

Operation and Methods Development for the Varian Saturn 2100D GC/MS

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ABSTRACT

Methods are built to integrate and control the Gas Chromatograph (GC) and Mass Spectroscopy (MS) detector. System Control houses the control panels, controls general maintenance and manual operation, and allows method guided procedures to be run. The Saturn View program is used to analyzed data with various search options. Results are formatted by MS Reports for printing. Guides, which were constructed to enhance the usability of the GC/MS, aid in building a method, injecting a sample, searching the libraries, building a compound table, identifying peaks, and troubleshooting printing problems. Methods were created to complement organic labs. How the settings in the methods effect the results is explained to give a better understanding of how the theory was applied.

Keywords: *Gas Chromatography; Mass Spectroscopy; GC/MS; Identification; Software; Operation*

INTRODUCTION

The role of analytical instrumentation in industry is growing increasingly important. A prime example is GC/MS, used for identifying drugs in urine, oil in leaves, toxins in water, gasoline in debris, and pesticides in soil to mention just a few (Varian GC/MS, 2002).

A GC/MS consists of two machines, the Gas Chromatograph (GC), and the Mass Spectroscopy (MS). The chromatogram, Fig. 1, is produced by the GC, showing the separation by number of molecules eluted over time and is a continuous line with peaks. The spectrum, Fig. 2, is produced by the MS, one for every second, and shows each identified ion mass and the relative number of ions found there. The flag in the chromatogram indicates the position at which the spectrum is taken. Large peaks, like in the chromatogram, give relatively little background noise, which is seen by the lack of small peaks in the spectrum.

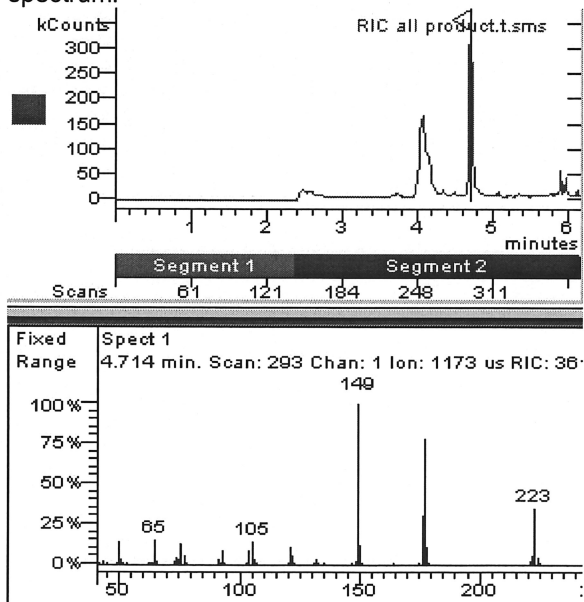


Fig.1

The GC works because of weak bonds made between molecules and the column walls, usually as a result of polarity. The non polar molecules are repelled by the polar coating on the column walls, making them move quickly through the column. Polar molecules form weak bonds with the walls, which explains the distinction in elution time between molecules. The number of collisions with and attachments to the walls influence the speed at which the molecules proceed through the column. The most common technique for increasing separation is to pack the column with coated beads to increase the surface area. Reducing the column diameter increases the surface to volume ratio exponentially (Skoog, et al, 1996). Some other influences on separation are the time the bond is maintained, the temperature, and the flow rate. The more polar the molecule, the stronger the bond with the column, and consequently the longer it takes for the molecule to detach. The flow rate and temperature determine how far molecules will go along the column between forming bonds. The slower the flow the more plates each molecule contacts, therefore the more distinct the separation becomes.

Chromatography gives us an indication of the polarity of the compounds and separates them. One of the identification techniques is to compare the elution time of known substances to that of an unknown using Flame Ionization Detectors, Thermal Conductivity Detectors, and Thermionic Detectors (Skoog, et al, 1996). This technique is used when building a compound table as well. A high degree of uncertainty exists in this technique; therefore other identification techniques are increasingly being coupled to GC to identify compounds, such as MS detectors. This combination allows library searches that accurately identify many compounds very quickly.

Traditionally, MS have worked by shooting an Electron Ionization (EI) beam at the molecules, which destabilizes them so that they break into ions of various sizes that reflect the structural characteristics of the molecule. Then these ions pass through a magnetic field that bends the particles trajectory in proportion to

their mass/charge ratio, allowing them to strike a detector at a position reflective of this ratio. Usually the individual ions or particles have a one-plus charge making this ratio the same as the ion mass. The proportions of the ions produced act like fingerprints allowing accurate identification. (Morrison, 1992)

EI is also used with this machine. The detection method works differently, by using an ion trap to collect the ions. The ions, except for those of the He carrier gas, are brought into orbit inside the trap. The orbit is based on the size and charge of each molecule. To analyze the trap contents, a radio frequency (RF) is sent through the trap and is ramped up to 1.1MHz. Each frequency corresponds to a specific mass/charge ratio. This kicks out ions, in order, to a detector that counts their concentration to generate the full mass spectrum. This entire process must happen for each MS spectrum, explaining why the shortest scan time attainable using this technique is around 0.4 sec. (Varian Software, 2001).

While the EI beam is the only ionization technique in the machine used for this project, it can splinter large molecules too much. Chemical Ionization (CI) is used for large compounds. In CI a solvent gas such as methane is ionized, which in turn ionizes the target compound in a softer way, to preserve the distinct spectrum it can produce.

Select Ion Storage (SIS) is also a powerful feature not included in the machine used for this experiment. The benefit of using a trap is the ability to link 2 or 3 traps together using SIS, which enables specific ion masses to be sent individually with a specific RF. The concentration of the target compound gets higher in each successive trap. Using this technique, background ions can be eliminated to purify a spectrum or search for specific peaks (Varian Tutorial, 1999). A well demarked peak and spectrum can be searched with the library using the NIST and Saturn Search algorithms.

MATERIALS AND METHODS

A Saturn 2100D GC/MS (Varian Inc.) with Saturn GC/MS WorkStation Version 5.5 is used for this experiment. The software is run by an Optiplex GX150 Dell computer with Windows 98. The GC column is a Chrompack Capillary Column, CP-Sil 8 CB LOW BLEED/MS, measuring 30m, ID 0.25mm, coated with 0.25 μ m particles. The MS uses an Ion Trap technique with both an internal diffusion pump and an external Varian DS 102 rotary vane pump. 99.999% grade He is used for the inert gas with a Chrompack Gas-Clean GC-MS Filter for oxygen and moisture. Stockroom chemicals of various grades are used for the runs.

In the process of learning to operate the GC/MS, the tutorial was read and practiced, the Ion Trap was dismantled and cleaned, and the operating system was reinstalled 7 times. From the tutorials Guides 1 through 7 were constructed containing the information needed to perform basic procedures on the GC/MS.

Two GC/MS methods were developed and are outlined as examples below.

Method 1

Developed for organic lab #728 (Simek, 1999)

Ketone and Aldehyde identification

GC-1.0ml/min. constant flow

300°C injector with 100 split ratio

column temperature 60°C for 1.5min.

ramp at 65°C/min. for 2.8min.

MS-data collection of none to 1.8min.

EI Auto 1.8 to 4.3min.

Compound Table included

2-Butanone, Cyclopentanone, Cyclohexanone,

2-hydroxy-Benzaldehyde, and Cinnamaldehyde

Print Options reduce to a 1 page Standard Report

Method 2

Developed for organic lab #713 (Wikholm, 1998)

Isopentyl Acetate Identification

GC-1.0ml/min. constant flow

150°C injector with 100 split ratio

column temperature 100°C for 1min.

ramp at 50°C/min. to 150°C and hold for 0.5min.

MS-data collection of none to 1.7min.

EI Auto 1.7 to 2.8min.

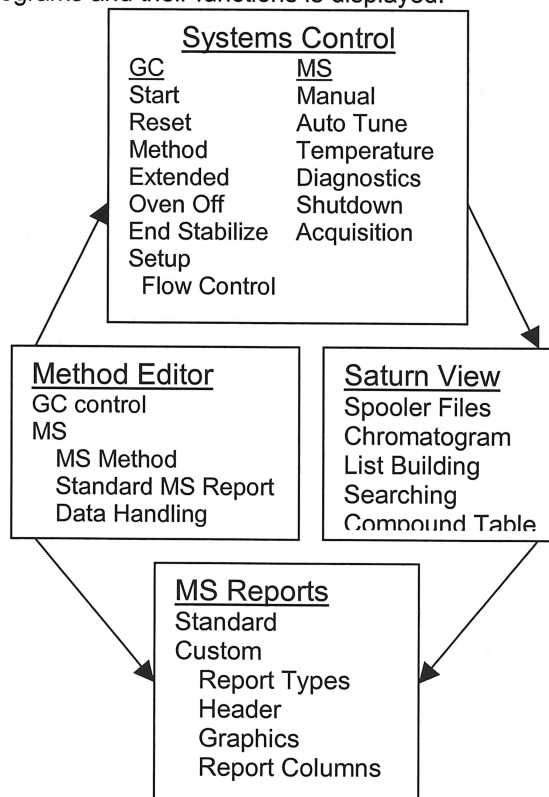
Compound Table included

1-Butanol-3-methyl-acetate, 3-methyl-1-Butanol

Print Options reduce to a 1 page Standard Report

SOFTWARE ANALYSIS

Below the relationships between the operating programs and their functions is displayed.



Method instructions control the entire system. Methods consist of sections for the GC, MS, and Results handling. The GC section controls the Injector Temperature, Split Ratio, Oven Temperature (with ramping capability), and the column flow. The Injector Temperature should be set approximately 20°C above the boiling point of the highest compound. This allows the solution to entirely vaporize soon after injection, ensuring that the split ratio will accurately combine the solution with the carrier gas of He. The unused solution leaves through the Septum Purge outlet into the air. The used portion flows into the column where it condenses on the column walls. The oven temperature offers best separation when ramped through the boiling points of the compounds. The MS module allows specific segments of runs to be analyzed individually. The solvent peak is typically the first peak eluted and overshadows the target peaks. The first time interval is set to cover the solvent elution with the Ionization Mode set to none. This eliminates the solvent peak so the target peaks on the chromatogram are prominent. Use EI Auto (Electron Ionization Automatic Gain Control) to collect spectra readings.

Standard reports can be automatically printed after runs by selecting the type of report in Print Options and manipulating the settings to produce the desired form. The software is wasteful when printing default reports, producing an average of fifteen pages per run. Often the header can be shortened to save paper. Another critical paper reduction option is in Results Format where Run Documentation elements should be turned off. User-defined Format gives the Landscape Mode option and controls the information given in the peak chart.

Data Handling primarily controls integration and Compound Table use. Compound Tables check for particular compounds at specific retention times to eliminate the uncertainty introduced by searches. Reverse Fit, Purity, and Amount are used to determine a compound's presence when using a compound table.

Opening System Control shows the various equipment and its relationships. This system contains the GC and MS as well as an auto sampler in most cases. The MS automatically opens up to Manual mode. Adjustments for Cal Gas and RF tuning are occasionally performed in this mode. Auto Tune controls Air/Water Check and Electron Multiplier Tune, which should be run before each set of samples or once a day, whichever comes less often. The Temperature section allows a Bakeout to be run. This should be done every month or so. Trap, manifold, and transfer line temperatures can also be controlled here but should not need to be. The Diagnosis section is unused under normal conditions and contains a variety of electronics and temperature tests. Shutdown window places the Mass Spectrometer in a safe state to be manually turned off. Varian suggests GC/MS machines remain on unless it will not be used for three months or longer. Acquisition is the most common operating mode. It displays the run time and the

chromatogram and/or the spectrum during runs. To inject a sample Inject is selected from the categories at the top of Systems Control; the Start button should not be used.

The chromatogram and spectrum can be watched from the Systems Control program, but is viewed best by clicking the Saturn View icon, thereby opening SatView with the current run displayed as the active window. Saturn View is only used when identifying new compounds or developing a Compound Table for a method. Several chromatograms can be simultaneously displayed and stacked or overlaid for comparisons. The active chromatogram is marked in the key, and can be changed. Clicking the active chromatogram displays the spectrum at that point. When searching several spectra from chromatograms, it is easiest to create a list to work with in the Spectra menu. Once a list is constructed and saved, it can be searched, act as a source for printing reports from, and be used in building Compound Tables. In addition to lists, searches on chromatograms or the Library allow the database to act like a chemical dictionary.

Saturn Search and NIST search are the two algorithms supplied by Varian corporation for searching GC/MS libraries. NIST search works, by comparing ion count between spectrum and determining the closest match by difference. It displays compound structures and raw numerical data in outputs. Saturn Search works on Fit (similar to NIST), Reverse Fit (what major peaks are missing), and Purity (amount of background noise per spectrum). Typically Saturn Target Search works with Reverse Fit on the largest well delineated peak of a compound yields the best results. Once the compounds present are identified, a method to optimize elution can be developed and a compound table built to check specifically for the compounds. Upon completing the compound table, it can be stored as a previously existing method; this will replace only the Compound Table section leaving the remainder of the method unchanged. A run containing the target compounds records a spectrum at the set retention time for the searching and naming of each target compound.

MS Reports combine information from the SatView in a format designated by the method. Methods only produce specified Standard Reports, Compound Reports, and Multi-Run Reports, not Custom Reports. Options for Standard Reports within the methods allows most information to be displayed in an acceptable format. For basic results, Standard Reports with restrictions on the number of peaks and eliminated Run Documentation provides the best printout. If printout is suppressed or not enabled at the completion of the run, printing a Standard MS Report will use the specifications from the active method. Customized reports offer one of six basic formats, depending on how the peaks are to be analyzed, and allows altering of each section.

RESULTS and DISCUSSION

Guides were created to increase the usability of the GC/MS. Instructions for the building of methods is the primary document shown in the attachment Guide 1. The first section sets up the module structure. Adjusting of the GC and MS settings for good peak elution comes next and is the most difficult aspect of method development. Several tips to guide development of these sections are included in the guide. A reference is made to building a Compound Table, though it is not necessary to run the method. The next section deals with controlling the format of the printed results. Turning off the Compound Reports and reducing the Run Documentation down to only the Error Log are the primary paper saving changes.

Guide 2 (Injecting a Sample) is the most common task. It is setup for single sample injections, since there is no auto sampler and typically single sample injections are most useful. Guides for Method Building and Injecting a Sample are all that is needed for basic running of the GC/MS.

Guide 3 (Searching Libraries) is very critical to interpreting results. Typically, a Chromatogram Search is done by selecting a peak and clicking it; then changing the settings to target the aspects that are known about the compound. If the major peak of a known compound is well separated, the correct compound can typically be identified in the top 2 or 3 of at least one search. Less defined peaks are often multiple compounds, at different concentrations, eluting simultaneously resulting in poor results. A Library Search allows the database to act as a type of chemical dictionary. List Search is a type of predefined chromatogram search.

Guide 4 (Building a Compound Table) is only used when specific compounds are being looked for, such as a lab where the product and reactants are known. Once samples of the compounds are run with the method, the SatView program is used to identify the compounds in the Build Compound Table mode. This is saved to the method and can be used for setting internal standards, changing integration parameters for individual peaks, or to use previous calibration settings.

Guide's 5 to 7 are to help with common problems that arise. Finding conditions that give proper separation requires developing a knack. When adjusting column temperature and flow rates does not work, the suggestions in Guide 5 (Misidentified Peaks) often helps. Each time a flow rate change is made, the GC and MS settings must be readjusted. For problems with injections and printing Guide 6 (Printing Problems ect.) details solutions. These are basic steps and will not fix program errors (such as Library NIST searching from SatView after changing specific Edit Constraints) or correct unusual method adjustments back to normal. Guide 7 instructs on list building to greater enhance SatView usage. This enables several peaks to be searched at the same time and speeds up the building of compound tables. A maintenance log is constructed

from instructions throughout the manuals. Several of the times suggested for performing tasks are lengthened to more realistic times and to reduce the amount of basic maintenance.

When forming a method, the first step is to identify all the compound names and their synonyms, their molecular weights, and boiling points. The boiling points are used to set the initial injector and column temperature. Methods for Organic Chemistry labs are created to identify products and reactants. The software is designed to identify specific compounds within a sample, as is shown in Method 1 (Simek, 1999). The concentration is 1 drop in 1ml of solvent allowing a split ratio of 100 to make the concentration entering the column 1 part per 2000 or 4 μ g. Reducing the flow rate to 1.0ml/min. gives separation good enough to delineate the five possibilities and their peaks, but not good enough to get good fit and purity. Identification between the 107,886 library compounds is not needed in Method 1, therefore poor certainty is accepted in the interest of creating a short practical run time for the method. Method runs in labs vary from 3 to 6 minutes, while industry runs are longer and more accurate (Varian GC/MS, 2002).

Method 2 identified Isopentyl Acetate and its reactant (Wikholm, 1998). When pure sources for all the compounds involved are obtainable before method development, accurate methods are easy to build. This is not true for all labs, however, making some labs impossible to analyze. Such situations emphasize the limitations of the machine. Other limitations are that it requires relatively long run times for accurate resolution, needs clear spectrums and limited searches to accurately identify some compounds, and is relatively expensive and time-consuming to maintain. On the other hand it can detect remarkably small concentrations, indicates the certainty of results, identifies molecular mass, and is very accurate at identification given a well-developed method.

ACKNOWLEDGEMENTS

Thanks to Dr. Allan van Asselt for assistance in solving problems and guidance, Dr. Jonathan Frye for reminding me of due dates, Dr. Tim Hubin for logistics assistance and suggesting applicable labs, Alfred Dutrow for sharing my excitement, Dr. Karrie Rathbone for explaining HPLC to me, Dr. Kent Noffsinger for contacting Abbott to get the HPLC, and finally my friends and family for relieving my irritation.

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ATTACHMENTS

Guide 1 Method Building

Open the Method Builder and select "Create a New
Method File" click OK

Click Next→ select "Instrument 1" (module 2000 and
3900 should be in the Configuration Description.)

Click Next→ Detector Modules should be 2000 Mass
Spec and should be selected.

Click Next→ in the left window "Channel 1=MS Data"
should be selected. In the right window "Standard
MS Reports" and "MS Data Handling" should be
selected.

Click Finish

◆2000 Mass Spec→ 2000 Mass Spec Control→ MS
Method Editor

Row 1— change the segment name to "solvent
elution", set End (min.) to cover the solvent peak
(about 1.8min. with a 1.0ml/min column flow).
Ionization Mode should be None. Turning Ionization
on during method development helps determine the
end of the solvent peak.

Row 2— change the segment name to "collection of
compounds", Start (min.) should be identical to End
(min.) for row 1, End (min.) should be changed to a
short time after the last peak is eluted, if known
enter the range of ions to be identified (note:
fragmenting of compounds requires including
smaller ions). Ionization mode should be set to EI
Auto (Electron Ionization Automatic Gain Control).
Ion Preparation feature is not on this machine so is
set on None.

Save

◆3900 GC→ GC Control

Constant Column Flow: turn Constant Flow to On.
Typically Column Flow works best if set at 1ml/min.

Injector Oven: select on. Change Injector Temperature
to 20°C above the highest boiling point in the
solution. Find the Split State column and change it
to On.

Column Oven Stabilization Time: change to 0.15 min.
Row 1— set initial temperature between the boiling
point of your solvent and that of your lowest
compound.

Row 2— Typically the temperature is ramped up
through the various boiling points, sometimes in
several separate rows. Save

◆Run solution/compounds

Alter the Split Ratio in the injector section of the GC
control module until the highest compound peaks
are between 300M Counts and 10K Counts.

Alter the column temperature until solution peaks are
well separated.

If peaks still do not separate well see Guide 5 on
Misidentifying Peaks

Build Compound Table if using one. Directions in
Guide 4

◆2000 Mass Spec→ Channel 1=MS Reports

Print Options → Single Run Reports: click Defaults
button

Sample Report: select Print Sample Reports (same
as default), click Title/Header, change format box
for desired elements (Operator, Acquisition Date,
and Data file work well) click OK.

Compound Report: unselect Printed Compound
Reports Save

Results Format: select User-Defined Format (this
should unselect Standard), click Select Fields, select
Landscape Mode (this should unselect Portrait Mode
and change the Current Width number in the box at
the bottom from red to black showing the parameters
will fit on the page.), change "Selected:" window to
desired elements (note Retention Time, Peak Name,
Fit, Reverse Fit, Purity, Area, and Amount work well
with room for other elements) click OK

Run Documentation: unselect all fields. Select Error
Log only. Save

Chromatogram Format: click Defaults button.

Plot Annotation→ General: unselect Integration
Events + Baseline

Plot Annotation→ Peak Annotation: unselect
Retention Time Save

◆2000 Mass Spec→ Channel 1=MS Data Handling
Calculations Setup: click Defaults button.

General: if no internal standard or compound table is
being used change Calibration Type to %(None) and
click OK to pop up box.

Chromatogram Processing→ Tentative Identification:
select Library parameters as desired, check Library
List for NIST98m.lbr, NIST98r.lbr, and labs.lbr at
least. If these are not present in that order click
Edit/Order Library List and Add or Up One to get this
configuration. It is not necessary to delete others
but it can be done. Save.

Chromatogram Processing→ Reporting Threshold:

select Largest N Peaks and change number to desired size (note: % of Largest Peaks is useful sometimes too.) Save

Compound Table: if one is being used it should have been built and be shown here. Peak adjustment can be used to better define peak integration if needed for identification. See other page for details.

Modules not listed should not influence single sample runs. If problems exist open each module and click Defaults button.

Guide 2 Injecting a Sample

System Control→ 2000.40 mass spec window.

Click the Acquisition button on the far right.

The active method is displayed in the toolbar. If it is not the correct method click the folder to its right and open the correct method. Click on the active method in the toolbar to Re-Activate the method before beginning.

Inject→ Inject Single Sample: change Operator to your name (leave Instrument #1 unchanged in above window)→ OK

Click Data Files button. If the folder you wish to save to is not the last open folder double click c:\ and open the folders below until where you wish to save data is the last open folder.

Data File Names box determines how your file is saved. To save information about the injection in addition to the default Sample ID (%s) put them in the text box. Ex. %t%d%s will display time, date, and sample ID in that order.

Sample Name (Sample ID) text box should be double clicked and changed to represent your sample.

The other windows should be Analysis, 1, none, none, 1, 0, 1, 1, none.

Click Inject.

Hold until "Waiting" is flashed in yellow in the toolbar in the main window.

Push the syringe into the injector with one hand while taping the plunger down immediately after the needle guide is pressed against the injector nut. (This will automatically start the method)

Guide 3 Searching Libraries

NIST Independent Name Search

My Computer→(C:)→NIST98→MS Search→NIST\$

SatView→ select chromatogram or File→Load Files→ select chromatogram.

◆Individual spectrum searching.

Click target peak in active window. (spectrum appears)

Search→Library Search or click L icon in toolbar.

Saturn or NIST Search in Target Mode gives possible identifications in order.

Editing search parameters can refine searches.

Clicking the icon L will automatically search using the last parameter settings.

◆Name or Formula searching.

Search→Library Search→ Saturn

Change the box to the right of the Saturn Search

button to "Seq. Library Search"→ click Saturn Search. Name Fragment, Element Equations, Mol. Weight Range, CAS Number, and High Weighted Ions can all be used in any combination to search by clicking the Use ---- box at the bottom of each section.

Search→ Library Search→ NIST

Change the box on the right of the NIST Search button to the desired search method. Name Search MainLib., Formula Search, Mol. Weight Search, Any Peaks Search, CAS Number Search can be searched as an individual element by selecting it. Seq. Library Search allows combinations of these searches by clicking the Edit Constraints button (this has a program error depending on the combination of constraints or specificity).

◆Search→ List Search

Click Select a File→ open the relevant list.

Search→ select a search and set parameters (ex. Saturn Target)If a compound is incorrect, highlight it and click Edit→ Select Different Match and identify the correct compound (researching spectrum may be needed)→ Done

Update→ Update all in current list file.

Export enables addition to Libraries.

◆Search→ Chromatogram Search

This is a type of List search. Once a list is created new chromatograms can be searched for the identified compounds at the retention times saved in the list file, like a compound table. Make sure the chromatogram to be searched is the active one. Make sure after Search is clicked an appropriate Spectra List File appears in the top left of the parameters box.

Guide 4 Building a Compound Table

Compound Tables check at several retention times for the corresponding compounds regardless of their present's in the solution. Looking at Amount, Purity, and Reverse Fit determines the presents or absence of the target compound.

At this point the GC and MS modules of the method should be completed.

◆Prepare solutions of the compounds that will be entered in the compound table and run them with the method (they should be saved as SatView chromatograms automatically).

SatView→ File→ Load Files→ place the chromatograms of the compound's in the chart→ Open Files (chromatograms are displayed stacked on each other)

Good to know features.

Chromatogram → Display Options → Overlay

Select an individual chromatogram by clicking on the square which corresponds in color to the desired chromatogram, as dictated by the key in the upper right.

◆Quantitation→ Build Compound Table→ Build

Meth→ Data File→ Select Data File→ find and open the first compound's chromatogram.
 Click on the apex of the compound peak. Click Add Peak Identify the known compound and select it (Seq. Library Search and name or formula search may be needed)→ Open.
 Repeat starting 4 lines up until all compounds have been added.
 Method File→ Save Peak Table→ select the method being developed (same method used to obtain the compound chromatogram)→ Save→ replace existing method (Yes)→ Click Done.

Guide 5 Misidentifying Peaks

Note: the GC/MS is not 100% accurate. If good separation is performed the correct compound is typically in the top 10 to 15 in a target search.

- ◆ Solvent elutes close to compound peaks
 Change solvent to something with a lower boiling point such as ether or methanol.
- Move the MS Method Editor segment for the solvent elution with Ionization Mode of None to the time covering the solvents' elution by changing the Start and End times.
- Lower Column Flow for better separation. This increases run time however.
- ◆ Two compounds elude simultaneously
 Hold the column temperature between the boiling points of the solvent and compounds for a time.
- Lower column flow; possibly change to pressure rather than column flow.
- Decrease time between scans (select MS segment by clicking on it, find Segment Set points→ Scan Time and lower the number.
- Integration Parameters editing: for all peaks go to 2000 Mass Spec→ Channel 1=MS Data→ MS Data Handling→ Calculations Setup or for individual peaks changes can be made in the Compound table.
- Change the column.

Guide 6 Printing Problems ect.

- ◆ System Control does not reach Waiting state
 3900.40 GC window→ Setup...→ click Close & Update to reset... wait a short time.
- Click method in toolbar and Reactivate or change method and change back.
- Close System control and reopen.
- ◆ Printing Report is not Automatic
 System Control→ Automation→ is Enable Automated Printing checked (if not click on it)
- Method Editor→ 2000 Mass Spec→ Channel 1→ Standard MS Reports→ Print Options
 Is the Print Sample Report box checked or at least one box on the left?
 Is the Suppress Printout on Injections box unselected (if not click it).
- Check Printer, manual switch between computers (A), cords & ports, plugged in, paper jams, default

printer, ect.

- Compound Table (Target Compounds) not printing.
 Method Editor→ 2000 Mass Spec→ Channel 1→ MS Data Handling→ Calculations Setup→ General→ Report Missing Peaks and Report Unknown Peaks should be selected. If still unsuccessful redo Building a Compound Table.
- ◆ Long Report Printed:
 Header is too large. Method Editor→ 2000 Mass Spec→ Channel 1→ Standard MS Reports→ Print Options→ Title/Header button→ remove elements from Format window. Note: the number of columns can be made to 3 by selecting the Landscape Mode under Peak Information.
- Chromatogram is too full. Method Editor→ 2000 Mass Spec→ Channel 1→ Standard MS Reports→ Chromatogram Format→ Plot Options→ unselecting in General & Plot Annotation helps reduce these features.
- Peak information is too wide. Method Editor→ 2000 Mass Spec→ Channel 1→ Standard MS Reports→ Results Format→ Select Fields (if grayed out click User-Defined Format)→ Current Width at bottom right must be black. If not select Landscape Mode at top and/or delete elements from the Selected box.
- Peaks list is too long. Method Editor→ 2000 Mass Spec→ Channel 1→ MS Data Handling→ Calculations Setup→ Chromatogram Processing→ Reporting Threshold→ select Largest N Pks. or select % of Largest Pks. and change number.
- Report Log is long. Method Editor→ 2000 Mass Spec→ Channel 1→ Standard MS Reports→ Results Format→ Run Documentation→ unselect all except Error Log
- Compound Report is printing. Turn off: Method Editor→ 2000 Mass Spec→ Channel 1→ Standard MS Reports→ Print Options→ Compound Report→ unselect Print Compound Report.
 Reduce: Method Editor→ 2000 Mass Spec→ Channel 1→ Standard MS Reports→ Compound Report

Guide 7 Building a List

- File→ Load Files→ Open chromatograms of interest Spectra→ click List #. If a list appears click Clear→ Done (this disconnects list files from List programs). If asked to create a list click yes→ type name and save in desired location.
- Spectra→ Auto Add (Disabled)→ click Confirm each addition, click the new List #.
- Click on the apex of interesting peaks to add them to the list; switch between chromatograms if needed.
- Search→ List Search or Spectra→ List #→
 Clear→Done will only disconnect the list, not erase or move the saved list.