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!!)

	Optic Wode. Schistivity of resolution (make sure tune me materies::)															
	А	В	С	D	E	F	G	H	I	J	K	L	М	N	0	
1_	# INITIAL PARAMETERS (for all fingerprints) ####################################															
2	Instrument Type	G2														
3	Combine ALL into 1 raw file?	FALSE														
4	TOF Cal File	F Cal File C:\MassLynx\IntelliStart\Results\Dan Pos Sen 100-10000-31.cal														
5	Save to MassLynx?	TRUE						_								
6	Masslynx Directory	C://MassLy	/nx//Dan.PRC)//ACQUDE	3											
7	Non-MassLynx Directory	C://MethodEditor//Outputs														-
8	Optic Mode	sensitivity														+
-																-
9	# INDIVIDUAL FINGERPRINT PA	RAMETERS #		##												_
		m/z to						Mass	Mass	TOTAL Collection	SCAN	Delay		Functions		
		select		Sample				range	range	time per Func	Time	Before	MS Tune	per Raw	Save DT	
10	# Use MSMS?	(MSMS)	Date	Name	CV Step	Start CV	End CV	low	high	(min)	(sec)	Start (min)	File	File	Func	
11	True	4000	2018_10_22	test1	5	10	200	100	8000	0.25	0.1	0	b-lac_l	20	false	
12	True	4200	2018_10_22	test2	5	10	200	100	8000	0.25	0.1	0	b-lac_l	20	false	
13	True	4400	2018_10_22	test3	5	10	200	100	8000	0.25	0.1	0	b-lac_l	20	false	
14																

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)

	Α	В	С	D	E	F	G	Н	I	J	K	L	М	N	0	
1	# INITIAL PARAMETERS (for all f	###														
2	Combine ALL into 1 raw file?	FALSE														
3	TOF Cal File	C:\MassLyr	nx\IntelliStar	t\Results\C	Dan_Pos_	Sen_100-1	10000-31.	cal								
4	Save to MassLynx?	TRUE														
5	Masslynx Directory	C://MassLy	/nx//Dan.PRC)//ACQUDE	3											
6	Non-MassLynx Directory	C://Metho	dEditor//Out	puts												
7	Optic Mode	sensitivity														
0																
9	# INDIVIDUAL FINGERPRINT PAI	RAMETERS #	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	##												
9		RAMETERS # m/z to	***************************************	##				Mass	Mass	TOTAL Collection	SCAN	Delay		Functions		
9			 	## Sample				Mass range		TOTAL Collection time per Func	SCAN Time	Delay Before	MS Tune		Save DT	
		m/z to	Date		CV Step	Start CV	End CV		range				MS Tune File		Save DT Func	
10		m/z to select (MSMS)		Sample Name	CV Step	Start CV		range low	range high	time per Func (min)	Time (sec)	Before Start (min)		per Raw File		
10 11	#Use MSMS?	m/z to select (MSMS) 4000	Date	Sample Name test1	CV Step 5	10	200	range low 100	range high 8000	time per Func (min) 0.25	Time (sec) 0.1	Before Start (min)	File	per Raw File 1 20	Func	
10 11 12	# Use MSMS? True	m/z to select (MSMS) 4000 4200	Date 2018_10_22	Sample Name test1 test2	5	10 10	200 200	range low 100 100	range high 8000 8000	time per Func (min) 0.25 0.25	Time (sec) 0.1	Before Start (min) 0	File b-lac_l	per Raw File 1 20	Func false	
10 11 12	# Use MSMS? True True	m/z to select (MSMS) 4000 4200	Date 2018_10_22 2018_10_22	Sample Name test1 test2	5	10 10	200 200	range low 100 100	range high 8000 8000	time per Func (min) 0.25 0.25	Time (sec) 0.1 0.1	Before Start (min) 0	File b-lac_l b-lac_l	per Raw File 1 20	Func false false	

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.

4	А	В	С	D	Е	F	G	Н	I	J	K	L	М	N	0	
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4	Save to MassLynx?	TRUE														
5	Masslynx Directory	C://MassLy	nx//Dan.PRC	//ACQUDB	3											
6	Non-MassLynx Directory	C://Metho	dEditor//Out	puts												
7	Optic Mode	sensitivity														
0																
9	# INDIVIDUAL FINGERPRINT PA															
		m/z to						Mass	Mass	TOTAL Collection	SCAN	Delay		Functions		
		select		Sample				range	range	time per Func	Time	Before	MS Tune	per Raw	Save DT	
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14																

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 tempalte 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