

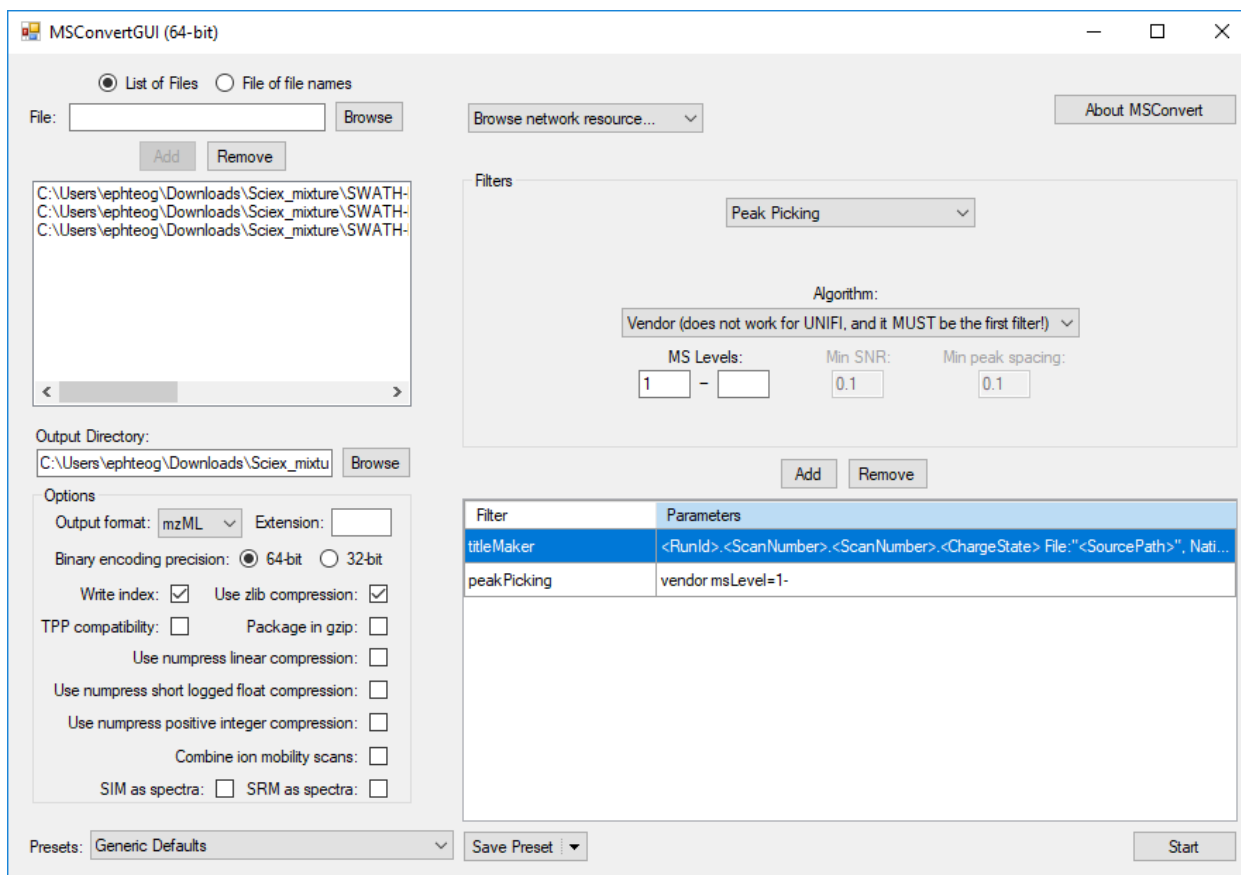
# MRMkit

July 7, 2020

## 1 Raw Data Conversion into mzML

The input files need to be in mzML format for MRMkit. MSConvert, provided through the ProteoWizard software suite, enables conversion of proprietary raw data files (.wiff for SCIEX, .raw files for Thermo Fisher instruments) into mzML.

1. Download and install a recent version ProteoWizard on a Windows computer.
2. Start the software by opening the Start Menu, type “MSConvert” in the search field and click on “MSConvert”.
3. In the MSConvert window, use the “Browse” button to select the raw files to be converted (the .wiff and .wiff.scan files need to be located in the same folder). Select “mzML” for “Output format”, “64-bit” for “Binary encoding precision”, check “Write index” and “Use zlib compression” checkbox (see figure below).



## 2 Input Parameters

Input parameters must be specified according to the user's preference for various aspects of the data processing. Input parameters are to be specified in the "param.txt" file.

MRMkit requires that the user provide the following options for data processing:

- **mzML\_files**: Names of the centroided mzML files. Use "\*.mzML" to select all mzML files in the folder.
- **batch\_info**: range of ion chromatogram of feature in seconds
- **length\_of\_ion\_chromatogram**: range of ion chromatogram of feature in seconds
- **transition\_list**: assay information with compound name, Q1, Q3, retention time and designated internal standards (ISTD).
- **ISTD\_trace\_all**: Set "1" to use the XIC shape of associated ISTD for peak integration for all transitions, "0" to directly take area under peak in the case for transitions with unimodal chromatogram.
- **batch\_correction**: Set "1" to enable batch effect correction, "0" to disable.

### 3 Analysis Output Table

- `batch_adjusted.txt` A table of quantification.

### 4 Example “param.txt”

`mzML_files`

`*.mzML`

`batch_info`

`batchinfo.txt`

`length_of_ion_chromatogram`

`4 40`

`transition_list`

`SP2 MRM list.txt`

`ISTD_trace_all`

`1`

`batch_correction`

`1`

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