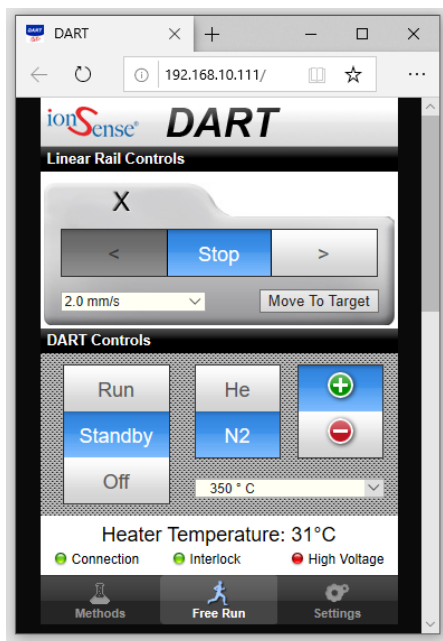


## **Department of Forensic Science**

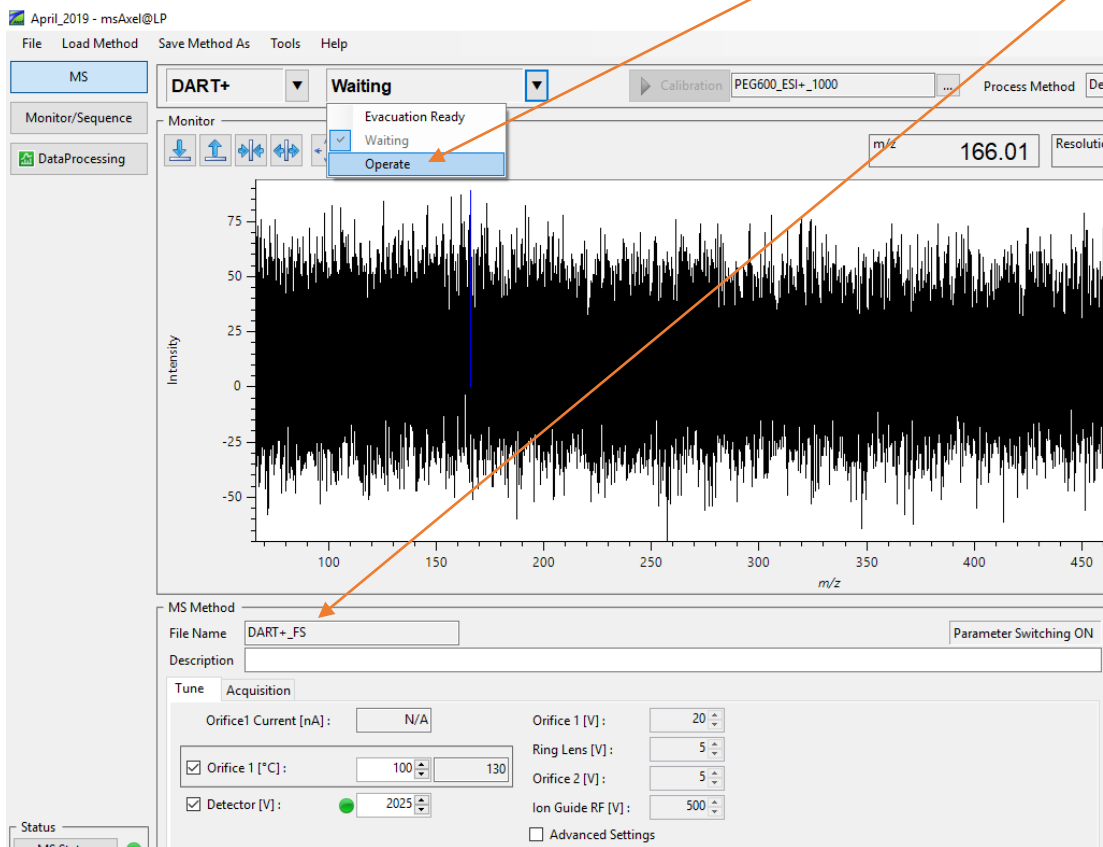
# **CONTROLLED SUBSTANCES INSTRUCTIONS FOR THE DART-TOF msAxel SOFTWARE**

## I. Acquiring Mass Spectral Data:

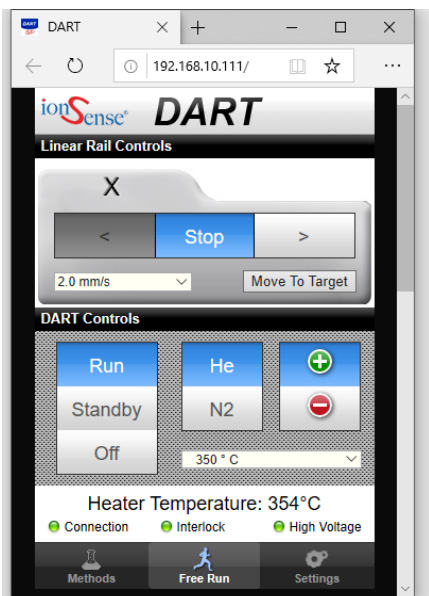
1. Set the DART Controller to Standby, with N2, and the temperature to 350°C.



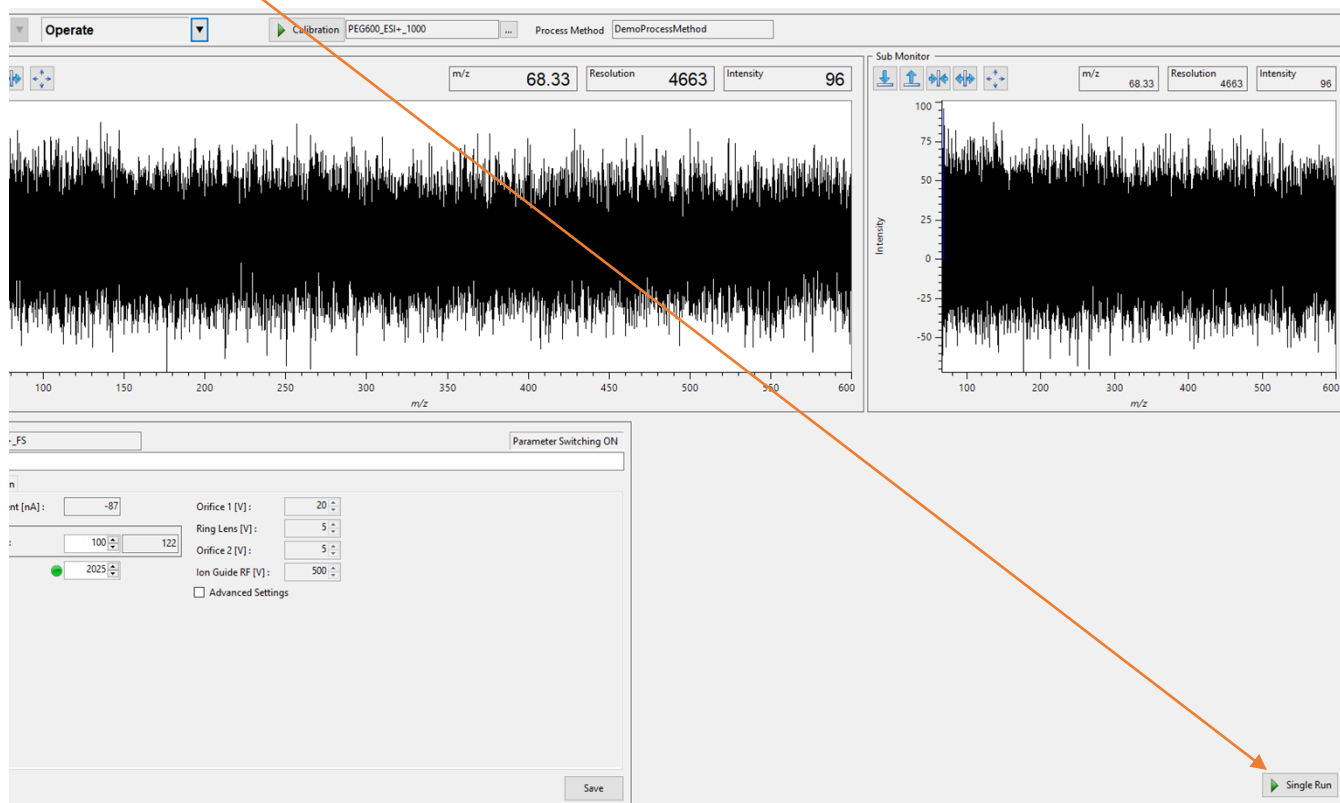
2. In the msAxel@LP window, change the instrument mode to Operate. Ensure the appropriate method is loaded.



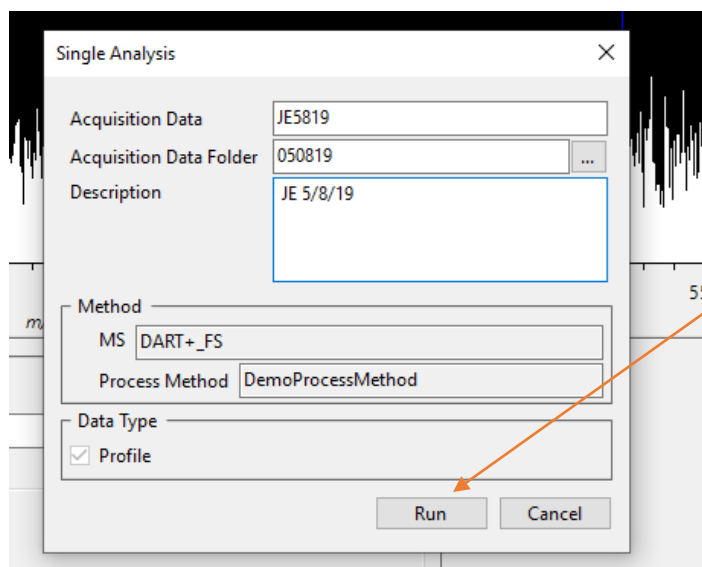
3. Once the DART temperature reaches 350°C, set it to run, with He.



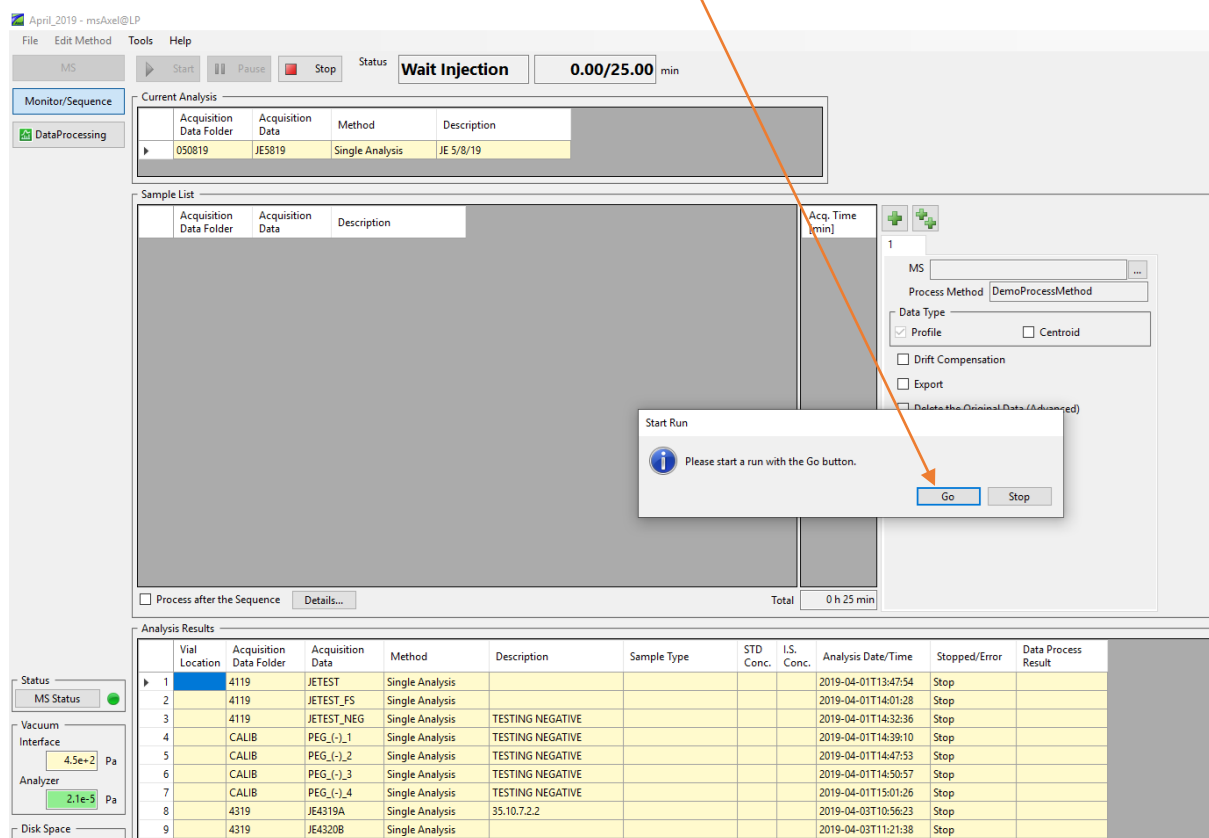
4. In the msAxel@LP window, click the Single Run button at the bottom right of the window.



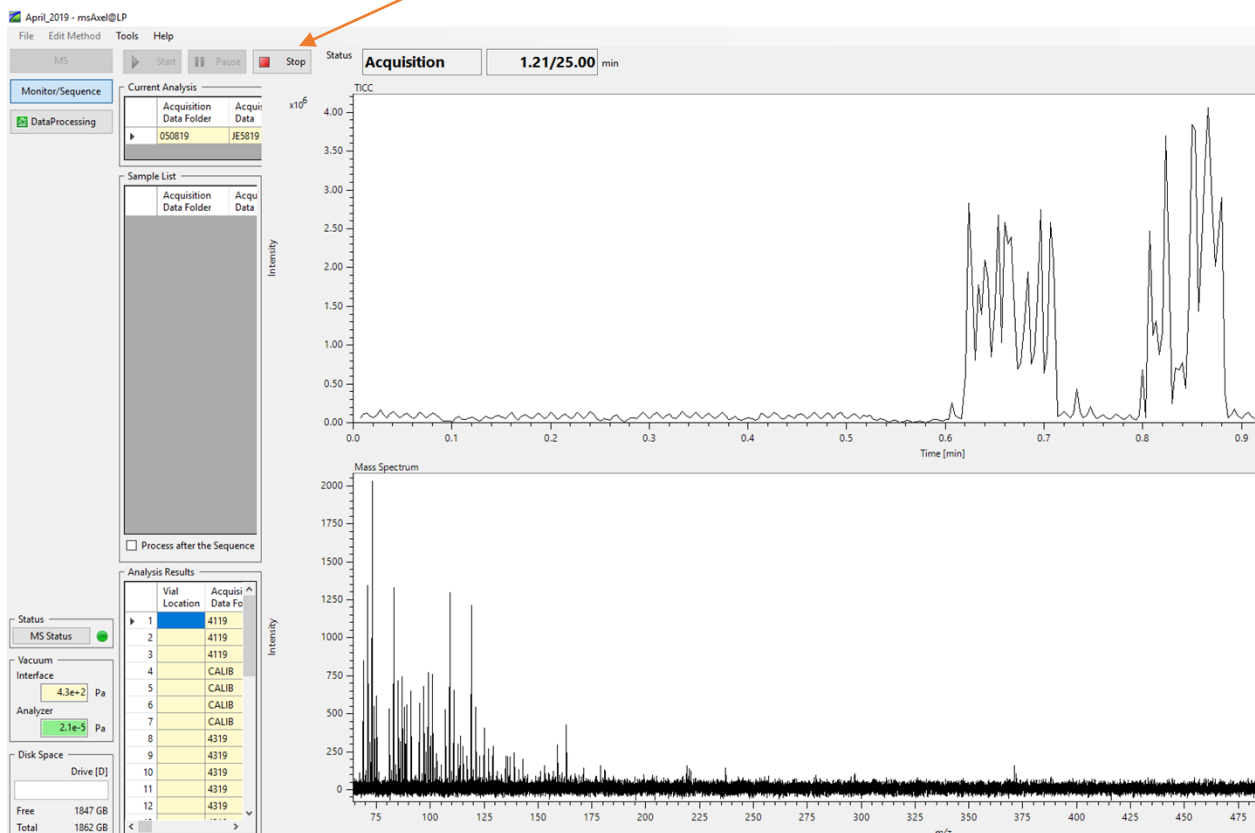
- In the window that appears, enter a filename in the Acquisition Data field. The name for the data folder in the Acquisition Data Folder field is already set at today's date during the daily calibration. You can also fill in the Description field. It is not necessary to adjust/change the other settings. Click the Run button.



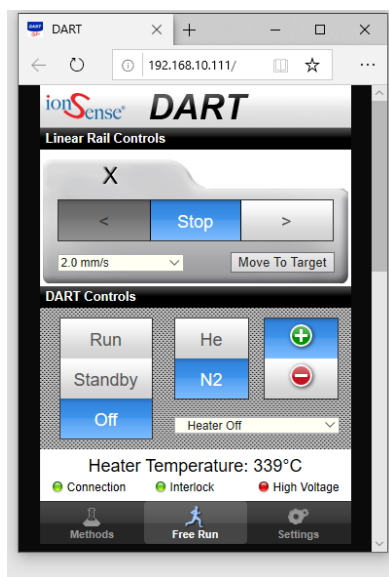
- You should now see msAxel switch to the Monitor/Sequence window along with a Start Run dialog box. When you are ready to start the run, click the Go button in the Start Run dialog box.



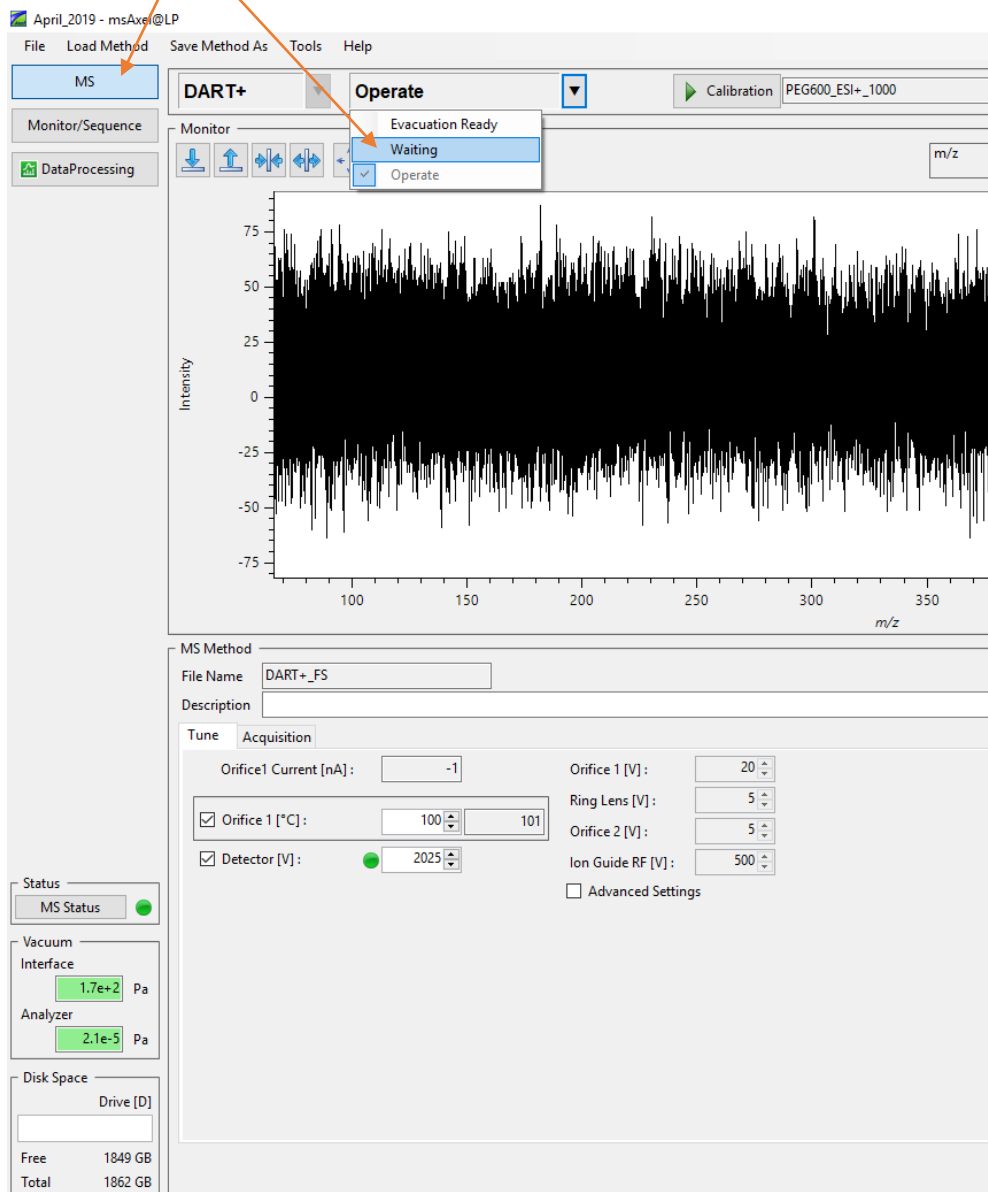
- Begin wadding samples and view the real time display to ensure the samples are analyzed. Once you are done analyzing samples, click the Stop button at the top of the msAxel@LP window.



- Set the DART Controller to Off mode. N2 will automatically switch on and the heater will automatically turn off. The N2 will remain on until the temperature is below 200°C, at which point it will automatically turn off.



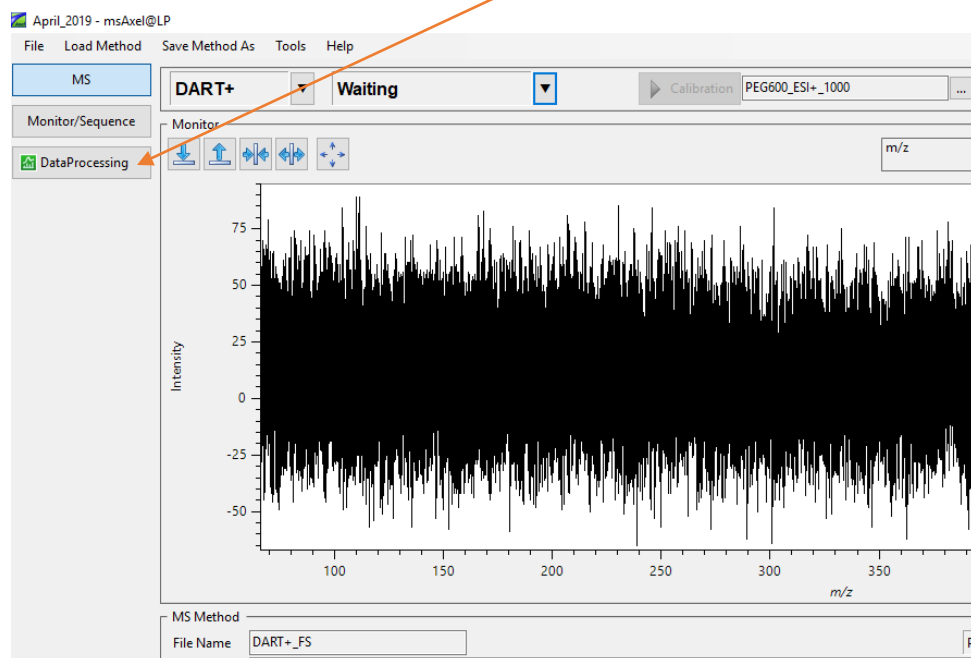
9. Select the MS button on the upper left side of the msAxel@LP window and change the instrument mode to Waiting.



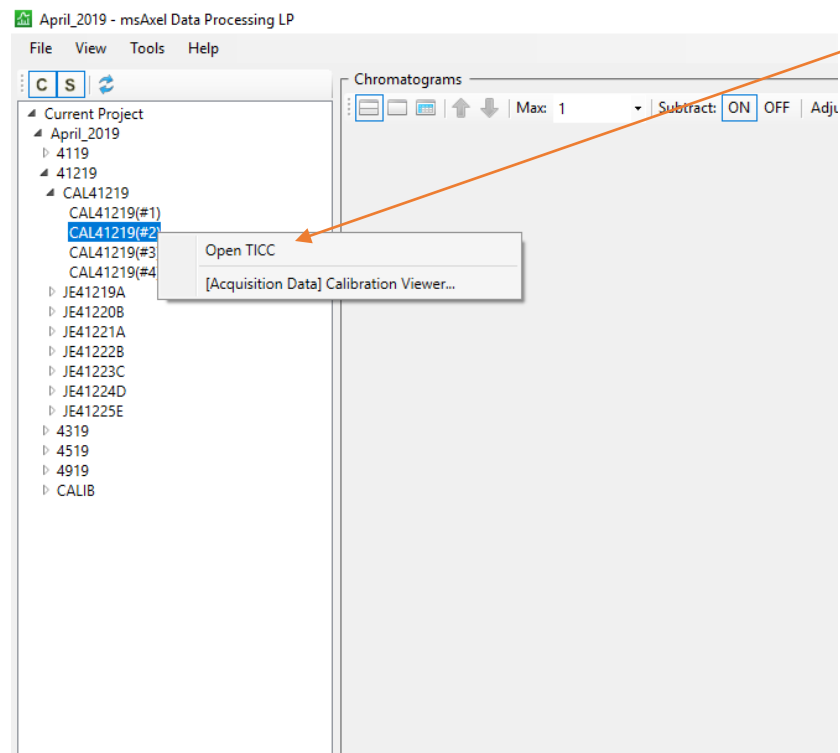
10. The data is now ready to be processed using the msAxel Data Processing software.

## II. Processing Mass Spectral Data:

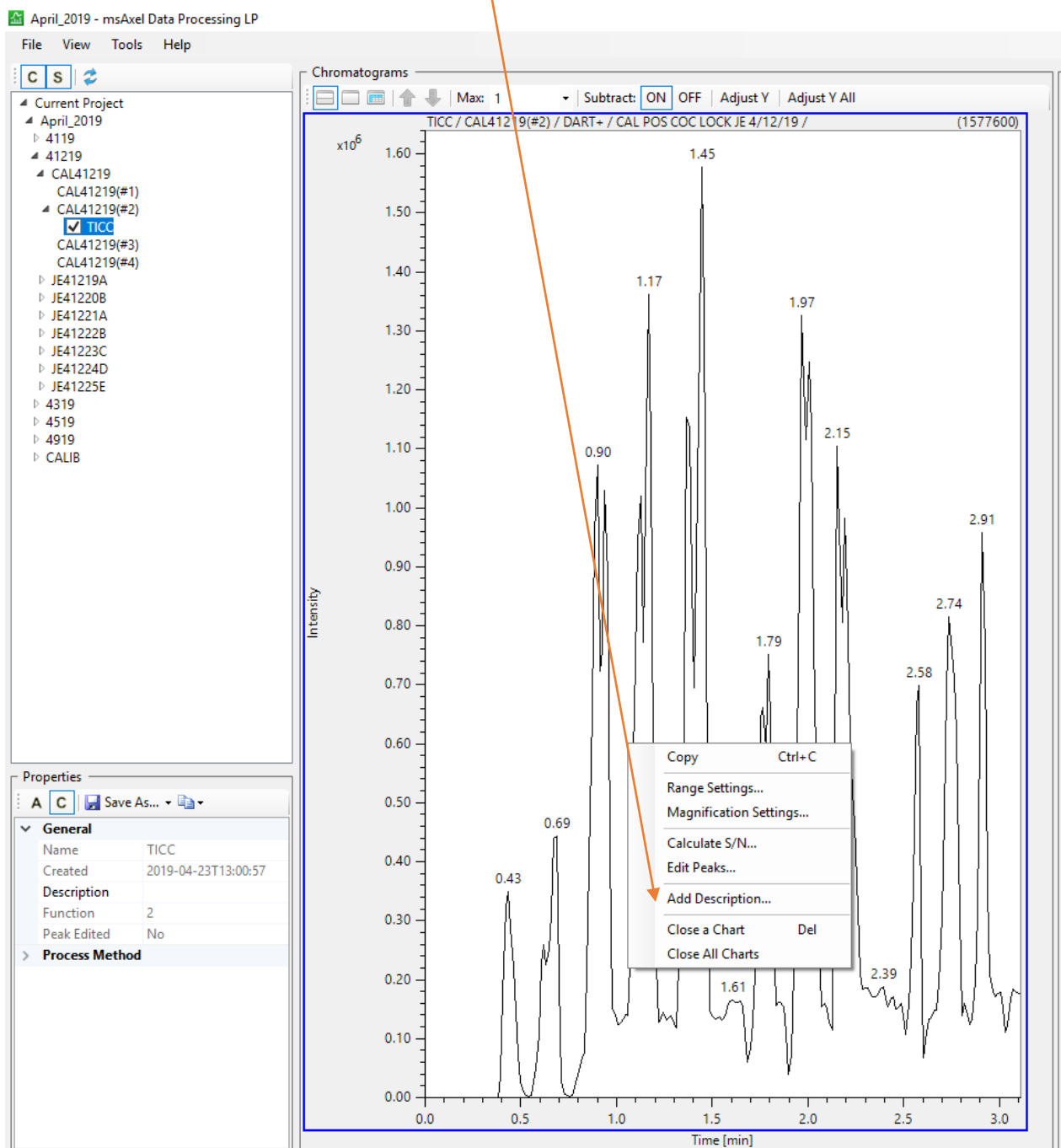
1. In the msAxel@LP window, click the Data Processing button on the upper left side.



2. In the Data Processing window, select the appropriate file in the list on the left side and then right click the highlighted data (#1 is 20V, #2 is 30V, #3 is 60V, #4 is 90V) and select Open TICC.

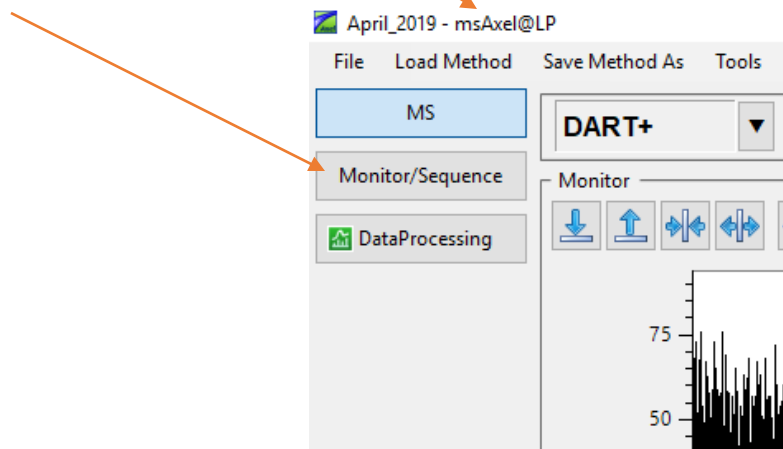


3. A Total Ion Current Chromatogram (TICC) will appear in the Chromatograms section of the Data Processing window that represents a time versus intensity plot for all of the ions generated during the analysis. (NOTE: The top left corner of the TICC indicates the chromatogram type, file name, and ionization technique to easily identify the currently viewed data.) You can label the TICC in the software: Right-click and select Add Description. (NOTE: wherever you right-click on the TICC is where the text box will appear.)





- The TICC will not print with a time stamp so it must be added manually using the Add Description feature. The time stamp can be copied from two places. On the upper left side of the MS Axel@LP window (not Data Processing window), select Monitor/Sequence.

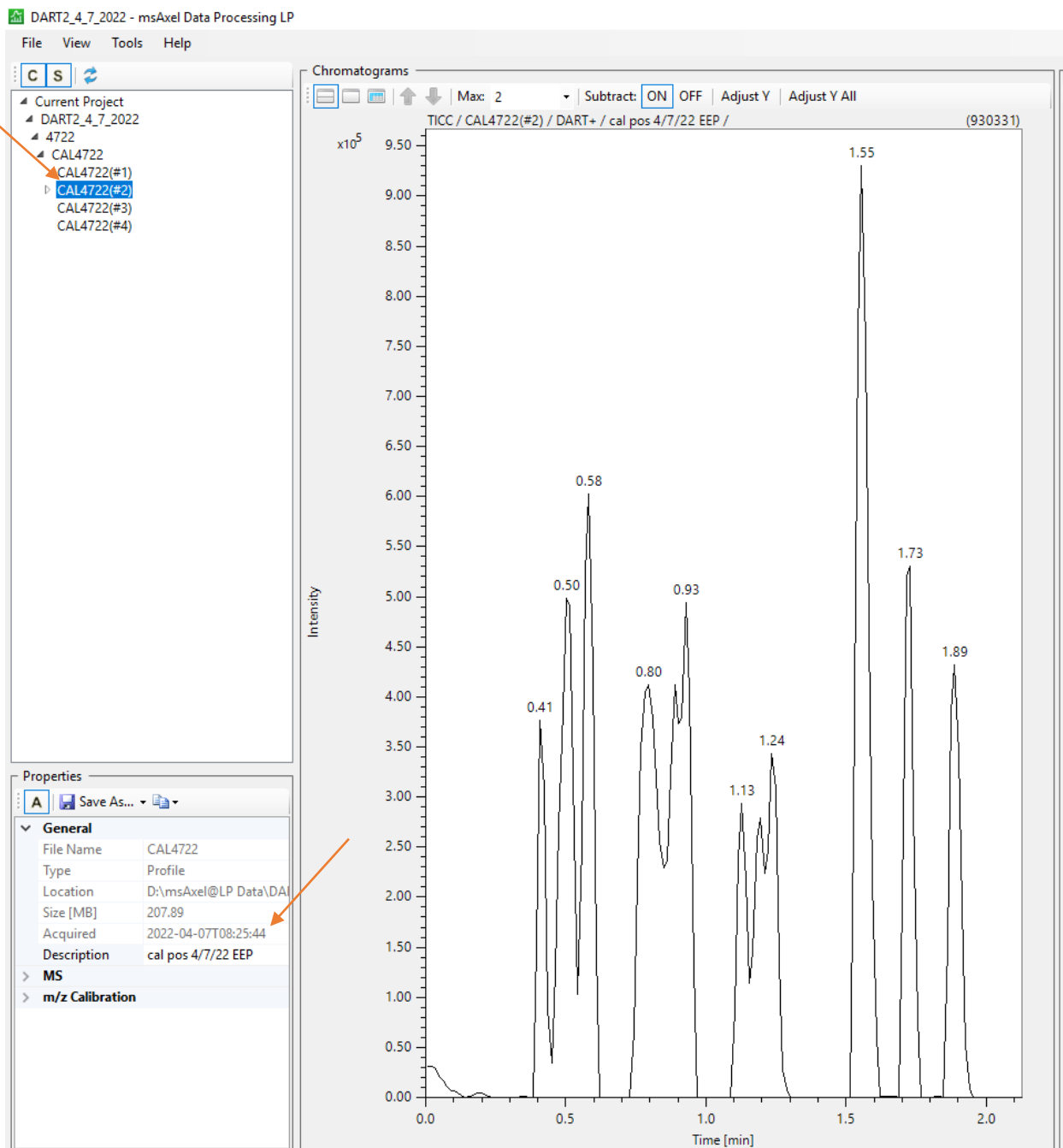


- In the Monitor/Sequence window, the time stamp information is located at the bottom. Find your Acquisition Data name in the table, and then right click on the corresponding Analysis Date/Time to Copy.

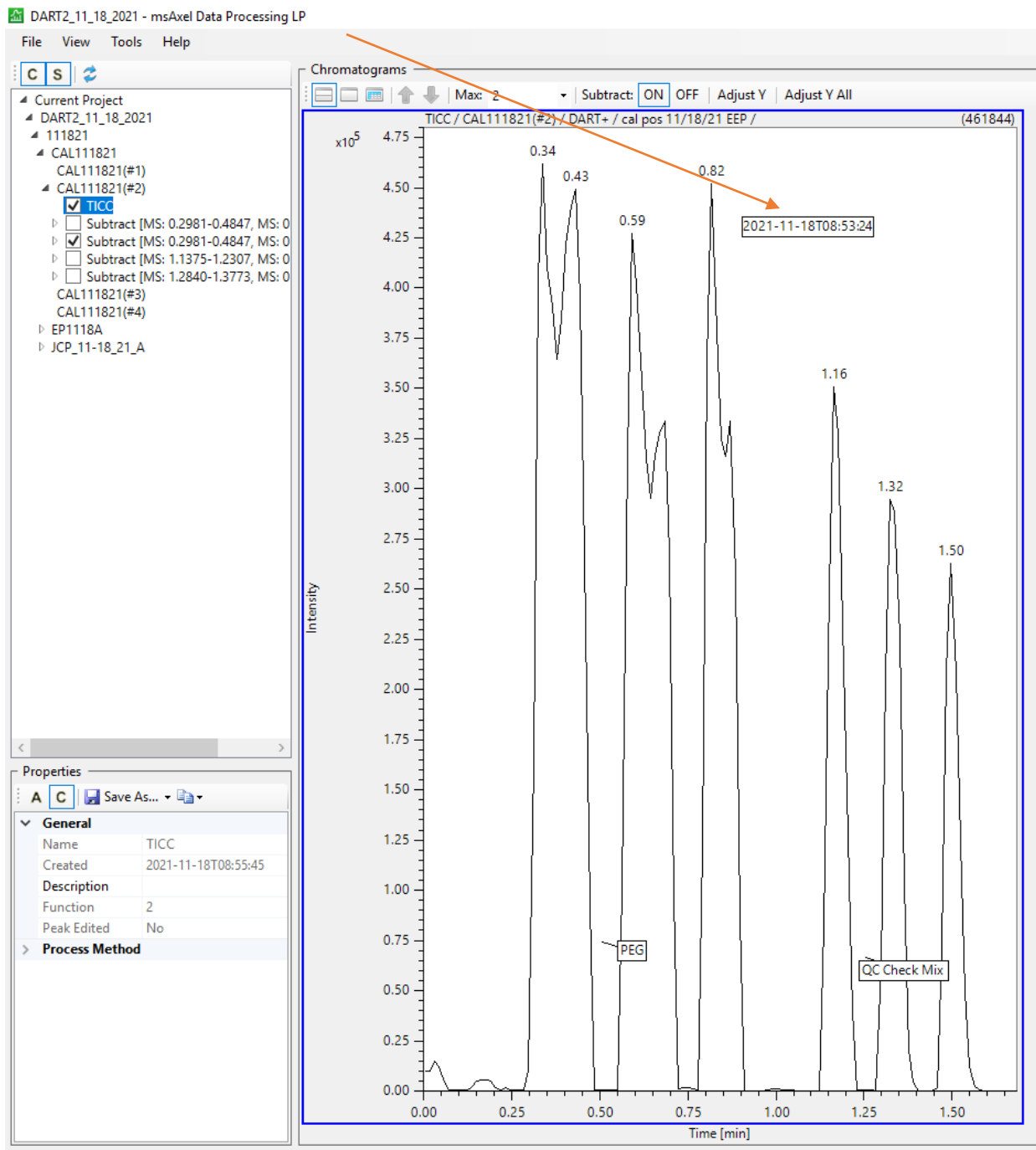
The screenshot shows the Monitor/Sequence window. On the left, there are status indicators for 'MS Status' (green dot), 'Vacuum Interface' (4.5e-2 Pa), and 'Analyzer' (2.1e-5 Pa). Below these is a 'Disk Space' section for 'Drive [D:]'. The main area is a table titled 'Analysis Results' with columns: Vial Location, Acquisition Data Folder, Acquisition Data, Method, Description, Sample Type, STD Conc., I.S. Conc., Analysis Date/Time, and Stopped/Error. An orange arrow points to the 'Acquisition Data' column, and another points to the 'Analysis Date/Time' column. The table contains 11 rows of data.

Vial Location	Acquisition Data Folder	Acquisition Data	Method	Description	Sample Type	STD Conc.	I.S. Conc.	Analysis Date/Time	Stopped/Error
1	4119	JETEST	Single Analysis					2019-04-01T13:47:54	Stop
2	4119	JETEST_FS	Single Analysis					2019-04-01T14:01:28	Stop
3	4119	JETEST_NEG	Single Analysis	TESTING NEGATIVE				2019-04-01T14:32:36	Stop
4	CALIB	PEG_(-)_1	Single Analysis	TESTING NEGATIVE				2019-04-01T14:39:10	Stop
5	CALIB	PEG_(-)_2	Single Analysis	TESTING NEGATIVE				2019-04-01T14:47:53	Stop
6	CALIB	PEG_(-)_3	Single Analysis	TESTING NEGATIVE				2019-04-01T14:50:57	Stop
7	CALIB	PEG_(-)_4	Single Analysis	TESTING NEGATIVE				2019-04-01T15:01:26	Stop
8	4319	JE4319A	Single Analysis	35.10.7.2.2				2019-04-03T10:56:23	Stop
9	4319	JE4320B	Single Analysis					2019-04-03T11:21:38	Stop
10	4319	JE4321C	Single Analysis	35.10.7.2.2				2019-04-03T12:44:41	Stop
11	4319	JE4322D	Single Analysis	35.10.7.2.3 RUIIN 1				2019-04-03T13:19:00	Stop

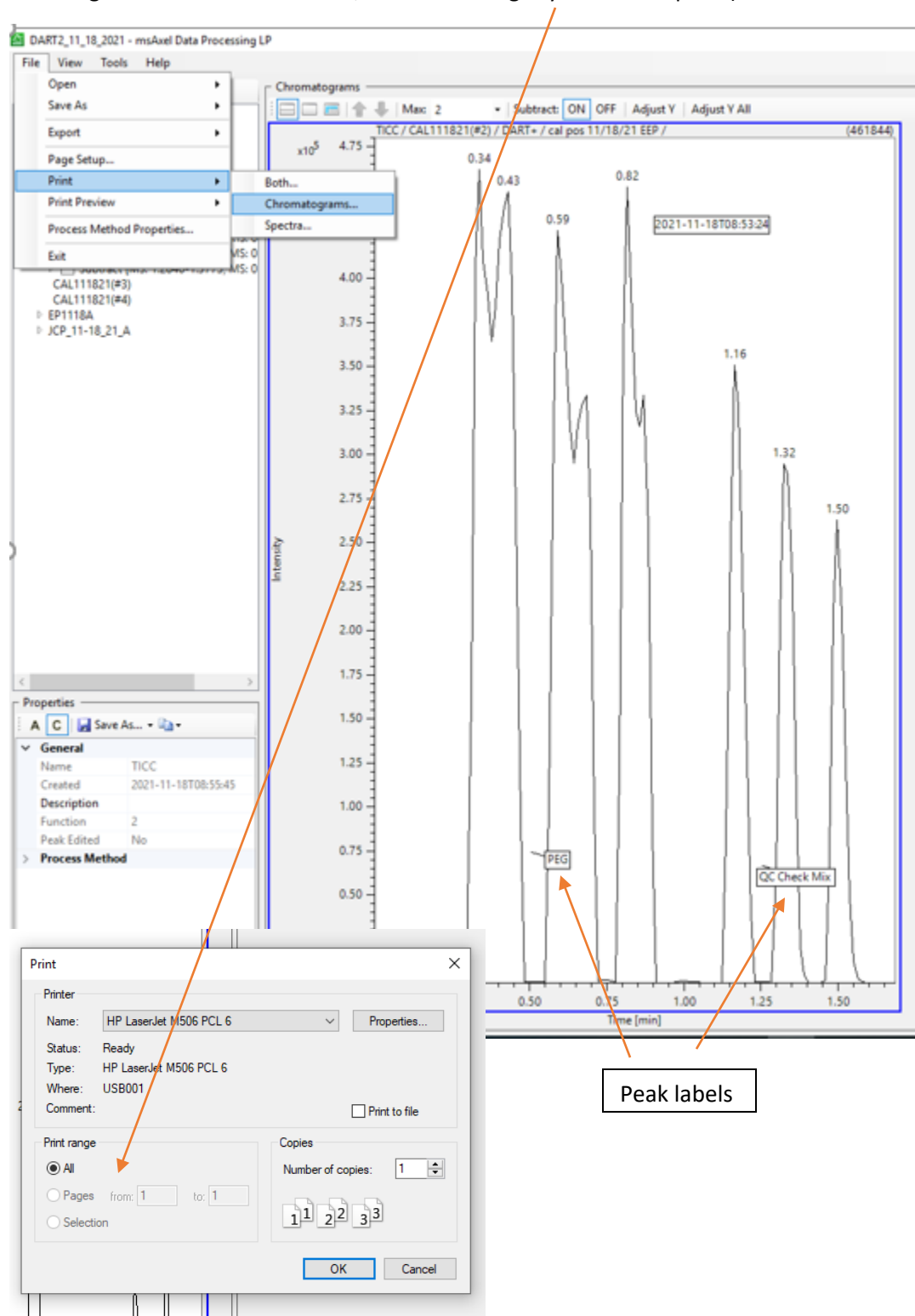
6. The time stamp can also be copied from the Data Processing window. After selecting the appropriate acquisition data file, the time stamp will be located in the 'Properties' box on the left-hand side. Highlight the time stamp and right click to copy.



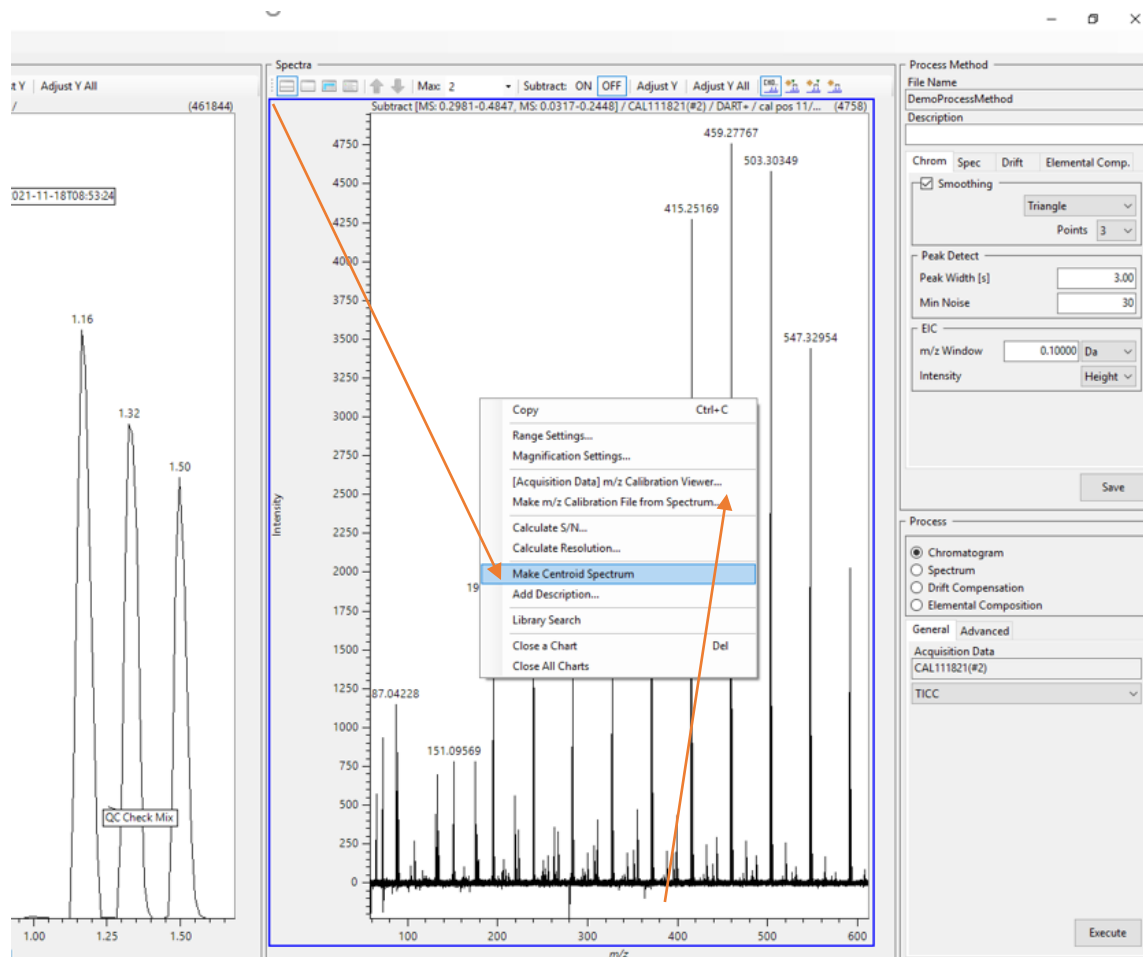
7. In the Data Processing Window, right click on the TICC in the upper right corner, click Add Description, and paste the time stamp.



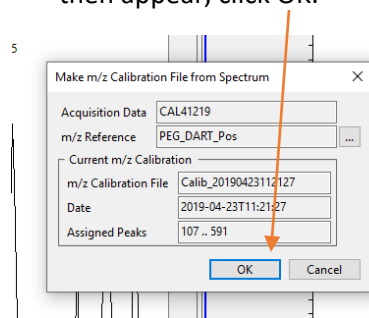
8. To print the TICC, File > Print > Chromatograms. Click OK in the box. (NOTE: Make sure you only have one TICC open. If you have multiple TICC's open, it will print all of them. To avoid this, in the Print Range section of the Print box, choose the Pages you want to print.)



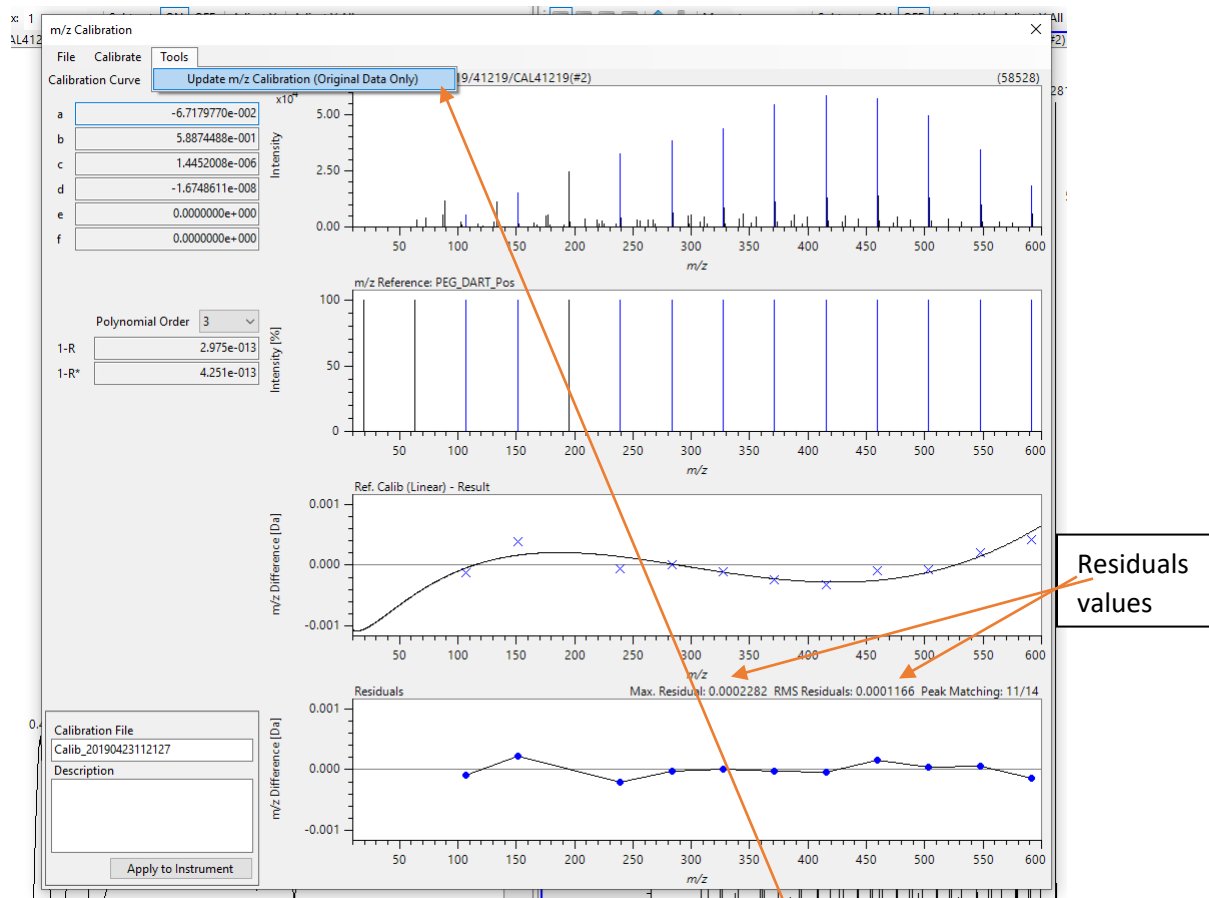
9. To create a mass spectrum from the Chromatograms window: Hold down the Control (CTRL) keyboard button. Press the left mouse button and drag over the peak of interest. Then hold down the SHIFT keyboard button. Press the left mouse button and drag over a background time region (NOTE: The created mass spectrum shows the time range for the mass data in the top left corner of the mass spectrum.). Create a mass spectrum of PEG600. Afterwards, right-click on the spectrum and select Make Centroid Spectrum.



10. Then left-click on the centroided spectrum to highlight it (the software doesn't default to "choosing" the centroided spectrum, you have to click on it or the mass calibration won't work). Right-click again on the spectrum and select Make m/z Calibration File from Spectrum. A dialog window will then appear, click OK.

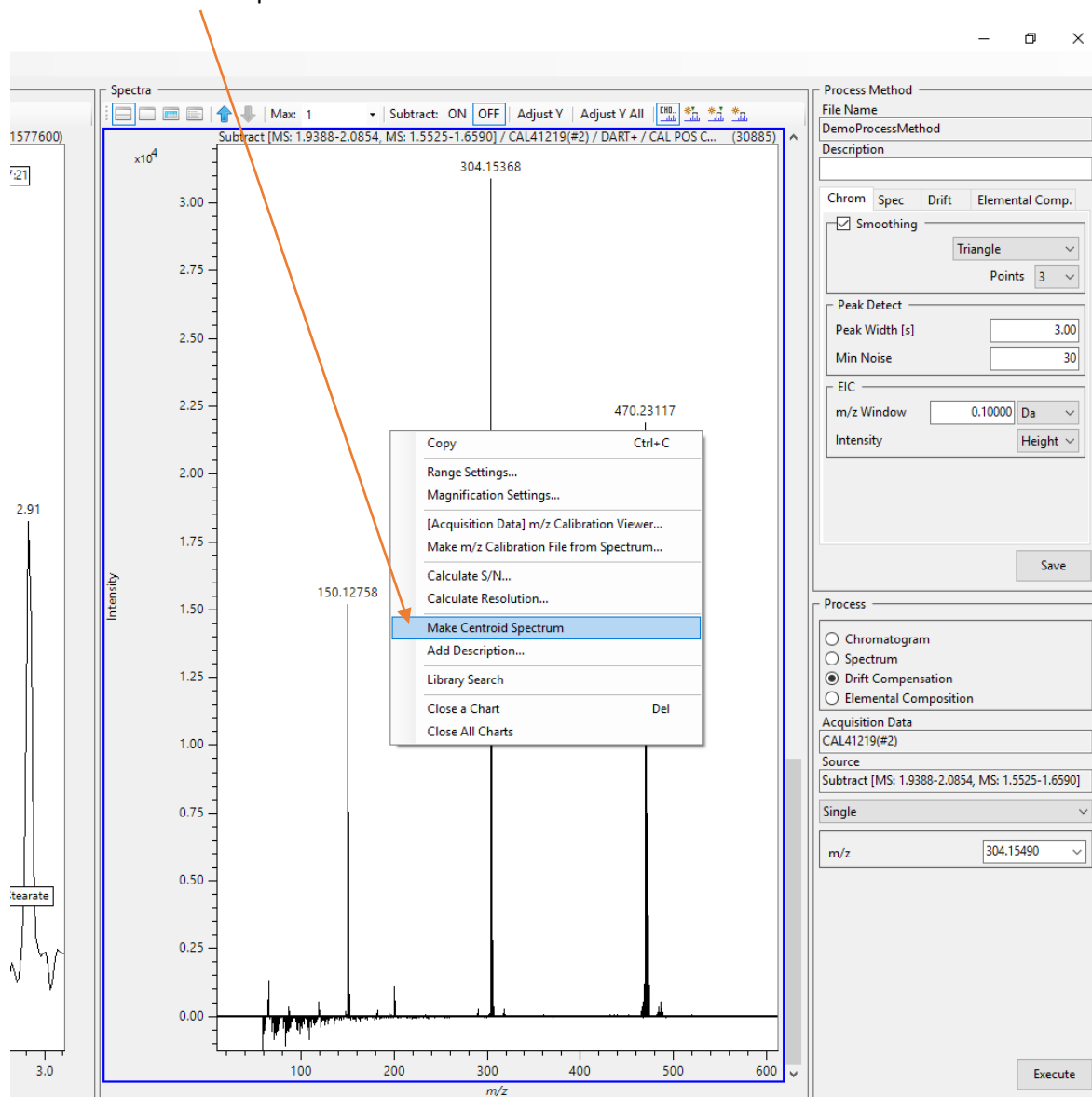


- The m/z Calibration window will appear. The max residual (max error in MassCenter) should be less than 0.003 and the RMS residual (standard error in MassCenter) should be less than 0.001. Also, the 1-R and 1-R\* should show values with e-012 for a good calibration. The polynomial order should remain at 3. Outlying data points can be removed on the PEG600 spectrum. Left-click on the data point, then right-click and select Release. No more than two, non-adjacent data points should be removed.



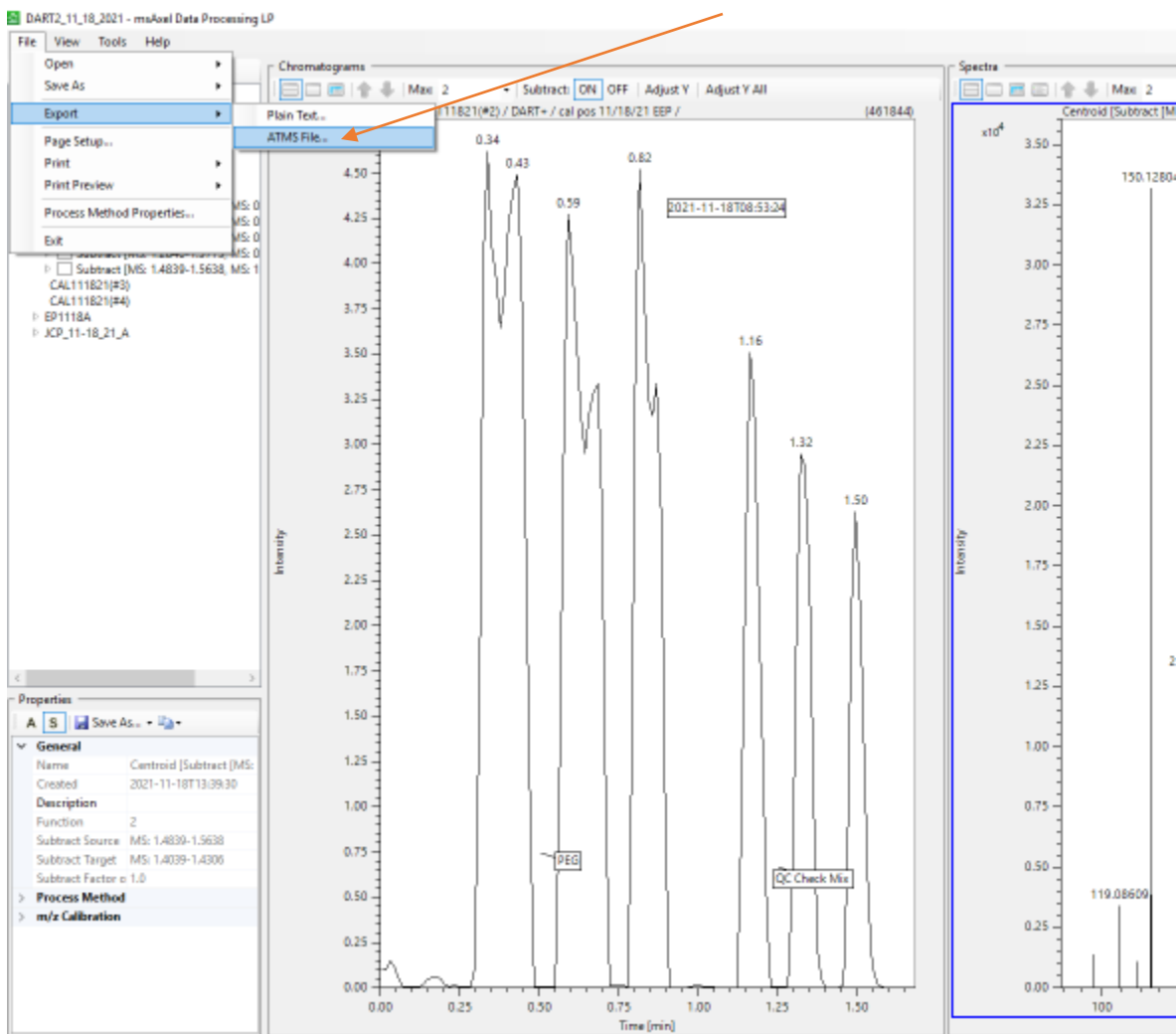
- Once you are satisfied with the curve fit, then click Tools > Update m/z Calibration (Original Data Only). Select Yes in the dialog box that appears to exit the m/z Calibration window. DO NOT CLICK APPLY TO INSTRUMENT. Make sure you apply the calibration to ORIGINAL DATA ONLY.
- The PEG600 calibration is now applied to all functions.

14. On the TICC, create a background subtracted spectrum of the QC Check Mix (CTRL + left-click and drag the peak, followed by SHIFT + left-click and drag the background). Right-click on the spectrum and centroid the spectrum.



15. Ensure the methamphetamine, cocaine, and nefazodone peaks are within  $\pm 5$  mDa of 150.1283, 304.1549, and 470.2323, respectively. To Print the spectrum, File > Print > Spectra. Once again, it will try to print all of the spectra you've created up to this point. In the Print Range section, choose the last page to print (7 of 7, or 5 of 5, depending on how many spectra you've created). Or, all previously created spectra can be deleted, then the centroided QC Drug Mix spectrum will print by default.

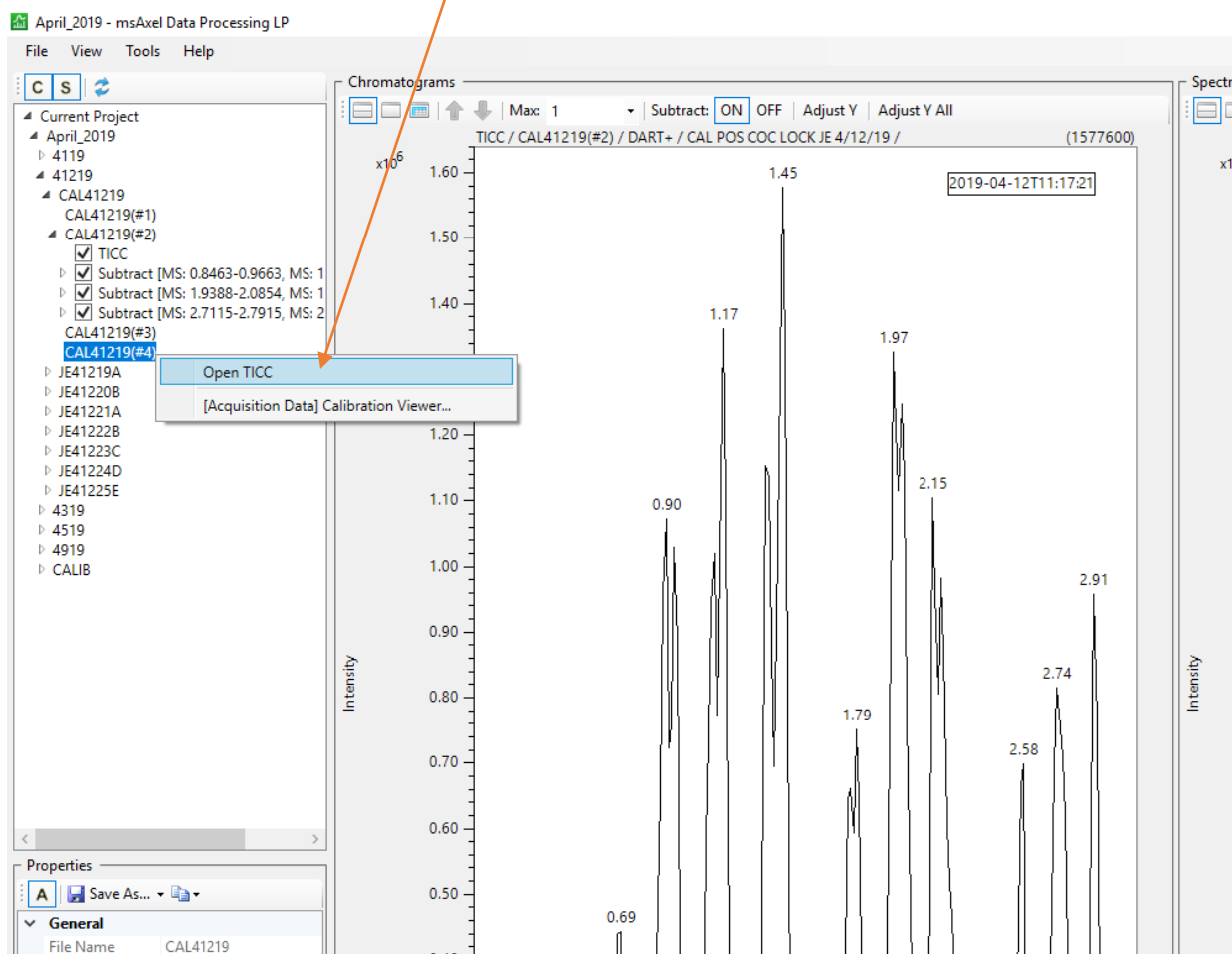
16. Begin processing data peaks, using CTRL + left-click and drag the peak, followed by SHIFT + left-click and drag the background. Right-click on the spectrum and choose Make Centroid Spectrum. Left-click on the spectrum to ensure it's highlighted before saving (or simply delete the previous, un-centroided, profile spectrum). To export for use in Mass Mountaineer, File > Export > ATMS File.



17. Make sure you save it as a .jsp! If you do not left-click on your sample spectrum after centroiding (or delete the previous, un-centroided, profile spectrum), it will want to save the previous, un-centroided, profile spectrum (.jpf). So, centroid spectrum, left-click on spectrum (or delete previous), then export. Save it in the current date's folder (initials, case #, item #, function).



18. To create a 90V spectrum, select the appropriate file in the list on the left side and then right-click the highlighted data (#4) and select Open TICC.



19. The PEG mass calibration is already applied to this function. Create a spectrum (using CTRL + left-click and drag the peak, followed by SHIFT + left-click and drag the background), centroid it, left-click it (or delete previous), and export it in the same manner as a 30V spectrum. All created TICC's (and added descriptions), calibrations, profile spectra, and centroided spectra are saved in the data folder. Should you need to go back to your data after someone else has run, or on a completely different day, simply open the correct date folder, and click on the arrow next to your data folder to see all TICC's and associated spectra. If new spectra need to be created, the PEG calibration does NOT need to be performed again. Once applied originally, it does not need to be applied again.