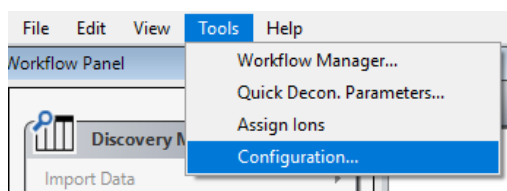


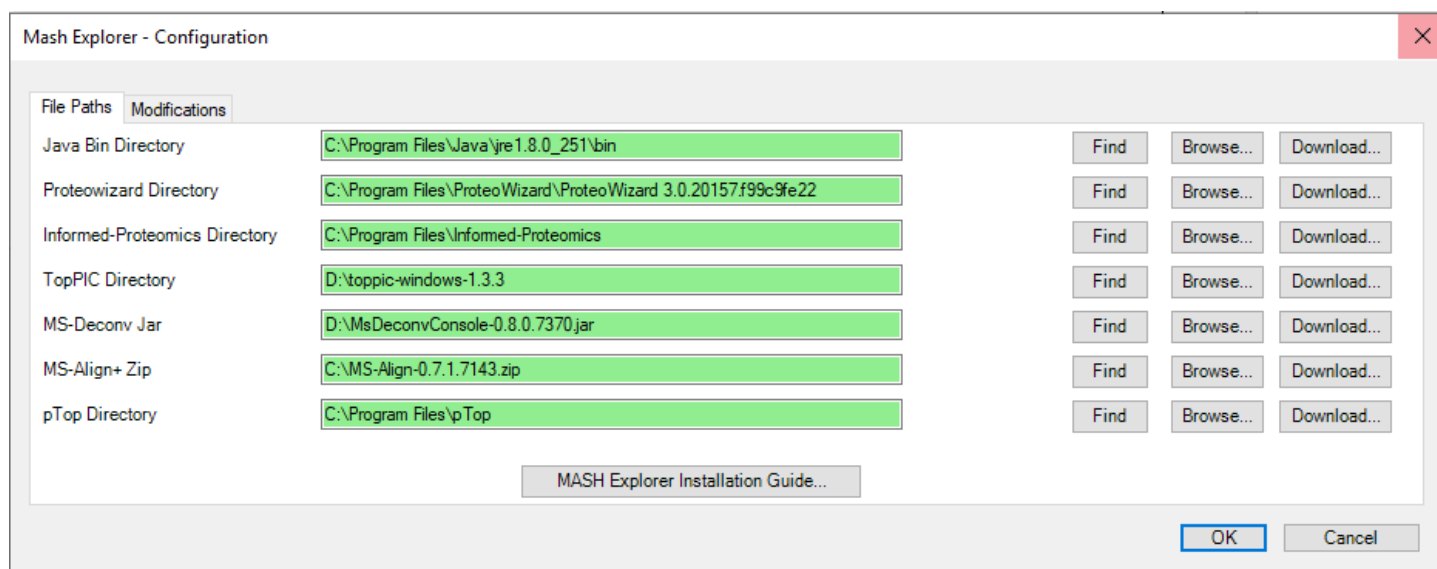
System Installation Guide

Version 2.0.2

We recommend downloading and installing supporting software as described in this document. This will allow MASH Explorer to automatically access the supporting software. If you wish to install supporting software in a location other than specified in this document, please use the “Configuration Tab” under the Tools Menu Item to configure supporting software.



Boxes in the configuration file will appear green if the selected file 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 a Windows operating system and is currently not functional on other operating systems.

2. Windows Offline (64-bit) Java

To use MS-Deconv and MS-Align+, 64-bit Java application needs to be installed in the system. 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:

Available Operating Systems

- » [Windows](#)
- » [Mac](#)
- » [Linux](#)
- » [Solaris](#)

Help Resources

- » [Troubleshoot Java](#)

Java 7

- » [Where can I get Java 7?](#)

JDK

- » [Looking for the JDK?](#)

Java Downloads for All Operating Systems

Recommended Version 8 Update 201
Release date January 15, 2019

Select the file according to your operating system from the list below to get the latest Java for your computer.

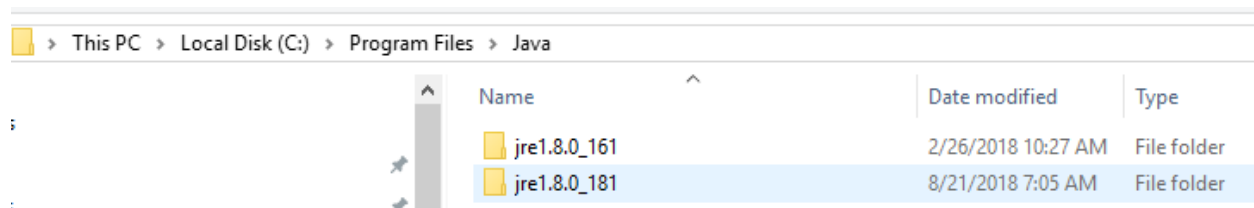
> [Remove Older Versions](#) > [What is Java?](#)

By downloading Java you acknowledge that you have read and accepted the terms of the [end user license agreement](#)

Windows	Which should I choose?
Windows Online filesize: 1.87 MB	Instructions
Windows Offline filesize: 63.53 MB	Instructions
Windows Offline (64-bit) filesize: 71.44 MB	Instructions

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:



3. 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.

4. .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.

5. 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 in some of our testing Thermo files. We recommend Thermo users to 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.

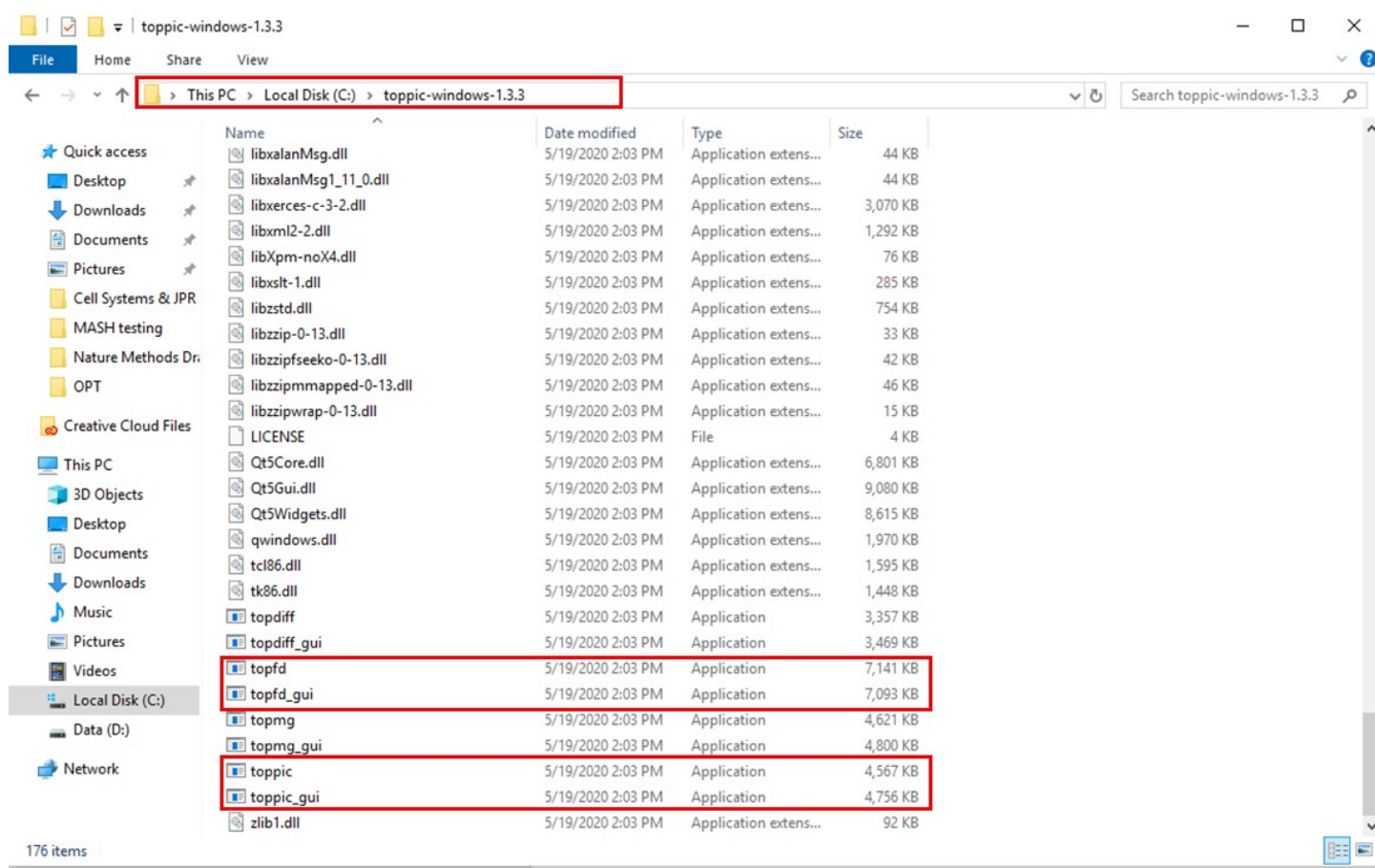
6. CompassXtract for Bruker data file import

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.

Search Algorithm Setup Guide

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:

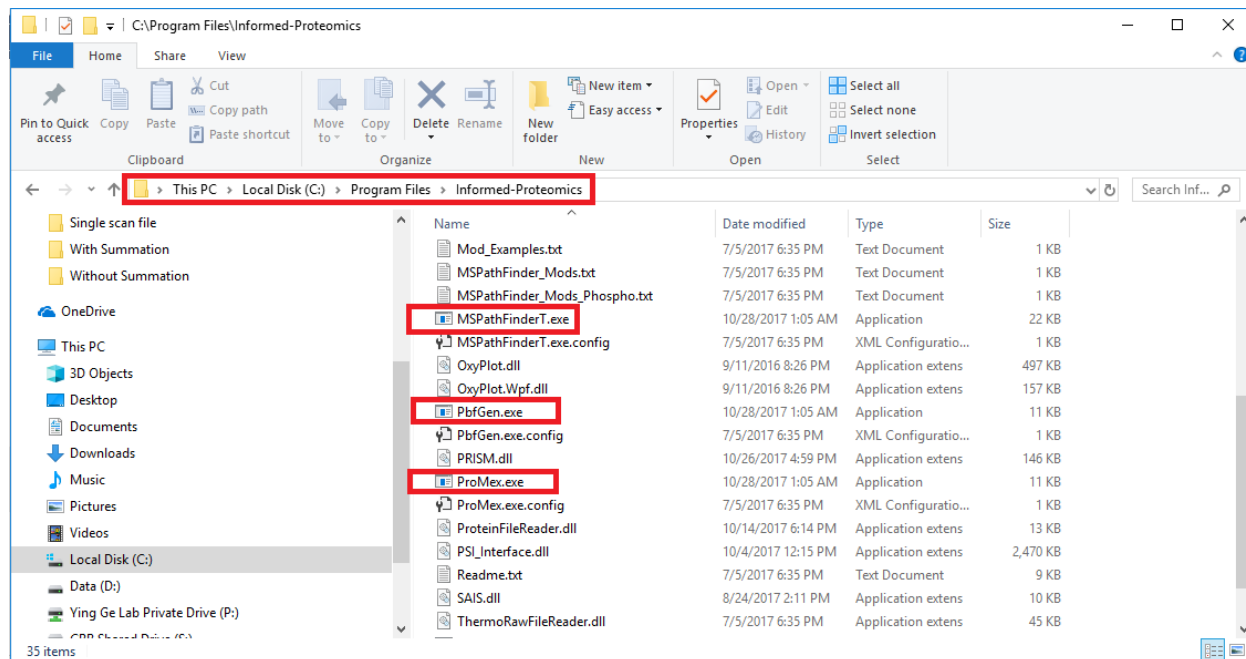


When using the TopPIC algorithm for searching in MASH Explorer software, please also acknowledge their paper (Bioinformatics, 32:3495-3497, 2016).

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 links 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).