

PMI Batcher

User's Manual

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PMI Batcher User's Manual

Introduction

The Batcher application allows the user to run multiple Byonic or Preview parameter and sample files as a single batch submission.

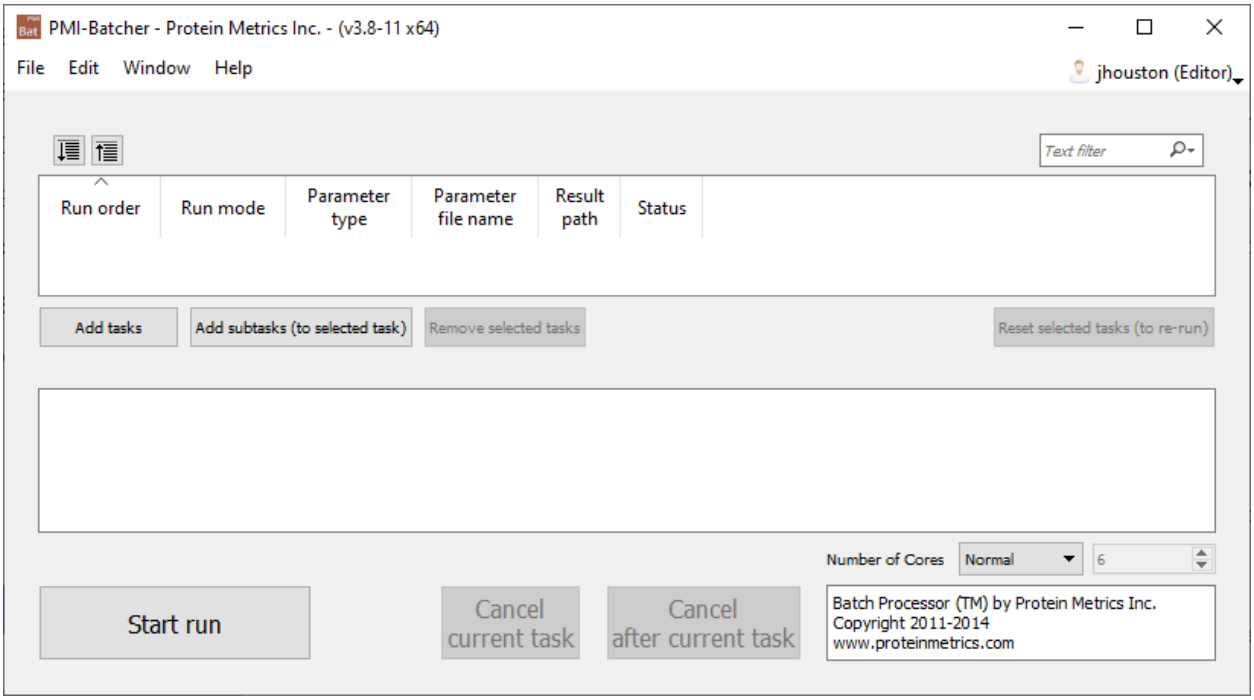


Figure 1: Batcher screen

Add Tasks

Tasks are parameter and sample files that are run sequentially. To create a task, click **Add tasks**.

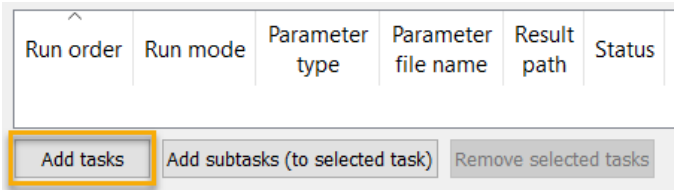


Figure 2: Add tasks button

The **Input options** dialog opens:

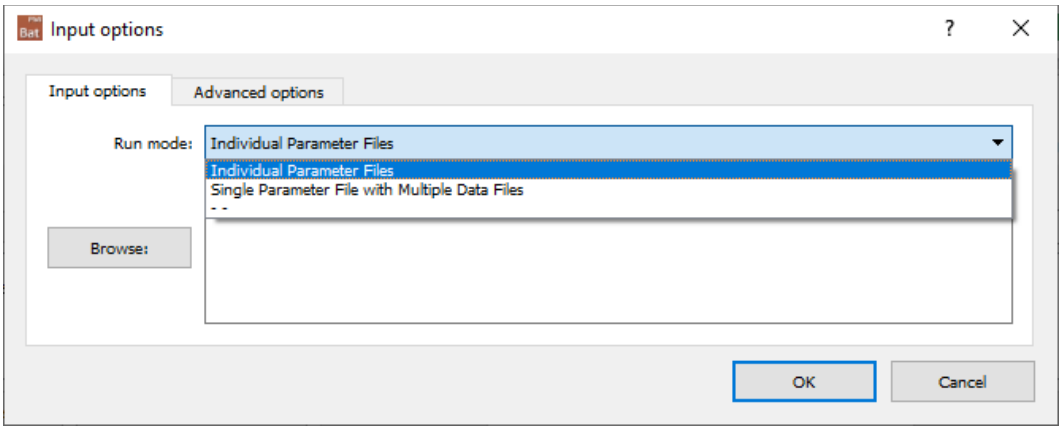


Figure 3: Input options dialog for creating tasks

There are three **Run mode** options:

- **Individual Parameter Files** runs any combination of related or unrelated parameter files.
- **Single Parameter File with Multiple Data Files** runs a parameter file associated with multiple MS spectra input files.
- The "**- -**" option allows entry of files of any type that support customized runs.

Individual Parameter File Runs

For this option, individual parameter files from Byonic (*.byparms) or Preview (*.prv) are added to the task to run one by one. The sample files and parameter settings need not be related. Each is treated as an individual run.

To load parameter files, click **Browse**, navigate to and select the desired parameter file(s) and click **Open**. Repeat for parameter files from other directories. The parameter files and their paths are listed in the window:

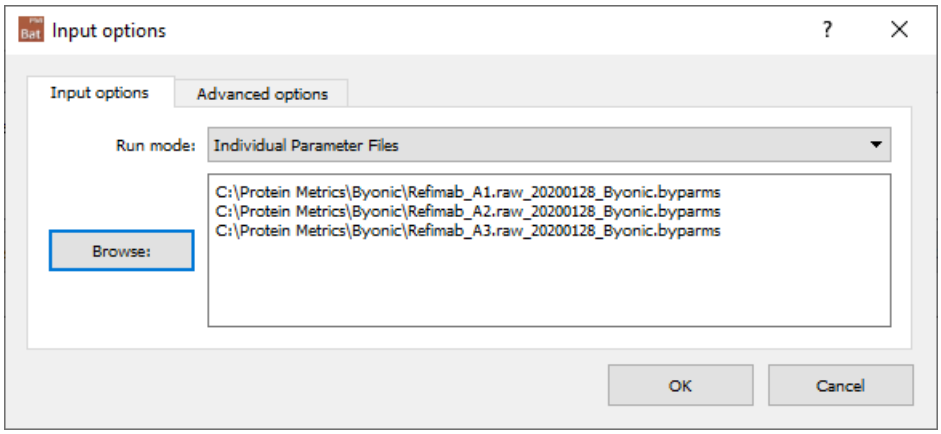


Figure 4: Individual Parameter Files option

When all the parameter files are loaded, click **OK** to add them as tasks in the batch queue.

Advanced options Tab

The **Advanced options** tab provides two options for more advanced cases:

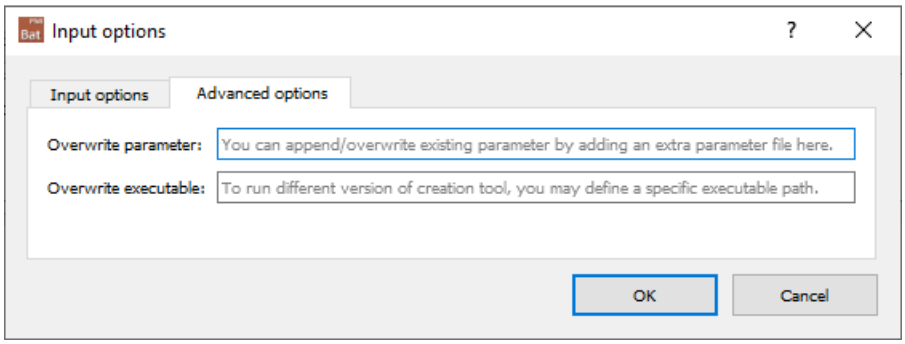


Figure 5 Input: Advanced options tab

Overwrite parameter allows users to manually assign a new set of parameters. **Overwrite executable** allows users to run a non-installed version of PMI software. Please contact support@proteinmetrics.com for instructions on how to run these advanced features in specialized cases.

Single Parameter File with Multiple Data Files

This option adds a single parameter file with multiple sample spectra files. These spectral files are all generated from different samples but from the same biological sample, with the same sample preparation and instrument settings defined by a single parameter file.

The same parameter file extensions are supported as with the Individual Parameter Files option described above. Click the ... button at the end of the **Parameter** box, navigate to and select the desired parameter file and click **Open**.

All of the sample data file types supported by PMI applications are supported by Batcher. This includes: Bruker: *.d, Thermo: *.raw, Waters: *.raw, Sciex: *.wiff, *.wiff2, Agilent: *.d, Shimadzu *.lcd, as well as *.mgf and *.mzxml. To load the sample data files associated with the selected parameter file, click **Browse**, navigate to and select the desired sample files and click **Open**. The user can also drag and drop the desired sample files. The list of sample files is added to the central window:

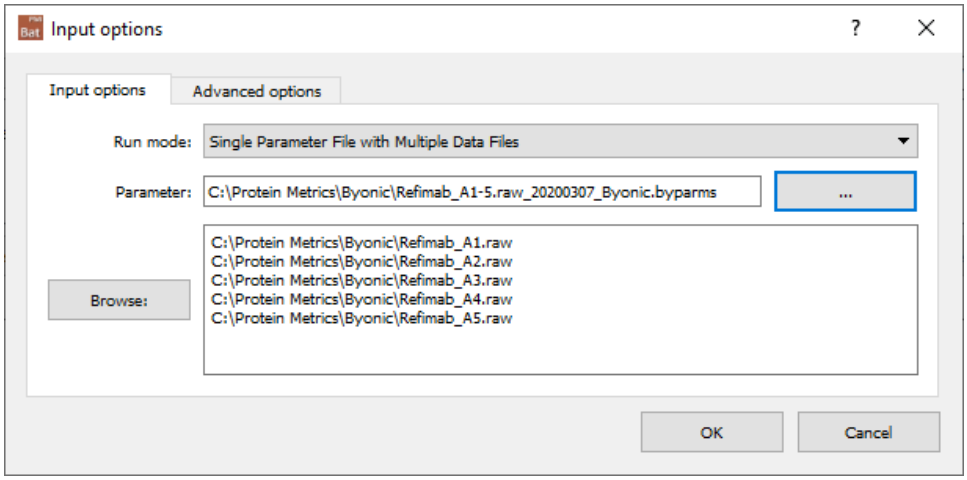


Figure 6: Single Parameter File with Multiple Data Files option

Click **OK** to add the sample files as a task set to be processed in the run queue:

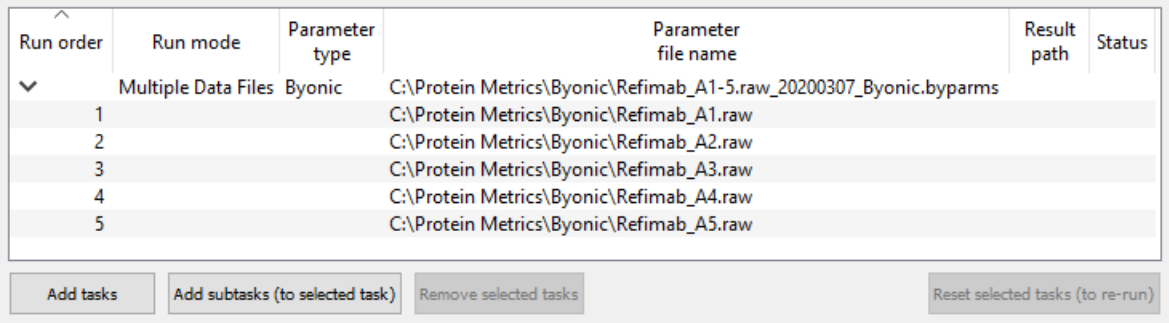


Figure 7: Created task parameter and sample files to be processed in the queue

To remove a task, select the parameter file task and click **Remove selected tasks**.

Add Subtasks

Subtasks are the sample data files that are added to an existing parameter file task. To add a subtask, select the associated parameter file and click **Add subtasks (to selected task)**.

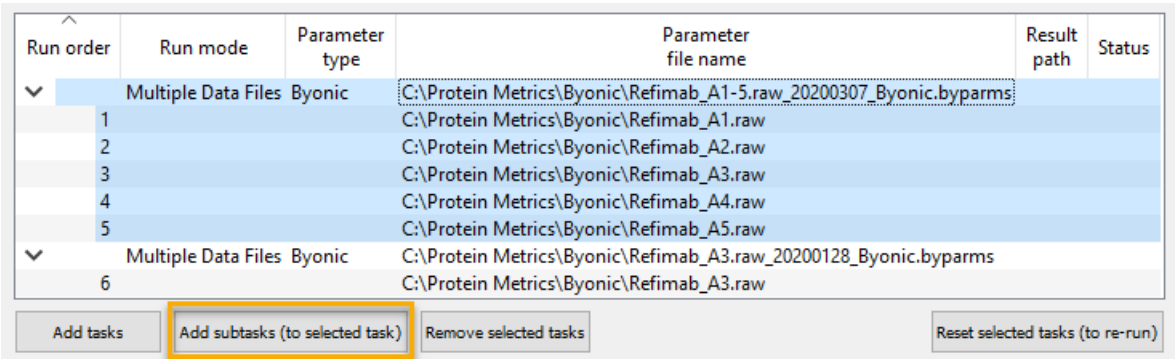


Figure 8: Add subtasks

An **Input options** dialog opens much like the one for tasks, except that the Run mode and Parameter settings are pre-populated and non-editable:

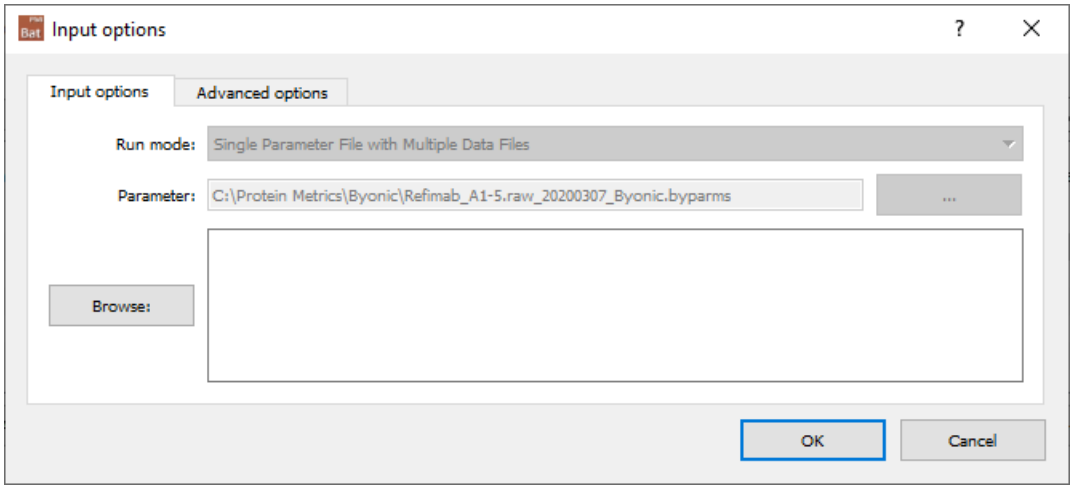


Figure 9: Subtask Input options

Click **Browse** to locate and add sample files to serve as subtasks. The user can also drag and drop the desired sample files. The same sample file types are supported as those for the Single Parameter File with Multiple Data Files option. Click **OK** to load the subtask(s). The subtask is appended to the subtask list under the parameter file task. To remove a subtask, select it and click **Remove selected tasks**.

Cores

The number of cores determines the proportion of computer power used to run the batch process. This setting determines how long the run will take, but also how much computer power is available for other uses. The options are:

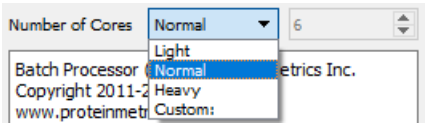


Figure 10: Number of Cores option

Light will use a single core, running the slowest but allowing the computer to perform other tasks unimpeded. **Normal** will use all cores less two, still allowing some light computer use. **Heavy** will use all cores; this assumes the machine will not be used during the run. **Custom** allows the user to choose the number of cores to run, for example, between that of Light and Normal. Normal and Heavy are the most commonly used settings.

Run the Batch

When the batch is ready to run, click **Start run**.

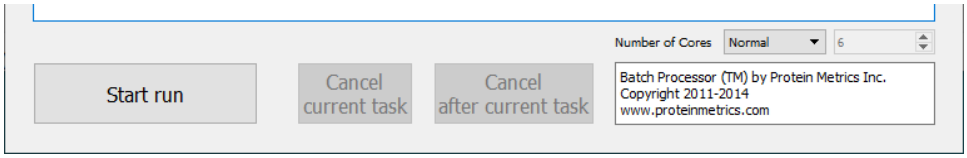


Figure 11: Run buttons

The Batcher will process the input files one by one. The directory of the output files is displayed after each sample file in the **Result path** column. The directory defaults to the path designated in the sample files. The run status is displayed in the **Status** column.

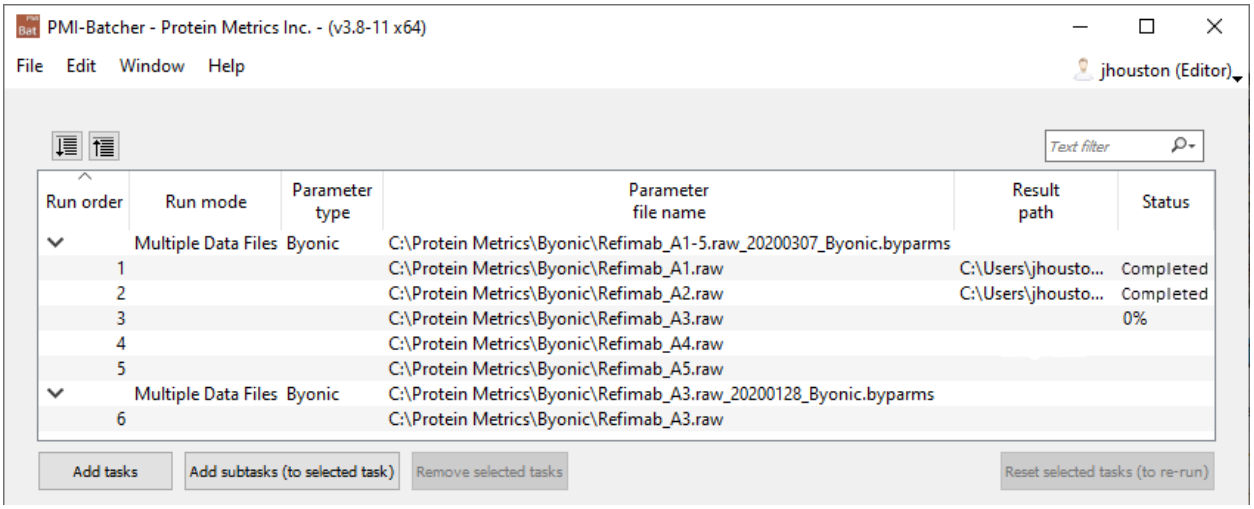


Figure 12: Result path and Status during a run

To cancel the batch run, click **Cancel current task**. To allow the current task to complete before cancellation, click **Cancel after current task**. To rerun one or more of the tasks, select those tasks and click **Reset selected tasks (to re-run)** and click **Start run.**

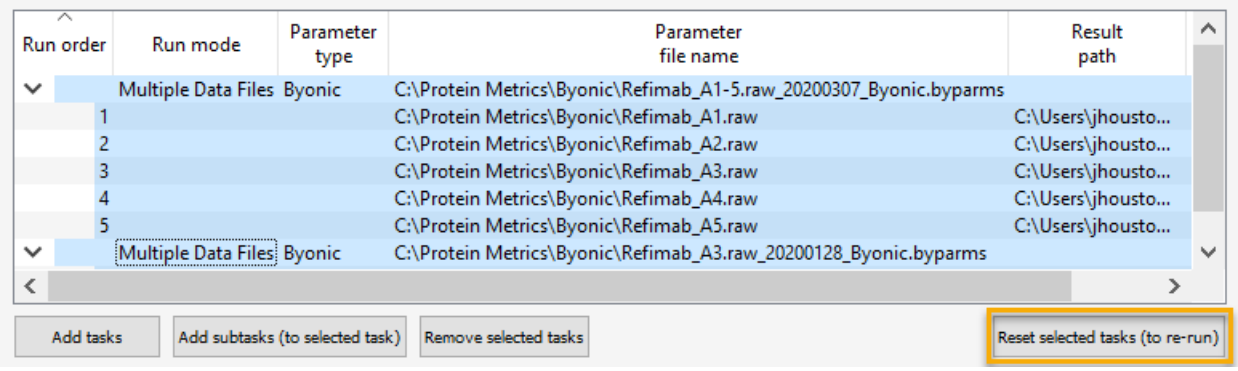


Figure 13: Reset selected tasks for a rerun

Additional tasks can be added to the Batcher queue after the batch process has started. Click **Add tasks** to append new parameter and sample files to the queue.

Main Menu Bar

The topmost menu bar includes four items: **File, Edit, Window,** and **Help**.

File Menu

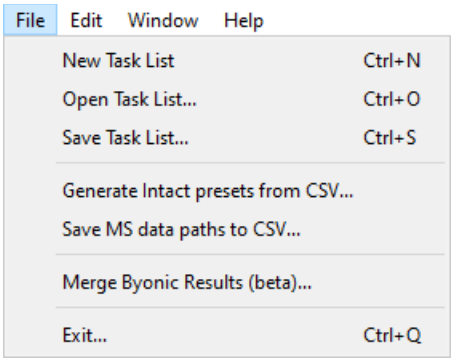


Figure 14: File menu

- **New Task List** clears out all tasks to allow a new set of parameter and sample files to be set.
- **Open Task List** opens a saved Batch task file (extension *.pmibat) of parameter and sample files saved in a previous session.
- **Save Task List** generates a Batch task file that can be reloaded to run at another time.
- **Generate Intact presets from CSV** is no longer supported in Batcher.
- **Save MS data paths to CSV** is no longer supported in Batcher.
- **Merge Byonic Results (beta)** is a preliminary function used to merge Byonic *.byrslt files.
- **Exit** closes the application.

Edit Menu

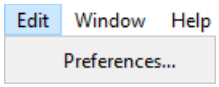


Figure 15: Edit menu

- **Preferences** identifies the relevant application executables (defaulting to installed versions), along with other pre-run settings:

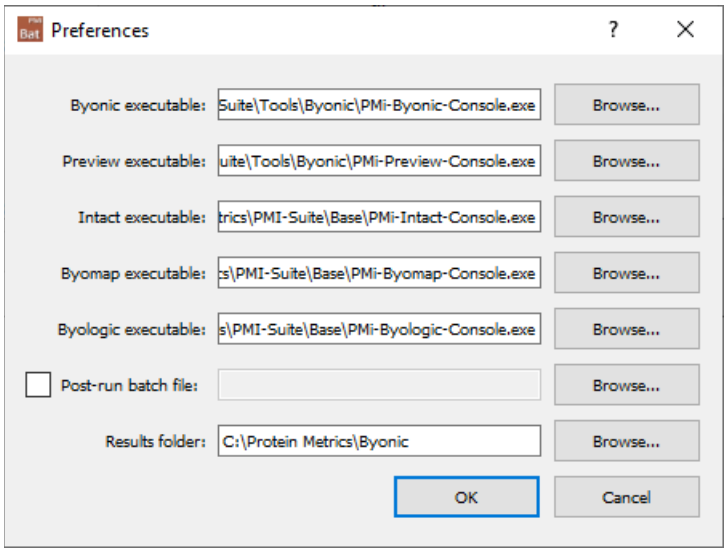


Figure 16: Preferences

  - The checkbox **Post-run batch file** allows the user to select a saved Batch task file (*.pmibat) to run after the current batch of tasks is run.
  - **Results folder** is no longer supported in Batcher. The output folder is set in the source sample files.

Window Menu

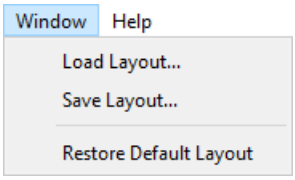


Figure 17: Window menu

- **Load Layout** opens a saved column layout.
- **Save Layout** saves the current column width and sorting layout to an *.ini file.
- **Restore Default Layout** applies the column layout used when Batcher first opens.

Help Menu

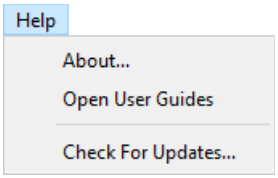


Figure 18: Help menu

- **About** menu shows the software version number, which is needed when reporting issues.
- **Open User Guides** opens the installed folder with the manuals and quick start guides for Protein Metrics software, including the PMI Batcher Manual.
- **Check For Updates** identifies whether a newer version of the Batcher application is available.

Task Table Management

- To change the width of a task table column, click the edge of the column to expose the icon. Without releasing the mouse, drag to the right or left to expand or shrink the column.
- To sort a task table column, click the column header. An up arrow appears, indicating that the column is sorted ascending. Click the column header again to sort descending, indicated by a down arrow.
- To collapse the tasks in one group, click the down arrow in the **Run order** column for that group. To expand the group again, click the left arrow for the group. To collapse the tasks in all the groups, click the button at top left. To expand all the groups again, click the button.
- To search for specific tasks in the task table, enter a term within the **Text filter** box at top right and click the button.