

MASH Explorer Release Notes

Version 2.2.1

July 30, 2021

Version 2.2.1 has some small improvements to version 2.2:

- Added support for MS3 data.
- Fixed a bug that could cause Index Out of Range errors when opening some Thermo .RAW files.
- Fixed an incompatibility with ProteoWizard 3.0.21193 that caused problems with importing experimental data.

Version 2.2

March 8, 2021

Version 2.2 introduces a number of new features:

- Added support for UniDec deconvolution.
- Added support for TopPIC 1.4.0 and later.
- Added the option to view fragment labels (see the View menu).
- Added the option to view fitting curves (see the View menu).
- Added the ability to re-run uploaded workflows.
- Added the ability to drag and drop workflow parameter files.
- Added a Workflow Manager button to automatically access workflow log files.
- Made opening of very large experiment files more reliable and responsive.
- Fixed problems parsing TopPIC output if the name of the experiment file contains a comma.
- Fixed a bug that would cause MASH Explorer to crash if you increased the number of workflow threads, and then closed and re-opened the Workflow Manager.
- Added contact/user support information to the About dialog.

Version 2.1.1

December 14, 2020

Version 2.1.1 fixes two bugs in version 2.1:

- Fixed a bug that prevented recent (1.3.0 and later) TopPIC versions from working if the generating function for E-value computation is enabled. (Note that there is apparently a bug in TopPIC version 1.3.5 that prevents it from working if the generating function is not enabled. We are anticipating a fix in a future TopPIC version.)
- Fixed the following bug: when the sequence table is generated from a match, if it has identified a modification from TopPIC, an extra amino acid is erroneously added to the sequence.

Version 2.1

November 23, 2020

Version 2.1 introduces a number of new features.

- Support for FLASHDeconv.
- Improved UVPD support.
- MzML file type supported.

- Fixed a problem that could cause importing of experiment files to fail if MASH Explorer is running on a computer that has its language set to something other than “English (United States)”.
- Fixed a number of bugs in multiple experiment support (including sequence table not being updated when switching experiments and problems importing results from a workflow not running on the currently-active experiment).
- Automatic cleanup of workflow working directories (removal of temporary files; can be disabled).
- Button to open workflow working directory.
- More improvements to the robustness of the workflow code.
- Added menu item to view the MASH Explorer log file.
- Fixed a bug in MSPathFinderT support (which caused some versions of MSPathFinderT to not work with MASH Explorer).
- Support for TopFD MS1 and MS2 s/n ratios.
- Support for fixed and variable mods in pTop 1.2.
- Color of status bar changed for better readability of messages.
- Minor improvements to MASH Explorer logging.

Version 2.0.2

August 24, 2020

Version 2.0.2 fixes a bug in the usage reporting introduced in version 2.0.1. This bug could potentially expose file paths when reporting exceptions.

Version 2.0.1

August 17, 2020

Version 2.0.1 introduces usage tracking and fixes a few issues found in 2.0.

- MASH Explorer optionally reports usage data to the MASH team. See the relevant privacy notice here: https://labs.wisc.edu/gelab/MASH_Explorer/doc/MASH%20Explorer%20Privacy_Notice.pdf.
- Note that the download links for MSDeconv and MSAlign+ have changed. The V2.0.1 installation guide has the correct links.
- We fixed several workflow-related bugs.
- We also fixed a bug that caused problems when multiple experiments are loaded.

Version 2.0

June 17, 2020

Version 2.0 introduces new functions and provides reliability and usability improvements from Version 1.2.

- MASH Explorer now supports opening multiple experiment files at the same time.
- Importing a data file can be done by dragging and dropping the data file on the MASH Explorer software.
- PTMs can be customized via the configuration dialog.
- The interface has changed from Docking Windows to Split Views.
- TopPIC up to version 1.3.3 is supported in MASH Explorer.
- New buttons were added in the Mass List panel to display the previous or next scan that has Mass List entries.
- The up/down keys change selection in the Mass List panel.

- The x- and y-axis coordinate for the mouse location in mass spectrum and chromatogram views is displayed. In the mass spectrum, the m/z value and intensity value are shown. In the chromatogram, the time value and intensity value are displayed.
- The “regular” and Quick Decon Workflow Managers are now unified.
- The adjustment of the theoretical spectrum (when an ion is selected) works much better (cleared up abundance vs. intensity confusion).
- The MS level of a scan can be manually specified.
- MASH Explorer can automatically detect activation type for search.
- Workflow folders are better-organized.
- The configuration dialog has buttons to automatically download third-party software.

Version 1.2

November 21, 2019

Version 1.2 is the maintenance upgrade of Version 1.1.

- There are a number of general stability and performance improvements.
- Workflow Manager is more useable and reliable.
- Users can now edit the parameters of queued and finished workflows, which will produce a new queued-to-run workflow.
- Ion assignments can now be filtered in the mass list using context menus by right-clicking the Ion column header.
- Zoom out functionality has been improved. Clicking the “zoom out” button multiple times will eventually show the full spectrum, even if the user has selected an ion from the Mass List.

Version 1.1

August 28, 2019

Version 1.1 is the maintenance release for Version 1.0.

- The Mass List has been re-worked. The Mass List is now displayed as table format.
- Stability has been significantly improved.
- A major bug in Version 1.0 for Mass List was fixed. In Version 1.0, the mass list refreshed every time an entry was edited.
- Stability of Workflow Manager has been improved.
- Users can now upload old workflows in Workflow Manager and use the tree view to import related deconvolution and database search result files.

Version 1.0

July 2, 2019

- A chromatogram scan can now be selected by double-clicking in the chromatogram view.
- Quick Decon now runs via a workflow, like "normal" deconvolution/search. (The old, non-workflow based Quick Decon is (temporarily) available via the Tools menu.)

- Quick deconvolution algorithm can now be any deconvolution algorithm that the user selects. This option is saved with the Quick deconvolution default parameters.
- Deconvolution results are automatically imported into the Mass List following completion of the run.
- Database search results are automatically imported into the Protein Search Results list following completion of the run.
- Citations have been added in the About dialog.
- Sample data is included with MASH Explorer installation.
- Configuration files to save user preferences are now available.
- The Ion Finder now displays a theoretical fit over the zoomed-in area.
- Calculate Fit button calculates theoretical scores for selected rows in the Mass List. • Maintenance updates

Version 0.2.1

April 15, 2019

- Users can now set MASH Explorer configurations in Configuration dialog under Tools menu item.
- Quick deconvolution algorithm and default parameters can be set within the Process Wizard (allows use of algorithms other than eTHRASH; and more control over the deconvolution parameters). Quick Deconvolution now runs as a workflow within the Workflow Manager.
 - The previous quick deconvolution function is still available (though deprecated) – via the Tools menu.
- Waters *.raw files can now be processed within MASH Explorer.
- pParseTD/pTop have been re-enabled.
- ProMex/MSPathFinderT have been re-enabled.
- Workflow Directories are now saved within a “MASH_Workflows” sub-folder within the folder containing the relevant data. This reduces clutter in the data folder.
- The Default Output Directory now contains deconvolution and/or search algorithm name.
- All log file entries now have timestamps.
- MASH Explorer log file and configuration file are now stored in the user’s “AppData\Local\MASH_Explorer\MASH_Explorer_LogBook.txt” folder. • Maintenance updates

Version 0.2

March 11, 2019

- Beta-version is released to enthusiastic users for testing.

