PolarisQ GC-MS Guide

Non-AS Version Revised 6-7-10 sbgb

Setting Up your run:

Open up Xcalibur
It will take a minute for the software to communicate with the instruments.



- 2. Click on Sequence Setup setup to set up your sequence.
- 3. A spreadsheet will open on the right side of the screen:

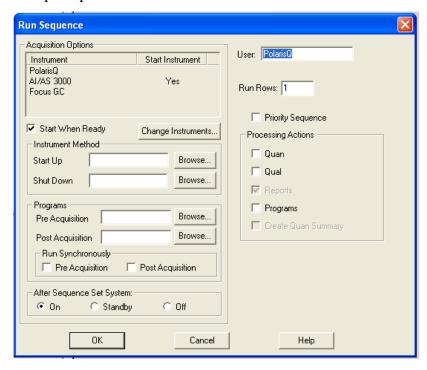
	Position	File Name	Comment	Inst Meth	Path	Inj Vol	Proc Meth
*						0.1	

- a. Enter "1" in the position box to start a new run line.
- b. Change your file name in the "File Name" column.
- c. Right-click in the box that says "Inst Meth", click on Browse, and open the method file "EI" if the instrument is in EI mode. This method has the latest MS tune/calibration file already put in it. You can also open any saved methods that you have had made for your specific conditions.
- d. The "path" should be set to C:\Xcalibur\Data already.
- e. Enter the injection volume (1.0 uL typical).
- f. You can leave the "Comment" and "Proc Meth" blank for manually run samples.
- 4. Click on File -> Save As, click OK, and then save over the Untitled sequence.

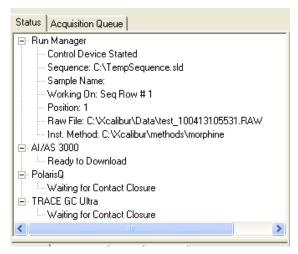
Running your Samples:

- 1. To run your sequence, highlight the row you want to run by clicking on the leftmost Excel column (the one you cannot edit) to turn the entire row black.
- 2. Click on the icon (looks like an arrow w/ a test tube on it). This will only run a SINGLE sample.

3. A box will open up:



- 4. Make sure that "AI/AS 3000" isn't listed as an instrument in the top box. If it is (as shown above) click on "Change Instruments" and click on the "Yes" in both columns next to AI/AS 3000" to remove the autosampler options.
- 5. Everything else should be OK do not make any changes to this screen!
- 6. Click on "OK"
- 7. When the GC-MS is ready for an injection, the box on the left side will look like this and say "Waiting for Contact Closure" on the PolarisQ and Trace GC:



Also, the "Ready to Inject" light on the GC keypad will be lit green.

- 8. When you inject your sample, press the START button on the GC keypad to start data acquisition.
- 9. You can click on the real time plot view while the sample is running to watch as the sample runs. YOU CANNOT PROCESS YOUR DATA IN THIS MODE!

Processing your data:

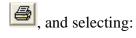


- 1. Click on Go To -> Qual Browser, or click on then select
- 2. Open your file (File -> Open or)
- To zoom in on the chromatogram, click and drag across a peak OR draw a box around a peak.
- 4. To zoom out click on .
- 5. To get a mass spectrum of a peak in the GC trace:
 - a. Pin the MS half of the screen by clicking the
 - b. Click and drag with the LMB across the GC peak you want to get MS information for.
 - c. To subtract the background MS, select the icon and click and drag in a SMALL REGION on the left and right baseline of the peak you want the MS data for.

6. To integrate your peaks:

- a. Click on the next to the chromatogram to make it active and zoom as needed.
- b. Click on to add peaks manually.
- c. To remove a peak or reintegrate a peak, click on 🚨
- d. To view your integrals, right click on the chromatogram, click on Display Options, then click the Labels tab and select Area. Click OK to close.

7. You can print the GC and MS information for each by clicking on File -> Print or





a. You will need to print each peak separately, if you have multiple GC peaks you want MS information for.