

Method Editor: Guide

- Installation

- From release (zipped PyInstaller file):
 - Unzip the files
 - Run MethodEditor_Main.exe
- From source code:
 - Clone github repository
 - Run MethodEditor_Main.py (“python MethodEditor_Main.py”)

Method Editor: Guide

- **THIS IS A USE-AT-YOUR-OWN-RISK PROGRAM!**
 - It is possible to crash MassLynx by providing inappropriate parameters/etc.
 - I've added some basic checking for illegal characters and bad file paths, but there are many ways to pass bad information to MassLynx. Always double-check all information you're providing to the method.

Method Editor: Guide

- To use:

1. Generate your template .csv file (see next slides)
2. Run the program (Start/MethodEditor_Main.exe)
 1. A file chooser will open, allowing you to select the template file you'd like to use
 2. Once a template file has been selected, the program will create your method files and sample list. A message box will pop up and say "success!" if the program finishes successfully
 3. Import the sample list into MassLynx (File/Import Worksheet). The sample list is saved as "csv-to-import.csv"
 4. Run the method in MassLynx

Template file

- Initial Parameters section is used for ALL runs
 - **Instrument Type:** G2, G2-Si, G1, or “G1neg” which means a G1 in negative mode.
 - Note: if you need other Waters instruments/modes added, let us know
 - Combine: generate a single raw file for ALL template lines list (max 30 functions)
 - **TOF cal file: calibration file to use (make sure this is correct)**
 - Save to MassLynx?: same as old method editor – usually true unless you want to do something fancy
 - **MassLynx Directory: Make sure this is your project**
 - Non-MassLynx directory: where the program saves outputs ONLY if not saving to MassLynx directory
 - Optic Mode: sensitivity or resolution (make sure tune file matches!!)

[illegible]

Template file

- Individual Runs Section: Each line is a new analysis (can have arbitrary number)
 - Use MSMS?: True means quad select, False means MS only (no selection).
 - m/z to select: only for MSMS mode. Gets ignored in MS mode
 - Date/Sample Name: what to name the output .raw file
 - CV step/start/end: trap collision voltage range/step to generate (can set start=end to do only one voltage)
 - Mass range low/high: TOF mass range
 - (ctd next slide)

[illegible]

Template file

- Individual Runs Section: Each line is a new analysis (can have arbitrary number)
 - Total collection time per Func: IN MINUTES – total accumulation time for each function
 - Scan Time: IN SECONDS – time per scan on the instrument. Must be between 0.1 and 5 seconds
 - Delay before start (min): whether to use a delay timer before this function (inserts an extra function at the lowest CV before starting the CV ramp. Intended for droplet or other automated sample introduction CIU)
 - **MS Tune File: IPR file to use for the analysis (filename only, not full path. Must include .ipr at the end)**
 - Save DT Func: Whether to save a mobility-specific function in addition to regular data. Usually unnecessary.

[illegible]

Troubleshooting

- Too Many Functions Error:
 - The EPC hardware is limited to 30 functions, so any method attempting to put more than 30 functions into a single raw file gets stopped. This is a STRICT limit, as going above 30 functions will crash the EPC and require a cold restart.
- The program said my Calibration File or Tune File does not point to a valid file path!?
 - This means the path specified for the cal or tune file is not correct (since there is no file at the destination). Check the spelling/formatting of the entry in the template (and make sure it includes the .cal or .ipr at the end)
- Illegal characters
 - MassLynx is very sensitive to special characters, so many are not allowed in the Date and Sample Name fields. If you see an illegal character message, remove any illegal characters from the template and try again.
 - Illegal chars: . , / \ ? * @ ~ () ; : < >
 - Double spaces are also illegal since they can crash MassLynx
- Inappropriate Parameter Value:
 - If a parameter is not within the required bounds, this message will appear. Ensure all parameters are within the noted bounds and try again.
- Other problems:
 - Ask Dan P