# Conversion to mzML Format for NIST26 Chromatogram Processing

## Video/Handout

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**Mass Spec Interpretation Services**
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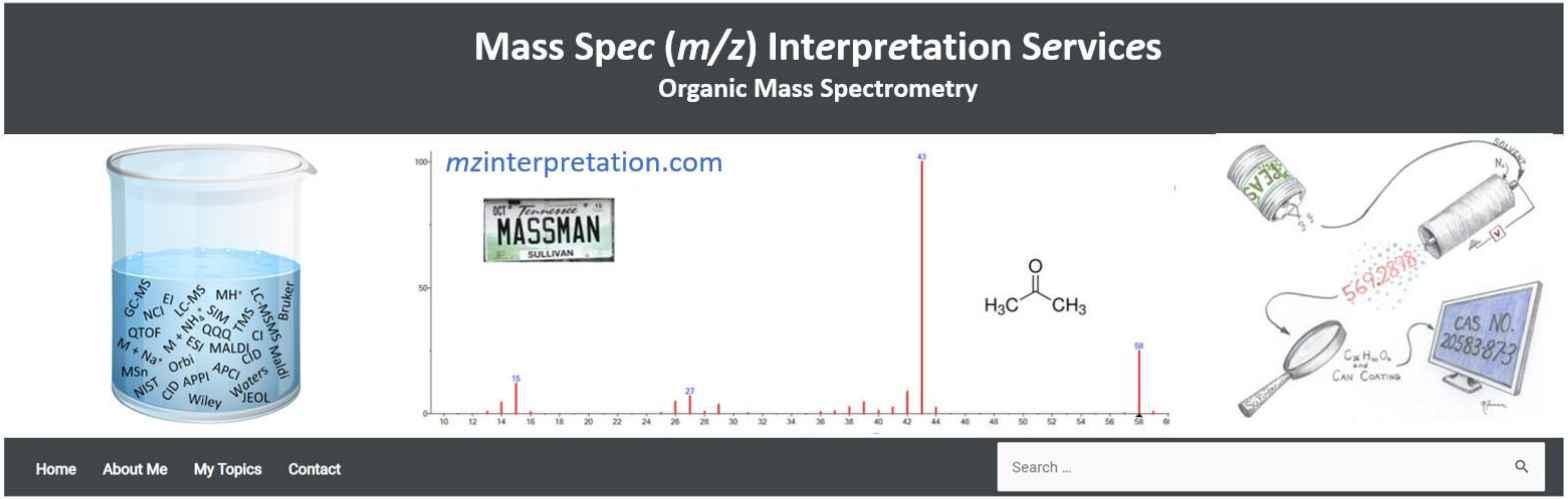
[mzinterpretation.com](mzinterpretation.com)

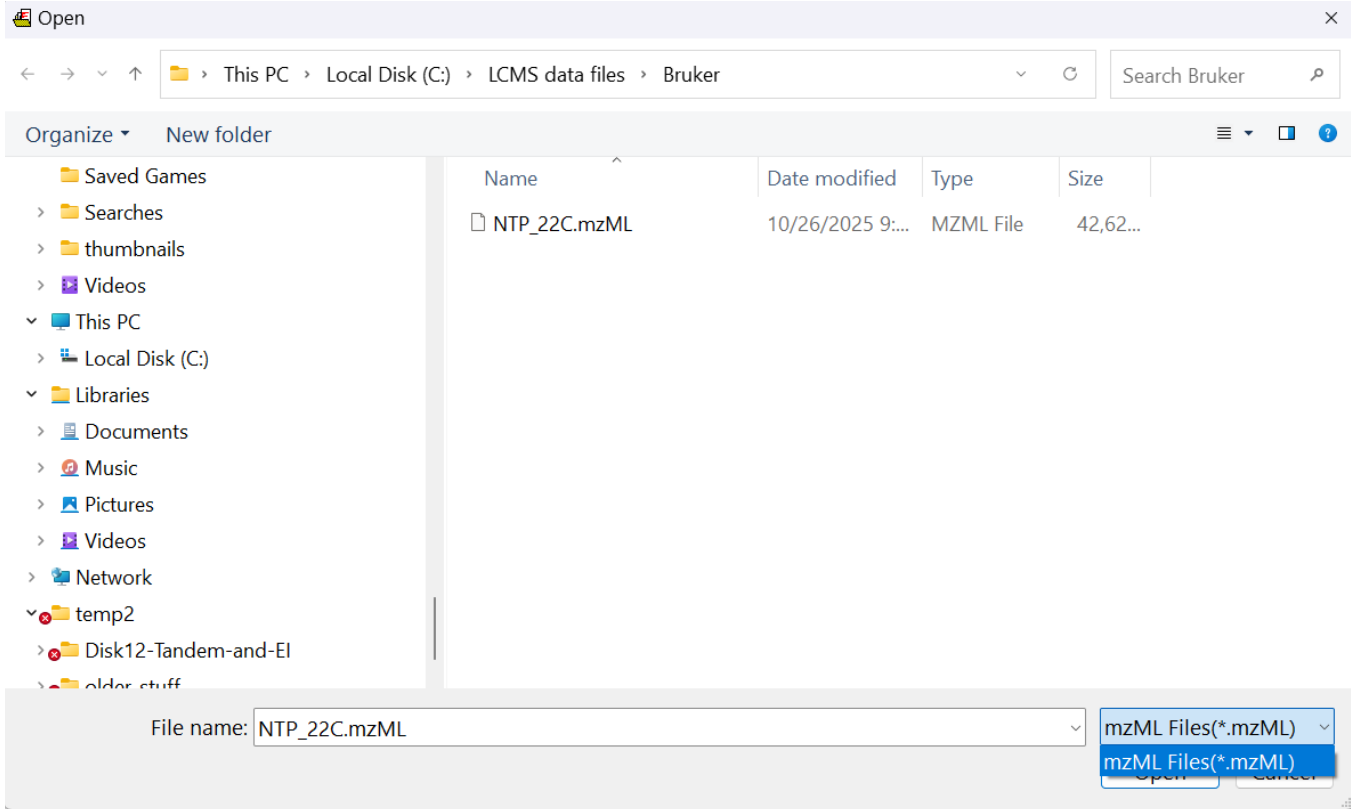
**See *Full Course* on NIST26 with new *Integrated* Deconvolution/Library Searching for *EI GC-MS* and *LC-MS/MS*!**



Mass Spec (*m/z*) Interpretation Services
Organic Mass Spectrometry

# Only Acceptable File Format is *.mzML

- Only acceptable file format is *.mzML
- Either obtain from a conversion by the vendor’s software
- Or use msconvert within Free ProteoWizard Software



| Name | Date modified | Type | Size |
|---|---|---|---|
| NTP_22C.mzML | 10/26/2025 9:... | MZML File | 42,62... |

File name: NTP_22C.mzML

mzML Files(*.mzML)

mzML Files(*.mzML)

Only mzML!

# Download of msconvert, Part of ProteoWizard

You download **MSConvert** as part of the full **ProteoWizard** package—there’s no separate installer just for MSConvert.

🔗 **Official download location**

Go to the ProteoWizard project page:

- [https://proteowizard.sourceforge.io/download.html](https://proteowizard.sourceforge.io/download.html)

**What to download**

- Choose the **Windows installer (.msi)** (most common for LC/MS work)
- File name typically looks like:

`ProteoWizard-x.xx.x-Setup.exe` or `.msi`

**After installation**

- MSConvert is installed automatically
- You’ll find it here:
    - Start Menu → *ProteoWizard* → **MSConvert (GUI)**
    - Or command line tool: `msconvert.exe`

**Versions to consider**

- **Stable release** → safest for routine workflows
- **Nightly build** → newer features (sometimes useful for newer vendor formats, but less tested)

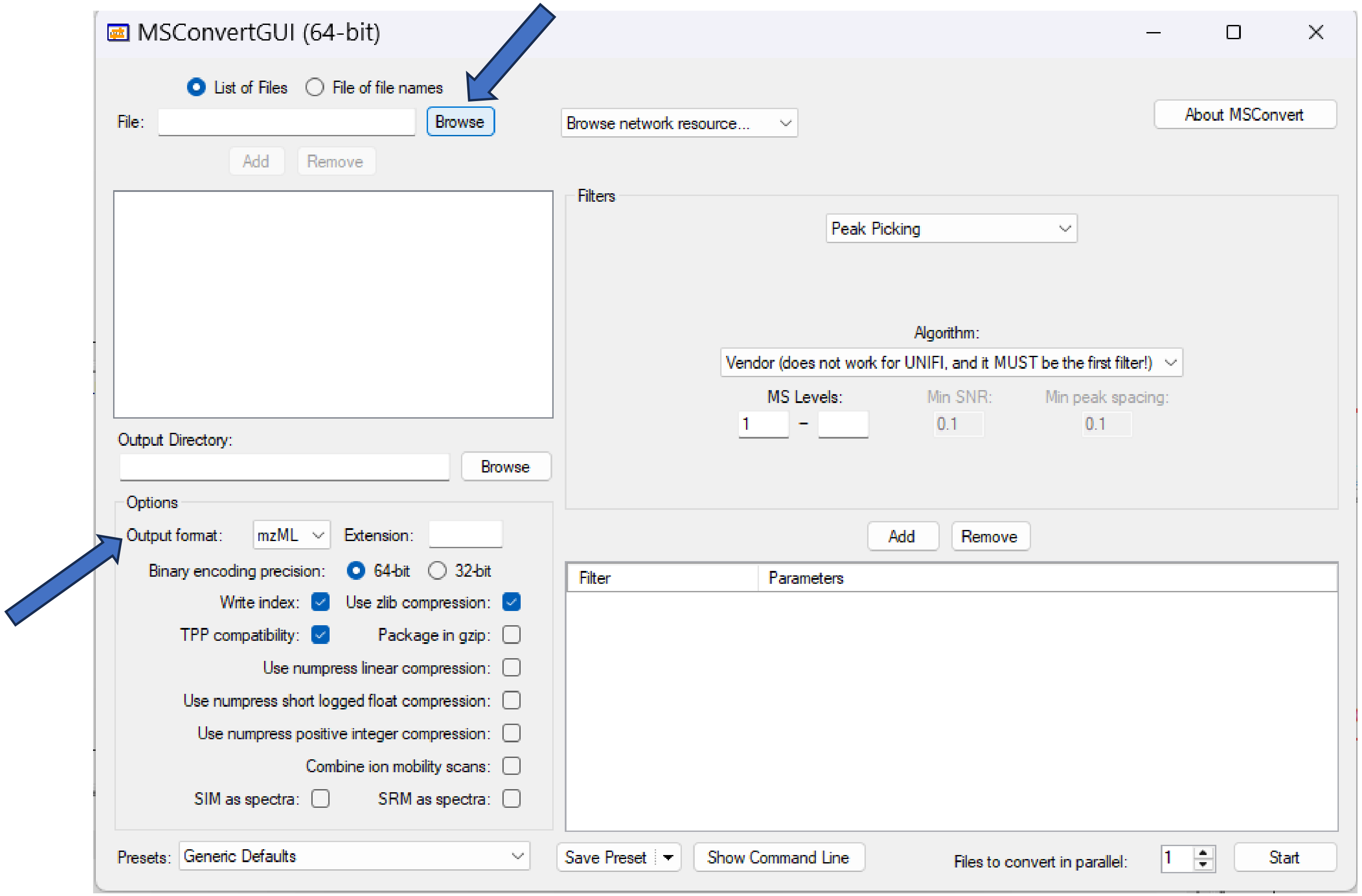
**Practical tip (relevant to your workflow)**

Since you’re working with **Agilent data and centroid/profile handling**, newer/nightly builds sometimes:

- improve vendor reader support
- give better control of **peak picking filters**

So if you run into odd behavior (especially with already-centroided Agilent data), it’s worth trying a **recent nightly build**.

# Start by Browsing Files with Output Format of mzML



MSConvertGUI (64-bit)

● List of Files ○ File of file names

File:

Filters

Peak Picking

Algorithm: Vendor (does not work for UNIFI, and it MUST be the first filter!)

MS Levels: 1 –

Min SNR: 0.1

Min peak spacing: 0.1

Output Directory:

Options

Output format: mzML

Extension:

Binary encoding precision: ● 64-bit ○ 32-bit

Write index: ☑

Use zlib compression: ☑

TPP compatibility: ☑

Package in gzip: ☐

Use numpress linear compression: ☐

Use numpress short logged float compression: ☐

Use numpress positive integer compression: ☐

Combine ion mobility scans: ☐

SIM as spectra: ☐

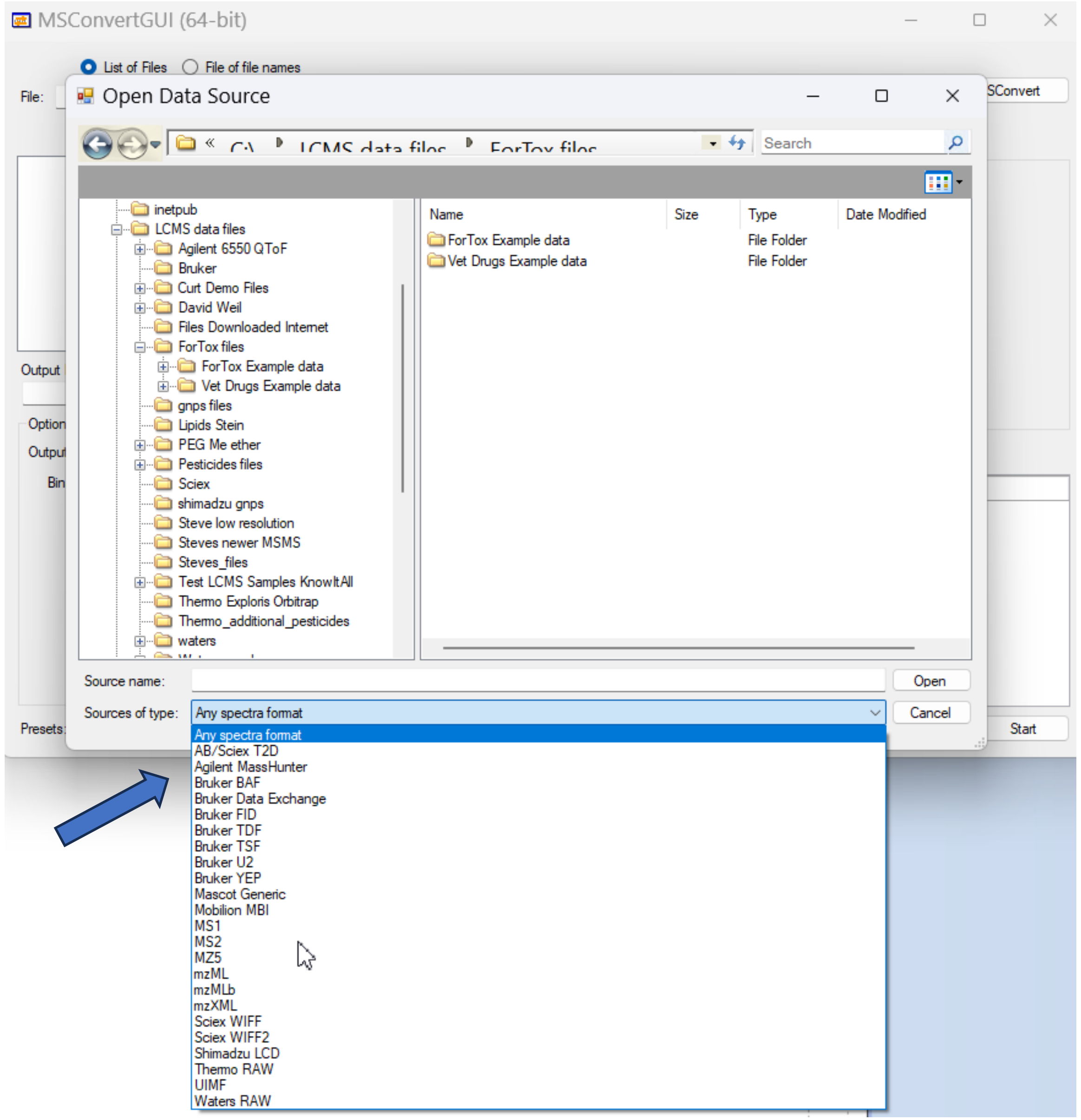
SRM as spectra: ☐

| Filter | Parameters |
|---|---|

Presets: Generic Defaults

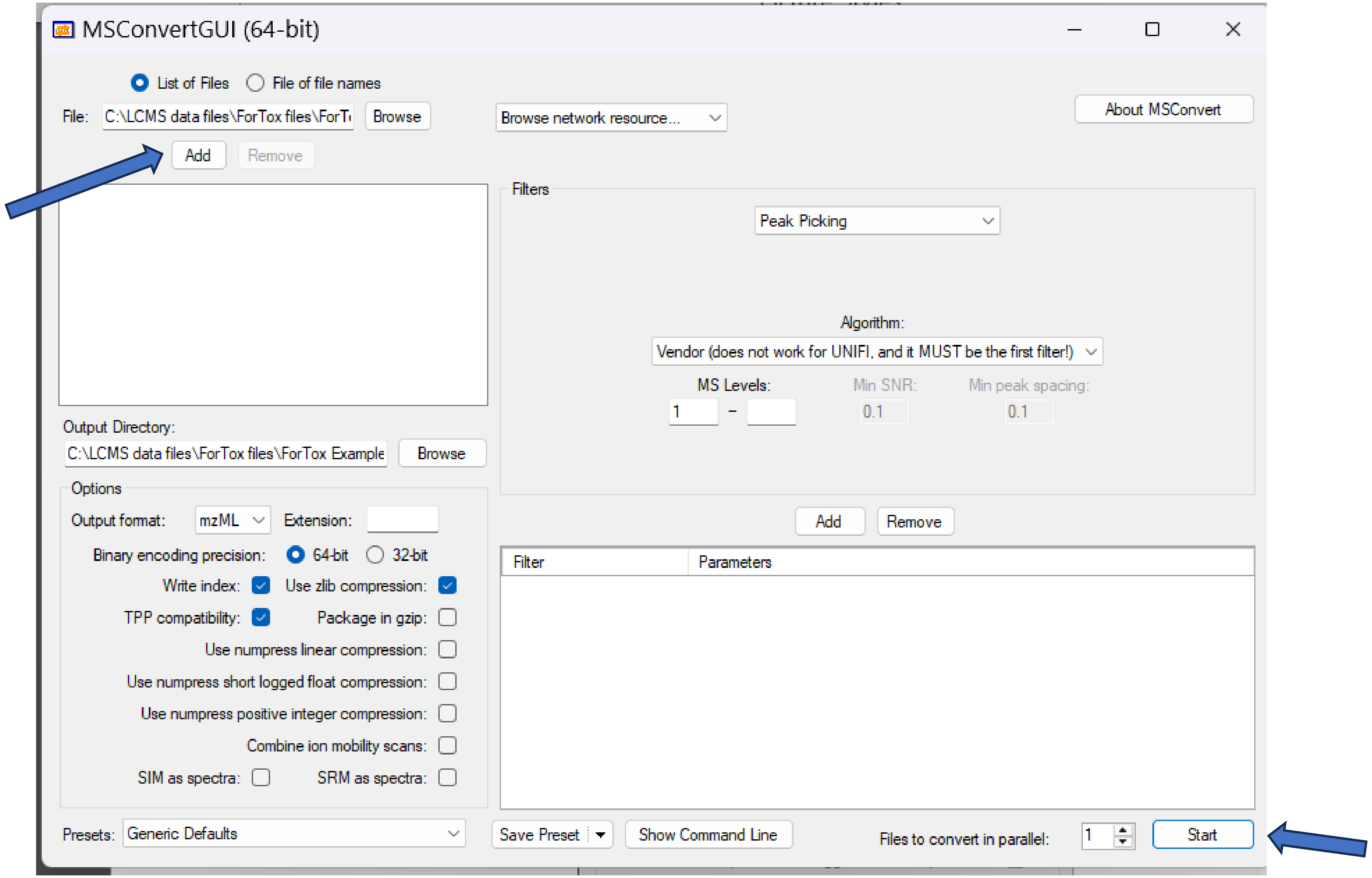
Files to convert in parallel: 1

# Can Select File Format or Any Spectra Format



Sources of type: Any spectra format

# Add then Start Conversion to mzML



● List of Files ○ File of file names

File: C:\LCMS data files\ForTox files\ForT

Output Directory: C:\LCMS data files\ForTox files\ForTox Example

Options

Output format: mzML

Extension:

Binary encoding precision: ● 64-bit ○ 32-bit

Write index: ☑ Use zlib compression: ☑

TPP compatibility: ☑ Package in gzip: ☐

Use numpress linear compression: ☐

Use numpress short logged float compression: ☐

Use numpress positive integer compression: ☐

Combine ion mobility scans: ☐

SIM as spectra: ☐ SRM as spectra: ☐

Presets: Generic Defaults

Peak Picking

Algorithm: Vendor (does not work for UNIFI, and it MUST be the first filter!)

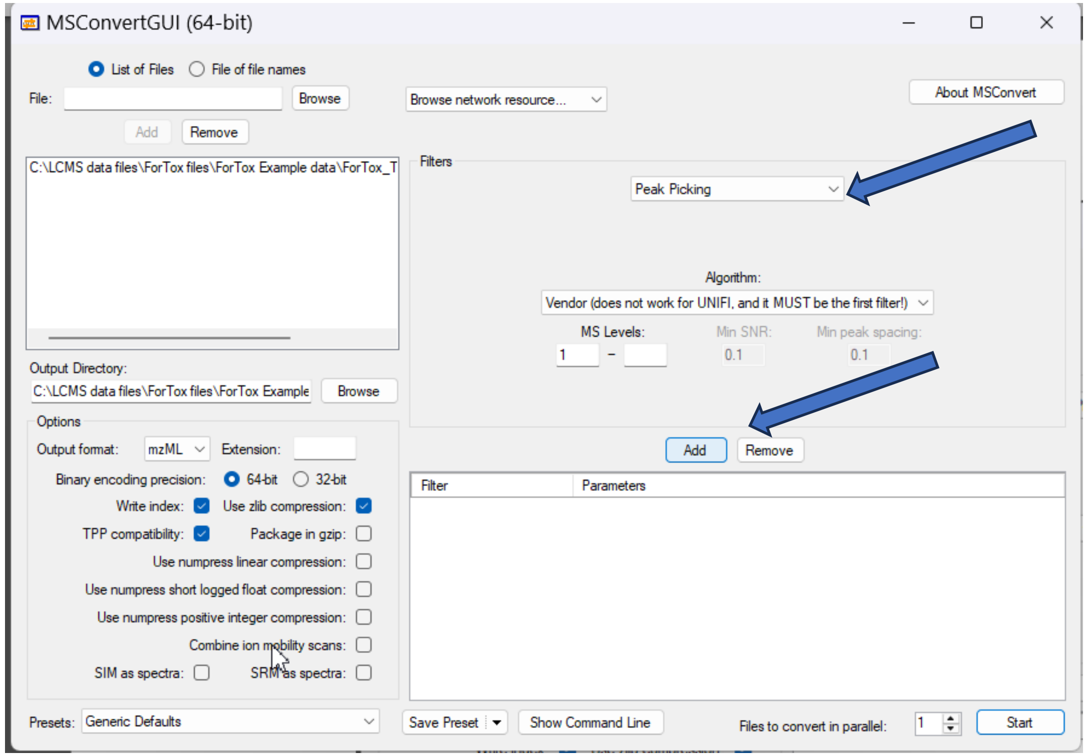
MS Levels: 1 –

Min SNR: 0.1

Min peak spacing: 0.1

Files to convert in parallel: 1

- Files MUST be in Centroided (Peak Picked Form), Profile Data NOT acceptable
- *Add* peak picking to the algorithm List
- File size will be dramatically increased if view in File Explorer
- *MUST* be first algorithm (function) in the list!
- If not sure if profile data, can add, will not change file if already centroided
- Can include MS levels
- Start to convert


MSConvertGUI (64-bit)

● List of Files ○ File of file names

File:

C:\LCMS data files\ForTox files\ForTox Example data\ForTox_T

Output Directory: C:\LCMS data files\ForTox files\ForTox Example

Options

Output format: mzML Extension:

Binary encoding precision: ● 64-bit ○ 32-bit

Write index: ☑ Use zlib compression: ☑

TPP compatibility: ☑ Package in gzip: ☐

Use numpress linear compression: ☐

Use numpress short logged float compression: ☐

Use numpress positive integer compression: ☐

Combine ion mobility scans: ☐

SIM as spectra: ☐ SRM as spectra: ☐

Presets: Generic Defaults

Files to convert in parallel: 1

Filters: Peak Picking

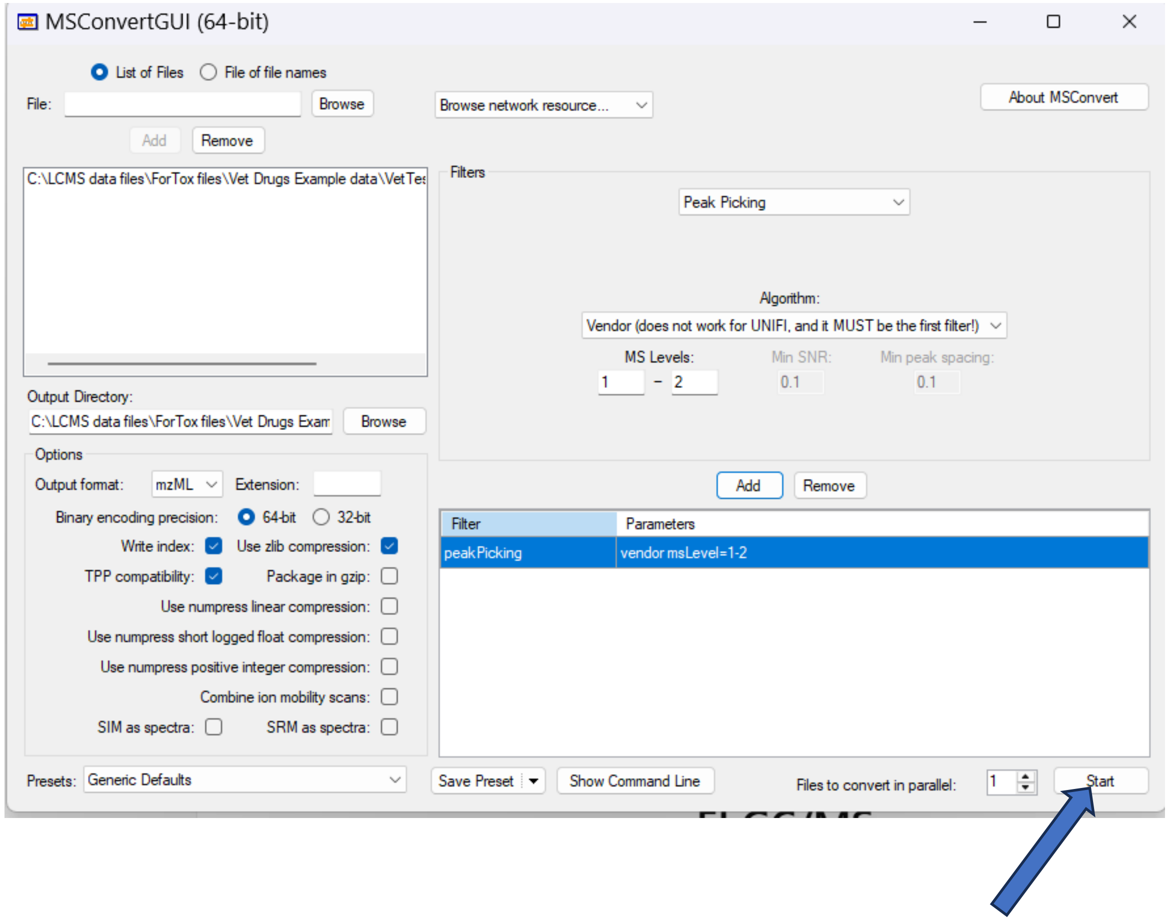
Algorithm: Vendor (does not work for UNIFI, and it MUST be the first filter!)

MS Levels: 1 –

Min SNR: 0.1

Min peak spacing: 0.1

| Filter | Parameters |
|---|---|


MSConvertGUI (64-bit)

● List of Files ○ File of file names

File:

C:\LCMS data files\ForTox files\Vet Drugs Example data\VetTes

Output Directory: C:\LCMS data files\ForTox files\Vet Drugs Exam

Options

Output format: mzML Extension:

Binary encoding precision: ● 64-bit ○ 32-bit

Write index: ☑ Use zlib compression: ☑

TPP compatibility: ☑ Package in gzip: ☐

Use numpress linear compression: ☐

Use numpress short logged float compression: ☐

Use numpress positive integer compression: ☐

Combine ion mobility scans: ☐

SIM as spectra: ☐ SRM as spectra: ☐

Presets: Generic Defaults

Files to convert in parallel: 1

Filters: Peak Picking

Algorithm: Vendor (does not work for UNIFI, and it MUST be the first filter!)

MS Levels: 1 – 2

Min SNR: 0.1

Min peak spacing: 0.1

| Filter | Parameters |
|---|---|
| peakPicking | vendor msLevel=1-2 |