Use of ExpressION **C**ompact single quadrupole **M**ass **S**pectrometer (CMS) With Liquid Chromatography and Autosampler Injection

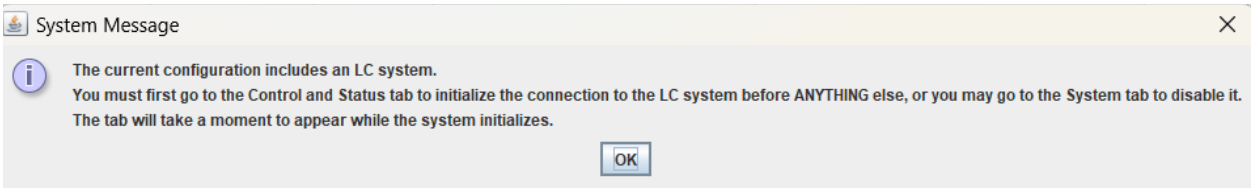
Picture Version 1.0 Green Circles Highlight key items for you!

This instrument is good when you know what ion you need to find, do not need a chemical formula, have an ion likely to be evident between 10 and 1,200 m/z as a single or multiple charge, have a compound that is soluble in water, acetonitrile, or methanol.

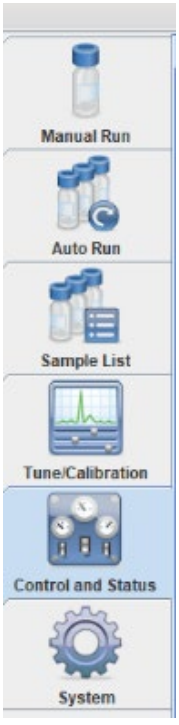
Ask Dr. Boersma for the default methods before using the instrument.

1. Login to the Lenovo laptop computer with your Auburn user ID and password. Complete the paper log-book.
2. Launch the Advion Mass Express software from the desktop.

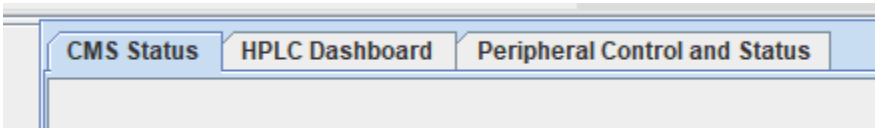
If a pop-up box indicates the software is already running, then the person before you did not log out of the computer. **Restart** the computer and repeat step 1.



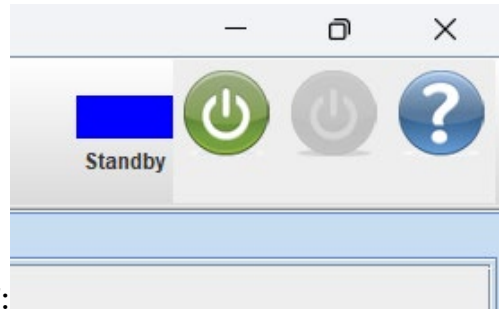
3. If this system message appears, click OK. If this message is not evident, go to the next step (4).
4. In the Mass Express software, go to the Control and Status icon on the left side of the software.

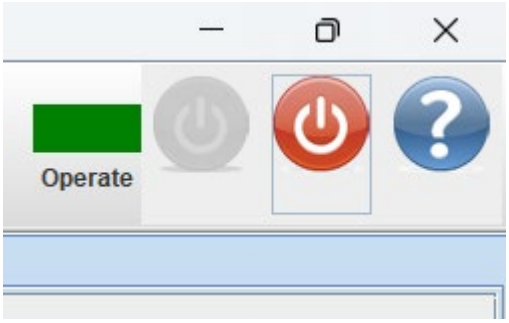


5. The window will probably show the CMS instrument. If not look for the folder structure on the top right within the software and click the CMS status tab.



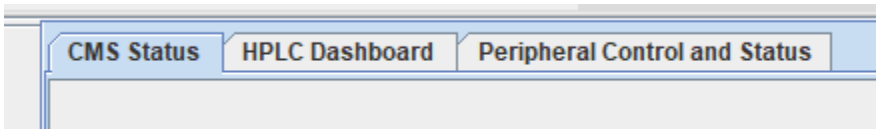
6. In the control and status page turn the CMS from OFF to ON by clicking the green button on the top right side of the Control and Status page. You may be able to hear the hiss of nitrogen gas as instrument starts.

OFF: 

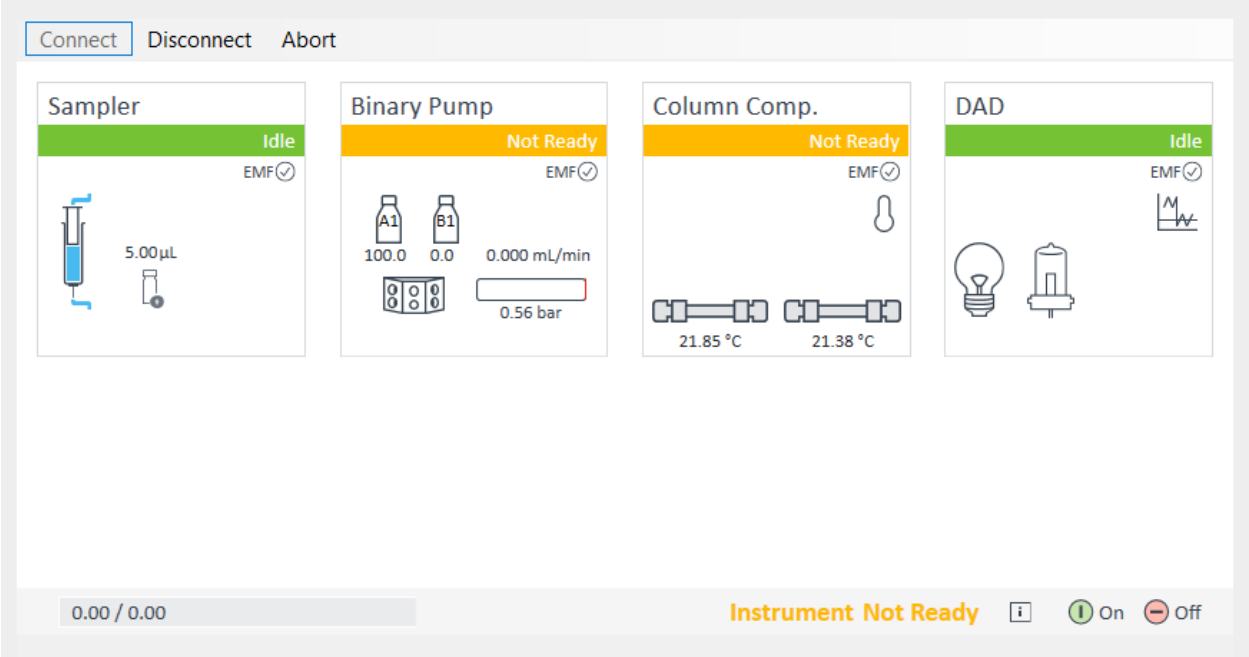
ON: 

YOU MUST TURN ON THE CMS BEFORE STARTING THE LC SYSTEM! If you turn on the LC without the CMS on, you will flood the source and potentially damage the instrument. You will be required to write a guide on how to clean a flooded source to show other students how to fix this mistake.

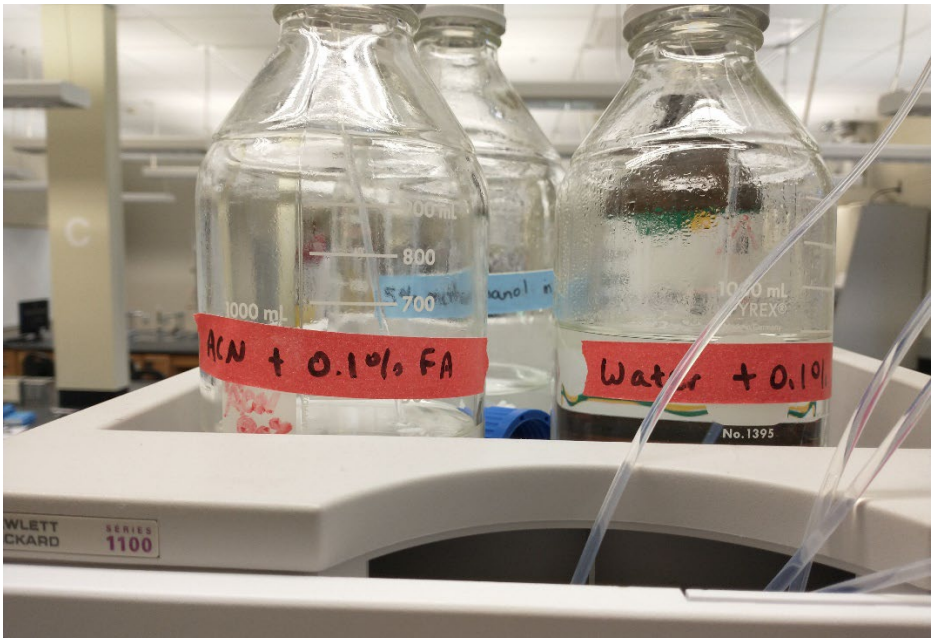
7. Go to the HPLC Dashboard by clicking on this tab.



8. You should see this view showing that the LC is not ready.

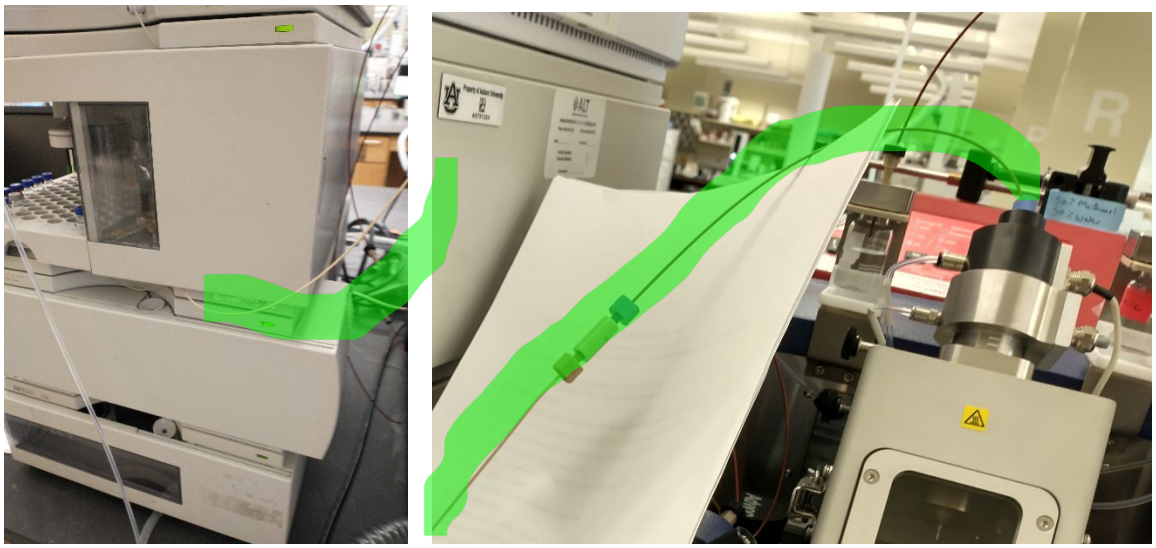


9. Verify there is fluid in the bottles on top of the LC stack. Determine if you are going to be using acid in your mobile phase or not. **Organometallic complexes should NOT** be analyzed with acid in the mobile phase, so use bottles A2 and B2. All others use acid and bottles A1 and B1. If the mobile phase volume is less than 200 mL, ask Dr. Boersma for more.

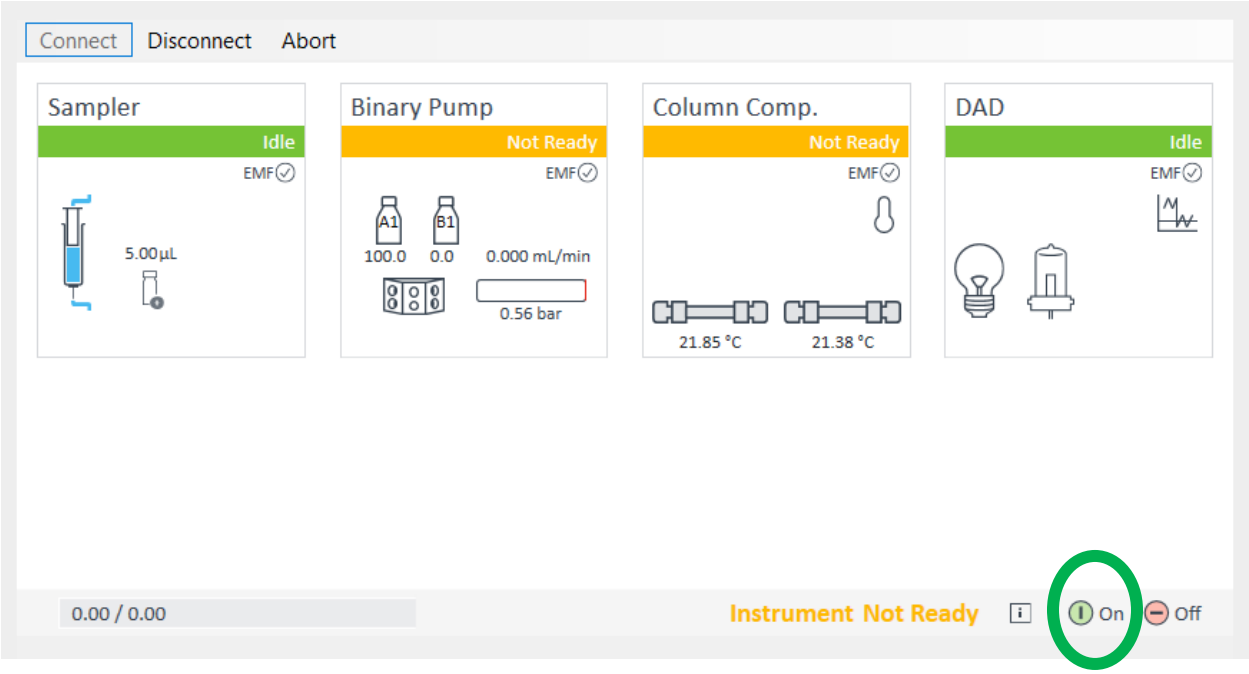


There must be adequate mobile phase on the system or you risk damaging the LC pump!!

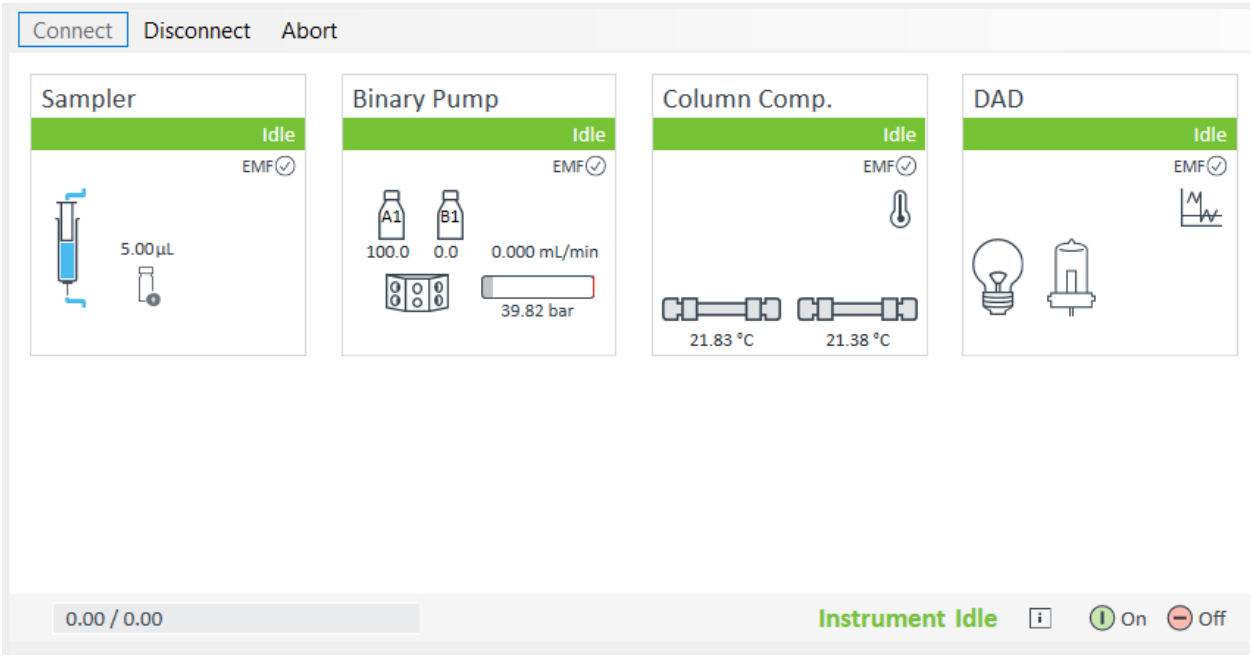
10. Verify the LC stack is connected to the Blue CMS instrument. The line should come from the autosampler, connect to a union, and be in the CMS source. Green highlights the tubing in pictures below

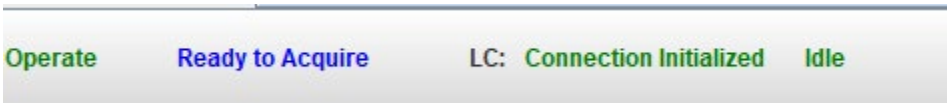


11. Once you have verified the instrument is correctly configured, click the green "On" button to start the LC system. You should hear the binary pump initialize.

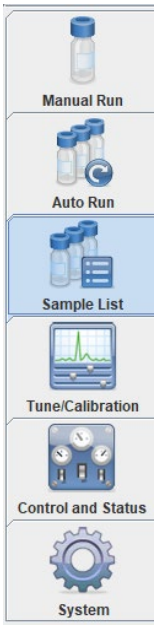


12. You should see the system go to green and the bottom left status change

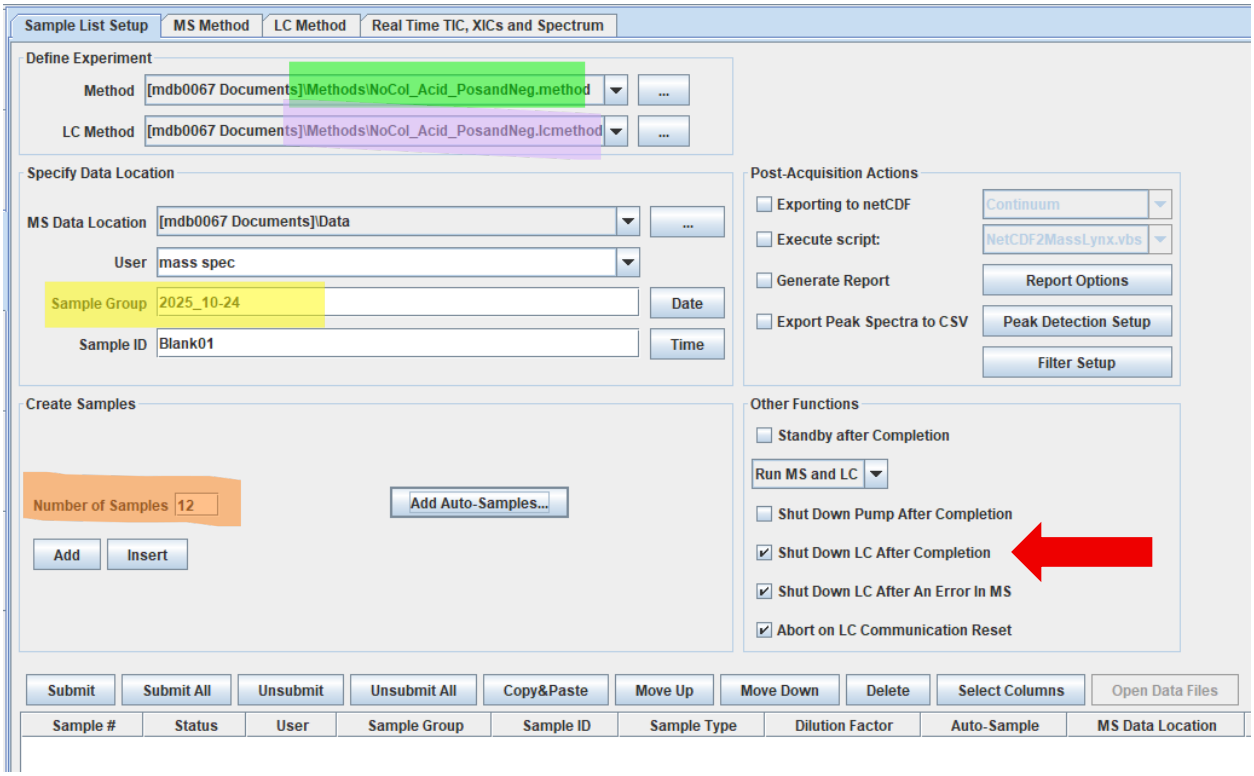




13. Next use the bar on the left to go to the Sample List.



14. You should see something like the image below. Dr. Boersma has provided you with 2 LC and 2 MS methods in your Box folder. Download those to the C:/Documents/Advion Mass Express/1.0/Methods folder. You will be logged in as your own user so you can organize your data as you see fit – but using the date as the sample group works well (yellow highlight)



In the Define experiment box click the … by method to select the mass spec method (green highlight). Then click the … to define the LC method (purple highlight). Acid should be used UNLESS your sample is an organometallic complex.

YOU MUST HAVE "Shut Down LC After Completion" set to ON with the checkbox otherwise you will flood the source and potentially damage the instrument. You will be required to write a guide on how to clean a flooded source to show other students how to fix this mistake. Refer to the red Arrow above.

15. Create a Sample ID. Blank is a good initial sample ID because **YOU MUST** have a blank before and after every sample. So the minimum number of samples (orange highlight) should be at least 3.
16. Click Add, and you should see 3 lines in the Sample list.
17. Click within the Sample ID to change the name to something that is meaningful to you. The data will be saved as the name you select in the Sample Group folder name that you have chosen. So, this step is shown in samples 2 and 4 of the list below.

Submit | Submit All | Unsubmit | Unsubmit All | Copy&Paste | Move Up | Move Down | Delete | Select Colum

Sample #	Status	User	Sample Group	Sample ID	Sample Type	Dilution Factor	Auto-Sample	MS Data
1	Unsubmitted	mass spec	2025_10-24	Blank01_1	Unknown	1.0	Vial 1	Data
2	Unsubmitted	mass spec	2025_10-24	NAKQ_DG_70...	Unknown	1.0	Vial 2	Data
3	Unsubmitted	mass spec	2025_10-24	Blank01_3	Unknown	1.0		Data
4	Unsubmitted	mass spec	2025_10-24	NAKQ_DG_80...	Unknown	1.0		Data

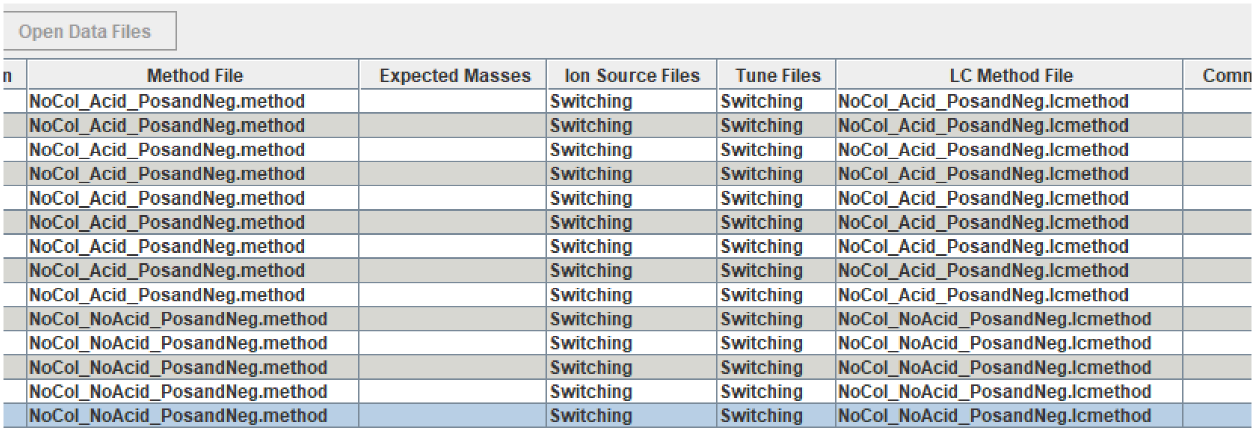
18. Click in the Auto-Sample box and you will briefly see “edit” and a pop up box. The image below shows the original sample list and the new box. The method volume is 0.5 microL. Change the location to where you put your vial and name it as Vial #.

Auto-Sample	MS Data Location	Method File
Vial 1	Data	NoCol_Acid_PosandNeg.method
Vial 2	Data	NoCol_Acid_PosandNeg.method
Vial 1	Data	NoCol_Acid_PosandNeg.method

Use Method Volume
Use This Volume (microL) 5 Check Volume
Injector Sampler 1
Location: Vial 3 Check Location
Save Remove Cancel

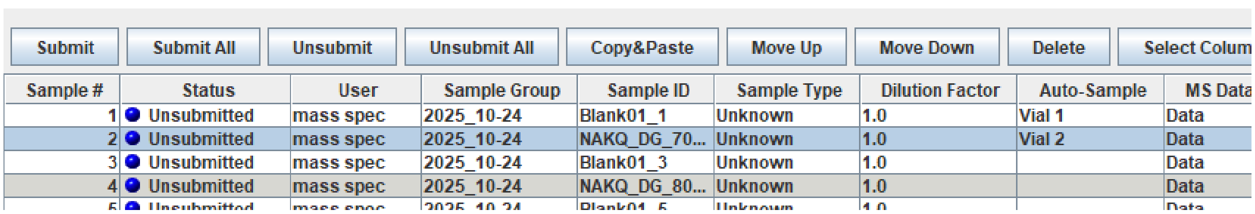
19. You know your vial number by where you placed your sample in the autosampler. Vial number 1 is always a blank and is in the front right position nearest you. That column is vials 1 to 10. The column to the right is vials 11 to 20. The next column is 21 to 30 and so on. Vial 81 is the autosampler wash vial. Make sure there is solution in Vial 1 and 81. There are solvents on the bench to the right to fill these vials with.

20. Verify that the correct method(s) have been chosen in your sample list.



n	Method File	Expected Masses	Ion Source Files	Tune Files	LC Method File	Comn
	NoCol_Acid_PosandNeg.method		Switching	Switching	NoCol_Acid_PosandNeg.lcmethod	
	NoCol_Acid_PosandNeg.method		Switching	Switching	NoCol_Acid_PosandNeg.lcmethod	
	NoCol_Acid_PosandNeg.method		Switching	Switching	NoCol_Acid_PosandNeg.lcmethod	
	NoCol_Acid_PosandNeg.method		Switching	Switching	NoCol_Acid_PosandNeg.lcmethod	
	NoCol_Acid_PosandNeg.method		Switching	Switching	NoCol_Acid_PosandNeg.lcmethod	
	NoCol_Acid_PosandNeg.method		Switching	Switching	NoCol_Acid_PosandNeg.lcmethod	
	NoCol_Acid_PosandNeg.method		Switching	Switching	NoCol_Acid_PosandNeg.lcmethod	
	NoCol_Acid_PosandNeg.method		Switching	Switching	NoCol_Acid_PosandNeg.lcmethod	
	NoCol_Acid_PosandNeg.method		Switching	Switching	NoCol_Acid_PosandNeg.lcmethod	
	NoCol_NoAcid_PosandNeg.method		Switching	Switching	NoCol_NoAcid_PosandNeg.lcmethod	
	NoCol_NoAcid_PosandNeg.method		Switching	Switching	NoCol_NoAcid_PosandNeg.lcmethod	
	NoCol_NoAcid_PosandNeg.method		Switching	Switching	NoCol_NoAcid_PosandNeg.lcmethod	
	NoCol_NoAcid_PosandNeg.method		Switching	Switching	NoCol_NoAcid_PosandNeg.lcmethod	
	NoCol_NoAcid_PosandNeg.method		Switching	Switching	NoCol_NoAcid_PosandNeg.lcmethod	

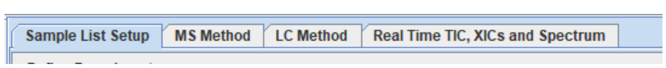
21. Highlight the rows you wish to inject by clicking in the Sample # and dragging down to highlight them (they will turn darker blue). Next click "Submit".



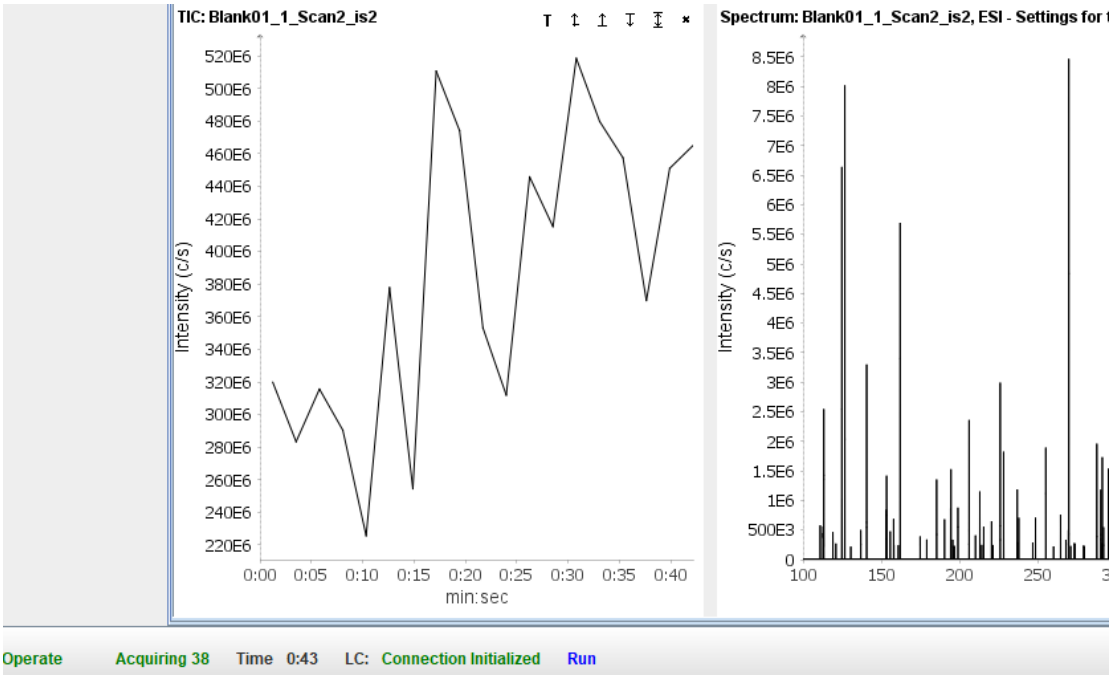
Sample #	Status	User	Sample Group	Sample ID	Sample Type	Dilution Factor	Auto-Sample	MS Data
1	Unsubmitted	mass spec	2025_10-24	Blank01_1	Unknown	1.0	Vial 1	Data
2	Unsubmitted	mass spec	2025_10-24	NAKQ_DG_70...	Unknown	1.0	Vial 2	Data
3	Unsubmitted	mass spec	2025_10-24	Blank01_3	Unknown	1.0		Data
4	Unsubmitted	mass spec	2025_10-24	NAKQ_DG_80...	Unknown	1.0		Data
5	Unsubmitted	mass spec	2025_10-24	Blank01_5	Unknown	1.0		Data

22. You should hear and see the autosampler begin to move to the first vial. You should also see the status bar on the bottom left change

23. Go to the Real Time TIC, XICs and Spectrum once the injection has been made.



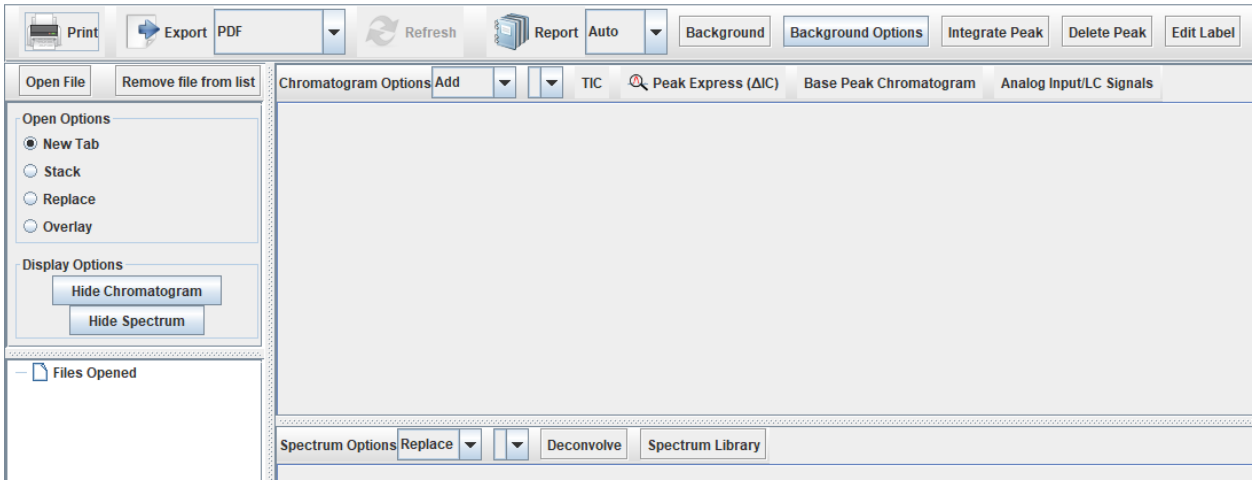
24. You should see the intensity (counts per second or c/s) and spectra as it is being acquired.



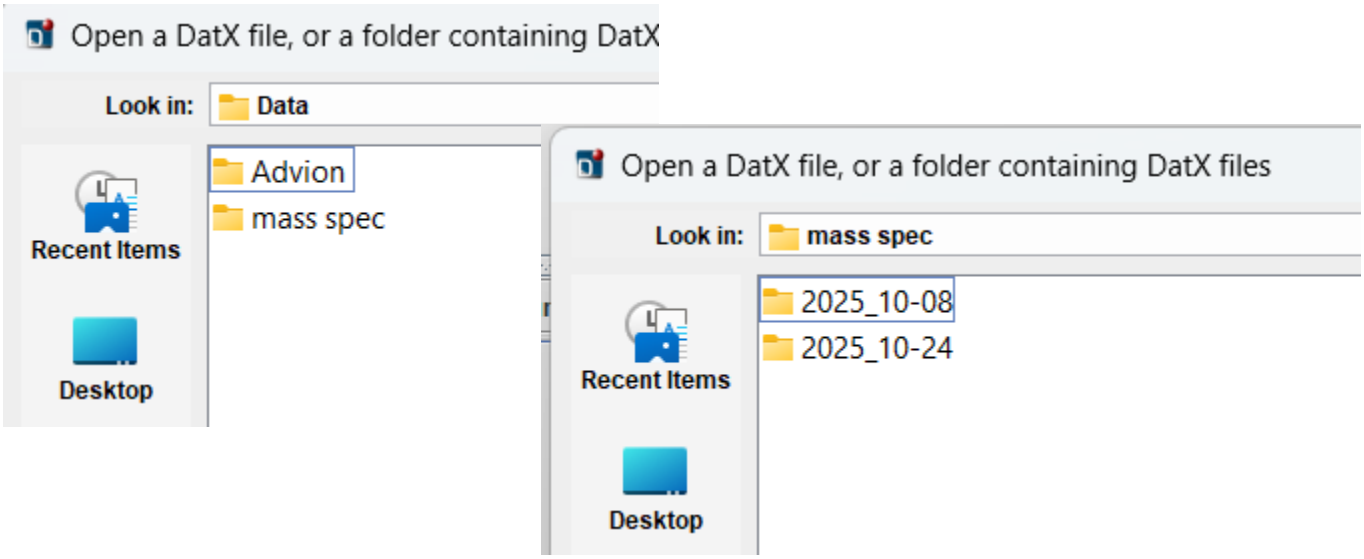
In the paper logbook, write down the background ions you see in the positive and negative mode spectrum for your first blank injection.

25. After your first sample has injected you can go to the Advion Data Express software to view your data. The icon is on your desktop.

26. The software will open and look like the image below. Click “OPEN FILE” and navigate to the data.

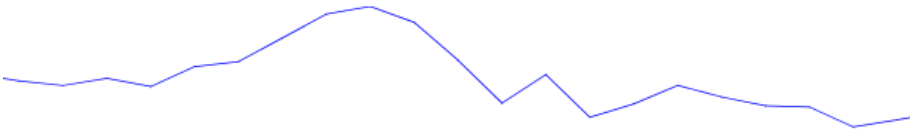


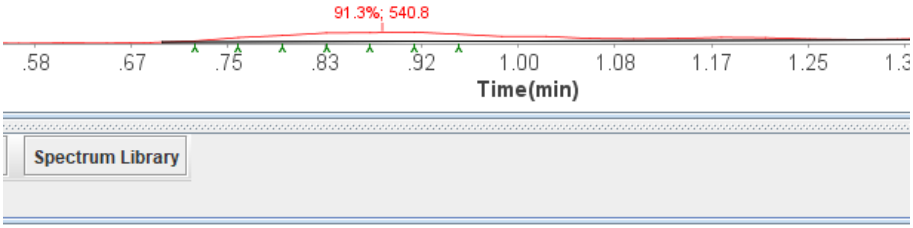
27. The data is usually in C:\Documents\Advion Mass Express\1.0\Data. If you used the date as the sample group, you will find the data within this folder. The location of the data can be found in your sample list.

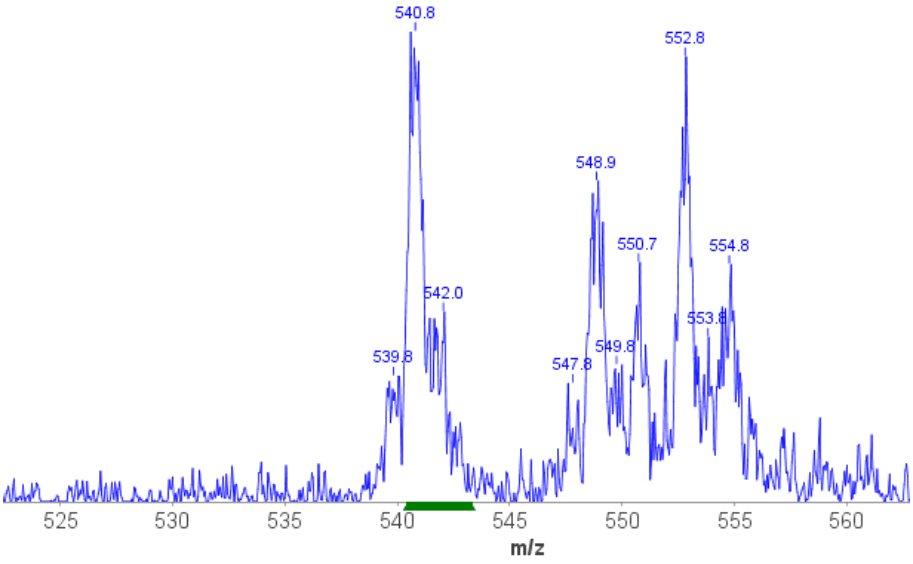


28. Generally the file ending in 1 is the positive mode data. You can see the mode is positive in the below with the ESI+ in the spectra (top right of Spectra). You can average spectra by using the right mouse and highlighting the time below the TIC (total ion chromatogram). You can see the green arrows where the time was highlighted below.

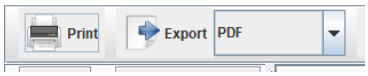
29. You can find your desired ion by right clicking inside the spectra to zoom to the region of interest. Then right click and drag below the m/z axis (x-axis) and the region in which the m/z will appear in the chromatogram.



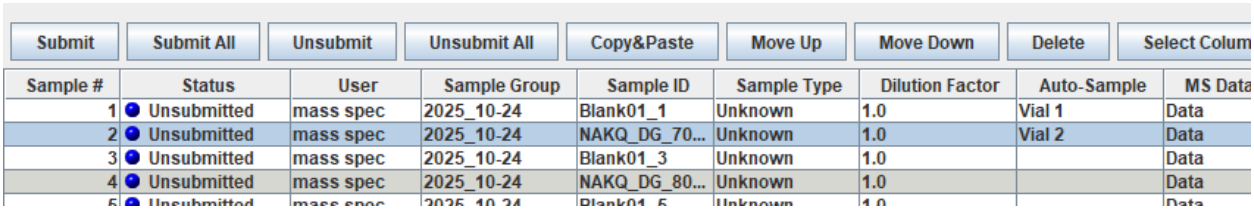




Here you can see that 540.8 is a contaminant in the blank injection. So a new wash solution should be added to vials 1 and 81. You can export your data as a .pdf or copy the data to your box folder and view at your leisure via your own copy of the software.



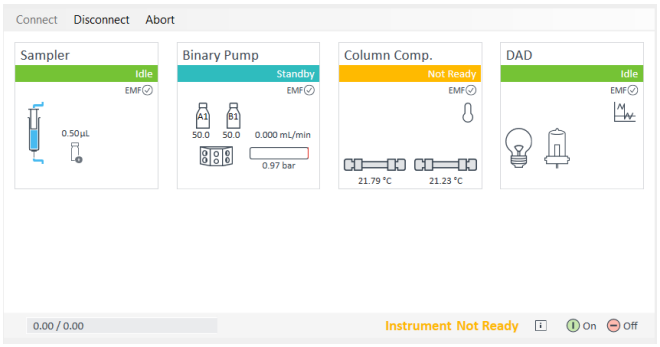
30. If you do not see your desired m/z do you see other new compounds in the data? Look at what is in the blank prior to your injection. If nothing has changed, you can go to the sample list, copy and paste the lines, and increase the injection volume in your sample list. Highlight those lines and click submit. ALWAYS start with a low injection volume and increase by 3 or 4-fold until you view data that differs from the blank. **DO NOT INJECT UNTIL YOU FIND YOUR DESIRED M/Z**, instead look at what is in the spectra. Is it your starting material? Is it a common contaminant? If you over-inject onto the system YOU and your Professor will be held responsible for cleaning it up and paying for repairs.
31. Once you have viewed all your data and printed the results, close Data Express and open Mass Express.
32. If your sample submittal list has completed, go to step 33. If not, you can wait or come back to the lab. You must come back before the lab closes at 5 pm. You can view the sample list by clicking on it and seeing what has been acquired in the Status column.



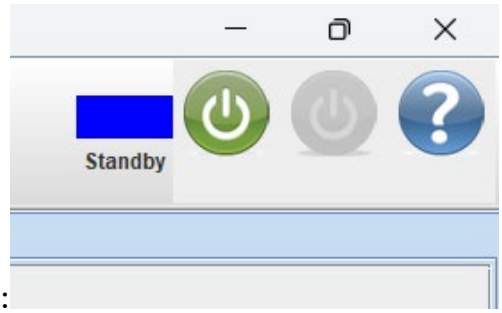
Sample #	Status	User	Sample Group	Sample ID	Sample Type	Dilution Factor	Auto-Sample	MS Data
1	Unsubmitted	mass spec	2025_10-24	Blank01_1	Unknown	1.0	Vial 1	Data
2	Unsubmitted	mass spec	2025_10-24	NAKQ_DG_70...	Unknown	1.0	Vial 2	Data
3	Unsubmitted	mass spec	2025_10-24	Blank01_3	Unknown	1.0		Data
4	Unsubmitted	mass spec	2025_10-24	NAKQ_DG_80...	Unknown	1.0		Data
5	Unsubmitted	mass spec	2025_10-24	Blank01_5	Unknown	1.0		Data

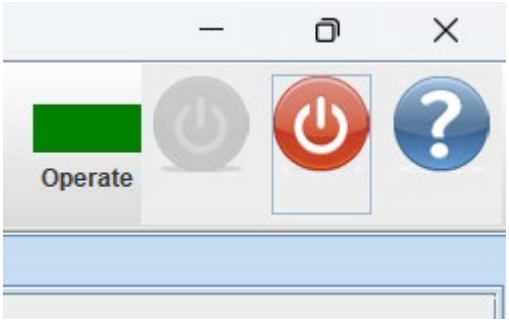
33. Go to the bar on the left and choose Control and Status

34. Verify the LC instrument is turned off.

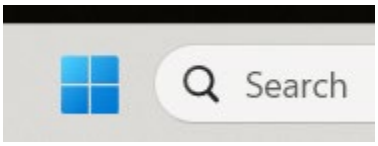


35. Turn off the CMS instrument by clicking the green symbol in the top left.

OFF: 

ON: 

36. Transfer the data from the mass spec computer to another location where you can review it easily, such as auburn.box.com or OneDrive.
37. Log OFF the computer by clicking the blue windows box bottom center and using sign-out.



38. Take any samples, solvents, and other items with you when you leave.