

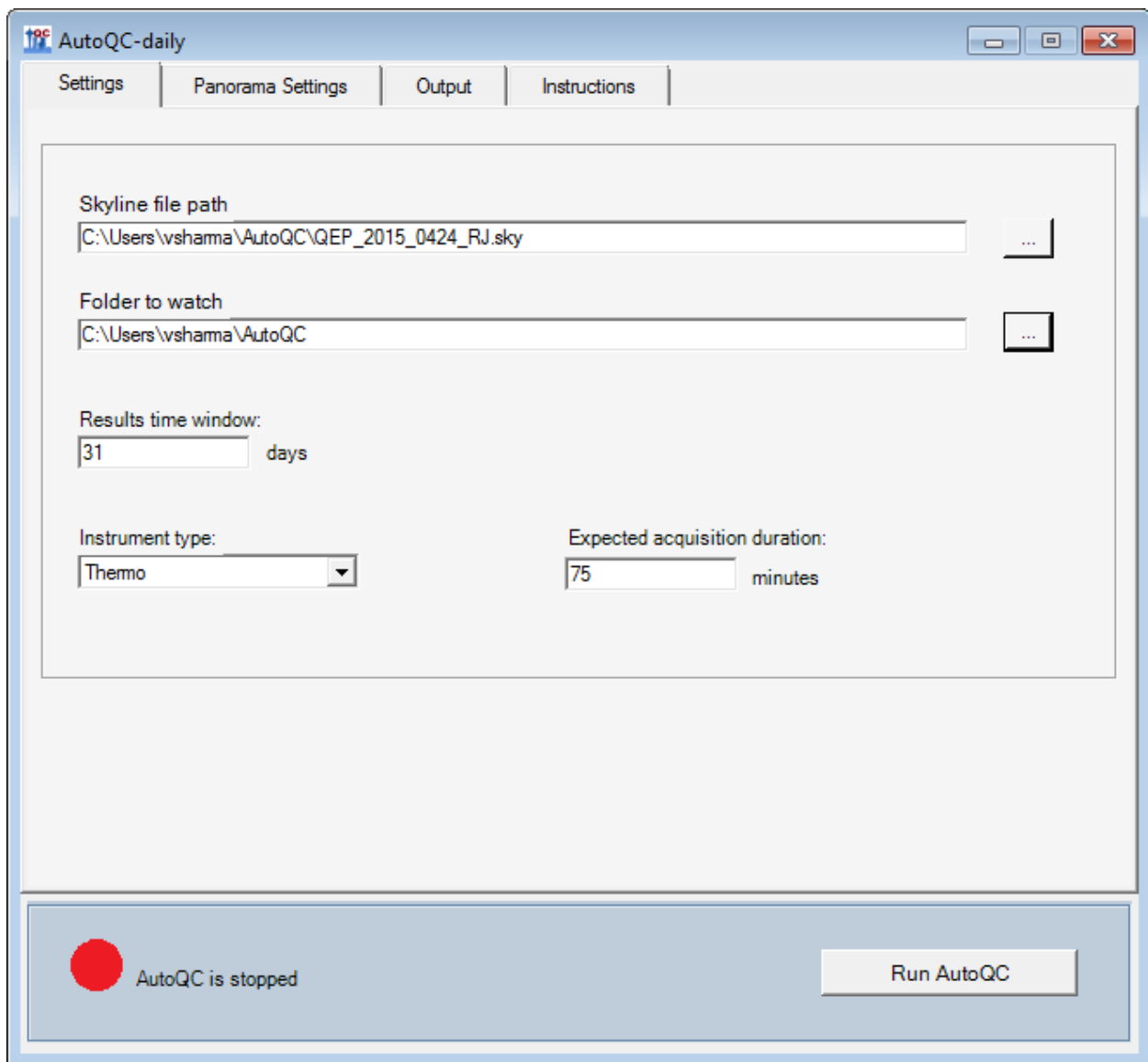
## Panorama AutoQC-daily

We are releasing a beta version of AutoQC (AutoQC-daily) that requires Skyline-daily (3.1.1.8694) or later. AutoQC-daily can be installed from this URL:

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

AutoQC 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.

Before starting AutoQC enter the appropriate settings in the **Settings** tab.



The screenshot shows the 'AutoQC-daily' application window with the 'Settings' tab selected. The window has a title bar with the application name and standard Windows window controls. Below the title bar are four tabs: 'Settings', 'Panorama Settings', 'Output', and 'Instructions'. The 'Settings' tab is active and contains the following fields:

- Skyline file path:** A text input field containing 'C:\Users\wshama\AutoQC\QEP\_2015\_0424\_RJ.sky' and a browse button ('...').
- Folder to watch:** A text input field containing 'C:\Users\wshama\AutoQC' and a browse button ('...').
- Results time window:** A text input field containing '31' followed by the label 'days'.
- Instrument type:** A dropdown menu with 'Thermo' selected.
- Expected acquisition duration:** A text input field containing '75' followed by the label 'minutes'.

At the bottom of the window, there is a status bar with a red circle icon and the text 'AutoQC is stopped'. To the right of the status bar is a button labeled 'Run AutoQC'.

**Skyline file path:** This is the path to the 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 will monitor for new QC runs. Any new runs added to the folder will automatically be imported into the given Skyline document. When AutoQC is started up, it will import all existing runs in this folder that are newer than the last imported run in the Skyline document. If the document does not have any imported results, AutoQC will import all existing runs in the folder.

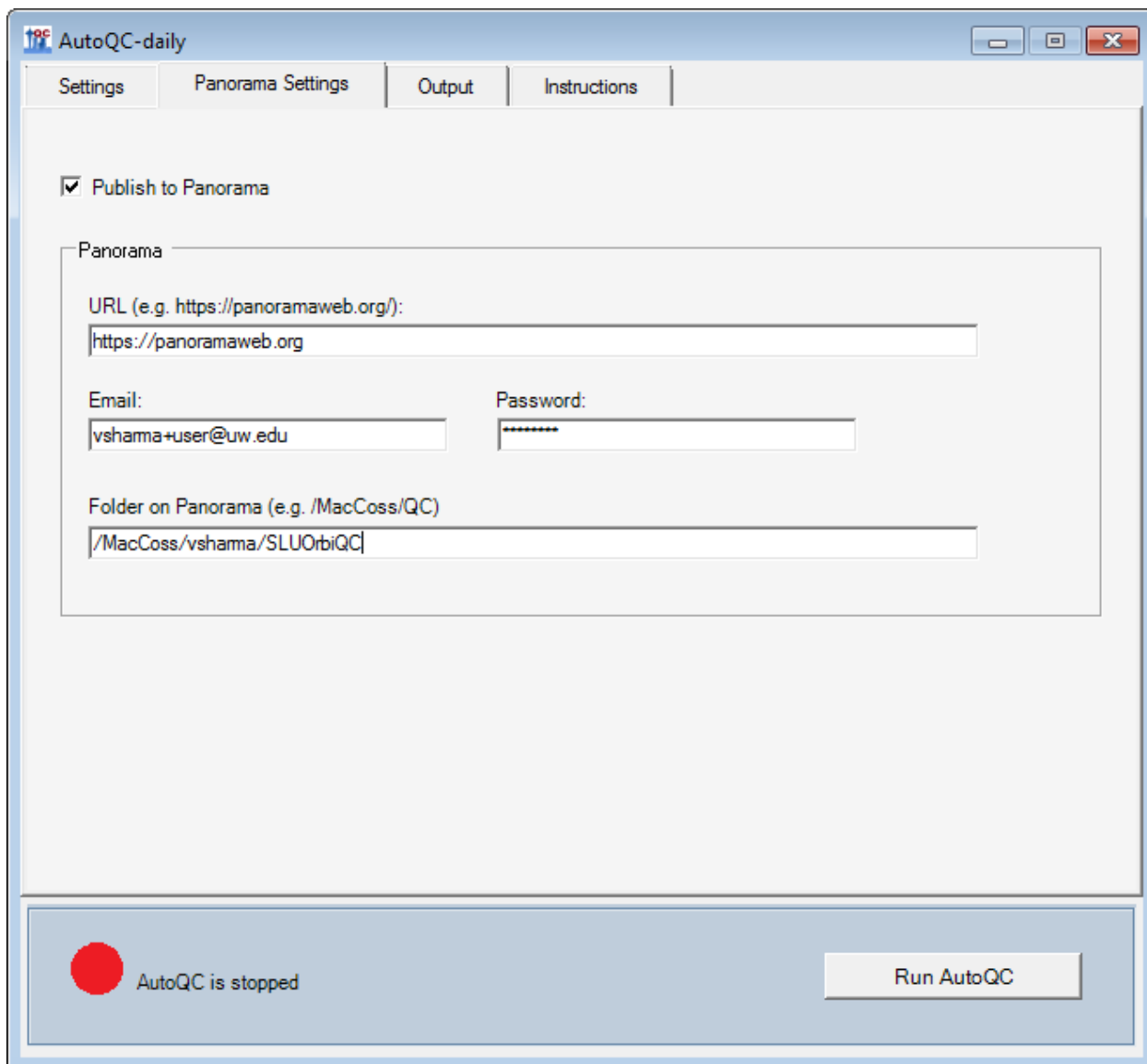
**Results time window:** The results time window determines how long imported results will be retained in the Skyline document. This is a rolling window and only results acquired within the last 'n' days, where 'n' is the width of this window in days, will be retained in the document. When a new run 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 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 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 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 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 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:

If you want to upload the Skyline document containing QC results to a Panorama server, check the **Publish to Panorama** checkbox in the **Panorama Settings** tab. AutoQC 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.



The screenshot shows the 'AutoQC-daily' application window with the 'Panorama Settings' tab selected. The 'Publish to Panorama' checkbox is checked. The 'Panorama' section contains the following fields:

- URL (e.g. <https://panoramaweb.org/>):
- Email:
- Password:
- Folder on Panorama (e.g. /MacCoss/QC):

At the bottom of the window, there is a red stop icon and the text 'AutoQC is stopped', and a 'Run AutoQC' button.

Click the **Run AutoQC** button once you have entered all the settings.

## **ARCHIVAL AND LOGGING:**

AutoQC 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.

In addition to displaying log messages in the **Output** tab, AutoQC writes to a log file in the directory that contains the Skyline document. This is a rolling monthly log file, e.g. AutoQC\_2015\_08.txt. A new log file is created each month. Please provide the latest log file to the developers if you run into any issues with AutoQC.

## **KNOWN ISSUES:**

1. AutoQC 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 and restart AutoQC.
2. AutoQC invokes Skyline (via SkylineRunner) to import runs to the Skyline document. If a user on the same computer updates Skyline while AutoQC is running, SkylineRunner will not be able to connect to Skyline and AutoQC will fail with a "Could not connect to Skyline..." message. In this case, finish the Skyline update and restart AutoQC. Any runs that may have been added to the QC folder while AutoQC was stopped, will be imported when AutoQC starts up.