

## Shimadzu GC-MS

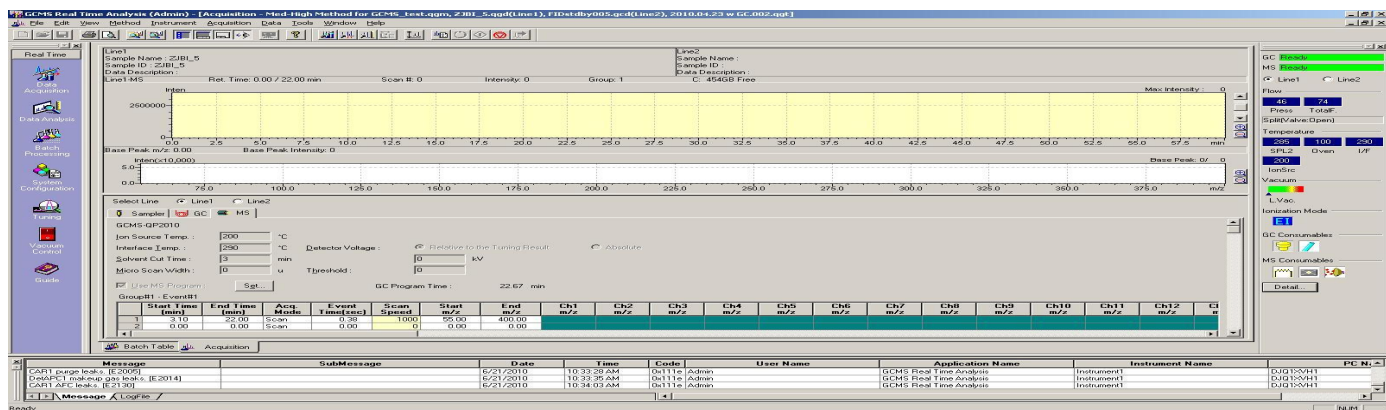
Please see Ariana for training before your first use.

### Sample Preparation

1. Your sample concentration should be no more than 5 mM (e.g., about <50  $\mu$ l of a 0.2M reaction).
2. Never put metals, strong acids, bases, oxidants, water, or samples with particulates on the GC!
3. Sample with metals: filter through silica.
4. Samples with Pd/C: filter through celite.
5. Sample with strong acids or bases: aqueous work-up.
6. Samples with strong oxidants (e.g., Oxone,  $\text{Br}_2$ ): quench with 10% aq  $\text{NaSO}_3$  solution and work-up.
7. Samples with particulates: filter through celite.
8. Always check and refill the wash vials from the bottles next to the GC. Make sure to push the wash vial rack into its original position after refilling wash vials, or the sample will not run.

### Running a Single Sample

1. Click to open the Shimadzu GCMS Real Time Analysis window.
2. Once the program has loaded, the screen should look like the picture below.



3. Click on the **Data Acquisition** icon, in the bar on the left side of the screen. If the **Data Acquisition** icon is not visible click on the **Top (arrow)** icon in the same bar until it appears.
4. Once you place the sample in the auto sampler, click on the **Sample Login** icon, enter Sample Name, ID, and Data Folder and change the vial number to where your sample is located in the autosampler. Click Ok.
5. In the main window, open the method you would like to use through **File > Open method file**.
6. Click on **Standby** icon . When it's done setting the instrument parameters, click on **Start** icon.
7. Once your run is done and both GC and MS are ready again, open the "GCMS sleep method" through **File > Open method file**. Then, click on **Acquisition > Download Initial Parameter** to put the instrument in energy saving mode.

## Running Multiple Samples

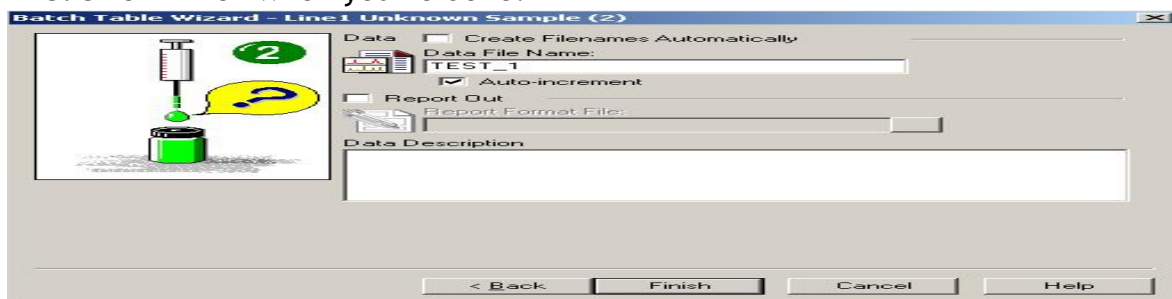
1. Click on the **Batch Processing** icon from the initial screen.
2. Then, click on the **Wizard** icon. Always use the wizard to run a batch file!!
3. You're now ready to make your sample batch.



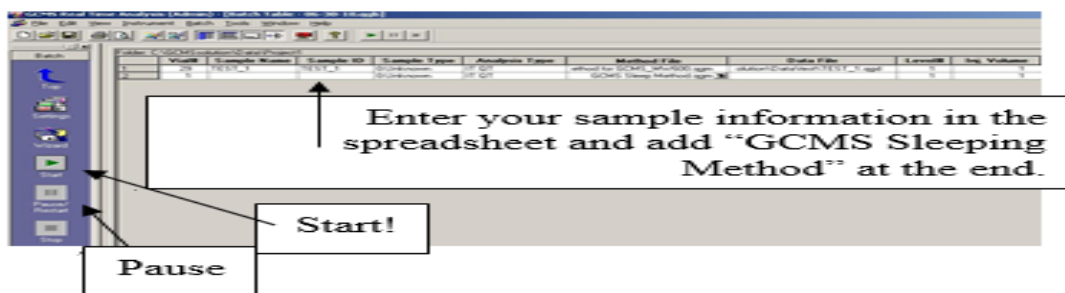
Batch Type: Line1 = GC/MS, Line2 = FID, Line1/Line2 = running both GC/MS and FID for a sample subsequently (not recommended) **Also, you can't run GC/MS of**

one sample and FID of another in the same batch!! Make sure to select correct method and click **Next**.

4. Enter the vial # and sample count (how many samples you have). The Sample Name and Sample ID should be the same. However, you will be able to change this information later. Click next.
5. Enter the Data File Name and make sure that "Report Out" is not selected. Click on Finish when you're done.



6. Now, the screen should look like the picture below. Click on **Data File** to designate the correct folder for your sample. At the end of the batch file, insert a new row by **right click > Insert Row** and set the Method File as "GCMS Sleep Method" Set the vial # to be zero (this will bypass the autosampler).



8. Click on the **Start** icon.

### *Adding a sample when it's already running*

1. Prepare the batch file as above using **GCMS Analysis Editor**.
2. In **Real Time Analysis**, click on **Batch > Batch Queue** and add the batch file you have made and hit Ok. Make sure to include the "GCMS sleep method" at the end.

### *Processing the data*

*For GC-MS data*

1. Open the **GCMS Postrun Analysis**, and click on the **Qualitative** icon.
2. Open the sample file you would like to process. Zoom into the region of interest by left click and drag. Double-left click on the peak of interest to analyze the MS. Or click and left click-drag within the GC peak to get average MS data.

*For GC-FID data*

1. Open the **Postrun** from GCsolution Operation and process it as you would with the GC.

## *Printing data*

In **GCMS Postrun Analysis**, click on **File > Print Image > Print** to print your data.