Shimadzu GCMS User's Booklet
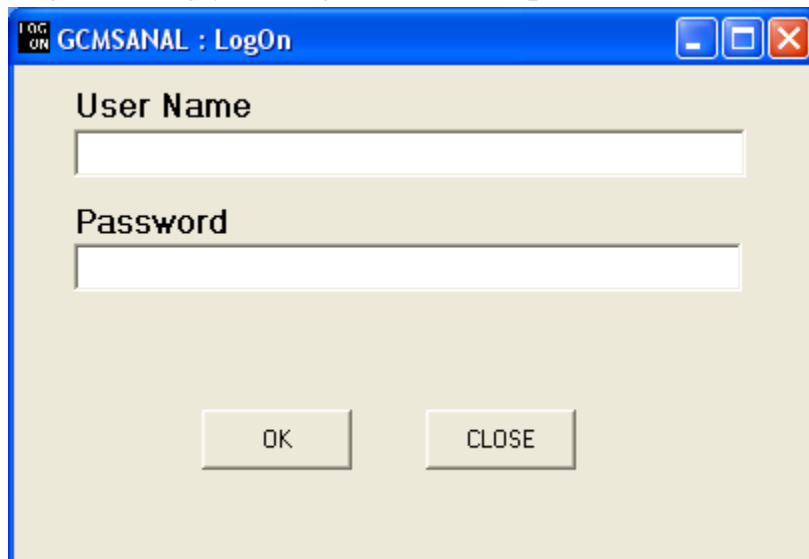
1) Log in, using your login name and password:

After you login, the data acquisition software will automatically come up. When you see this box, just click OK:

2) After the data acquisition software comes up, click on File, and Open Method, in order to choose and open a data acquisition method. Two common methods already created for you are Student_Default_Split, and Student_Default_Splitless.

Use the "Student_Default_Split" method for samples which are concentrated (around 1mg/ml).

Use the "Student_Default_Splitless" method for samples which are dilute (around 10 nanograms/microliter).

You can change or edit the Method file to suit your experiment. If you change the method, please save it as your method, by clicking on "File", and "Save Method File As".

There are 3 tabs for entering information in the method.
The first tab has parameters for the auto-injector.
The second tab has parameters for the gas chromatograph.
The third tab has parameters for the mass spectrometer.

3) Be sure to remember to put your vial in the autosampler carousel. You need to use a 2 ml autosampler vial with a Teflon-lined cap, such as Fisher Scientific part # 03-391-15.


The minimum volume of solution is 450 ul. If you cannot spare that much solution, you can use a conical glass insert in the vial, so that the solution level will be high enough for the syringe needle to enter it.

When you put the sample in the carousel, please note the number of the well in which you place the vial.

4) Make sure that the solvent rinse vials contain the solvent you are using. The purpose of each vial in the injector tray is shown here:
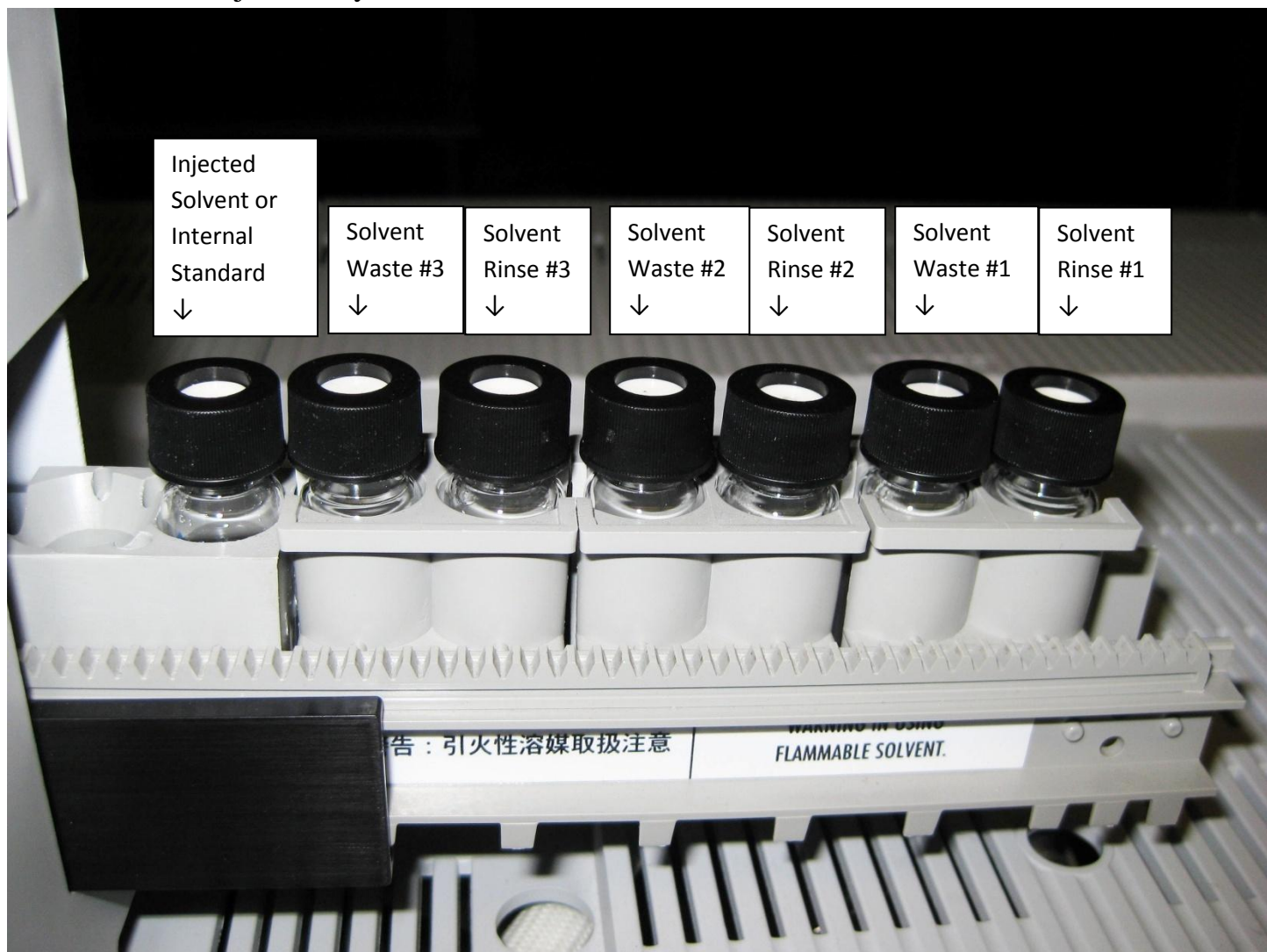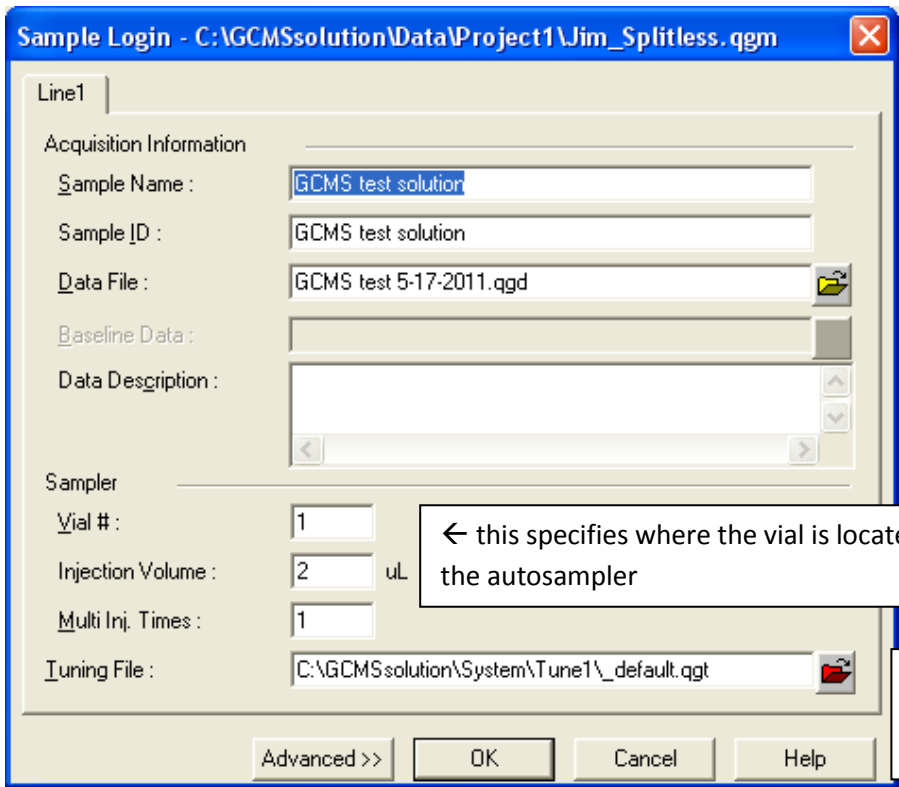

The vials in the injector tray are 4 ml autosampler vials with a Teflon-lined cap, such as Fisher Scientific part # 03-391-22.

5) On the left hand side, click on the "Sample Login" icon to enter sample information.

Acquisition

Top

Wizard

Sample Login

← Click on the Sample Login icon to enter sample information for individual (non-batch) runs.

Standby

Start

Stop

Method Detail

Snapshot

Guide

Sample Login - C:\GCMSsolution\Data\Project1\Jim_Splitless.qgm

Line1

Acquisition Information

Sample Name : GCMS test solution

Sample ID : GCMS test solution

Data File : GCMS test 5-17-2011.qgd

← Enter a data file name, and a location for the file.

Baseline Data :

Data Description :

Sampler

Vial # : 1

← this specifies where the vial is located in the autosampler

Injection Volume : 2 uL

Multi Inj. Times : 1

Tuning File : C:\GCMSsolution\System\Tune1_default.qgt

← The tuning file should remain as the default.

Advanced >>   OK   Cancel   Help

6) Click on the "Standby" icon to download your acquisition method parameters to the instrument. When the "Start" icon becomes active, you can click on it to start your run.

← Click on the "Standby" icon to download the acquisition parameters.

← When the "Start" icon turns green and becomes active, click on it to start the run.

7) When the data acquisition is complete, click on "Top" icon on the left hand side to move up one level. Then, click on the "Data Analysis" icon.
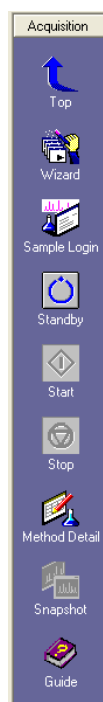
← Click on the Top icon, to move up one level.

← Then click on the Data Analysis Button, to launch the data Analysis program.

8) The last data file acquired automatically comes up. If you wish to view a different file, just double-click the one in the list you want.

To display a mass spectrum of a chromatographic peak: right-click the mouse anywhere in the chromatogram to obtain a menu. Then left-click on "Average Spectrum" to get a cursor. Left-click and drag the cursor across the chromatographic peak, and its mass spectrum will be displayed.

To perform a library search on the mass spectrum: right-click the mouse anywhere on the spectrum to obtain a menu. Then, left-click on "Similarity Search".
A list of possible matches will be displayed.

Similarity Search Results

Report View Compound Info Process Help

Hit#	Similar	Regis	Compound Name	Mol Wt	Formula	Library
1	96	☑	Benzaldehyde $$ Artificial Almond Oil $$ Benza	106	C7H6O	NIST05s.LIB
2	96	☐	Benzaldehyde $$ Artificial Almond Oil $$ Benza	106	C7H6O	NIST05.LIB
3	96	☐	Benzaldehyde $$ Artificial Almond Oil $$ Benza	106	C7H6O	NIST05s.LIB
4	95	☐	Benzaldehyde $$ Artificial Almond Oil $$ Benza	106	C7H6O	NIST05s.LIB
5	89	☐	Benzeneacetonitrile, .alpha.-hydroxy- $$ Benza	133	C8H7NO	NIST05.LIB
6	89	☐	1,2-Benzenedicarboxaldehyde $$ Phthalic dica	134	C8H6O2	NIST05s.LIB
7	89	☐	Bis[4-acetamidophenylsulfonyl]phenyl methane	486	C23H22N2O6	NIST05.LIB
8	88	☐	1,2-Propanedione, 1-phenyl- $$ Acetylbenzoyl	148	C9H8O2	NIST05.LIB
9	88	☐	1,2-Propanedione, 1-phenyl- $$ Acetylbenzoyl	148	C9H8O2	NIST05s.LIB
10	87	☐	Ethanone, 2-amino-1-phenyl- $$ Acetophenon	135	C8H9NO	NIST05.LIB
11	87	☐	1,2-Benzenedicarboxaldehyde $$ Phthalic dica	134	C8H6O2	NIST05s.LIB
12	87	☐	Ethanone, 2,2-dihydroxy-1-phenyl- $$ .alpha.,.a	152	C8H8O3	NIST05.LIB

←The list of possible library spectra matches.

Target:

Your mass spectrum.

1 : 106 : Benzaldehyde $$ Artificial Almond Oil $$ Benzaldehyde FFC $$ Benzenecarbonal $$ Benzenecarboxaldehyde $$ Benzoic aldehyde $$ Phenylmethanal $$ Almond artific

The highlighted library spectrum.

Subtraction Result

The difference between your spectrum and the library spectrum.

To manually integrate the area under a chromatographic peak, click on the Qualitative menu. Then click on Manual Peak Integrate, and then on TIC. Then left-click and drag the cursor across the chromatographic peak.

To display a mass chromatogram, right-click anywhere on the chromatogram, to obtain a menu. Then left-click "Fragment Table…."
You will see this box:
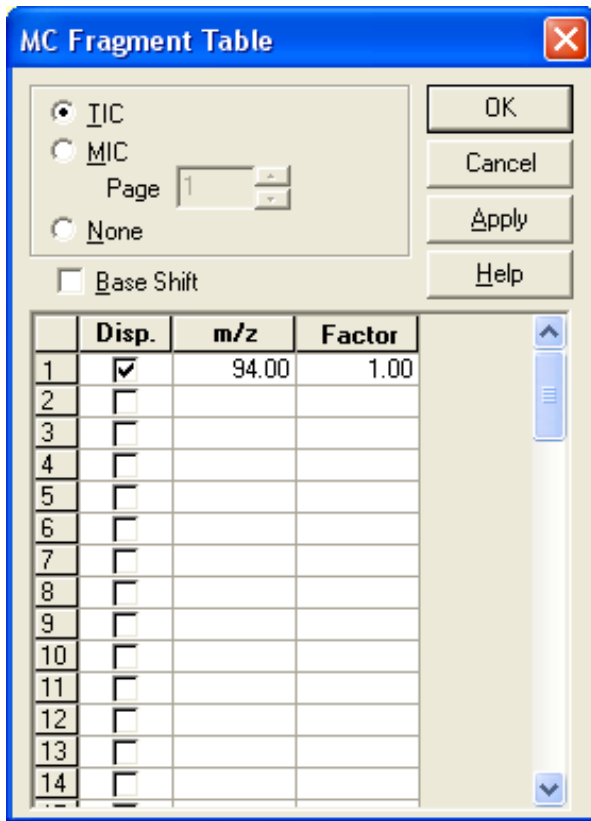
Type in the m/z values that you want to display. You can enter a multiplying factor to scale up the signal if you wish. Click on the Disp. option, and click ok.
Both the TIC and the mass chromatogram will be displayed on the same graph.
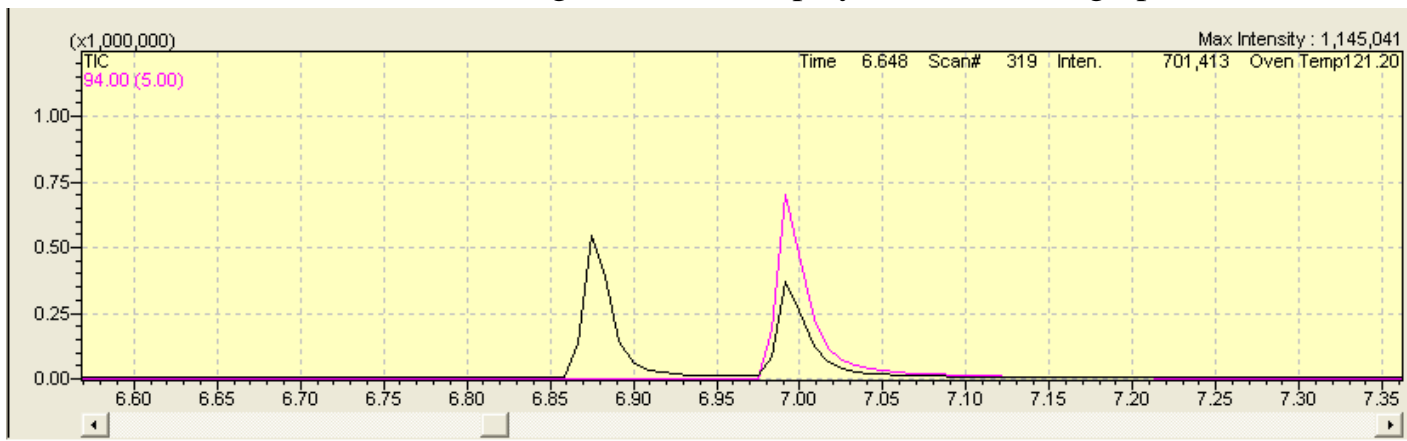
Optional:

How to acquire batch runs of large numbers of samples.

← Click on the Batch Processing Icon.

← Then click on the Wizzard Icon to set up the batch table.
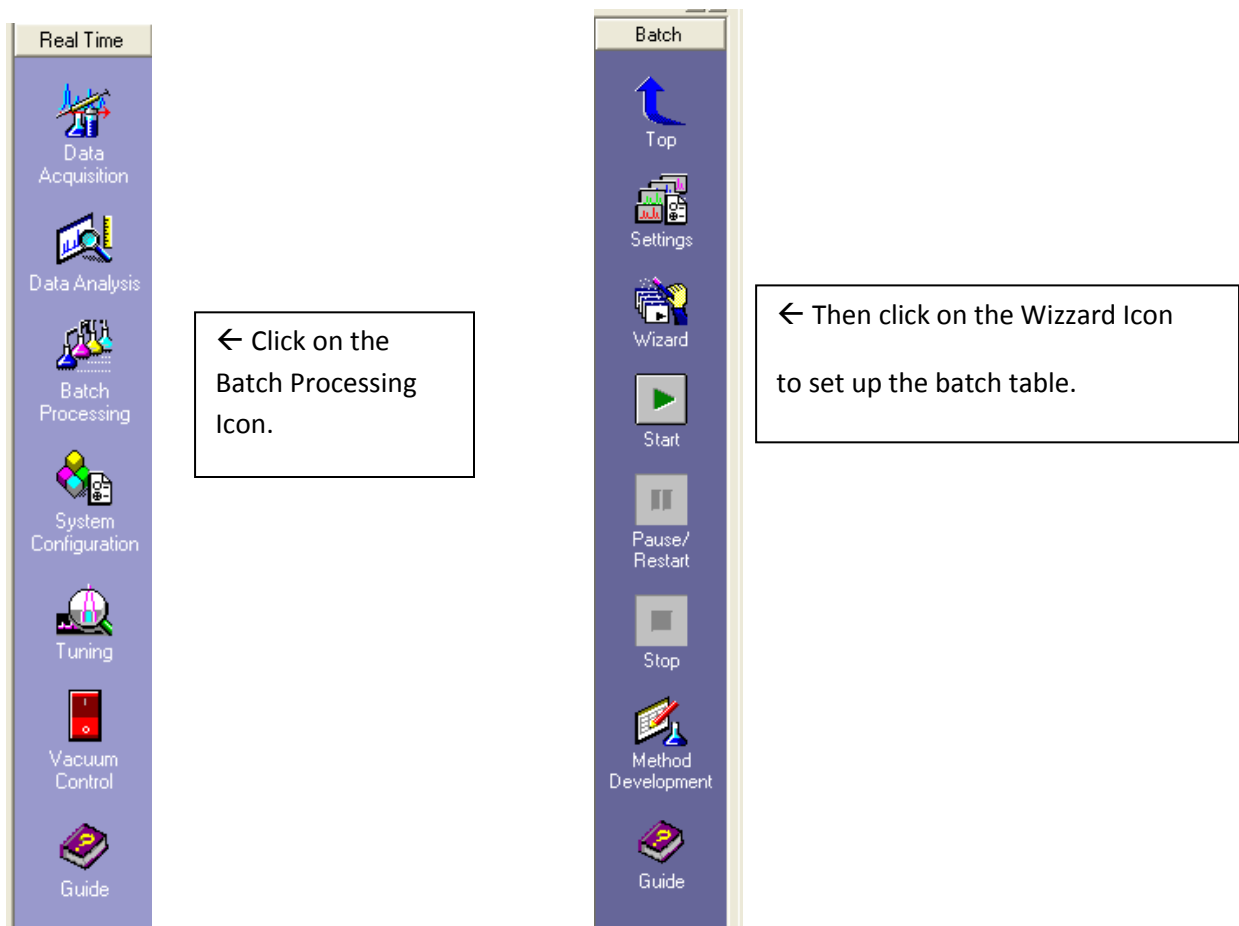
After the batch table has been set up, put your samples into the auto-sampler carousel, and click on the Start icon to start the batch.

How to shut down the instrument when you are finished:

1) Make sure that no data acquisition is in progress. Stop any data acquisition.
2) Close the data acquisition program. Closing this program will log you off, so that you will not be billed for any more instrument time.
3) Close any other software, such as the GCMS Postrun analysis program.
4) Remove your samples from the autosampler carousel.