

Agilent Technologies

Environmental
Analysis Software

Getting Started

Environmental Software

Overview

The Environmental software is a data acquisition and data analysis package designed to assist you in complying with United States Environmental Protection Agency (US EPA) data analysis protocols.

The software is driven by user-customized methods specifying instrument parameters for data acquisition and all the quantitation information needed to perform target compound analysis, including integration information and the calibration table. Methods for various EPA protocols along with their corresponding compound lists are included with the software.

A separate Environmental Forms software package lets you generate forms from your data that are based on the Contract Laboratory Program (CLP) Statement of Work, August 1991. The Environmental software does not provide CLP disk-deliverable capabilities.

The Custom Reports software lets you transfer quantitative results from Data Analysis into the Custom Reports spreadsheet program where you can create your own custom reports and databases.

Software Menus

The software menus shown in this booklet are for a system configured with an 6890 GC and a 5973N MSD.

Online Help

This booklet lets you see the software menus and buttons at a glance and gives an overview of target compound analysis. However, most of the information you will need to use the Environmental software is provided in the online help. The online help is divided into task (how to) and reference information. The tutorials use demo files supplied with the software to demonstrate environmental data analysis tasks.

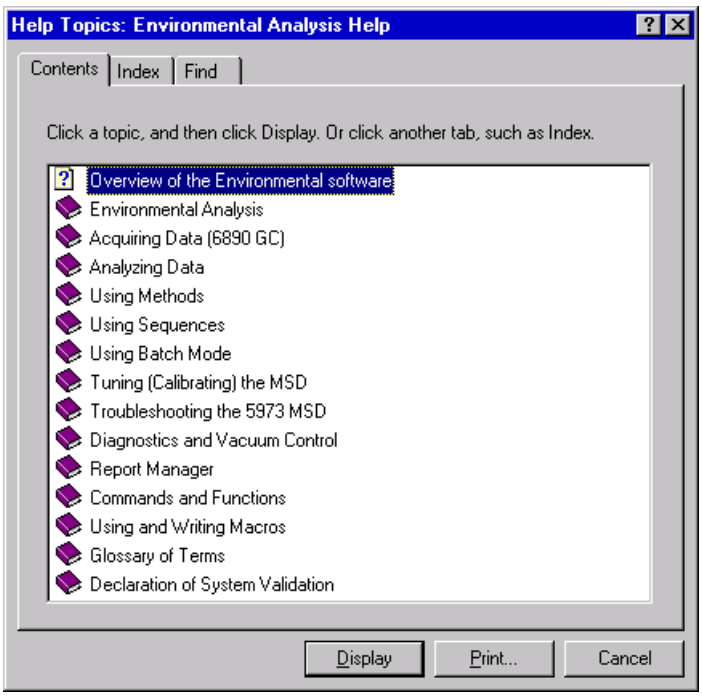
The Environmental software can be configured to support GC/MS or GC-only mode. A GC-only system will have some menus and menu items that differ from those on a system configured with a mass spectrometer. These differences will be pointed out in the online help for menus.

Because some screens are shared by both GC and GC/MS systems, some fields intended specifically for mass spectral information will not apply to GC data analysis. In these cases, the specific fields are labeled in the help as being for mass spectra only.

Using Online Help

To access the online help, select ***Contents*** from the Help menu in any window, or click the ***Help*** button on any dialog box.

When you jump to a help topic, it is displayed in another help window. Click the Contents button in that window to return to this list of help topics.



Item	*Description*
Contents	Displays the list of help topics (shown to the right).
Index	Lets you use keywords to search the help index for a particular topic.
Find	Lets you type a word or phrase and then displays a list of all the topics in the online help that contain those words.
Open	Opens the selected book or help topic. When you open a book or select a book that is already open, this button changes to Close.
Print	Prints the selected book or help topic for future reference. If you select a book, then all the help topics contained in the book are printed. To print a popup, click on it with the right mouse button and select Print from the menu.
Cancel	Closes the Help Topics window.

Help Icons



Indicates a book containing more help topics. To open a book, select it then double-click or click the ***Open*** button.



Indicates an open book of help topics. To close an open book, select it then double-click or click the ***Close*** button.

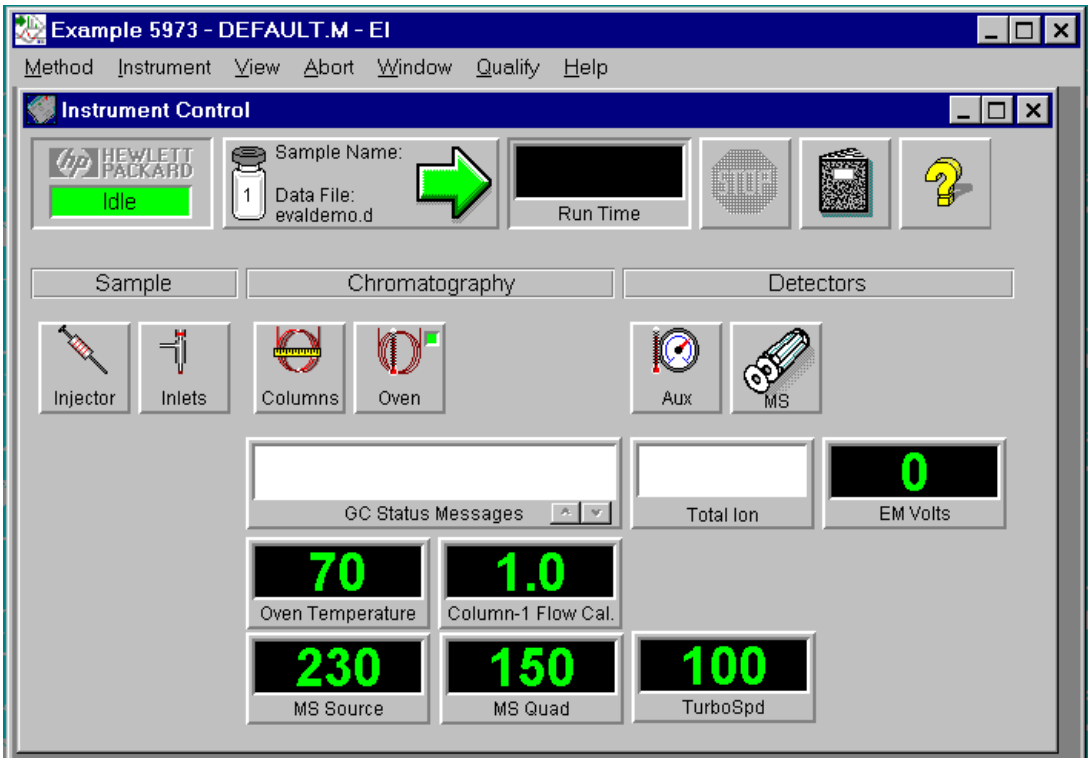


Indicates a help topic. To jump to a help topic, select it then double-click or click the ***Open*** button.

Instrument Control View

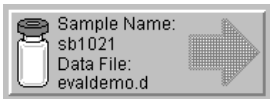
The Instrument Control view is displayed when you start up the Environmental software. This is where you set and monitor instrument parameters. If you are in some other view, select ***View / Instrument Control*** when you are ready to set up the system for data acquisition.

The picture shown below is an example of a system configured with a 5973 MSD. The menu items and monitors may be slightly different on other instruments.





Acquisition Status Lets you tell at a glance the status of the current instrument or run (if any).



Start Button Lets you start a run (acquisition only). When a run is not in progress, the arrow is green. When a run is in progress or the instrument is offline, the arrow is gray.

This button also shows the current data file name, sample information (if any), and the vial number (1 if no ALS).



Run Time Clock Shows the elapsed time since the beginning of the run if a run is in progress. The scheduled run time is shown below the digital clock.



Stop Button Lets you stop the system when it is in Pre-Run, Run, or Post-Run mode. The stop sign is red when a run is in progress and gray when a run is not in progress or the instrument is offline.



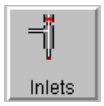
Logbook Button Displays a menu where you can choose to view, open, clear, save, or print a particular logbook.



Help Button Displays a menu where you can select an online help topic for the Instrument Control view. Choose Help Topics to go to the online help for the entire system.



Injector Button Lets you set parameters for the injector when you have configured your system with an ALS.



Inlets Button Lets you set parameters for the GC inlet (injection port) that is configured on your system.



Columns Button Lets you configure columns and set up ramped flow and pressure programs.



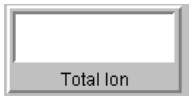
Oven Button Displays a menu that lets you edit GC oven parameters or GC monitor parameters. When the GC is ready, the small square in the upper right corner is green. When the GC is not ready or the instrument is offline, the square is red.



Aux Button Lets you set the temperature of the GC/MSD interface.

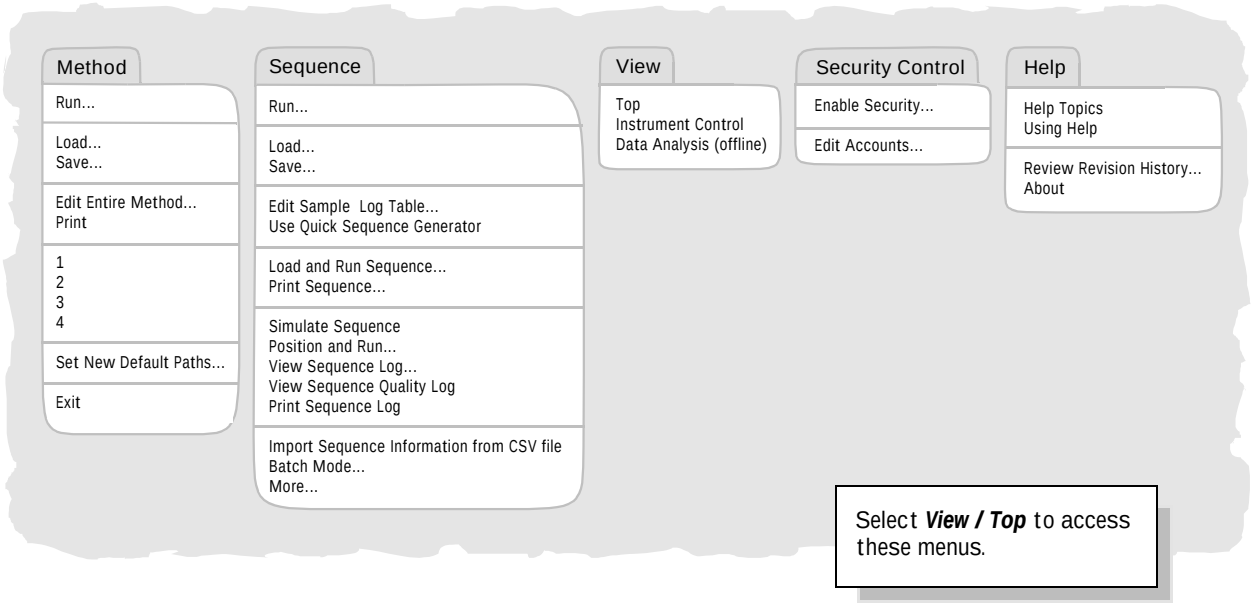


MS Button Displays a menu that lets you edit MS acquisition parameters, select another tune file, or edit MS monitor parameters. Not available on a GC-only system.



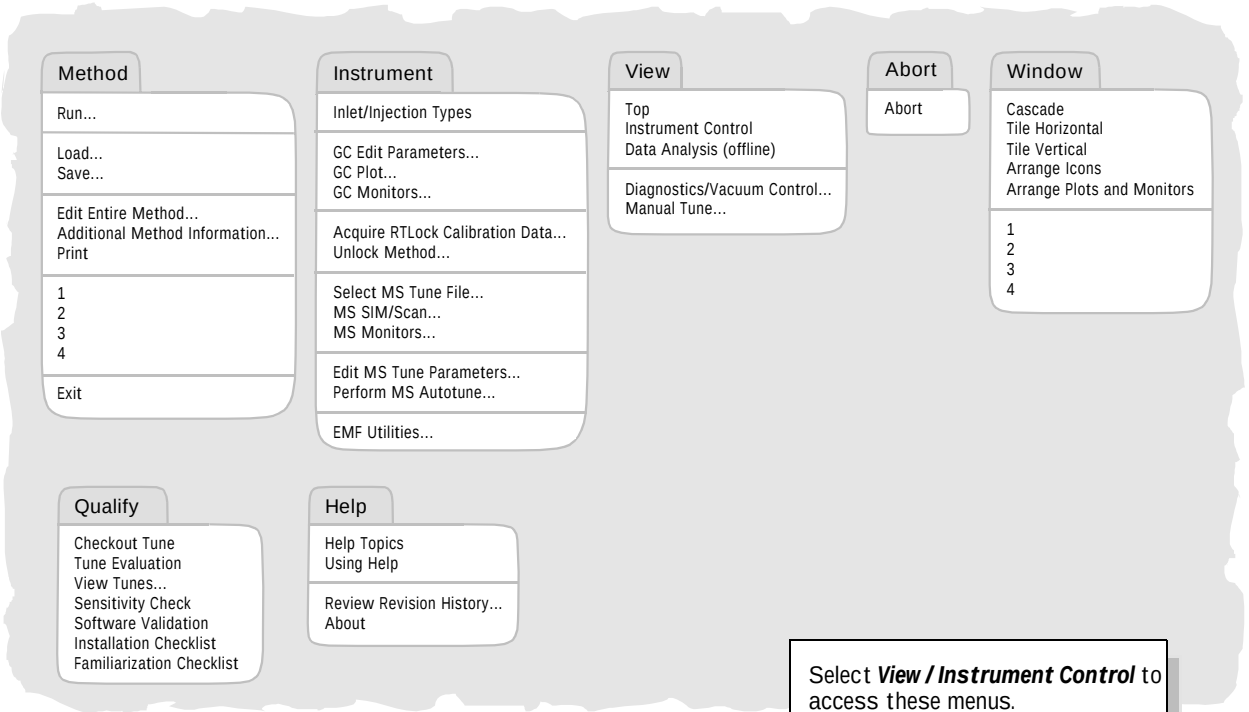
Monitor Each monitor displays one instrument parameter. See the online help for a description of the instrument monitors.

MS Top Menus



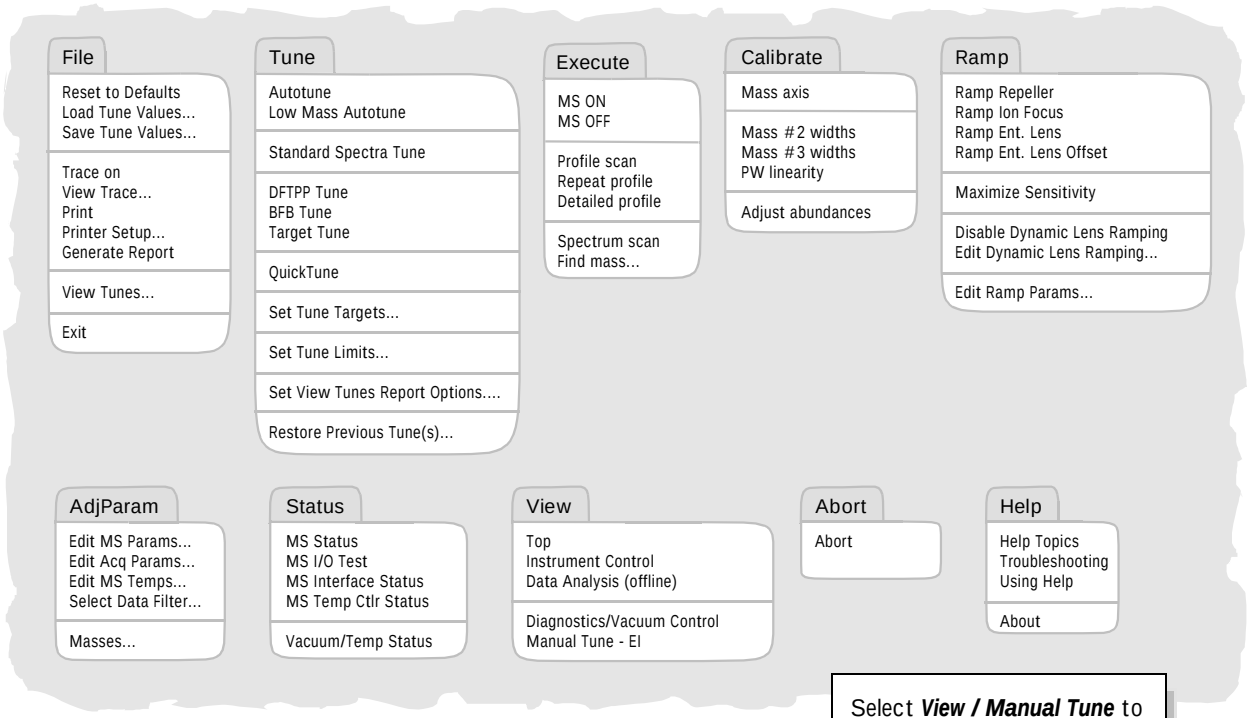
Select ***View / Top*** to access these menus.

Instrument Control Menus



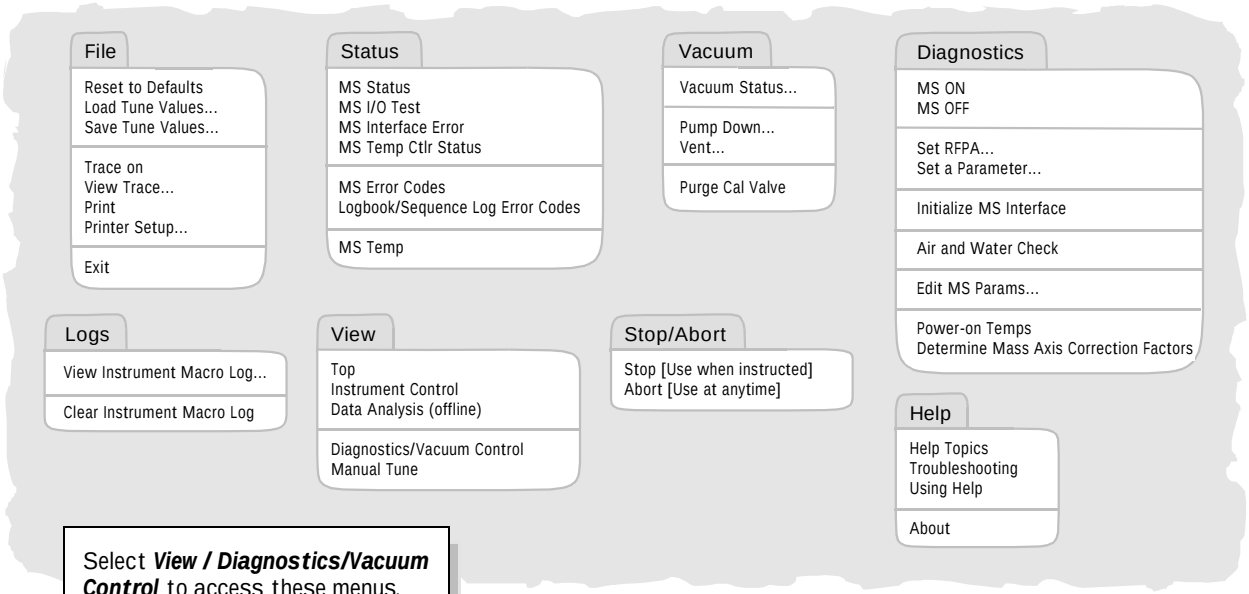
Select ***View / Instrument Control*** to access these menus.

Manual Tune Menus



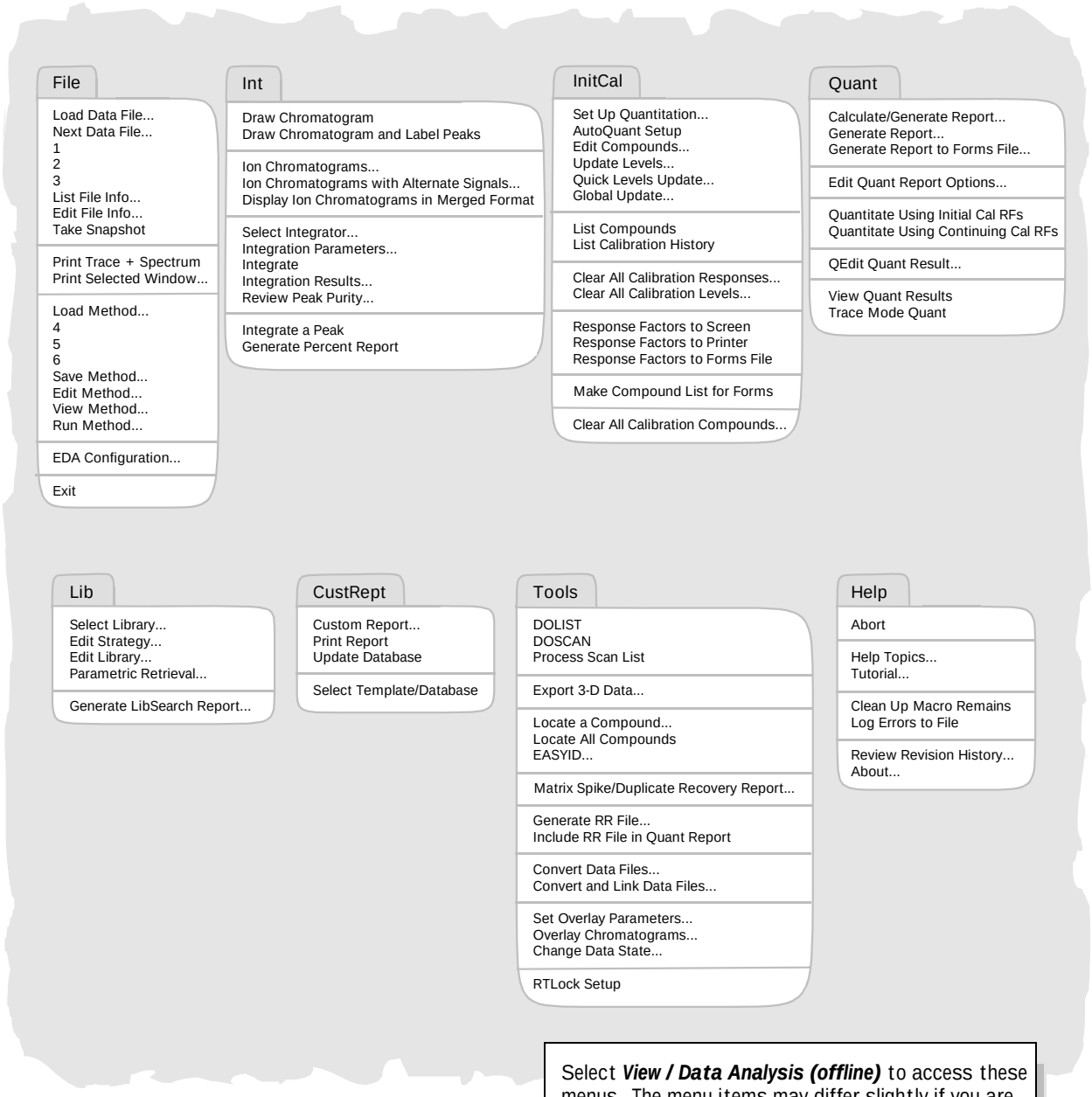
Select ***View / Manual Tune*** to access these menus.

Diagnostics/Vacuum Control Menus



Select ***View / Diagnostics/Vacuum Control*** to access these menus.

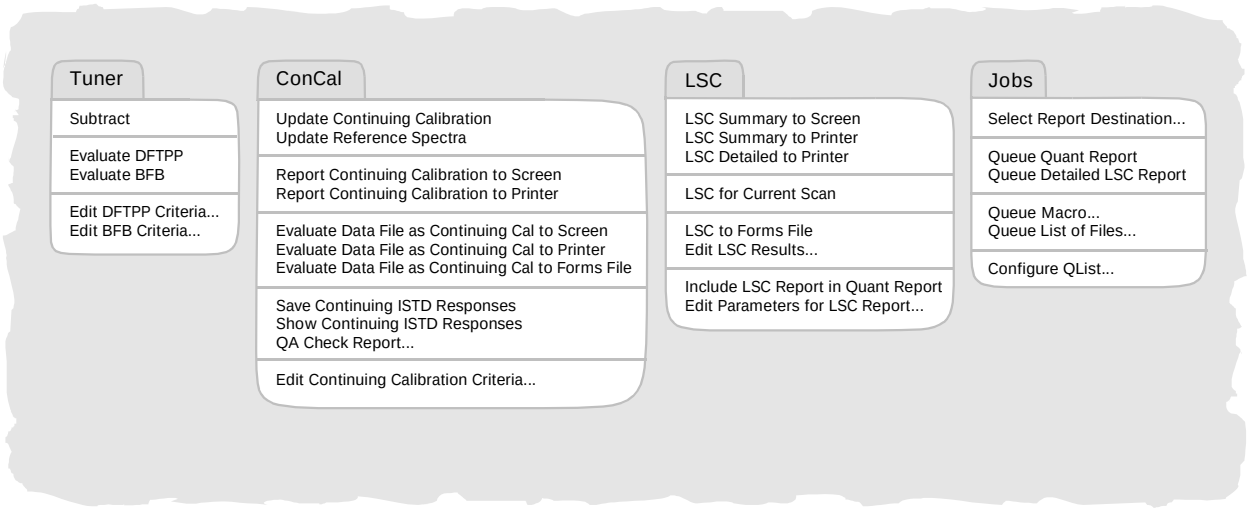
Environmental Data Analysis Menus



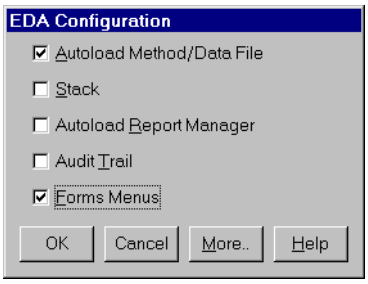
Select ***View / Data Analysis (offline)*** to access these menus. The menu items may differ slightly if you are using GC-only mode.

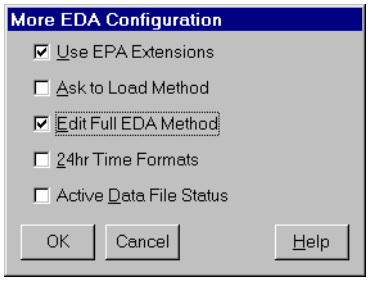
The Forms menu items are available when the Environmental Forms software is installed and configured.

Additional Data Analysis Menus

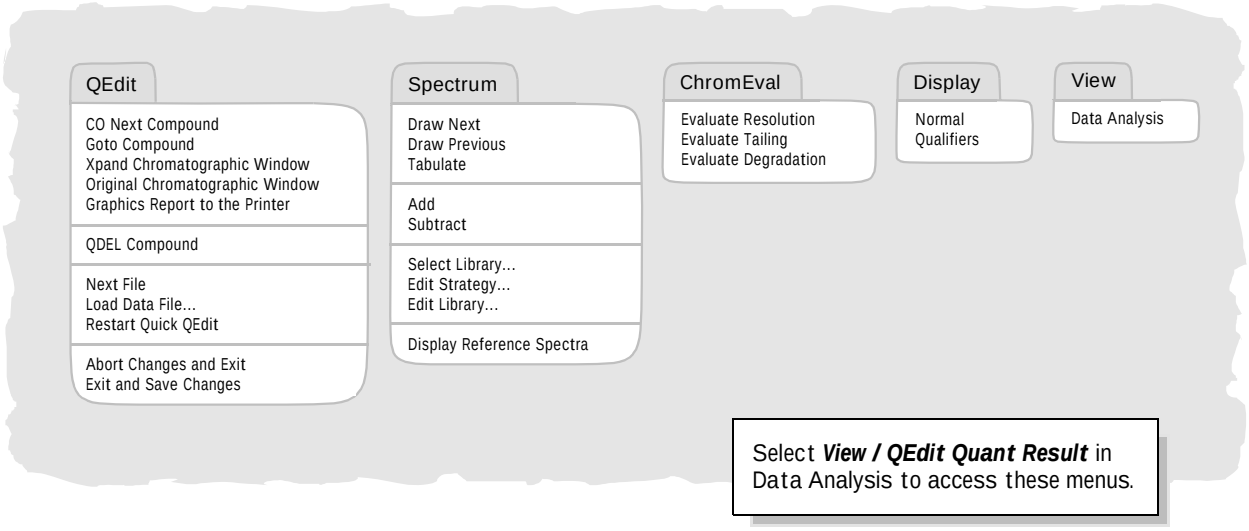


To configure Environmental Data Analysis, select ***File / EDA Configuration***. Select the options you want to use.

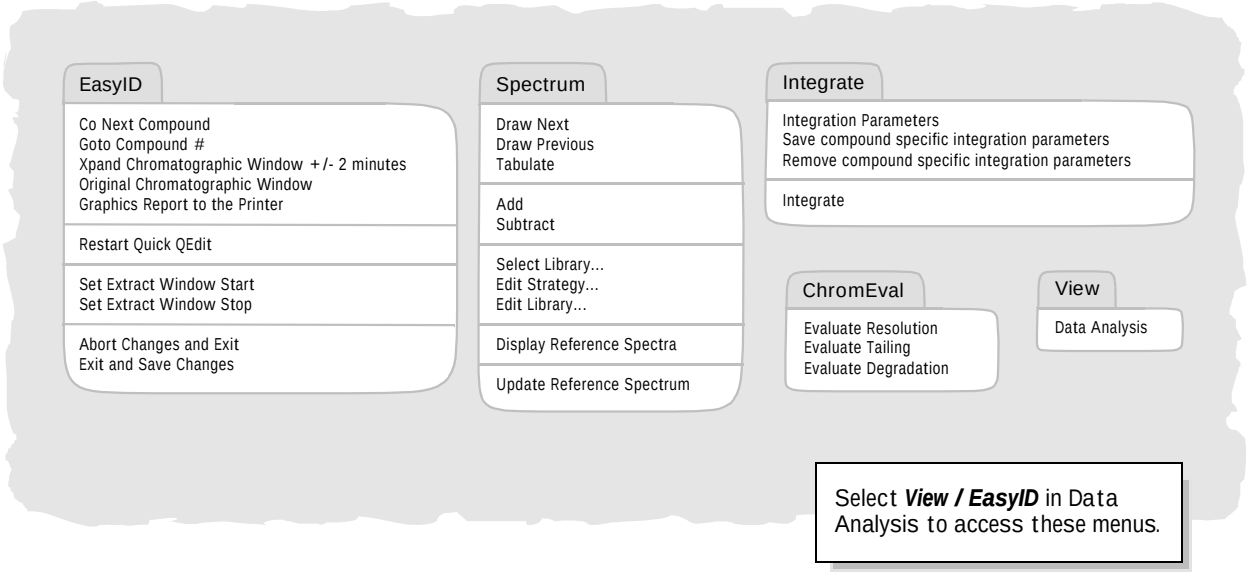




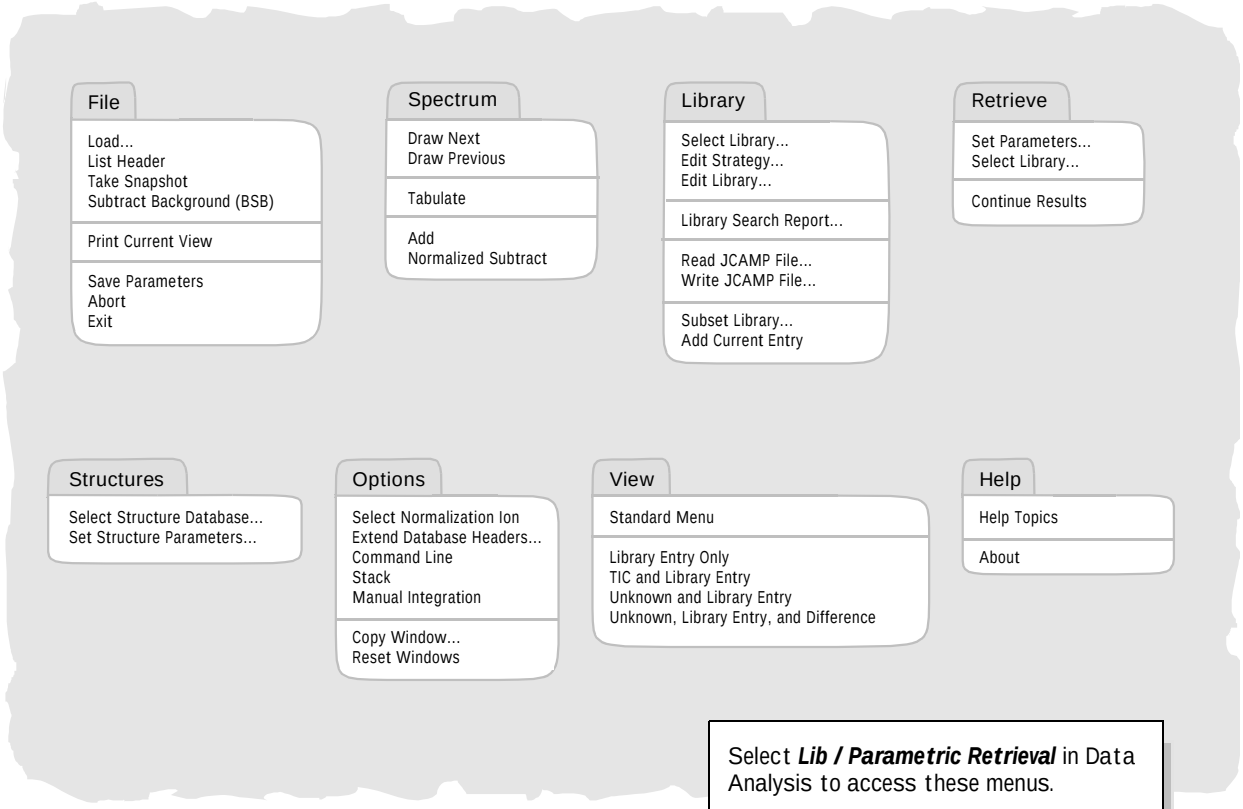
QEdit Menus



EasyID Menus



Parametric Retrieval Menus



Select ***Lib / Parametric Retrieval*** in Data Analysis to access these menus.

Select ***View / Standard Menu*** to return to Data Analysis.

Overview of Target Compound Analysis — EPA Protocol

Tuning and Tune Evaluation (MS Only)

1 Tune the MSD using ***Target Tune***, ***BFB Tune*** or ***DFTPP Tune***. Use the Tune report to verify that the tune meets your lab standards.

2 Load an appropriate method from ***\MSDchem\envdemo*** to use as a template.

3 Save the method with a new name.

4 Set up acquisition parameters for tune evaluation.

5 Run the tune evaluation compound (run the method).

6 In Data Analysis, verify Tune criteria (***Tuner / Edit DFTPP*** or ***BFB Criteria***).

7 Evaluate the tune (***Tuner / Evaluate DFTPP*** or ***BFB***, then ***Autofind***. If you are using Forms, after you have evaluated the tune and it is acceptable, select ***Tuner / Autofind to Forms***. If this is a daily tune evaluation, go to ***Run Samples***, step 2, on page 13.

Set Up Quantitation Database — Part 1

1 Load an appropriate method from ***\MSDchem\envdemo*** to use as a template.

2 Save the method.

3 From the Instrument Control view, set up acquisition parameters for calibration standards.

4 Run calibration standards in correct concentrations.

5 (GC-only) Load a data file for a mid-level concentration standard and select ***Int / Integrate***. Verify that all peaks are correctly integrated.

6 Select ***InitCal / Clear All Calibration Levels***.

7 Use ***Tools / EasyID*** to correct the retention times for all compounds.

8 Quantitate (***Quant / Calculate/Generate Report***).

9 If all compounds were identified, go to step 10.

Otherwise, use QEdit (***Quant / QEdit Quant Results***) to manually integrate "missing" peaks.

10 Select ***InitCal / Update Levels***, then select ***Add New Level***. Enter level ID and compound and ISTD concentration information.

Set Up Quantitation Database — Part 2

1 Load the data file for the next level. If there are no more levels, go to Part 3.

2 Quantitate (***Quant / Calculate/Generate Report***).

3 If all compounds were identified, go to step 4.

Otherwise, use QEdit (***Quant / QEdit Quant Results***) to manually integrate "missing" peaks.

4 Select ***InitCal / Update Levels***, then select ***Add New Level***. Enter level ID and compound and ISTD concentrations.

5 Repeat steps 1 – 4 for each additional level you want to add.

Note One level should correspond to continuing calibration. Add this level using any level ID you choose and then add it again using a level ID of CC. This CC level ID is used if you quantitate using continuing calibration response factors.

6 If there are exceptions to global entries, select ***InitCal / Edit Compounds*** and make any necessary changes.

7 If you will be using Forms, select ***InitCal / Make Compound List for Forms***.

8 Save the method and go to Part 3.

Set Up Quantitation Database — Part 3

1 Evaluate response factors (select ***InitCal / Response Factors to Screen*** or ***Printer***). If response factors are correct, go to step 2.

If response factors are not correct, use QEdit (***Quant / QEdit Quant Results***) to manually correct integration then select ***InitCal / Update Levels*** and ***Replace Responses***.

If manual integration does not correct the response factors, you may need to rerun the standards.

2 If you will be using Environmental Forms, load the data file for each standard and select ***InitCal / Response Factors to Forms***.

3 If you want to store reference spectra (GC/MS only), select ***ConCal / Update Reference Spectra***.

4 Save the method.

Set Up Reports

1 Select ***File / Edit Method***. The Select Report Options dialog box is displayed.

2 Select the reports you want to use and click ***OK***.

If Edit Full EDA Method is configured (see page 11), a series of dialog boxes lets you edit report options. Make any necessary changes and click ***OK***. You can click ***Cancel*** at any time to stop the editing process.

3 If you want to print an LSC report when the method is run, select ***LSC / Include LSC Report in Quant Report***.

4 If you need to quantitate using the initial calibration, select ***Quant / Quant Using Initial Cal RFs***.

5 If you need to quantitate using the continuing calibration response factors, select ***Quant / Quant Using Continuing Cal RFs***.

6 Save the method.

Run Samples

1 Make sure you have not exceeded the time allowed between tune evaluations (MS only). If OK, go to step 2.

If not OK, go to Tuning and Tune Evaluation on page 12.

2 Inject and analyze continuing (daily) calibration.

- Run the continuing calibration standard.
- Load the data file in Data Analysis.
- Select ***Quant / Calculate/Generate Report***.
- Verify continuing calibration criteria (select ***ConCal / Edit Continuing Calibration Criteria***).
- Select ***ConCal / Evaluate Data File as Continuing Cal to Screen***.
- Verify relative response factors, retention times, and areas are correct.
- Select ***ConCal / Update Continuing Calibration***.
- If you are using Forms, select ***ConCal / Evaluate Data File as Continuing Cal to Forms File***.

3 Run your samples.

4 Use Data Analysis to review the results.

Overview of Target Compound Analysis — Non-EPA Protocol

Tuning and Tune Evaluation (MS Only)

1. Tune the MSD using ***Autotune***
2. Use the Tune report to verify that the tune meets your laboratory standards.

Set Up Quantitation Database — Part 1

1. In Data Analysis, load the method ***envdef.m*** (located in the directory ***\MSDchem\instrument #\methods***) to use as a template.
2. Save the method with a new name.
3. From the Instrument Control view, set up acquisition parameters for calibration standards.
4. Save the method.
5. Run calibration standards in correct concentrations. The highest and lowest levels should bracket expected sample concentrations.
6. (GC-only) Load a data file for a mid-level concentration standard and select ***Int / Integrate***. Verify that all peaks are correctly integrated.
7. Select ***InitCal / Set Up Quantitation***. Select peaks (for GC/MS, also select target and qualifier ions).
8. Quantitate the data file (select ***Quant / Calculate/Generate Report***).
9. If all compounds were identified, go to step 11.

   Otherwise, use QEdit (***Quant / QEdit Quant Results***) to manually integrate "missing" peaks.
10. Select ***InitCal / Update Levels***, then select ***Add New Level***. Enter level ID and compound and ISTD concentration information.
11. Save the method.

Set Up Quantitation Database — Part 2

1. Load the data file for the next level. If there are no more levels, go to Part 3
2. Quantitate (***Quant / Calculate/Generate Report***).
3. If all compounds were identified, go to step 4.

   Otherwise, use QEdit (***Quant / QEdit Quant Results***) to manually integrate "missing" peaks, then select ***Quant / Generate Report***.
4. Select ***InitCal / Update Levels*** then select ***Add New Level***. Enter level ID and compound and ISTD concentration information.
5. Repeat steps 1 – 4 for each additional level you want to add.
6. If there are exceptions to global entries, select ***InitCal / Edit Compounds*** and make any necessary changes.
7. Save the method and go to Part 3.

Set Up Quantitation Database — Part 3

1. Evaluate response factors (select ***InitCal / Response Factors to Screen*** or ***Printer***). If response factors are correct, go to step 2.

   If response factors are not correct, use QEdit (***Quant / QEdit Quant Results***) to manually correct integration and then select ***InitCal / Update Levels*** and ***Replace Responses***.

   If manual integration does not correct the response factors, you may need to rerun the standards.
2. Save the method.

Set Up Reports

1. Select ***File / Edit Method***. The Select Report Options dialog box is displayed.
2. Select the reports you want to use and click ***OK***.

   If Edit Full EDA Method is configured (see page 11), a series of dialog boxes lets you edit report options. Make any necessary changes and click ***OK***. You can click ***Cancel*** at any time to stop the editing process.
3. Save the method.

Run Samples

1. See Tuning and Tune Evaluation on page 14.
2. Run your samples.
3. Use Data Analysis to review the results.



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