

This guide is intended as a quick reference for people who have already been trained in the use of this instrument.

If you have not used this GC-MS system before, please contact Allis Chien (Keck 313, x3-0710, [allis@stanford.edu](mailto:allis@stanford.edu)) for training before you attempt anything.

## GENERAL REMINDERS

- Create a logbook entry record in the “GC-MS Logbook” database.
- Any problems or feedback should be recorded in the Notes field of the database record.
- Make sure the solvent vials have enough solvent, as indicated on the vial. Solvent A is acetone, Solvent B is diethyl ether.

## QUEUE MODE

As long as there is room in the autosampler tray, more samples may be added to the queue at any time, even if a prior analysis is in progress.

1. In the “Queue Mode” window, select “run individual sample” or “run batch of samples” and click “OK”, then follow the prompts. Use “batch sample” only if you want to use the same sample name and method for multiple vials.
2. You will be asked for your username and password.
3. Select an analysis method. Methods are posted on the GC oven door.
4. Place vial in the indicated position in the autosampler tray. To override the position assignment, click “cancel”, then enter the desired position.
5. Enter sample title and description, if desired
6. Check vial position
7. If you have only one sample, answer “no” to “Another Autoqueue?” If you have additional sample(s) to run, click “yes” and repeat steps 2-5.
8. Click on the “Report Manager” in the taskbar, and check the status of the instrument by double clicking on the “MS-1” line. If the window on the top right reads “status standby”, click on the “resume” button and enter “osesame” at the password prompt.
9. In Report Manger, be sure to note the filename that has been assigned to your sample; it consists of “P” followed by 4 numerals, then “.D”, e.g. “P1024.D”.
10. When a run is finished, a report will be printed automatically. The report consists of the total ion chromatogram (TIC), percent report, and library search results. If you want printouts of the mass spectra, they can be obtained through the Data Analysis module.

**DURING THE RUN**

- No need to wait around; you can come back later to pick up your printouts.
- If you want to watch the data as it is generated, click on “GC/MS Instrument #1” and maximize the “Total Ion Chromatogram” window. If the peaks go off-scale at the default attenuation (2.0E6), then your sample is too concentrated.
- Time elapsed/remaining can be viewed on the GC: press “time” on the GC keypad (top gray key on the far left)
- Use the standalone Data Analysis software module to take snapshots, etc.

**ANALYZING DATA**

1. If the “Enhanced Data Analysis” module is not already in the taskbar, a shortcut to the program (“Instrument #1 Data Analysis”) is located in the Windows XP Start menu.
2. Enter the same username and password as previously.
3. Select Load under the File menu
4. Select the data file, and the chromatogram will be displayed.
5. To expand a portion of the chromatogram or mass spectrum window, use the *left* mouse button to click and drag the cursor over the region of interest.
6. To zoom out to the entire range, double click the *left* mouse button.
7. To display the mass spectrum of a peak, place the pointer over the peak and double-click the *right* mouse button.
8. To display an averaged mass spectrum across a peak, click and drag the *right* mouse button across the region of interest.
9. To search the MS library, double click the right mouse button on the mass spectrum of a compound. (“Wiley275” must be selected as the library; this setting is in the “select library” option in the “Spectrum” menu.)
10. To print your data, select Print from the File menu. Either or both the TIC and MS windows may be printed.

**SAMPLE PREPARATION**

Certain classes of compounds are unsuitable for gas chromatography, and can damage the GC column. The following should never be injected: metals, strong acids or bases, salts, oligomeric and polymeric material.

**Solvents:** Ether and methanol are the recommended solvents for sample preparation. Other options are acetone, pentane, and hexane, i.e. low-boiling solvents.

**Sample Concentration:** Sample solutions should be approximately 100 ppm (0.01%). Abundances of over  $10^6$  on the TIC indicate that sample are too concentrated.

**DATA FILES**

Data files are saved into a folder named for the current month. These folders will remain on the hard drive for approximately 4 months before they are removed; e.g. the “May” folder will be deleted in September. If you wish to save your data, bring your own 5¼” floppy disk or CD, and use Windows Explorer to copy your files. The full path for the data files is “C:\MSDchem\1\data\” then the month. See item #9 under “queue Mode” on individual data file names.