



MRMPilot™ Software

Version 2.1

Release Notes

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Introduction

This document describes version 2.1 of the MRMPilot™ software, an application for developing MRM-based methods for identification or quantitation of peptides.

System Requirements

MRMPilot software has been tested with Windows® XP Service Pack 2; Windows NT® is not supported. A minimum of 1 GB of RAM is recommended.

Before installing the program, ensure that the Analyst® software has been installed and that a hardware profile is active. The software has been tested with both Analyst 1.5.1 and Analyst TF 1.5.

To enable peak review of MRM when importing data into MRMPilot software, installation of MultiQuant™ software is required.

System Recommendations

A screen resolution set to 1280x1024 or higher, with Normal size (96 DPI).

Installation

If you have installed a previous version of the program, you must remove it before installing the latest version. It can be uninstalled using the Add/Remove Programs wizard in the Microsoft Windows Control Panel. Click the old version of the program in the list and click the Remove button.

To install the program, extract the downloaded .zip file to a folder, then double-click the Setup.exe installer in that folder and follow the instructions presented on-screen.

Activation

If you already have a valid license for version 1.0 of MRMPilot software, then you do not need to acquire a new license for this version. The software will attempt to find your 1.0 license file the first time you run the program. (Your 1.0 license file is not deleted when uninstalling the 1.0 version.) If it cannot find the license file, you will see the activation dialog box. Click “Install License File...” and browse to the license file in the bin folder where the 1.0 version of MRMPilot software was installed.

If you do not already have a valid license for MRMPilot software, then you will be prompted for a license to activate the software the first time you run the program. Follow the directions in the activation dialog box for obtaining a license.

Documentation

There are two main help documents installed with the program. To view either of the help documents, on the Windows Start menu, click All Programs, and then MRMPilot, and then Help.

The User Manual document is the main users manual. This manual provides a good introduction to all of the main features of the program. If you have not previously used MRMPilot software it is suggested that you start with this document.

The Reference Manual document describes all of the features of the program in detail. Unlike the User Manual, this document does not provide worked examples; instead, it describes the various menu items and other features in relative isolation.

Known Problems and Limitations

The following known problems currently exist:

MultiQuant 2.0:

1. MRMPilot uses parts of MultiQuant 2.0 to integrate and import MRM data. MultiQuant 2.0 requires that data files are located within the Analyst Data project folder hierarchy. Wiff files must be located under a projects 'Data' folder. Results files will be created in a projects 'Results' folder. The current Analyst project will be the project used by MRMPilot when importing MRM data. To change the current project, select the desired project in Analyst before importing MRM data in MRMPilot.
2. MRMPilot can import data from older MultiQuant results files (version 1.2), however the 'Review Data' feature will not work correctly. Data imported to MRMPilot directly from a wiff file or from a MultiQuant 2.0 results file has full functionality, including 'Review Data'.

Installation:

3. The software requires Microsoft .NET 3.5 SP1 to be installed. If the installer is launched by running the setup.exe, then the .NET framework will be automatically downloaded and installed if necessary. Do not launch the installer by running the .msi file. This can lead to an install without .NET 3.5 SP1, which will result in various crashes during operation.

Importing Proteins:

4. Importing very large lists of proteins may result in unacceptable performance. To build large assays, it is recommended to develop assays for smaller numbers of proteins, save the assays to the ProteinAssay Catalogue, and then build a final assay for many proteins using the catalogue.
5. After deleting a protein, the feature to add proteins by accession number may not function correctly. The proteins will be added, but selected peptides may not be added. Restart the application to fix this problem.
6. The software will not prevent adding the same protein multiple times. Be sure to avoid this to prevent wasteful MRM methods.

7. The automatically generated short names for proteins are not guaranteed to be unique, but can be edited to make them unique. To edit the short name for a protein, select it, then click on View Sequence and Info under the Protein menu.

Peptides:

8. Theoretical spectra are not created for peptides longer than 50 amino acids.
9. Contact support (email support@absciex.com) in order to create peptides with custom modifications.

Other Data Import Issues:

10. The software may crash if asked to import data from a file that is open in another application. If this happens, close the software, close the open file, then restart the software and try again.
11. The ability to import proteins and peptides from other software has only been tested with certain versions of output from each other software. The import may not work with different versions of these formats. Listed below are some sources of proteins and peptides and the versions tested.
 - o Mascot: Version 2.1
 - o X!Tandem: Unknown. No version information found in output file.
 - o Sequest: Version 28 rev 13
 - o Spectrum Mill: pepXML v1.8 and mzXML v3.0, with the parameter 'parentFileName' in the tag 'scanOrigin' within the mzXML file matching the parameter 'spectrum' in the tag 'spectrum_query' within the corresponding pep.XML file.

General Issues:

12. The software will not work for users with a “limited user” account in Windows XP SP2. It is recommended to use the software from a Windows account with administrator privileges.
13. Occasionally UI items such as Selected MRM count or graph panels will not be updated with current values. The work-around for this issue is to select another item (protein, peptide, or MRM) and then re-select the desired item. If this does not work, save the .choose file, exit the software, then re-launch and open the .choose file again.
14. When browsing for a folder (not a file) where the full name, including all its parent directories, is very long, the program will crash. You can either move your files further up the directory structure or download a patch from Microsoft at: <http://www.microsoft.com/downloads/details.aspx?familyid=a8f5654f-088e-40b2-bbdb-a83353618b38&displaylang=en>

Instrument-Specific Issues:

15. QTRAP® 5500 System: The software will attempt to build methods for QTRAP 5500 systems with MRMs up to 1250 Da. Successful method building up to this mass range requires installation of either the Analyst 1.5 Software Components for 5500 Systems HotFixes to April 2009. Without this, methods may fail to build without the cause of failure being clearly reported. Contact support (email support@absciex.com) to get the HotFixes release if you do not already have it.