

Panorama AutoQC

The Panorama AutoQC pipeline enables mass spec laboratories to evaluate LC MS/MS performance over time, and quickly identify potential issues. This pipeline comprises three components: Skyline, Panorama and AutoQC Loader, a utility program that automates the processing and uploading of QC results from the instrument computer to a Panorama server. The pipeline is initialized by specifying a 1) template document with target QC peptides into which data files should be imported as they are acquired, 2) a local folder where QC data files are written, and 3) a folder on the Panorama server where data should be uploaded.

After the Skyline documents containing QC results are uploaded to Panorama, users can examine instrument performance through a variety of charts that track several metrics such as retention time, peak area, FWHM etc. More information on the QC capabilities in Panorama can be found on this page:

<https://www.labkey.org/wiki/home/Documentation/page.view?name=panoramaQC>

AutoQC Loader 1.1

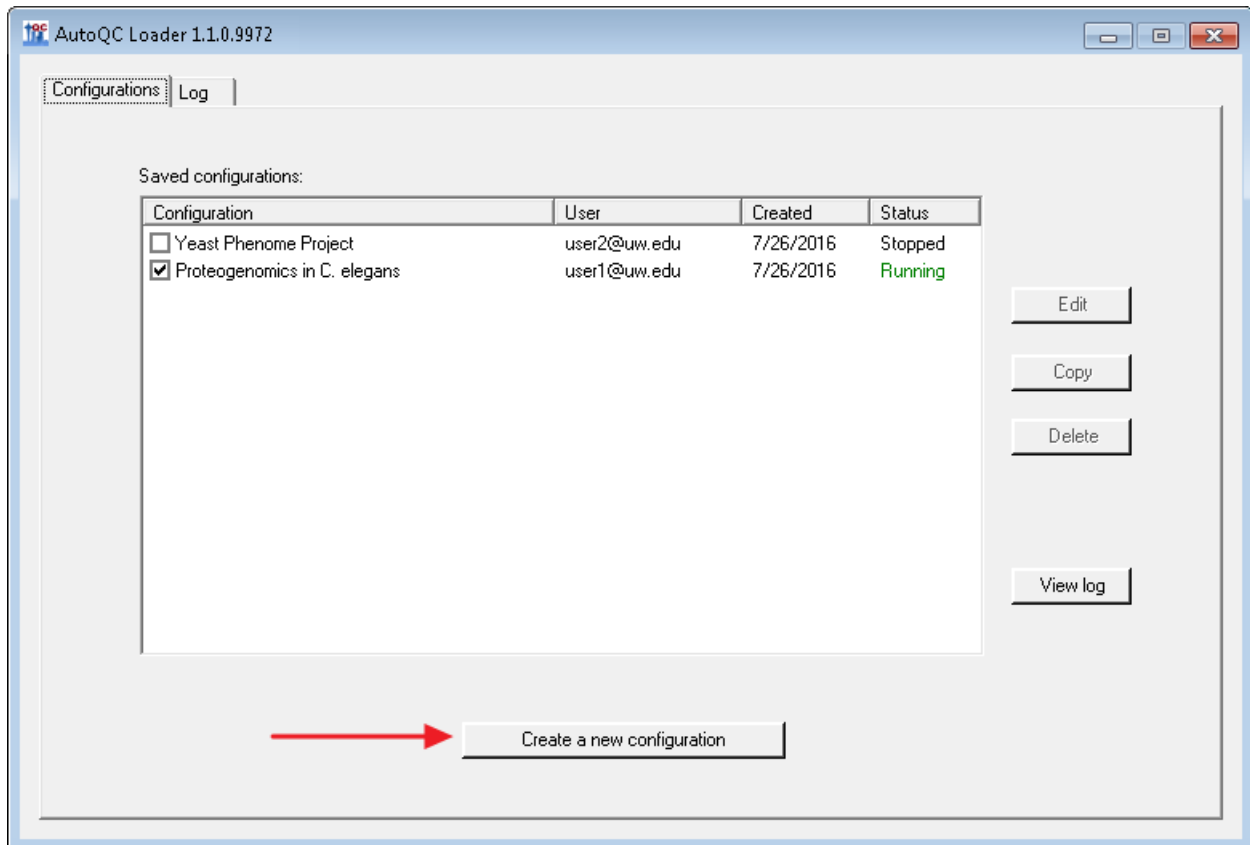
AutoQC Loader automates importing QC results file to a Skyline document and uploading the document to a Panorama server. It uses SkylineRunner to launch Skyline without showing the Skyline window, passing command-line arguments to this invisible instance of Skyline to import runs and publish documents to a Panorama server. SkylineRunner is automatically installed along with AutoQC Loader.

AutoQC Loader can be installed from this URL: <http://skyline.gs.washington.edu/software/AutoQC/>

If you are using Skyline-daily, install AutoQC Loader-daily from:

<http://skyline.gs.washington.edu/software/AutoQC/daily/index.html>

To start monitoring a local folder for QC results, create a new configuration in AutoQC Loader by clicking on the **Create a new configuration** button. Each configuration is a combination of settings that include the location of the template Skyline document, the local folder where QC results will be written, and the folder on a Panorama server where the results will be uploaded. Multiple configurations can be enabled allowing users to monitor more than one QC data folder at the same time. Configurations are saved so instrument operators can enable a previously created configuration if they are acquiring data for an on-going project with intermittent breaks in data acquisition.



In the **AutoQC Configuration** form enter the appropriate settings in the **Settings** tab.

AutoQC Configuration

Settings | Panorama Settings

Configuration name

Skyline file path: [] ...

Folder to watch: [] ...

Include subfolders

File filter: [All]

Results time window: [31] days

Instrument type: [Thermo]

Expected acquisition duration: [75] minutes

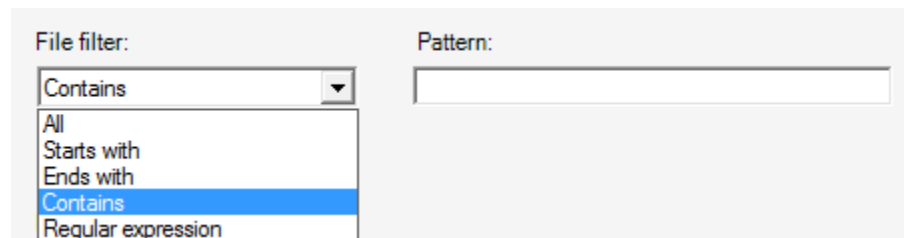
[Save] [Cancel]

Configuration name: This can be the name of the project or study for which data is being acquired.

Skyline file path: This is the path to the template Skyline document into which QC runs will be imported. Please note that the **Integrate all** setting (**Settings > Integrate all**) must be checked for Skyline documents that contain QC results. This setting forces Skyline to calculate areas for all fragment ions between the integration boundaries and gives better quantitative results.

Folder to watch: This is the folder that AutoQC Loader will monitor for new QC runs. Any new runs added to the folder will automatically be imported into the given Skyline document. When a configuration is enabled or started, all existing runs in this folder that are newer than the last imported run in the Skyline document will get imported. If the document does not have any imported results, AutoQC Loader will import all existing runs in the folder.

File filter: One of the options in this combo-box can be used to apply a filter on the QC files that will be imported to the Skyline document. Only files with names that match the selected option will be imported. The default option (**All**) will import all data files added to the QC folder without applying any filters.



The image shows a software interface with two input fields. On the left, there is a 'File filter:' label above a dropdown menu. The dropdown menu is open, showing a list of options: 'All', 'Starts with', 'Ends with', 'Contains', and 'Regular expression'. The 'Contains' option is currently selected and highlighted in blue. To the right of the dropdown menu is a 'Pattern:' label above an empty text input field.

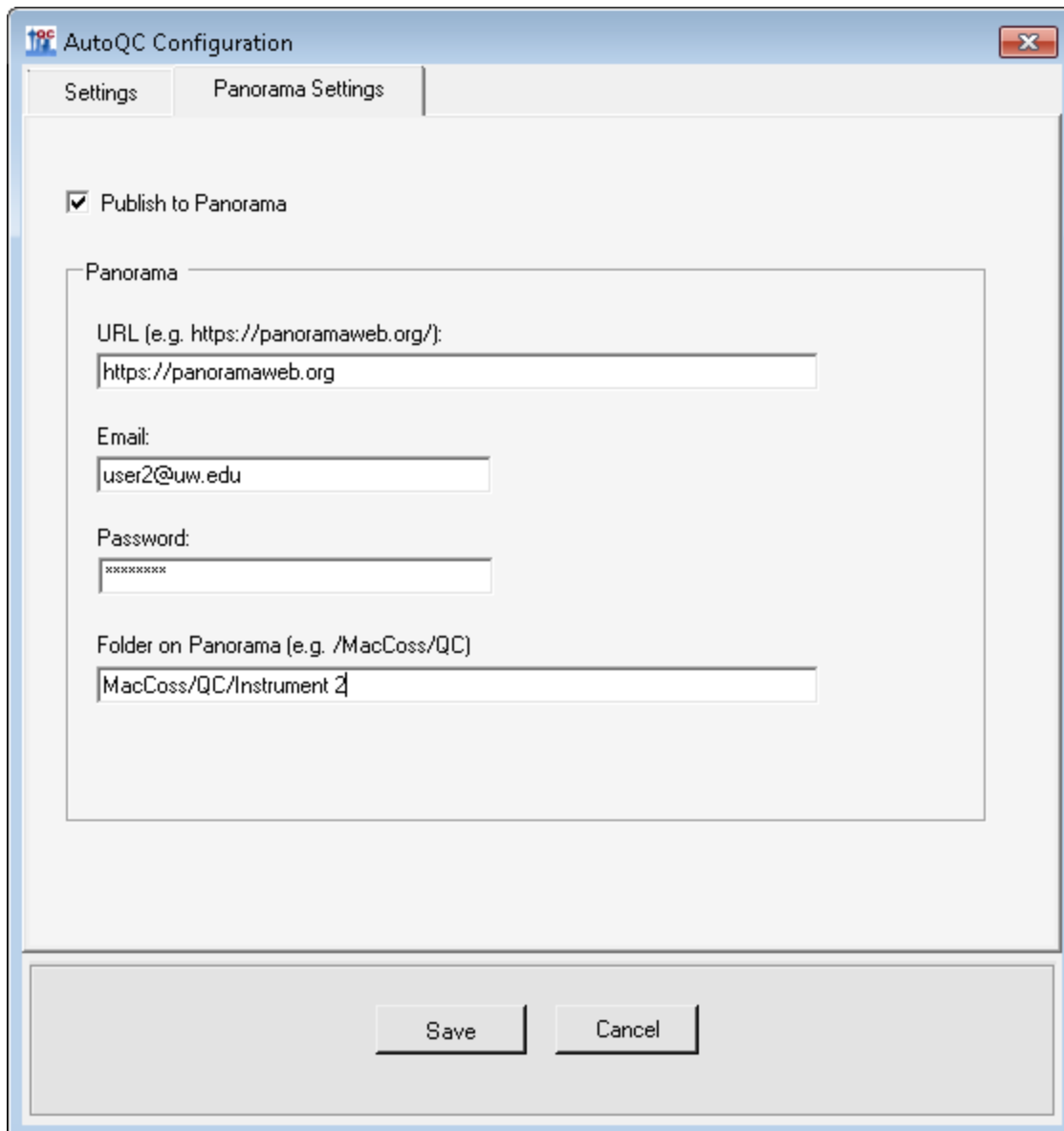
Results time window: The results time window determines how long imported results will be retained in the Skyline document. This is a rolling window and only results acquired within the last 'n' days, where 'n' is the width of this window in days, will be retained in the document. When a new run is imported into the document any results that no longer fall within this time window, ending on that day, will be removed from the document. The default (and minimum) width of the window is 31 days. Please note that AutoQC Loader does NOT delete any raw data files. Only results imported into the document that are older than the current time window are removed from the document. AutoQC Loader also keeps local archival documents to which you can refer for older runs that have been removed from the active document (See ARCHIVING AND LOGGING).

Instrument type: The instrument type setting tells AutoQC Loader the type of files (e.g. *.raw for Thermo instruments, *.wiff for SCIEX instruments etc.) to look for in the **Folder to watch**.

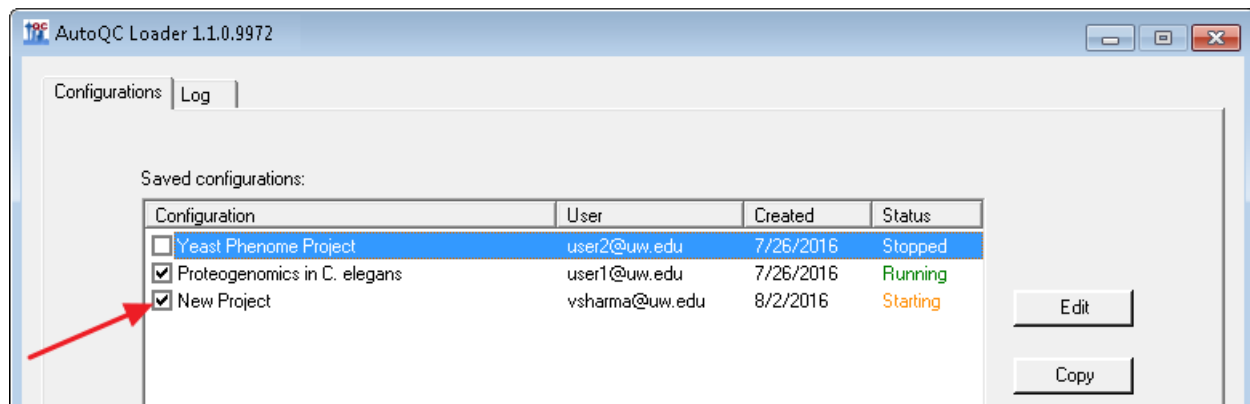
Expected acquisition duration: The expected acquisition duration tells AutoQC Loader how long to wait before attempting to import a QC run. Most instruments write directly to the output raw data file during acquisition and, except for Thermo instruments, we do not have a good way to determine programmatically when file acquisition has completed. When AutoQC Loader detects a new run in the QC folder, it will wait for the duration specified in this setting before attempting to import the run. The default value for this setting is 75 minutes (10 min. trapping time + 60 min. gradient + 5 min. extra).

PANORAMA SETTINGS:

To upload the Skyline document containing QC results to a Panorama server, check the **Publish to Panorama** checkbox in the **Panorama Settings** tab. AutoQC Loader will upload the document to Panorama server each time a new run is imported into the document. Note that Panorama will handle the redundancy of importing documents where most of the runs may have already been imported.



Click **Save** to save the settings, and in the main AutoQC Loader window check the box next to the configuration name to enable the configuration. AutoQC Loader will start the monitoring the local folder specified in the configuration for new results files.



ARCHIVAL AND LOGGING:

AutoQC Loader creates a monthly archive (*.sky.zip) of the Skyline document. Archive creation is triggered when the first run is imported into the document in a given month. For example, when the first run is imported into the Skyline document, QC_doc.sky, in the month of August 2015, an archive file, QC_doc_2015_07.sky.zip, is created in the same directory as QC_doc.sky.

AutoQC Loader writes to a log file (AutoQC.log) in the directory that contains the template Skyline document. Please provide this log file to the developers if you run into any issues with AutoQC Loader.

KNOWN ISSUES:

1. AutoQC Loader will fail to import runs to the Skyline document if the document is also open in an instance of Skyline. If this happens close the Skyline instance.
2. AutoQC Loader invokes Skyline, via SkylineRunner (or Skyline-daily via SkylineRunnerDaily) to import runs to the Skyline document. If a user on the same computer updates Skyline while AutoQC Loader is running, SkylineRunner will not be able to connect to Skyline and running configurations will fail with a "Could not connect to Skyline..." message. In this case, finish the Skyline update and restart any running AutoQC Loader configurations.