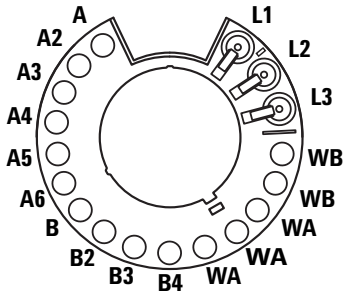
DMS Agilent GCMS

Pre-run checks

Helium is the carrier gas for the separation so make sure you have enough helium. The helium tank has a regulator on it that has two circular gauges. The right gauge tells you how much helium you got left. If the right gauge is less than 500 psi then you need to inform the stockroom to replace the helium tank.

On the circular *transfer turret,* which sits over the injector port, there are two spots, one marked **A** and one marked **B**. These spots are where you place the solvents for rinsing your syringe between samples. Make sure **A** is full of toluene (or acetone) and **B** is full of methanol before you start a run. Also make sure that the vials marked **WA** & **WB** are empty. The **WA** and **WB** vials are where the waste from the rinses are deposited.



Transfer turret

Clean off all the previously ran samples from the *Agilent 7693* autosampler, except leave the blank vial in position 150.

Running the samples

If it's not already running launch the acquisition software by clicking on the yellow *gcms #3* (or *gcms #4* in room 309) shortcut on the desktop

Put your samples onto the autosampler tray. If you fill up the first tray and need to get the robot out of the way press the black key on the front of the autosampler. The robot will move all the way to the left and the black key will light up with a **P** on it, indicating the autosampler is in the *Parked* position. When you're done loading the samples press the black button again to put the autosampler in the *Home* position. Note: the instrument will <u>not</u> run samples if the autosampler is in the Parked position.

Figure 57 Tray in Park position

Figure 58 Tray in Home position

To run samples you must create a sequence table that lists all your samples and the method you want to use for each sample.
Open a run sequence by going to Sequence → Edit Sequence

Under Data Path make sure the path is D:\Data\OChem_LABS\run*Date*

Where run*Date* is a folder that you create when you click the **Browse** button (click on OChem_Labs folder then click Make New Folder, then rename folder). For example if today was 4/8/2011 then you're path would be D:\Data\OChem_LABS\run040811

So all your runs for that day will be in a folder called something like *run040811* on the D drive.

For each sample you plan to run add a line in the sequence table. Each line consists of the following information

Type Choose Sample from the drop-down box, after you click on Type cell
Vial is position on autosampler (1 though 150)
Sample is the sample name, use only alphanumeric, underscore, and dash
Method is OChem (right click on the cell and choose *Browse for Method…*)
Data File copy sample name over to here

To delete a line right click on the leading line number and select Delete Row

Make sure the last line of your sequence is

Type	**Vial**	**Sample**	**Method**	**Data File**
Sample	150	standby	STANDBY	standbyDATE

If it were 4/08/2011 you'd enter **standby040811** for the entry under Data File in the above sequence line.

Running the STANDBY method as the last sample in your sequence will put the instrument in standby mode (lower temperature and gas flow rates) after all the samples have been ran.

Once you're done filling out the sequence table click OK.

To run the sequence go to *Sequence* → *Run Sequence*
A Dialog box will open up. Enter in your name as the operator and then click **Run Sequence**.

Data Analysis

Once a sample has finished running you can analyze its data.

Launch the data analysis software by clicking on the *gcms #3 Data Analysis* (or *gcms #4 Data Analysis* in room 309) icon on the desktop.

Using the *Browse* button on the left-hand side of the data analysis screen and go to the data folder. It should be on the D drive under something like D:\Data\OChem_LABS\run040811

Double click on a file to bring up its GC chromatogram. Double **right-click** on a peak in the GC chromatogram to bring up that peaks mass spectrum.

(If you want to you can double-click anywhere in the mass spectrum window and it will bring up a library search. Note, the library is limited and will not have every compound.)

Currently there is no printer configured for the system. You'll need to print to a pdf. Go file print, select *TIC and spectrum* and then give it a name and save it under **~/My Documents/Ochem_pdfs** .The pdfs can then be copy to a USB drive and printed elsewhere.

Fixing Errors

1) The autosampler will go into an error state if the following scenario happens: You load several samples on the autosampler tray and the robot picks up a sample, for example the first sample, and starts processing it. Meanwhile, someone comes along and sees the first position is empty and places their sample in the first position. When the autosampler robot is done processing the first sample it will want to put it back in the first position but there is a sample in that spot so it stops and generates an error.

To fix this error remove the sample from position one then press the black button on the front of the autosampler. The button will light up with a **P** on it and the autosampler robot will put the sample that it is holding back in position one and then move the arm out of the way (the autosampler is now in the *Parked* position and will not run samples). You'll then need to press the black button with the lit **P** on it again to move the autosampler into the *Home* position. You'll notice the autosampler robot will move to the front of the autosampler tray.