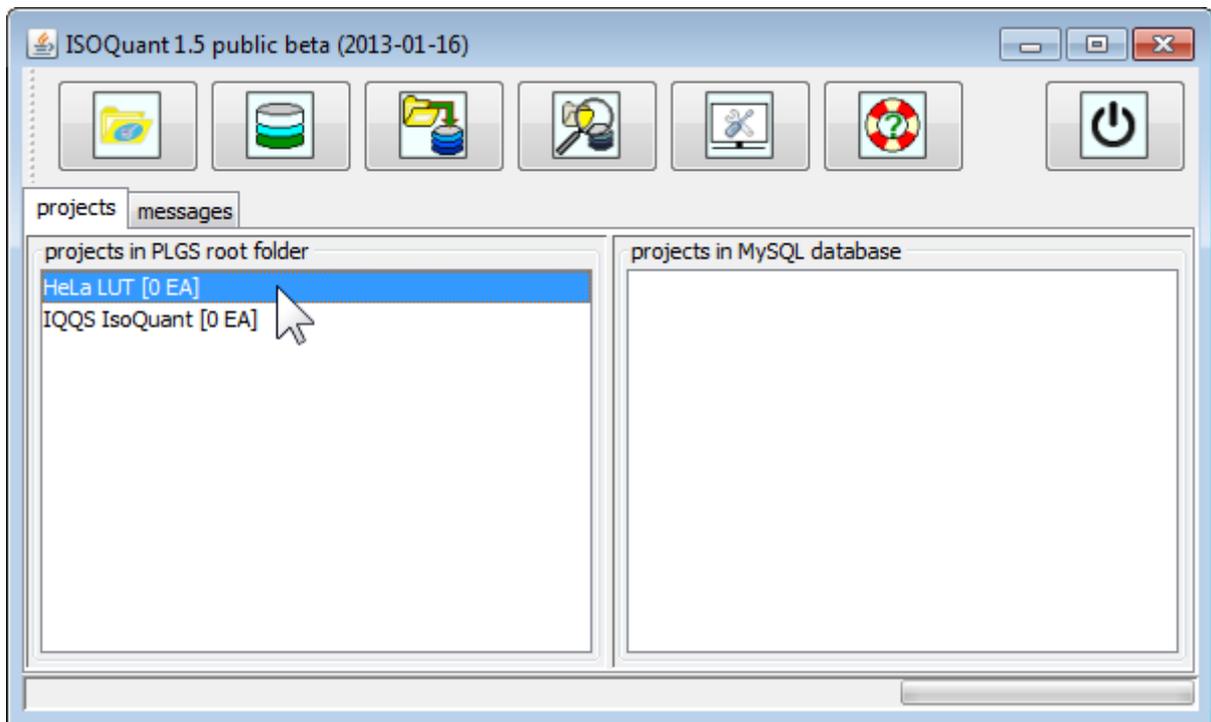
Select your PLGS root folder, this folder is typically located inside of PLGS installation folder, e.g. D:\PLGS\root



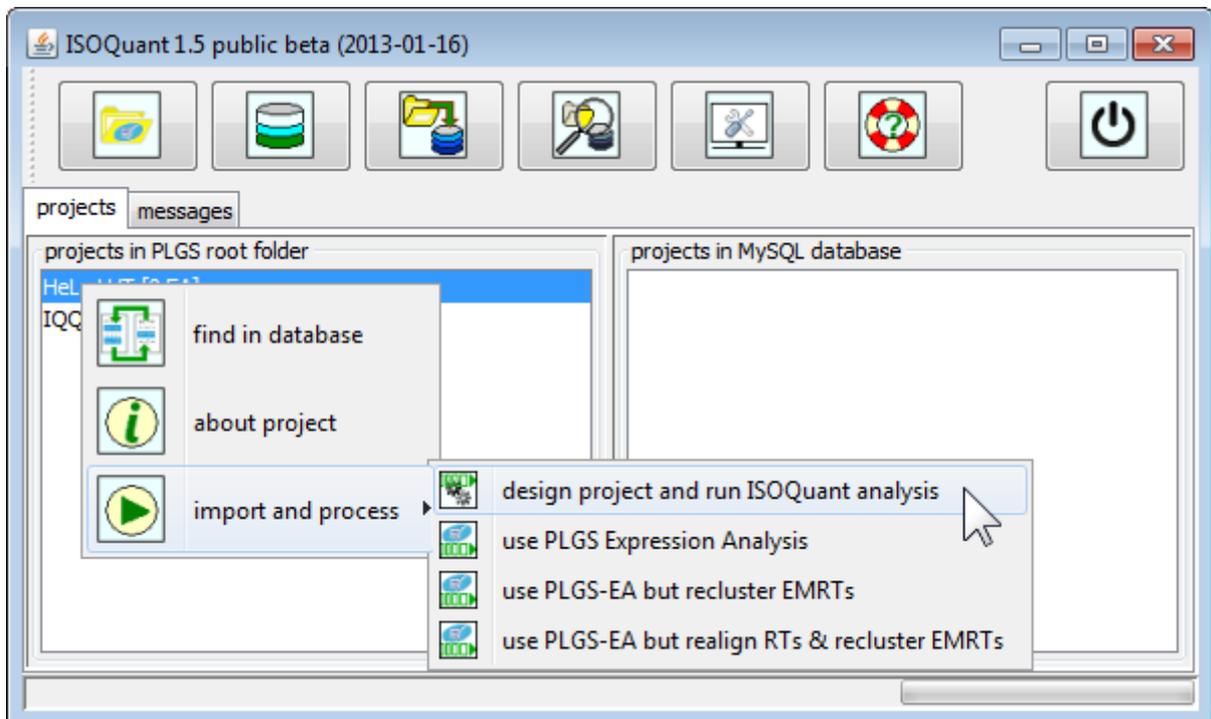
After first time successfully choosing a PLGS root folder, ISOQuant will store its location for future usage.

ISOQuant will list Projects found in selected PLGS root folder on the left side of main window in the pane labeled „projects in PLGS root folder“.

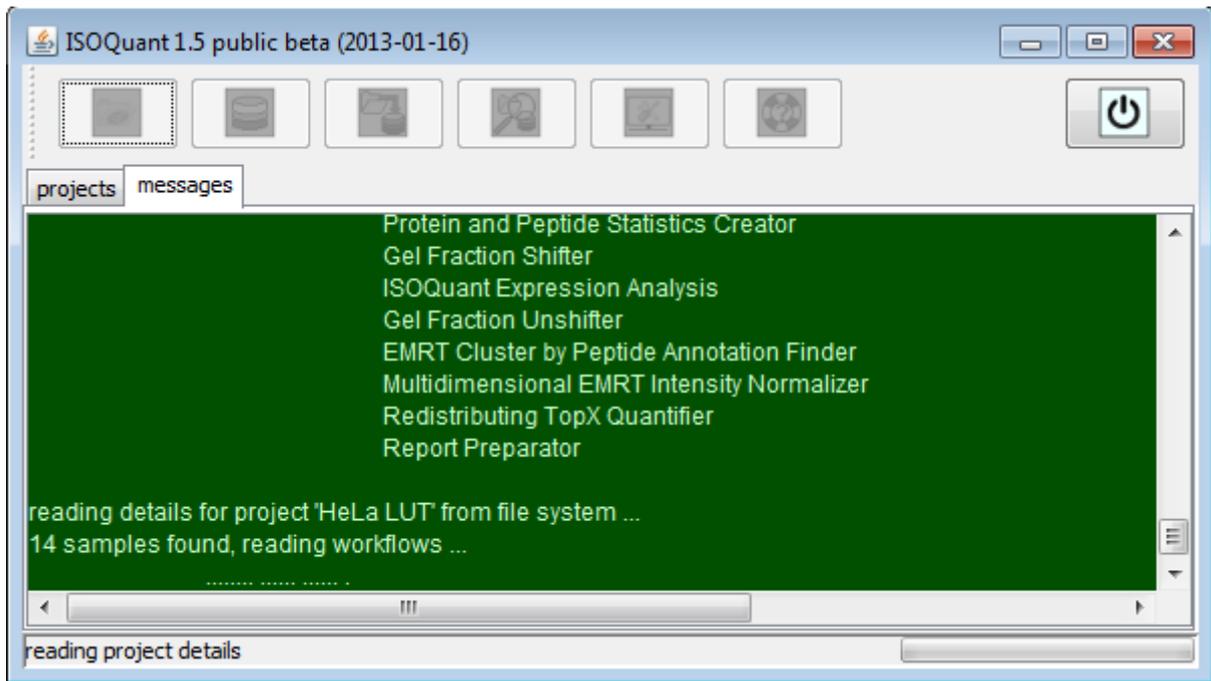
Select a project of your choice from this list.



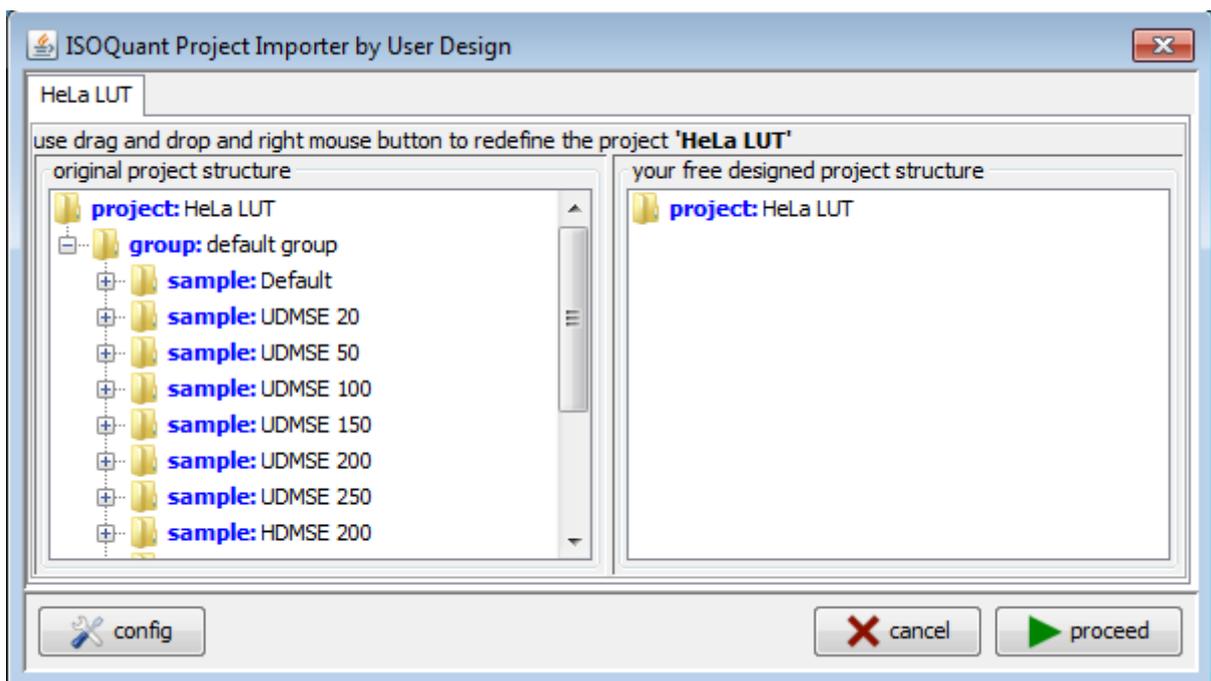
After right clicking selection, a context menu will appear.



Select “design project and run ISOQuant analysis” submenu item from “import and process” context menu item.

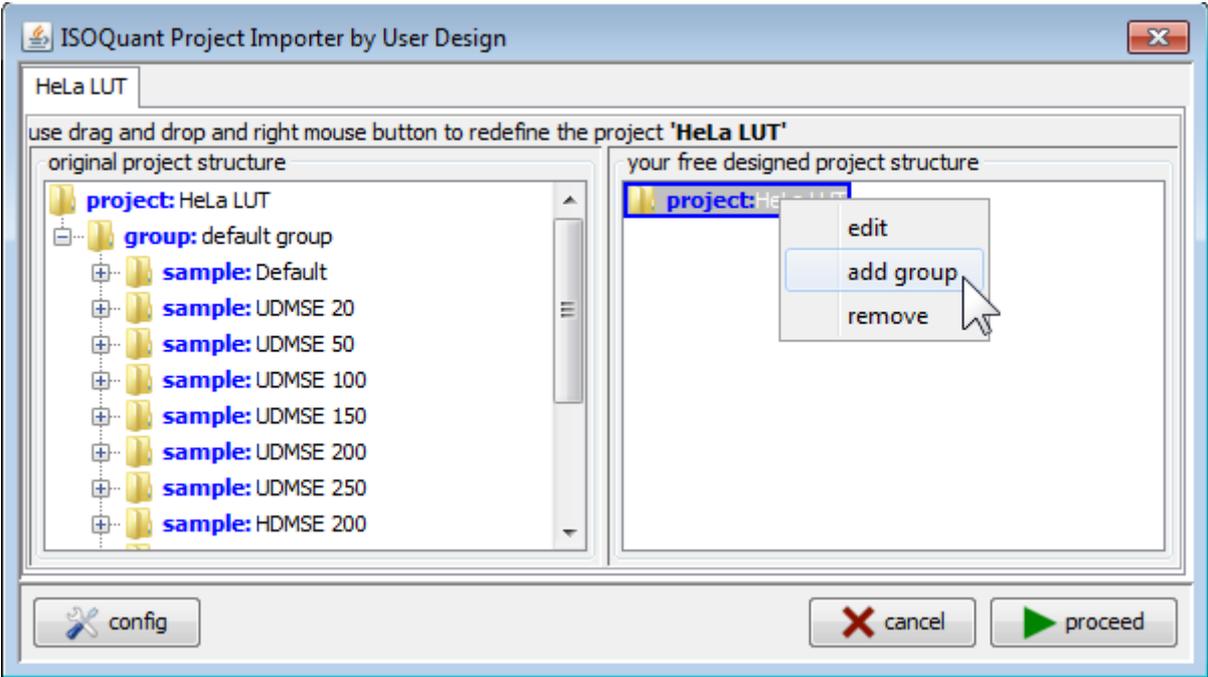


Next, ISOQuant will automatically read and show PLGS project structure in Project Designer window:

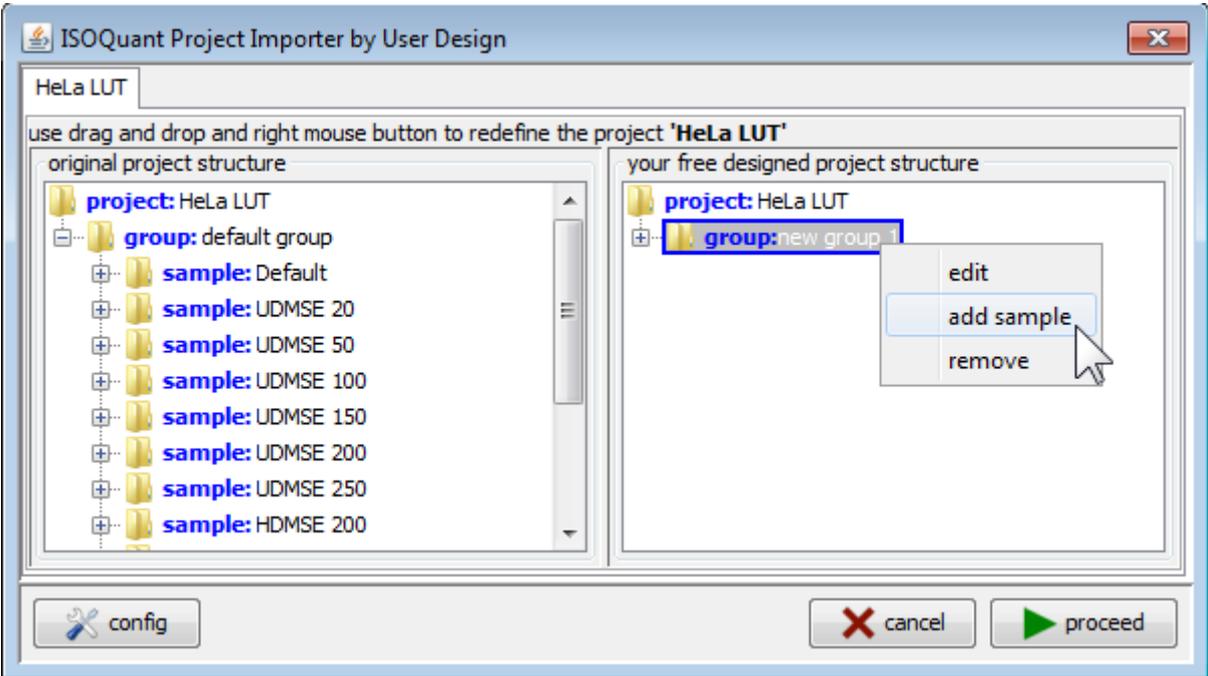


Project Designer window contains the original PLGS project structure on the left and user designed project structure on the right.

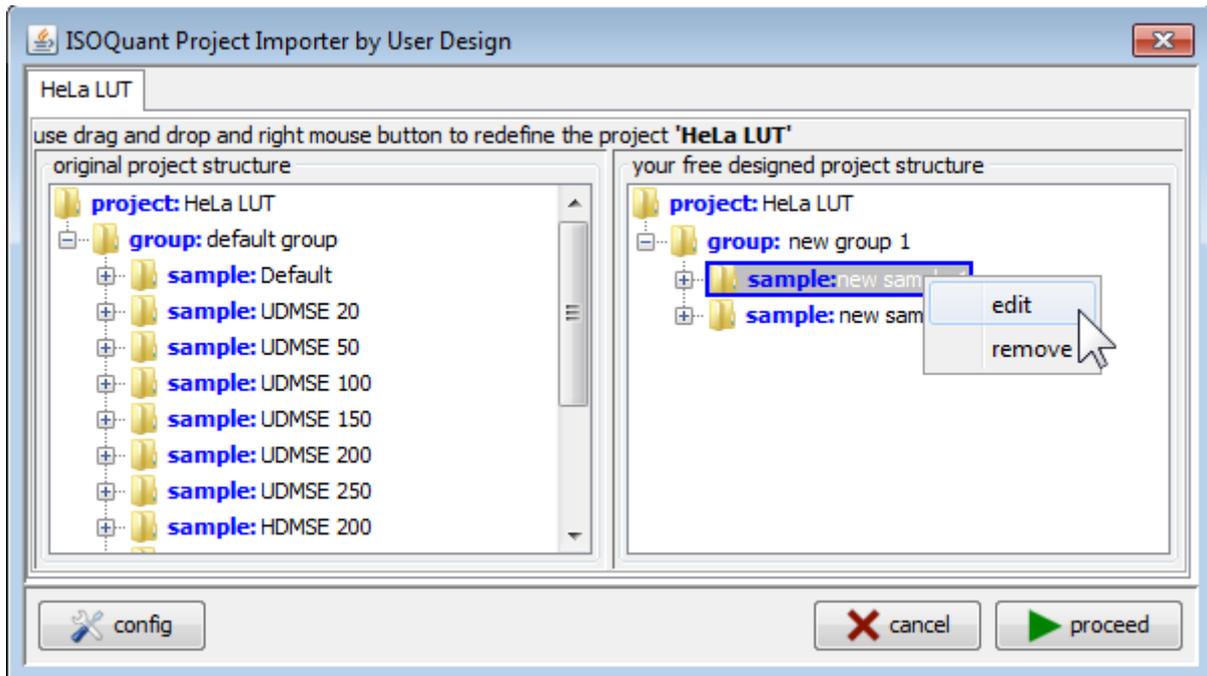
Right clicking objects on the right will show context menu enabling creation of user defined hierarchical project structure.



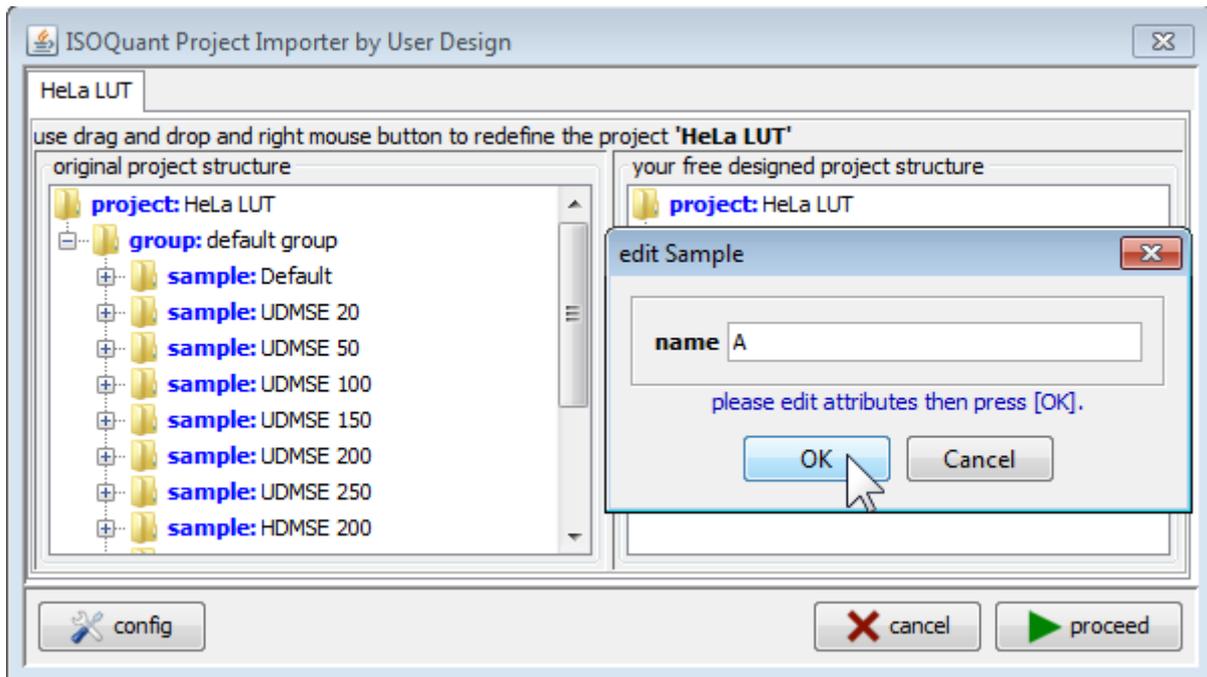
Sample groups and samples may be either created manually or by “drag and drop” elements from the original project structure.



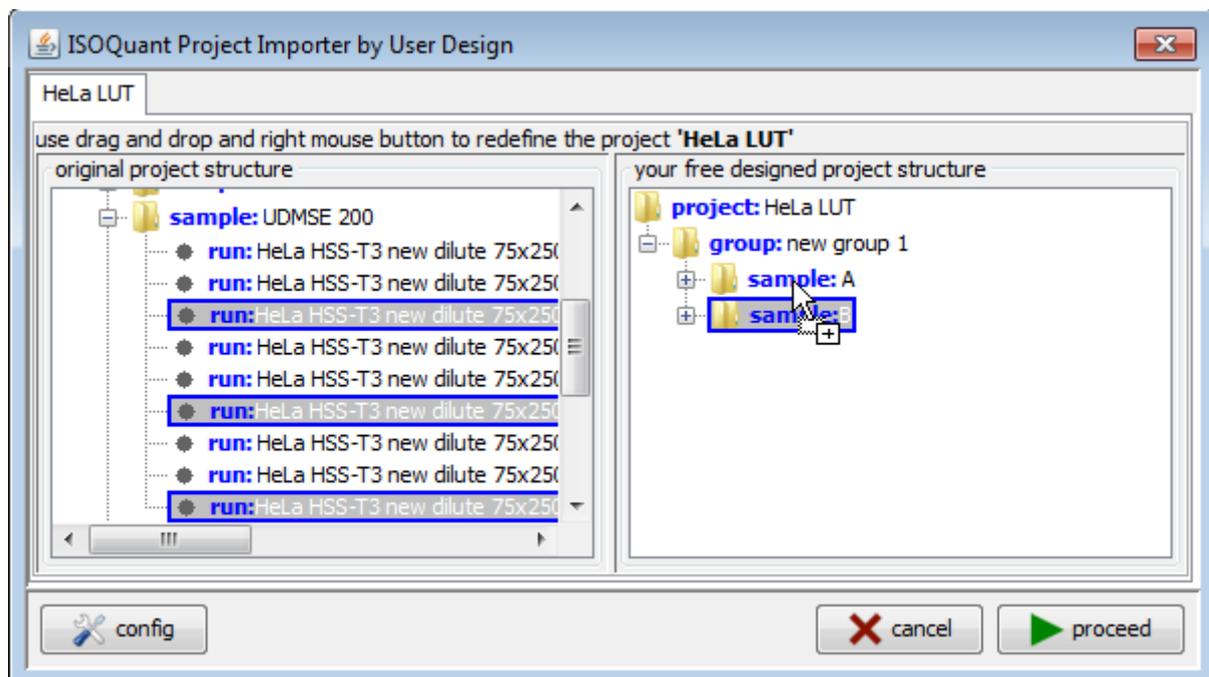
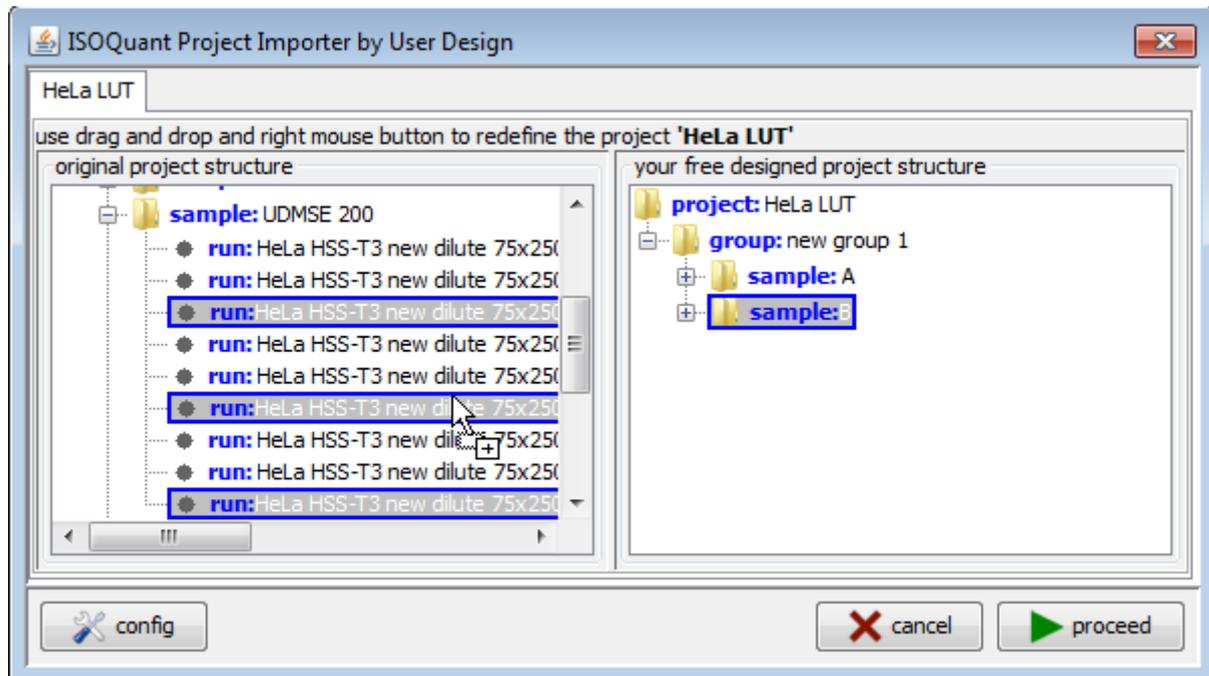
Created elements can be edited



enabling the assignment of user defined names to groups or samples.



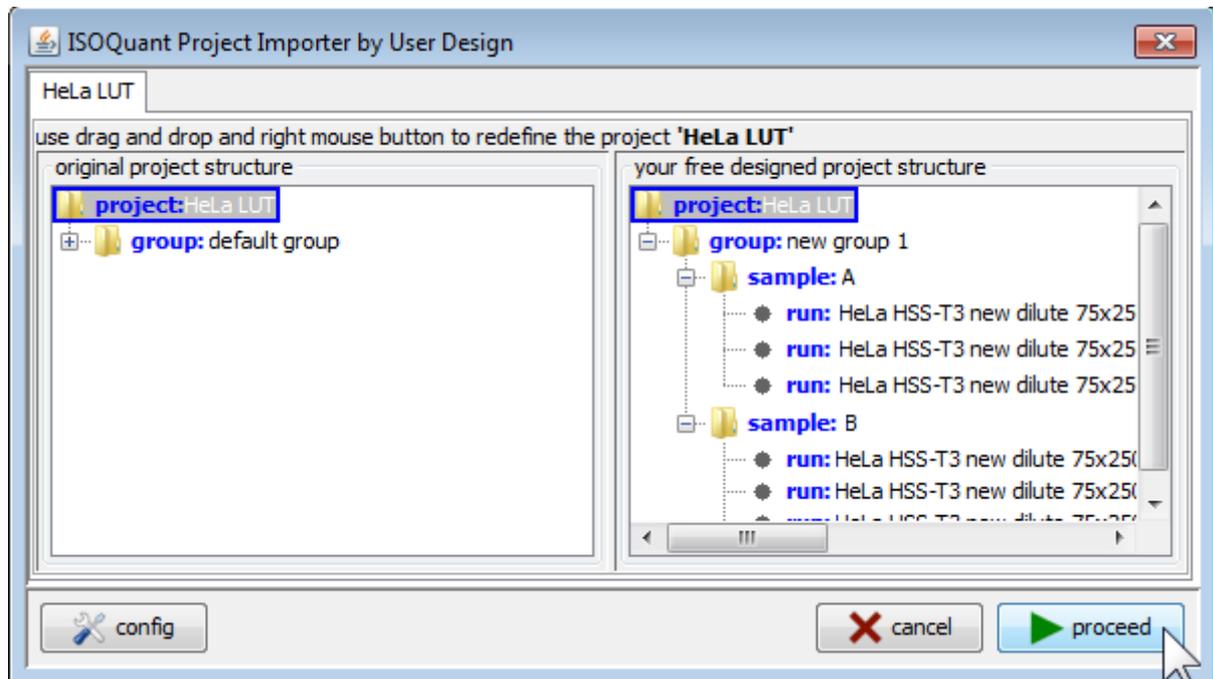
After creating target project structures, just drag and drop LC-MS runs from the original PLGS project to the target project.



carefully check:

- designed project contents ...
(wrong project structure will make difficult to interpret results)
- current ISOQuant configuration ...
(clicking config button will show ISOQuant configuration editor window)

and click button “proceed” to start processing designed project.

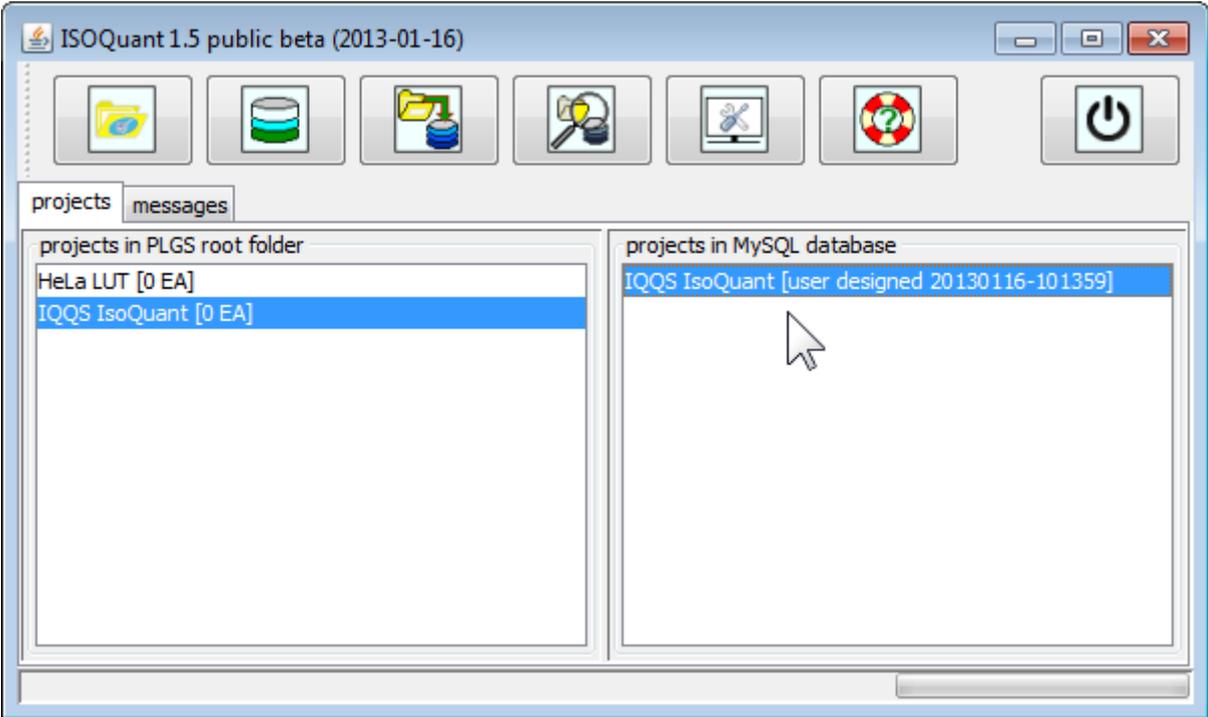


ISOQuant will start processing data.

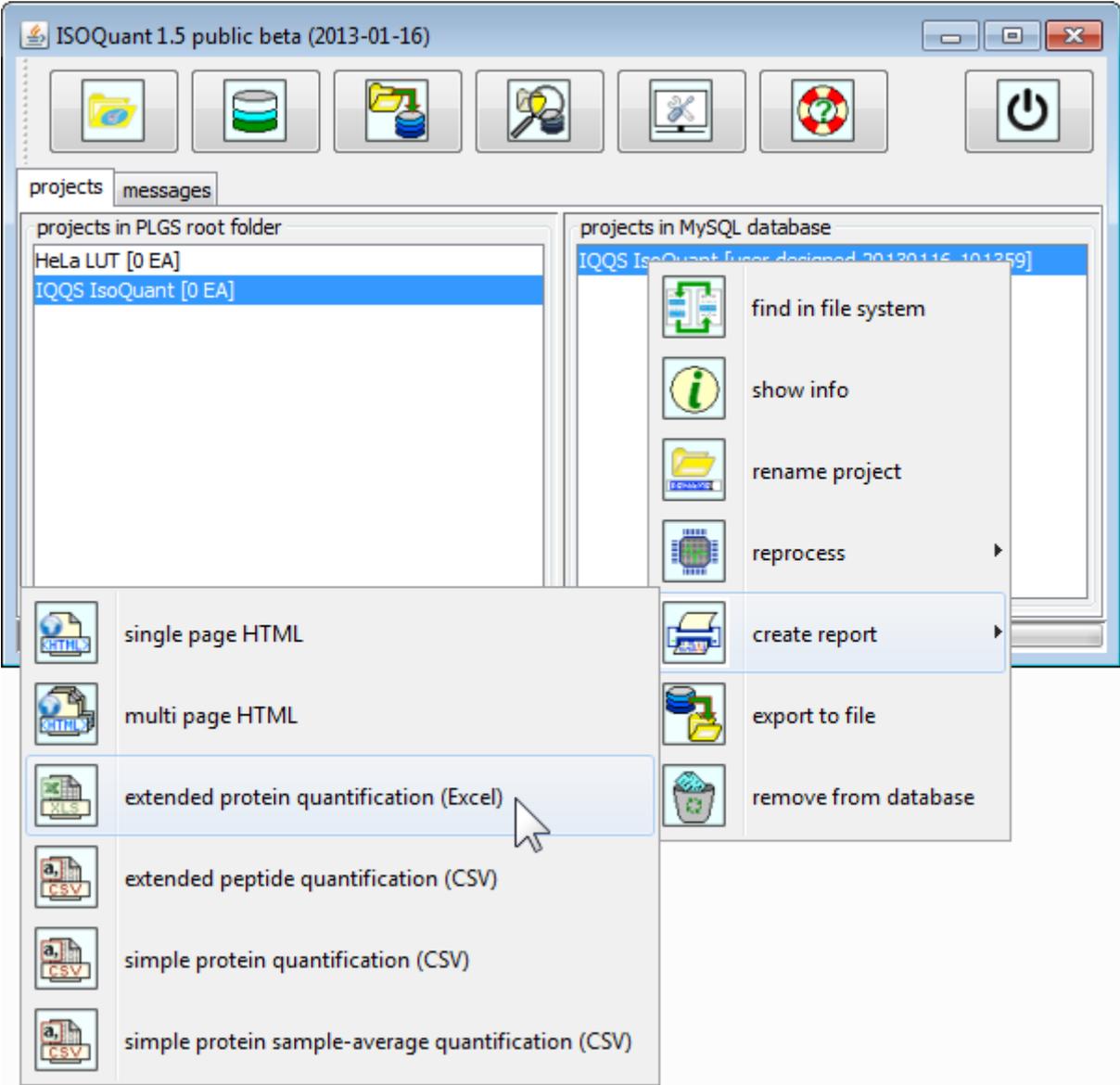
Processing duration mainly depends on database and host PC system performance and also project size and complexity.

ISOQuant will include processed projects inside of “projects in MySQL database” pane.

Select a project and right click it.



Context menu will appear, select "create report" submenu



from this submenu, selecting one of the report items will start report creation generating chosen reports.

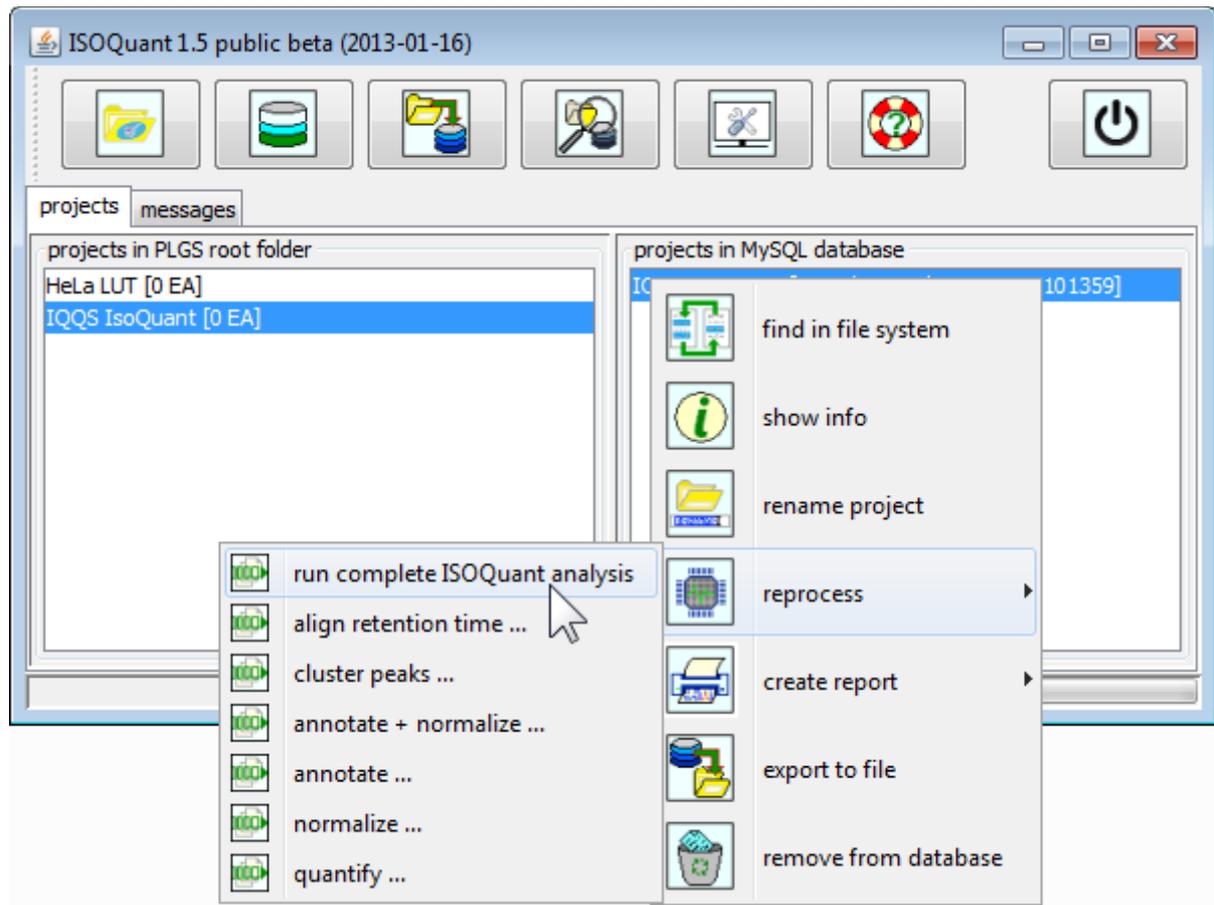
Processed projects may be reprocessed starting from different stage.

This feature is useful if you want to test different ISOQuant settings.

Example: testing other emrt clustering settings:

- adapt clustering settings using Configuration Editor
- select a processed project
- right click it
- select "reprocess" -> "cluster peaks"

ISOQuant will redo all needed processing steps starting from emrt clustering ...



After reprocessing project data, you can recreate reports on your need.