

ISOQuant usage guide

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1 About usage guide

This document describes how to operate ISOQuant.

2 Installation

For installing ISOQuant application, please read ISOQuant installation guide and follow instructions.

3 Purpose of ISOQuant

The basic idea behind ISOQuant is to reduce data analysis time and also to ensure constant analysis quality by automating standard analysis steps applied to LC-MS based label-free proteomics data.

4 Workflow

4.1 Overview

ISOQuant extracts preprocessed data from vendor software (Waters PLGS), and transfers extracted information into a relational MySQL database. Once data is transferred, ISOQuant applies a set of statistical analysis steps to it and reports analysis results in human readable, common file formats.

4.2 Steps

Main workflow contains following steps:

- PLGS root folder selection
- MySQL database connection
- Parameter configuration
- Project selection
- Processing type selection
- Project design or Expression Analysis selection
- Automated processing
- Report creation

5 Workflow steps explained

5.1 PLGS root folder selection

On the main view of ISOQuant, click on ‘select PLGS root folder’ button (figure 1, item 3) to initiate root folder selection. From the appearing folder selection dialog, choose the correct path to PLGS root folder, e.g. C:\PLGS2.4\root. Do not select the PLGS folder, nor one of the project folders inside the root. When you have selected a valid root folder, ISOQuant explores contained projects and shows them as a list inside the projects in PLGS root folder container.

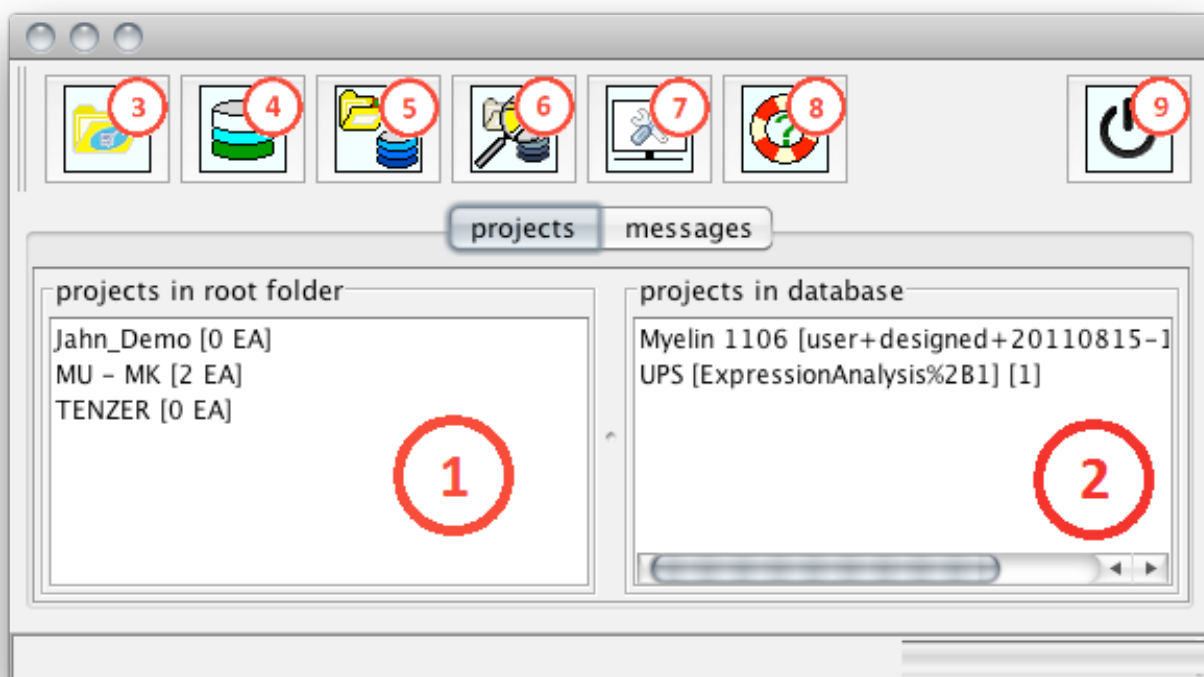


Figure 1: the main view of ISOQuant

5.2 MySQL database connection

On the main view of ISOQuant, click ‘connect database’ button (figure 1, item 4) and type requested accession data into appropriate fields on appearing dialog (figure 2). Once ISOQuant has successfully connected to a MySQL database, it shows a list of previously imported projects inside the projects in MySQL database (figure 1, item 2) container.

5.3 Parameter configuration

The behavior and the appearance of ISOQuant as well as the attributes of its processing steps may be adapted by editing ISOQuant’s configuration file `isoquant.ini`. The easiest way to edit the configuration file is to use the built-in configuration editor (figure 3). Which is accessible from ISOQuant’s GUI by clicking edit configuration button (figure 1, item 7) . Please see ISOQuant configuration guide for detailed explanation of attributes and possible values.

5.4 Project selection

Projects to be processed with ISOQuant may be selected from projects in PLGS root folder container (figure 1, item 1) by left clicking them. Multiple projects could be selected by holding Shift or Control and left clicking them.

5.5 Processing type selection

Right click on selected projects and choose import and process from appearing context menu (figure 4). The appearing submenu offers a set of predefined processing pipelines for processing data in different ways depending on user choice and preprocessing status.

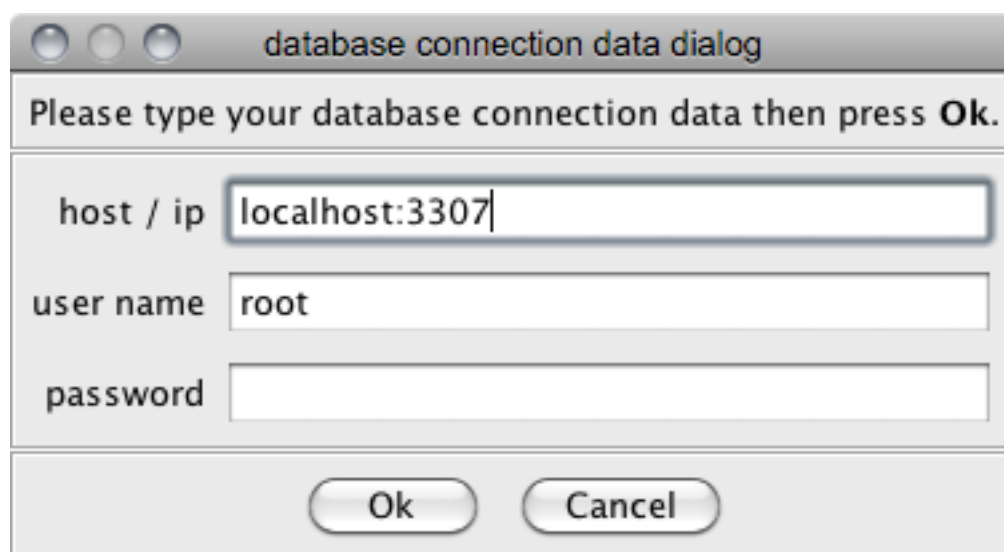


Figure 2: database connection dialog

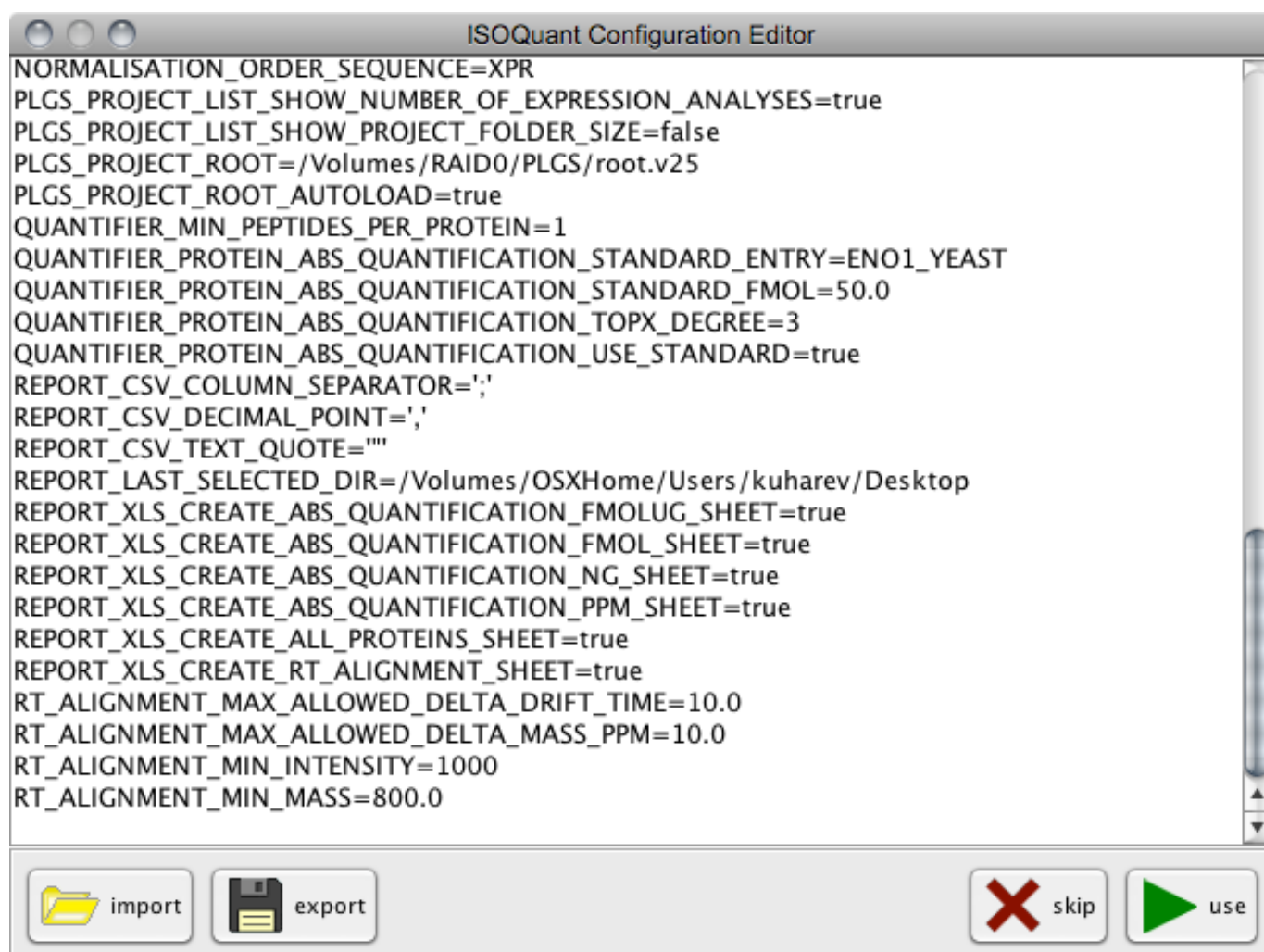


Figure 3: built-in configuration editor

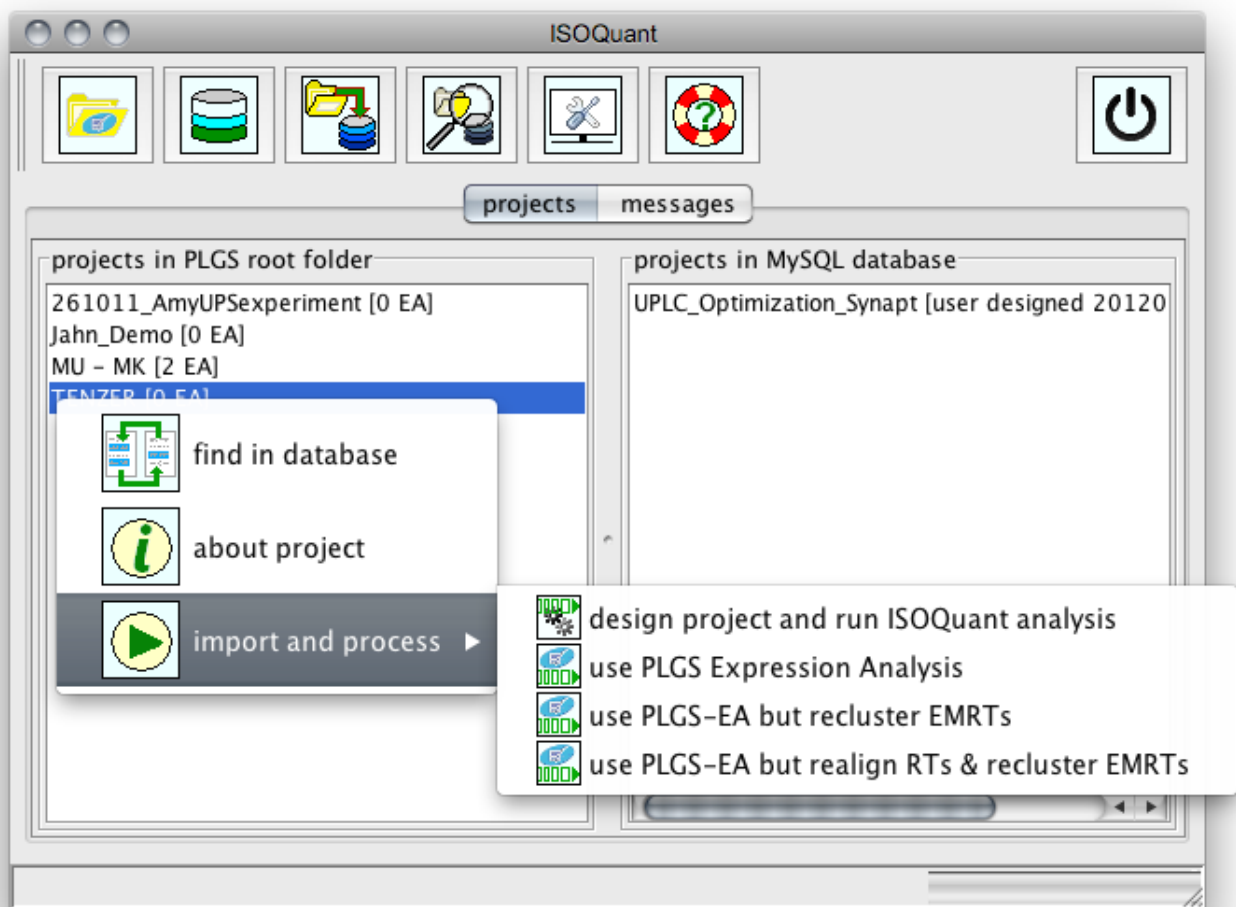


Figure 4: context menu for projects in PLGS root folder

5.6 Project design or Expression Analysis selection

5.6.1 Project design

Project designer dialog (figure 5) shows for each selected project the original PLGS project structure and the targeted ISOQuant project structure, which is redefineable by drag-and-drop.

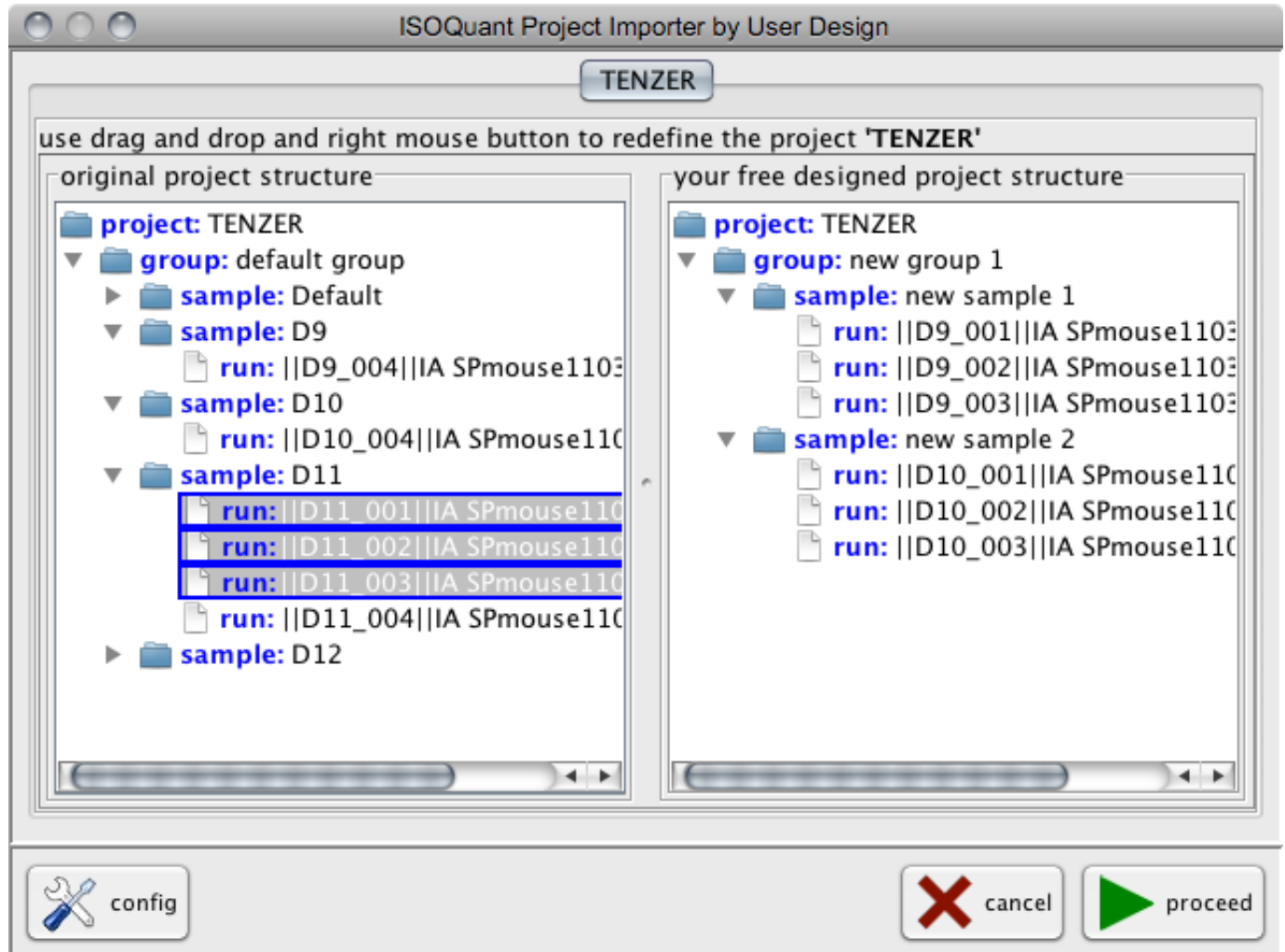


Figure 5: project designer

5.6.2 Expression Analysis selection

For each selected project every contained Expression Analysis may be selected to be imported and processed by ISOQuant by using Expression Analysis Selector (figure 6).

5.7 Automated processing

Automated processing of user chosen contents is initiated after project design or Expression Analysis selection is done. Depending on user choice, data is processed by different predefined analysis pipelines.

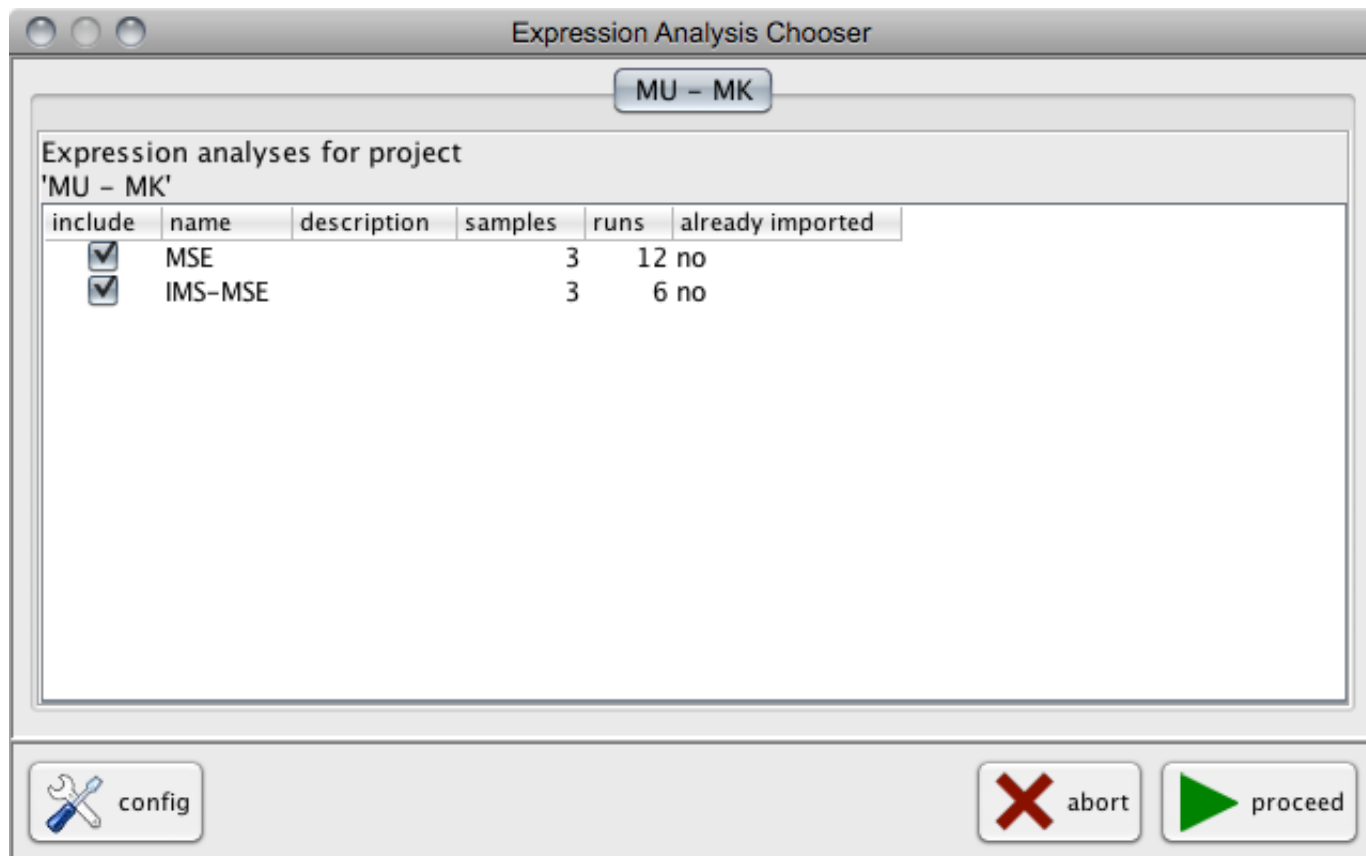


Figure 6: Expression Analysis Selector

5.8 Report creation

After successfully importing and processing data, newly processed projects appear inside projects in MySQL database container (figure 1, item 2). By selecting and right clicking on one of them, its processing results may be reported to a file (figure 7). Different types of report are available offering different points of view at the analysis results.

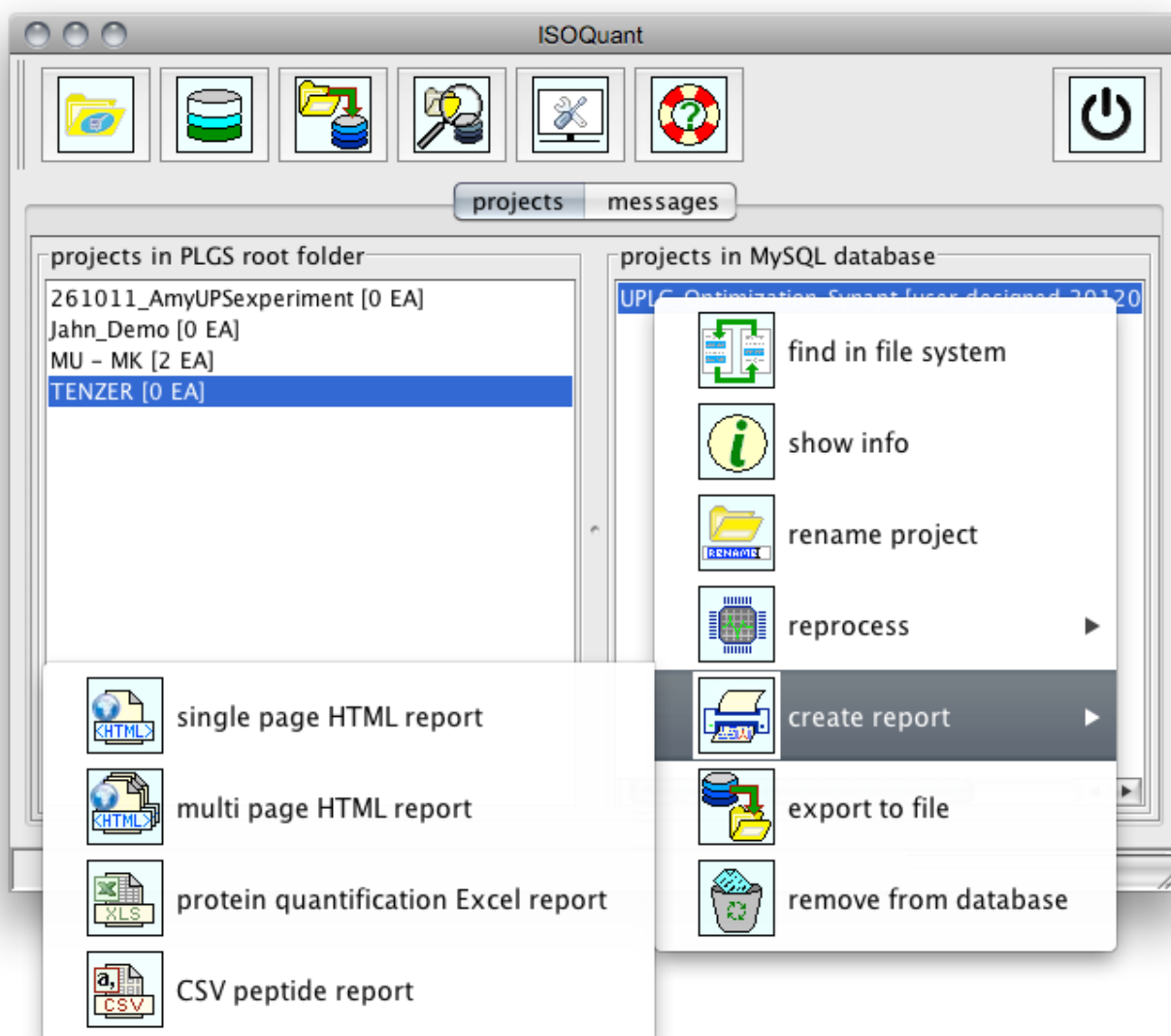


Figure 7: context menu for projects in ISOQuant database