

# Skyline Command-Line Interface

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The command-line interface for Skyline is called SkylineRunner.exe. It is a tiny shim executable less than 10 KB in size. It requires a full Skyline installation on the computer on which it is run. SkylineRunner simply starts Skyline running without any user interface, pipes the parameter options from the command-line to the running Skyline instance, and prints output from Skyline to the command console. At present, only one instance of SkylineRunner may be executed at a time.

The Skyline instance started by SkylineRunner is independent of any other instances that may already be running on the same machine. It is not necessary to have a visible instance of Skyline running on your computer for SkylineRunner to work.

SkylineRunner is intended for automating tasks, such as quality control, scheduling and refinement, during acquisition. SkylineRunner can open a Skyline document, import a newly acquired data file, and export a report or new method.

## Parameter Options:

The current implementation of SkylineRunner offers the following options:

### General input/output

--in=path/to/file.sky	Open a Skyline file
--save	Saves any changes to the file
--out=path/to/file.sky	Same as save except writes to the specified file
--share-zip[=path/to/file.sky.zip]	Saves document and supporting files into a .sky.zip sharing file. If no path is provided the file name will be generated based on the document file name with a date-time stamp appended.
--batch-commands=path/to/file	Runs a file line by line treating each line like a SkylineRunner input. Useful for automating the execution of multiple commands. The open Skyline file remains active through all commands.
--dir=path/to/folder	Used to specify a default root directory for all other path arguments, other than the directory in which the command is run.
--timestamp	All logging output will be preceded by a time and date.
--memstamp	All logging output will be preceded by two memory usage values managed and process private bytes in MB, rounded to the nearest MB.

Until the section titled *Settings Customization* all other command line parameters rely on the “in” parameter because they all rely on having a Skyline document open.

### Importing results replicates

<code>--import-file=path/to/file</code>	Attach a replicate to the open document
<code>--import-replicate-name=&lt;name&gt;</code>	Name to give the new replicate in an <code>--import-file</code> operation.
<code>--import-optimizing=&lt;ce   dp&gt;</code>	Indicates the data being imported contains extra transitions for detecting optimal collision energy or declustering potential.
<code>--import-append</code>	Append the import-file to the given replicate. This is an intention check in case the document already has a replicate with the given name. By default this is set to false. This option only works with the <code>--import-file</code> option.
<code>--import-all=path/to/folder</code>	Imports from a folder all files or sub-folders which are not already in the document, naming each with the base-name of the file or sub-folder, unless the <code>--import-naming-pattern</code> parameter is also supplied. If <code>--import-replicate-name</code> is supplied, then all files are added to one multi-injection replicate.
<code>--import-all-files=path/to/folder</code>	Imports from a folder all files but not subfolders which are not already in the document, naming each with the base-name of the file, unless the <code>--import-naming-pattern</code> parameter is also supplied. If <code>--import-replicate-name</code> is supplied, then all files are added to one multi-injection replicate.
<code>--import-naming-pattern=&lt;reg-ex&gt;</code>	A regular expression from which the first group will be used to name replicates in an <code>--import-all</code> operation (e.g. <code>[^_](.*)</code> for everything after the first underscore).
<code>--import-before=&lt;date&gt;</code>	When importing from a folder, only import from files with modified time before the given date.
<code>--import-on-or-after=&lt;date&gt;</code>	When importing from a folder, only import from files with modified time after the given date.
<code>--import-no-join</code>	Import results files to individual .skyd files without joining them to the main document .skyd file. This is useful for distributed

	processing, as on HPC cluster.
--import-process-count=<num>	A number of sub-processes will be run for single-file import, after which the results from each single file will be joined by the main process. This can produce 10x performance gains on 24-core NUMA servers and 3-4x even on i7 processors, under the right conditions. Be sure to test with your system.
--import-threads=<num>	A number of files will be imported in parallel using threads in the main process (equivalent to "Files to import simultaneously" in the user interface), after which the results from each single file will be joined. This can produce 2-4x performance gains under the right conditions. Be sure to test with your system.
--import-lockmass-positive=<m/z>	Waters lockmass correction $m/z$ for positive ion scans.
--import-lockmass-negative=<m/z>	Waters lockmass correction $m/z$ for negative ion scans.
--import-lockmass-tolerance=<m/z>	Waters lockmass correction tolerance ( $m/z$ ).

### Reintegrate with advanced peak picking models

--reintegrate-model-name=<name>	The name of a scoring model to use for the reintegrate operation. The model can either be pre-defined (e.g. using the Edit > Refine > Reintegrate form) or created automatically during this operation by using --reintegrate-create-model.
--reintegrate-create-model	This option will cause a new model to be created, using the mProphet algorithm with all available scores for the results found in the document. (requires --reintegrate-model-name)
--reintegrate-overwrite-peaks	Existing manually integrated peaks will be overwritten with peaks chosen by the reintegration model. (requires --reintegrate-model-name)

### Removing results replicates

--remove-before=<date>	Remove all results from the open document with an acquired time before the given date.
--remove-all	Remove all results from the open document.

## Importing other Skyline documents

<code>--import-document=path/to/file</code>	Import another Skyline document file into the open document. This may be specified multiple times for multiple files.
<code>--import-document-results=remove merge_names merge_indices add</code>	Determines how any results in the imported document are handled. The default is to remove them.
<code>--import-document-merge-peptides</code>	Matching peptides are merged if used, otherwise not.

## Importing FASTA files

<code>--import-fasta=path/to/file</code>	Import a FASTA file into the open document.
<code>--keep-empty-proteins</code>	Keeps any empty proteins in the open document after importing a FASTA file.

## Importing peptide searches

<code>--import-search-file=path/to/file</code>	Import a peptide search results file into the open document, building a document-specific spectral library. This may be specified multiple times for multiple files. Use <code>--import-fasta</code> argument to add matched peptides as targets.
<code>--import-search-cutoff-score=&lt;cutoff&gt;</code>	Defines a cutoff score (between 0 and 1) to be used when building a spectral library from peptide search results files, where 1 is for highest confidence matches and 0 includes everything. [default 0.95]
<code>--import-search-add-mods</code>	Adds all modifications found in peptide search results files to the open document.
<code>--import-search-include-ambiguous</code>	Prevent spectra with multiple ambiguous peptide matches from being discarded when building the spectral library.

## Importing transition lists and assay libraries

<code>--import-transition-list=path/to/file</code>	Import a simple transition list with Q1, Q3 and peptide sequence. Also supports small molecule transition lists in CSV format with suitable headers.
<code>--import-assay-library=path/to/file</code>	Import an assay library transition list with columns for iRT and relative product ion abundance to create an iRT calculator and spectral library for enhanced peak picking.
<code>--ignore-transition-errors</code>	When present imports all recognized transitions from a transition list or assay library, with error rows reported as warnings.

<code>--irt-standards-group-name=&lt;name&gt;</code>	The name of a protein or peptide list containing the iRT standards within an imported assay library. (optional)
<code>--irt-standards-file=path/to/file</code>	The path to a separate assay library containing the iRT standards to be applied to an imported assay library. (optional)
<code>--irt-database-path=path/to/file</code>	The path to an existing iRT calculator (.irtdb file) to be used with an imported assay library. Or, if <code>--irt-standards-group-name</code> or <code>--irt-standards-file</code> are used, then this is the output path for the created .irtdb file. (optional) The default iRT calculator path is <code>path/to/document.irtdb</code>
<code>--irt-calc-name=&lt;name&gt;</code>	The name for the iRT calculator created during assay library import. (optional) The default name is the document base name.

### Adding spectral libraries

<code>--add-library-path=path/to/file</code>	Specify a spectral library to be added to the open document.
<code>--add-library-name=&lt;name&gt;</code>	Name to give the spectral library in an <code>--add-library-path</code> operation.

### Adding decoy peptides

<code>--decoys-add[=reverse   shuffle]</code>	Add decoys to a template document for reintegrate model generation with mProphet. (decoy generation method is optional and defaults to "reverse")
<code>--decoys-add-count=&lt;number&gt;</code>	A number of decoys to add. (optional – default is to generate as many decoys as targets)

### Exporting reports

<code>--report-name=&lt;name&gt;</code>	The name of a report to export as it appears in the Skyline Export Report form
<code>--report-file=path/to/file.csv</code>	The path to export the report to. Required if <code>--report-name</code> is specified.
<code>--report-format=&lt;CSV   TSV&gt;</code>	CSV for comma-separated reports (or semicolon separated, depending on your localization) or TSV for tab separated reports [default CSV]
<code>--report-invariant</code>	Exports the report with the "Invariant" language setting, using English (US) number formats and header text without spaces, ideal for use with the R statistical programming environment.

## Exporting chromatograms

<code>--chromatogram-file=path/to/file.tsv</code>	The path to the tab delimited file where to export chromatograms.
<code>--chromatogram-precursors</code>	Export precursor ion chromatograms.
<code>--chromatogram-products</code>	Export product ion chromatograms.
<code>--chromatogram-base-peaks</code>	Export base peak chromatograms.
<code>--chromatogram-tics</code>	Export total ion current chromatograms.

## Exporting isolation/transition lists

<code>--exp-isolationlist-instrument=&lt;AB SCIEX TOF   Agilent TOF   Thermo Q Exactive   Thermo Fusion   Waters Synapt (trap)   Waters Synapt (transfer)   Waters Xevo QTOF&gt;</code>	Export an isolation list. This option is required for exporting an isolation list and has no default. This option cannot be used with <code>--exp-translist-instrument</code> or <code>--exp-method-instrument</code> , because you cannot export an isolation list and a transition list or method simultaneously.
<code>--exp-translist-instrument=&lt;AB Sciex   Agilent   Bruker   Shimadzu   Thermo   Thermo Quantiva   Waters&gt;</code>	Export a transition list. This option is required for exporting a transition list and has no default. This option cannot be used with <code>--exp-isolation-list</code> or <code>--exp-method-instrument</code> , because you cannot export a transition list and an isolation list or method simultaneously.
<code>-exp-polarity=&lt;all   positive   negative   separate&gt;</code>	Controls export behavior for documents with both positive and negative transitions. Allows for output of only positive or only negative transitions, or creates separate outputs for each polarity. Defaults to all, and is ignored for single polarity documents.

## Vendor-specific transition list options

AB Sciex	<code>--exp-dwell-time=&lt;millis&gt;</code>	Dwell time per transition. This option is required for unscheduled transition lists.
Agilent	<code>--exp-dwell-time=&lt;millis&gt;</code>	Same as above.
Thermo Scientific	<code>--exp-add-energy-ramp</code>	Adds an extra column for energy ramp to the transition list. Optional. Defaults to false.
Waters	<code>--exp-run-length=&lt;minutes&gt;</code>	Run length of the entire gradient in minutes. This option is required for unscheduled experiments.

## Exporting native instrument methods

<p>--exp-method-instrument=&lt;AB SCIEX QTRAP   AB SCIEX TOF   Agilent 6400 Series   Bruker TOF   Shimadzu   Thermo TSQ   Thermo LTQ   Thermo Quantiva   Thermo Fusion   Waters Xevo TQ   Waters Quattro Premier&gt;</p>	<p>Export a method. This option is required for exporting a method and has no default. This option cannot be used with --exp-isolationlist-instrument or --exp-translist-instrument, because you cannot export a method and an isolation/transition list simultaneously.</p>
<p>--exp-template=path/to/file.meth exp dam m</p>	<p>Path of the method template. This can be a file or a directory depending on your instrument. This option is required for method export.</p>

## Vendor-specific method options

<p>AB Sciex Qtrap</p>	<p>--exp-dwell-time=&lt;millis&gt;</p>	<p>Dwell time per transition. This option is required for standard (unscheduled) methods.</p>
<p>Agilent (all instruments)</p>	<p>--exp-dwell-time=&lt;millis&gt;</p>	<p>Same as above</p>
<p>Thermo (all but LTQ)</p>	<p>--exp-run-length=&lt;minutes&gt;</p>	<p>Run length of the entire gradient in minutes. This option is required for unscheduled experiments.</p>
<p>Waters (all instruments)</p>	<p>--exp-run-length=&lt;minutes&gt;</p>	<p>Same as run length above</p>

## Method and transition list options

<p>--exp-file=path/to/file</p>	<p>Path to the method or transition list file (or directory) to export to. This option is required for method and transition list export.</p>
<p>--exp-strategy=&lt;single   protein   buckets&gt;</p>	<p>Strategy for dividing a method into injections. The default is "single".</p>
<p>--exp-method-type=&lt;standard   scheduled   triggered&gt;</p>	<p>Sets a standard, scheduled or triggered method. The default is "standard".</p>
<p>--exp-max-trans=&lt;number&gt;</p>	<p>Maximum number of transitions per injection for export strategies "protein" and "buckets" OR maximum number of</p>

	simultaneous transitions for scheduled methods. The default is 100.
--exp-optimizing=<ce   dp>	Export a method with extra transitions for finding optimal collision energy or declustering potential.
--exp-scheduling-replicate=<name>	Use this only if creating a scheduled or triggered method. The default is to schedule based on an average of all replicates, but if you specify one, the method will be scheduled based on that replicate.
--exp-ignore-proteins	Ignore protein boundaries in creating methods.
--exp-primary-count=<number>	For --exp-method-type=triggered specifies the number of transitions to make primary.

### Publishing to Panorama

--panorama-server=<server url>	URL of the Panorama server to which the --in file is to be published. The URL should contain the protocol (http or https), hostname and port, if required. Examples: <a href="https://panoramaweb.org">https://panoramaweb.org</a> or http://localhost:8080
--panorama-username=<username>	The username/email address for a user with access to publish to the Panorama server.
--panorama-password=<password>	The password for a user with access to publish to the Panorama server.
--panorama-folder=path/to/folder	The path to a folder on the Panorama server to which the file is to be published (e.g. MyProject/MyFolder).

*If the parameters above are used along with parameters to import results files into the document (--import-file or --import-all) the Skyline document will be uploaded to the given Panorama server only if new results are added to the document.*

### Settings Customization

*The below commands do not rely on the "in" parameter because they modify the user settings that are independent of a specific Skyline document.*



<code>--full-scan-precursor-res=&lt;resolving power&gt;</code>	Resolving power of the precursor mass analyzer.
<code>--full-scan-precursor-res-mz=&lt;m/z value&gt;</code>	The m/z value at which the precursor mass analyzer resolving power is specified. (applies only to orbitrap and ft_ocr mass analyzers)
<code>--full-scan-product_res=&lt;resolving power&gt;</code>	Resolving power of the product mass analyzer.
<code>--full-scan-precursor-res-mz=&lt;m/z value&gt;</code>	The m/z value at which the product mass analyzer resolving power is specified. (applies only to orbitrap and ft_ocr mass analyzers)
<code>--full-scan-rt-filter-tolerance=&lt;minutes&gt;</code>	The number of minutes on either side of the predicted time or MS/MS IDs, i.e. ± minutes. Defaults to.
<code>--tool-arguments="&lt;arguments&gt;"</code>	Optional command-line arguments for the tool to be added, used when the tool is executed. (Not applicable to web URL commands)
<code>--tool-initial-dir=path/to/dir</code>	Optional initial directory for the tool to be added, used when the tool is executed. (Not applicable to web URL commands)
<code>--tool-conflict-resolution=&lt;overwrite   skip&gt;</code>	Tells the SkylineRunner how to resolve a tool name conflict, by either overwriting an existing installation or skipping installation of the new tool.
<code>--tool-report=&lt;report-name&gt;</code>	The name of a report in the settings to use as the input report for the tool.
<code>--tool-output-to-immediate-window</code>	When present the tool output is piped to the Immediate Window at runtime.
<code>--report-add=path/to/file.skyr</code>	Adds the report formats from a skyr file. If there are name conflicts the <code>--report-conflict-resolution</code> parameter is required.
<code>--report-conflict-resolution=&lt;overwrite   skip&gt;</code>	Tells the SkylineRunner how to resolve a report name conflict, by either overwriting the existing report or skipping adding the new report.
<code>--tool-add-zip=path/to/file.zip</code>	Import tools from a tool installation ZIP file.

<pre>--tool-zip-conflict-resolution=&lt;overwrite   parallel&gt;</pre>	<p>Specify whether tool conflicts from the provided ZIP file should be resolved by overwriting or installing in parallel. This is for conflicts related to tool versioning and report names.</p>
<pre>--tool-zip-overwrite-annotations=&lt;true   false&gt;</pre>	<p>Specify whether conflicting custom annotations from the provided ZIP file should overwrite (true) existing annotations or be skipped (false).</p>
<pre>--tool-program-macro=&lt;programTitle&gt;</pre> <p>Or</p> <pre>--tool-program-macro=&lt;programTitle&gt;,&lt;programVersion&gt;</pre> <p>Eg.</p> <pre>--tool-program-macro=R,2.15.2</pre>	<p>Specifies a program title and version to use with the <code>--tool-program-path</code> command. Together these commands are for importing tools from a ZIP file that use the <code>\$(ProgramPath())</code> macro as their command. For more information see the documentation on External Tools.</p>
<pre>--tool-program-path=path/to/file</pre>	<p>Specifies the path to an executable on the local machine for the program title and version specified by the <code>--tool-program-macro</code> flag.</p>
<pre>--tool-ignore-required-packages</pre>	<p>Ignore required packages when installing a tool from a ZIP file.</p>