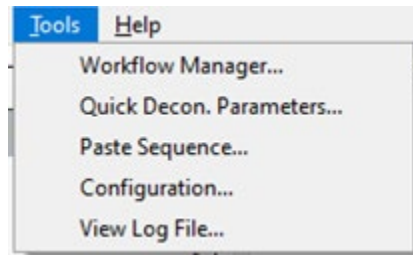


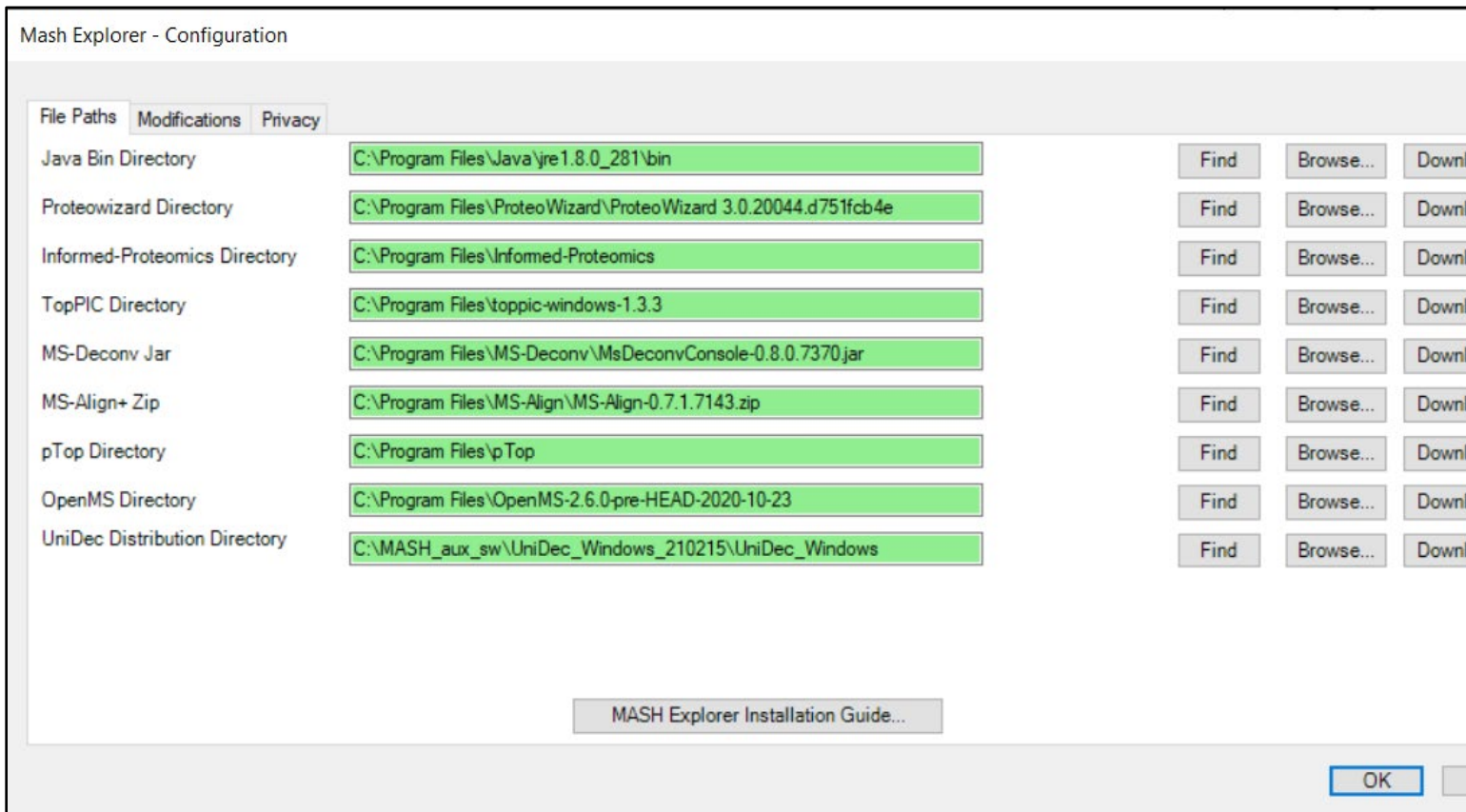
System Installation Guide

Version 2.2

This document gives information on downloading and installing MASH Explorer and its supporting software. Note that when you install supporting software, you need to use the Configuration dialog in MASH Explorer to specify where MASH Explorer should find the supporting software. Access the Configuration dialog via the Tools menu:



Boxes in the Configuration dialog will appear green if the specified file path exists and red if it does not. Use “Find” to automatically find supporting software, and “Browse” to set the file path yourself.



Please note that Windows has a 270 character path limit. Please keep all file paths to supporting software and raw data well below this limit, as MASH Explorer automatically creates new directories for your workflows.

1. Windows Operating System

MASH Explorer requires the Windows operating system and is currently not functional on other operating systems.

2. MASH Explorer

You can obtain the MASH Explorer software here:

https://labs.wisc.edu/gelab/MASH_Explorer/MASHSoftware.php.

To install MASH Explorer itself, run the Windows installer executable file (for example, "MASH_Explorer_App_x64_V2.1.exe"). (You will need administrator permission to install MASH Explorer.)

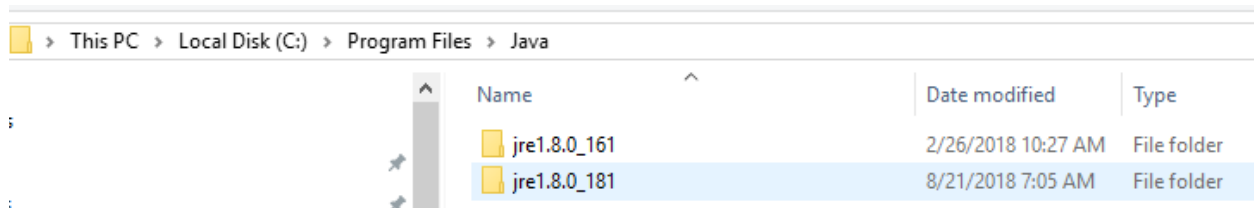
Note that if you have a previous version of MASH Explorer installed, you must manually uninstall that version before installing the new version (see Settings->Apps by right-clicking on the Windows icon in the lower left corner of the screen). You do not have to uninstall any of the supporting software to upgrade MASH Explorer itself.

3. Java (64-bit)

To use MS-Deconv and MS-Align+, 64-bit Java needs to be installed on your computer. You can download the Java software with the following link <https://www.java.com/en/download/manual.jsp>. Download the Windows offline (64-bit version), seen below:

The screenshot shows the Java website's download page. The main heading is "Java Downloads for All Operating Systems" with a sub-heading "Recommended Version 8 Update 201". A sidebar on the left lists "Available Operating Systems" (Windows, Mac, Linux, Solaris), "Help Resources" (Troubleshoot Java), "Java 7" (Where can I get Java 7?), and "JDK" (Looking for the JDK?). The main content area lists three download options for Windows: "Windows Online" (1.87 MB), "Windows Offline" (63.53 MB), and "Windows Offline (64-bit)" (71.44 MB). The "Windows Offline (64-bit)" option is highlighted with a blue box. Below the list, there is a note: "If you use 32-bit and 64-bit browsers interchangeably, you will need to install both 32-bit and 64-bit Java in order to have the Java plug-in for both browsers. » [FAQ about 64-bit Java for Windows](#)".

Follow the Java installation setup and copy Java into the following directory into the system drive shown below:



4. ProteoWizard, Windows 64-bit Installer

MASH Explorer has integrated ProteoWizard for convenient data import and data conversion. Download ProteoWizard 64-bit with vendor libraries from their website (<http://proteowizard.sourceforge.net/>).

ProteoWizard is not a requirement to run the MASH Explorer application, but it is a requirement to load Thermo and Bruker files into the application.

5. .NET Framework 3.5 SP1 and .NET Framework 4.7.2

These .NET Framework 4.7.2 can be downloaded at <https://dotnet.microsoft.com/download/dotnet-framework-runtime>. The .NET Framework 3.5 SP1 can be downloaded from <https://dotnet.microsoft.com/download/dotnet-framework/net35-sp1> MASH Explorer requires the .NET Framework 3.5 SP1 or above. ProteoWizard requires both .NET Framework 3.5 SP1 and .NET Framework 4.7.2 or above.

6. Xcalibur 2.0.7+ or MSFileReader x64 for Thermo Data File Import

During our testing and development of the MASH Explorer using the ProteoWizard library, we encountered trouble parsing some of our testing Thermo files. We recommend that Thermo users install either Xcalibur version 2.0.7 or above (please consult with your vendor regarding this software), or MSFileReader x64 (available from Thermo website upon account registration, <https://thermo.flexnetoperations.com/control/thmo/login?nextURL=%2Fcontrol%2Fthmo%2Fsearch%3Fquery%3DMSFileReader>). If your computer requires any administrative access when downloading applications select “Run as Administrator” when installing MSFileReader. Please download any version of MSFileReader except MSFileReader 3.1 SP4. Neither Xcalibur nor MSFileReader is not required to run MASH Explorer but one or the other is required for loading Thermo files into MASH Explorer.

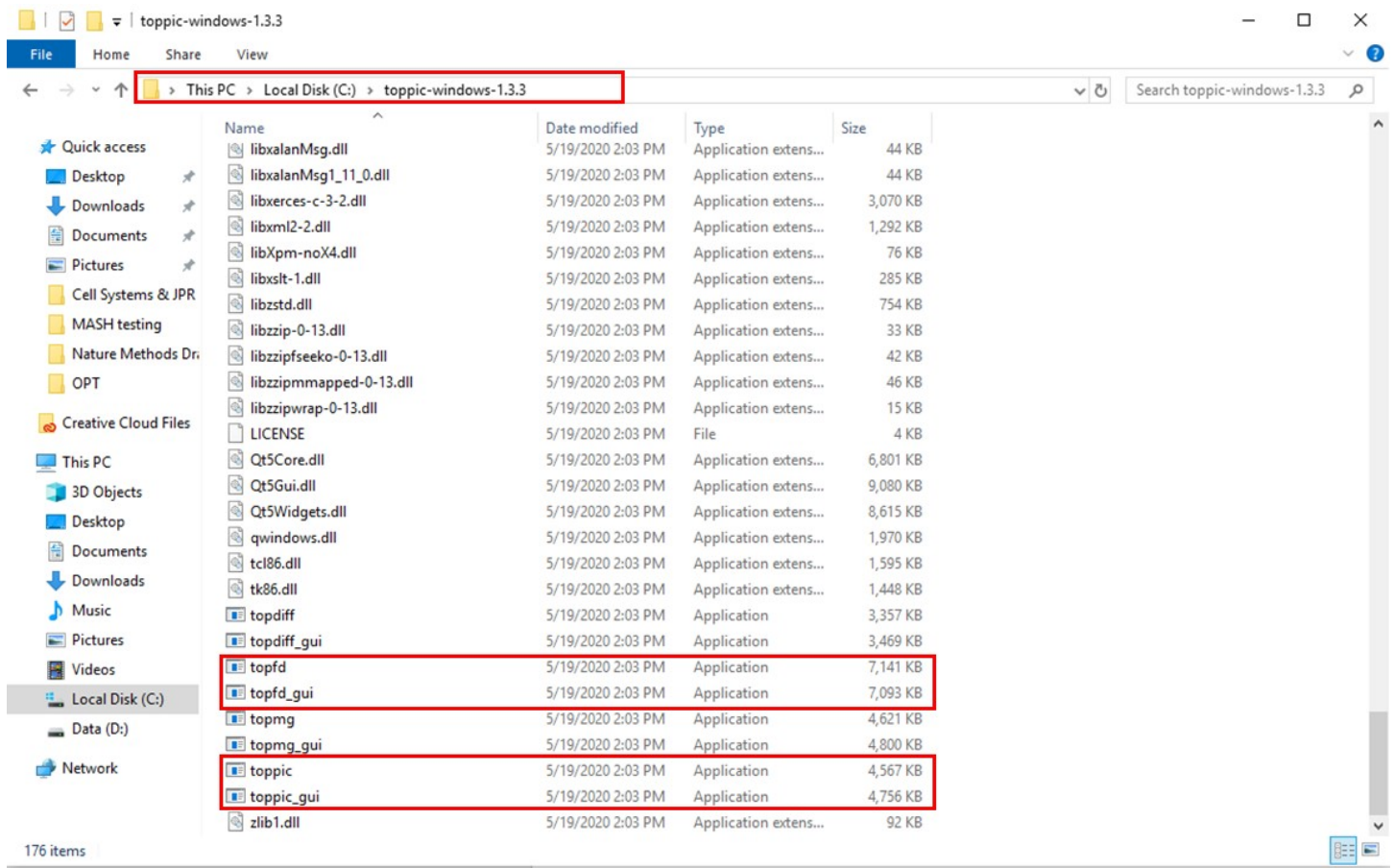
7. CompassXtract for Bruker data file import

Similar to the case in Thermo data import, sometimes ProteoWizard has trouble parsing some of the Bruker files. We recommend Bruker users install CompassXtract (available from Bruker, <https://www.bruker.com/service/support-upgrades/software-downloads/mass-spectrometry/compass-tools.html>; free registration needed). CompassXtract is not a requirement to run MASH Explorer, but it is a requirement to open Bruker data files within the application.

Deconvolution and Search Algorithm Setup

1. TopPIC Suite

MASH Explorer can interface with an installed version of TopPIC developed by Xiaowen Liu's research group in Indiana University - Purdue University Indianapolis. Download the TopPIC Suite software package (including TopFD for deconvolution algorithm and TopPIC for database search algorithm) from their website (<http://proteomics.informatics.iupui.edu/software/toppic/register.html>). Copy the folder containing the topfd.exe and toppic.exe to system drive (C:) shown below:



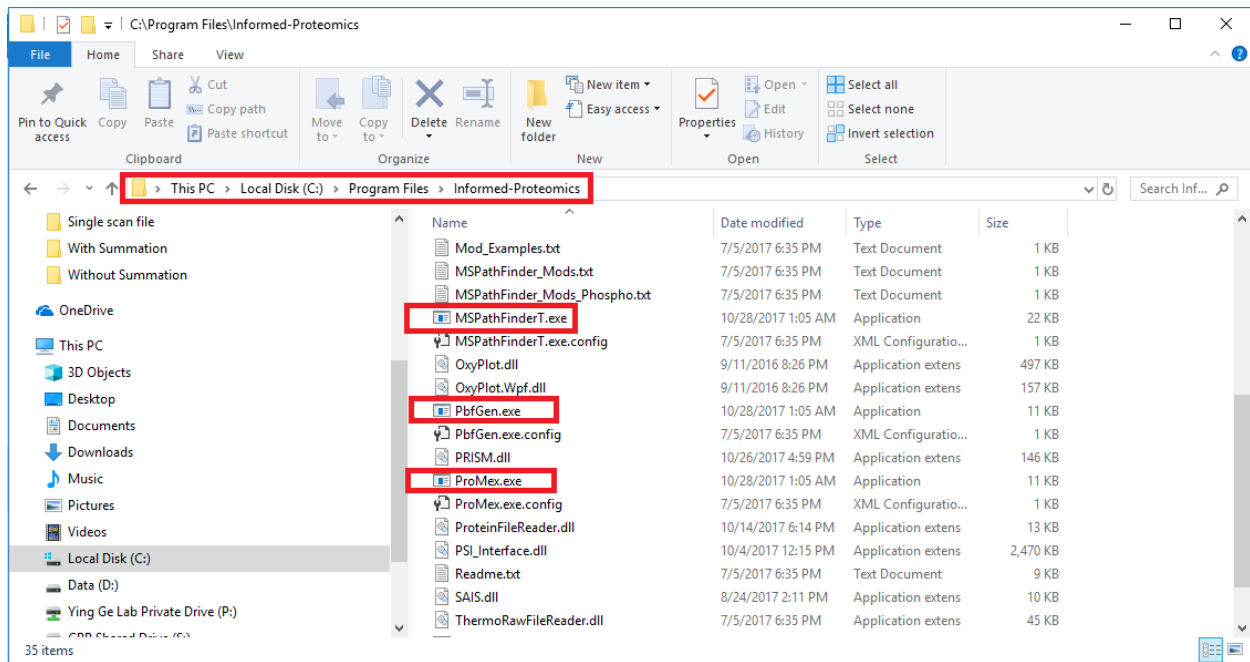
When using the TopPIC algorithm for searching in MASH Explorer software, please also acknowledge their paper (Bioinformatics, 32:3495-3497, 2016).

We recommend using TopPIC 1.3.2 or later.

2. Informed-Proteomics Package

MASH Explorer can interface with the installed version of the Informed-Proteomics software package. Download the Informed-Proteomics package from (<https://github.com/PNNL-Comp-Mass-Spec/Informed-Proteomics/releases>) and install the software package using the Informed-Proteomics_Installer.exe. Before using

this package for database search, make sure that the three executable files (MSPathFinderT.exe, PbfGen.exe and ProMex.exe) are included in the system as shown below:



When using the Informed-Proteomics for database search, please acknowledge their paper (Nature Methods volume 14, pages 909–914 (2017)).

3. MS-Deconv/MSAlign+

Download MS-Deconv 0.8.0.7370 from their website (<https://xwliu.pages.iu.edu/msdeconv/download.html>). Download MS-Align+ 0.7.1.7143 from their website (<https://xwliu.pages.iu.edu/msalign/download.html>). Move the MsDeconvConsole-0.8.0.7370.jar and MS-Align-0.7.1.7143.zip to a local drive (C:) from your Downloads folder, and use the configuration tool to set these file paths. MASH Explorer will unzip MSAlign+ for you.

If using MS-Deconv or MSAlign+, please cite respective publications MS-Deconv (Mol Cell Proteomics 2010;9:2772-2782) and MS-Align+ (Mol Cell Proteomics 2012;11:M111.008524).

4. pParseTD/pTop

Please use the following link to download pTop (<http://pfind.net/software/pTop/index.html>). pParseTD is an embedded algorithm which is installed at the same time. Run the downloaded executable file, pTop1.2_x64.exe (at the time of writing this document). Running pTop workflow will require installation of Xcalibur software.

When using this software package, please cite their publication (Anal. Chem., 2016, 88 (6), pp 3082–3090).

5. OpenMS (for FLASHDeconv)

Please use the following link to download OpenMS (for FLASHDeconv) (<https://abibuilder.informatik.uni-tuebingen.de/archive/openms/OpenMSInstaller/experimental/feature/FLASHDeconv/OpenMS-2.6.0-pre-HEAD-2020-10-23-Win64.exe>). Note that FLASHDeconv is not currently included in the official OpenMS release, so you should download the pre-release version from the link provided here. Download the Windows installer executable (for example, OpenMS-2.6.0-Win64.exe) and run it to install OpenMS.

When using FLASHDeconv, please cite their publication (K. Jeong, J. Kim, M. Gaikwad, S. N. Hidayah, L. Heikaus, H. Schlüter, and O. Kohlbacher, “FLASHDeconv: Ultrafast, high-quality feature deconvolution for top-down proteomics,” *Cell Systems*, vol. 10, iss. 2, p. 213–218, 2020).

6. HDF5 (for UniDec)

Please use the following link to download the HDF5 libraries (<https://www.hdfgroup.org/downloads/hdf5/>). You will have to register on the HDF5 group website in order to download the libraries. We suggest you use the `hdf5-x.x.x-Std-win10_64-vs14.zip` file. After downloading, unzip the file and run (double-click) the associated msi file to install the HDF5 libraries.

7. UniDec

Use the following link to download the latest version of the UniDec release (<https://github.com/michaelmarty/UniDec/releases>). Version 4.4.1+ is needed in order for MASH Explorer and UniDec to work in the interactive mode; earlier versions will work in non-interactive mode. Download the `UniDec_Windows_XXXX.zip` file. Unzip the file into the desired location on your computer. Inside MASH Explorer, point the configuration dialog to the file folder that contains `GUI_UniDec.exe` and `UniDec.exe`.

When using UniDec, please cite their publication (M. T. Marty, A. J. Baldwin, E. G. Marklund, G. K. A. Hochberg, J. L. P. Benesch, and C. V. Robinson, “Bayesian Deconvolution of Mass and Ion Mobility Spectra: From Binary Interactions to Polydisperse Ensembles”, *Anal. Chem.* vol. 87, iss. 8, p. 4370-4376, 2015).