

Tutorial to convert wiff to mzml

DMS Data Extraction Toolkit was created to enable users to easily batch extract data from .jdx or .mzml files and populate .csv sample datasets in the format used by [iDMS](#).

DMS data collected on a Sciex® SelexION Differential Mobility Separation device is acquired in proprietary .wiff and .wiffscan format. These data can be converted to .jdx or .mzml files for batch processing using the DMS Data Extraction Toolkit. JCAMP-DX is an ASCII-based format (1-3). MZML is an open-source XML-based format (4,5). Both formats are used to store and share mass spectrometry data across platforms and manufacturers.

This tutorial is meant as a helpful guide for users new to transforming Sciex® .wiff and .wiffscan to .mzml using their existing Analyst software.

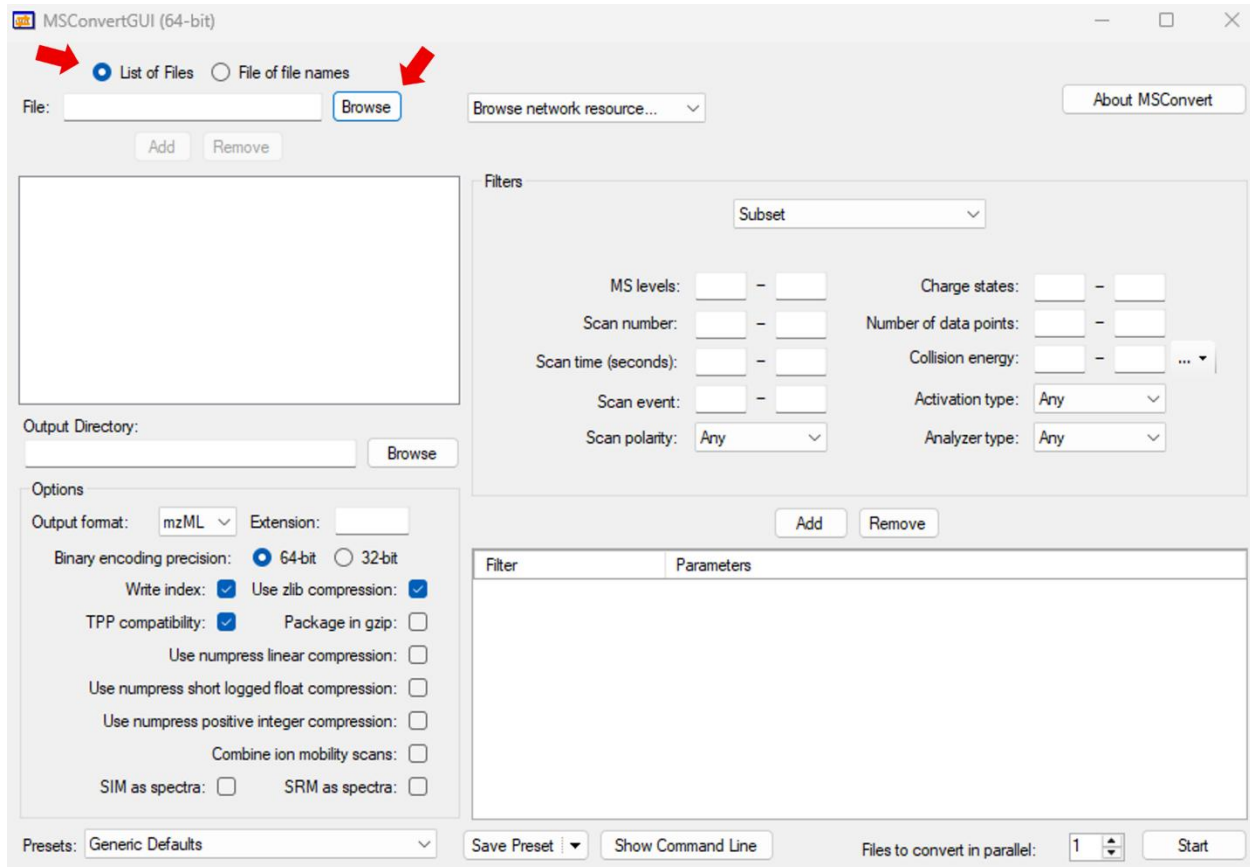
Tutorial

1. Download Proteowizard

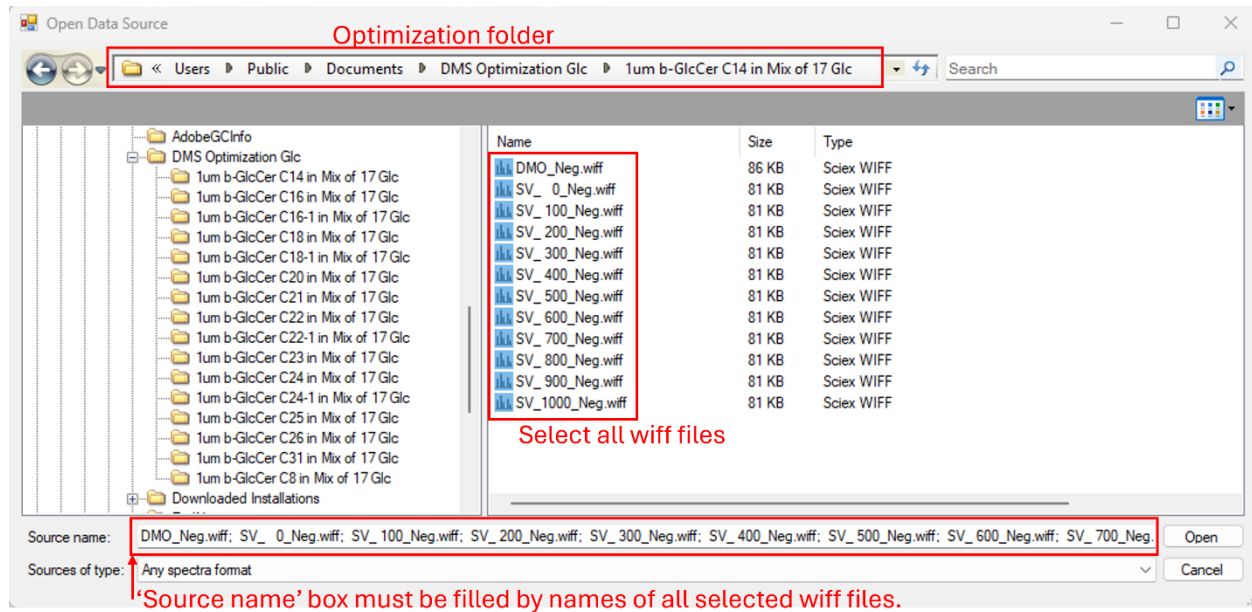
- Access Proteowizard website at <https://proteowizard.sourceforge.io/download.html>.
- Choose “Proteowizard” in “Project”.
- Enter in the Download form the information appropriate to your computing platform.
- Read and accept the license agreements to Download.
- Install Proteowizard on your computer

2. Convert .wiff files to .mzml files

- Open msconvert on your computer.
- Select “List of Files”, then choose “Browse” (Figure below).



- Navigate to each optimization folder, press and hold “Ctrl” (PC) to select all the .wiff files corresponding to that single optimization experiment (Figure below).



- Click "Open" when finished.
- By default, the "Output Directory" is the same as the input directory (ie. the selected optimization folder). For file organization simplicity, leave this as default.
- Choose "mzML" for Output format.
- Binary encoding precision: 64-bit
- Select: "Write index", "Use zlib compression", "TPP compatibility".
- Leave the rest as is (default).
- Select "Start" in the bottom right corner.
- Progress is indicated in the "Conversion progress" window (Figure below).

Conversion Progress	
Name	Progress
C:\Users\Public\Documents\DMS Optimization Glc\1um b-GlcCer C14 in Mix of 17 G...	Finished
C:\Users\Public\Documents\DMS Optimization Glc\1um b-GlcCer C14 in Mix of 17 G...	Finished
C:\Users\Public\Documents\DMS Optimization Glc\1um b-GlcCer C14 in Mix of 17 G...	Finished
C:\Users\Public\Documents\DMS Optimization Glc\1um b-GlcCer C14 in Mix of 17 G...	Finished
C:\Users\Public\Documents\DMS Optimization Glc\1um b-GlcCer C14 in Mix of 17 G...	Finished
C:\Users\Public\Documents\DMS Optimization Glc\1um b-GlcCer C14 in Mix of 17 G...	Finished
C:\Users\Public\Documents\DMS Optimization Glc\1um b-GlcCer C14 in Mix of 17 G...	Finished
C:\Users\Public\Documents\DMS Optimization Glc\1um b-GlcCer C14 in Mix of 17 G...	Finished
C:\Users\Public\Documents\DMS Optimization Glc\1um b-GlcCer C14 in Mix of 17 G...	Finished
C:\Users\Public\Documents\DMS Optimization Glc\1um b-GlcCer C14 in Mix of 17 G...	Finished
C:\Users\Public\Documents\DMS Optimization Glc\1um b-GlcCer C14 in Mix of 17 G...	Finished
C:\Users\Public\Documents\DMS Optimization Glc\1um b-GlcCer C14 in Mix of 17 G...	Finished

Starting...
 Opening file "C:\Users\Public\Documents\DMS Optimization Glc\1um b-GlcCer C14 in Mix of 17 Glc\DMO_Neg.wiff" for read...
 Calculating SHA1 checksum...
 Processing...
 Note: input contains only chromatogram data.
 Writing "C:\Users\Public\Documents\DMS Optimization Glc\1um b-GlcCer C14 in Mix of 17 Glc\DMO_Neg-TuneSampleName.mzML"...
 Finished.

- Repeat the above steps for each optimization folder.
- Each optimization folder now will have a .mzml file as well as the original .wiff and .wiff.scan files for each optimization acquisition.

Naming convention for converted files

After conversion, confirm that each file name is the following format before proceeding to use DMS Data Extraction Toolkit. Input files for the DMS Data Extraction Toolkit must be named with the following convention, such that underscores are used to delimit the SV value of a given run.

[text]_[SV value]_[text].mzml

For example: SV_200_Pos.mzml

If not, user must change filename to assume this format.

References

- (1) Gasteiger, J., B. M. P. Hendricks, Hoever P., Jochum C., and Somberg H. 1991. "JCAMP-CS: A Standard Exchange Format for Chemical Structure Information in a Computer-Readable Form." *Applied Spectroscopy* 45 (1): 4–11.
- (2) Lampen, P, H Hillig, AN Davies, and M Linscheid. 1994. "JCAMP-DX for Mass Spectrometry." *Applied Spectroscopy* 48 (12): 1545–52.
- (3) Baumbach, JI, AN Davies, P Lampen, and H Schmidt. 2001. "JCAMP-DX. A Standard Format for the Exchange of Ion Mobility Spectrometry Data - (IUPAC recommendations 2001)." *Pure and Applied Chemistry* 73 (11): 1765–82.
- (4) Orchard, S., Hermjakob, H., The HUPO proteomics standards initiative—easing communication and minimizing data loss in a changing world. *Brief. Bioinformatics* 2008,9, 166–173.
- (5) Deutsch, E., mzML: A single, unifying data format for mass spectrometer output. *Proteomics* 2008, 8: 2776-2777.