

The following table lists the folders that are created within Projects:

Folder Name	Type of information stored in the folder
Acqudb	Acquisition defaults and saved tune page settings, calibrations etc. Inlet method files.
Curvedb	Quantify calibration curve data.
Data	Raw data files.
Peakdb	Peak list data.
Methdb	Method files.
Sampledb	Sample Lists.

## Data File Structure

Data acquired from the mass spectrometer is saved into data files on the computer's hard disk. These data files may contain more than one acquisition function and may also contain processed data derived from the original raw data, for example refined spectra.

All files are acquired to the data directory of the current project


For example if the **file name** is specified as **test2** then the data files are stored in the directory **c:\MassLynx\currentproject\data\test2**. If the data file contains 2 acquisition functions and 2 sets of processed data then the directory listing will be as follows:

_Header.txt	Data file header information
_Funcs.inf	Information on functions acquired
_history.inf	Information on how data has been processed
_expment.inf	Experimental record information.
_Func001.dat	Data file for first function (one for each function)
_Func001.idx	Data file index for first function
_Func002.dat	Data file for second function
_Func002.idx	Data file index for second function
_proc001.dat	First processed data file (one for each process)
_proc001.idx	Index for first processed data file
_proc002.dat	Second processed data file
_proc002.idx	Index for second processed data file

## Displaying Spectra

There are several ways in which you can display the Spectrum window.

- **To select a Spectrum using the MassLynx menu**



Choose **Spectrum** from the **View** menu or press the  toolbar button. The spectrum displayed will be the current default spectrum (this will be either the last spectrum viewed, or if acquisition is in progress the last spectrum acquired). If the Spectrum window is already on display, it becomes the current window.

- **To select Spectra using the Sample List**

If whole rows are selected in the Sample List editor, Spectra from the data files represented by these rows will be displayed.


- **To select a Spectrum from Chromatogram**

Double click on the chromatogram at the retention time in which you are interested. The spectrum displayed will be the spectrum closest in retention time to the click. If the Spectrum window is already on display, the selected spectrum will either

- Be added to the one currently on display.
- Replace the one currently on display if the  Spectrum Toolbar button is activated.
- Be displayed in a new document window of its own if the  Spectrum Toolbar button is activated.

- **To Remove Spectra and document windows**


To remove a particular spectrum, click on the spectrum with the mouse to make it the currently selected spectrum and press the **DELETE** key. You will be prompted to confirm the deletion, press **OK** to confirm the delete.

To close a particular Spectrum document window press the Windows close button  at the top right hand corner of the document window.

## Displaying Chromatograms

There are several ways in which you can display the Chromatogram window:

- **To select Chromatogram using the MassLynx menu**

Choose **Chromatogram** from the **View** menu or press the  toolbar button. The chromatogram displayed will be the Total Ion Current (TIC) chromatogram of the current data file (unless Mass Chromatogram has been selected on the System Globals page and the files selected contain MUX data. See page 54 for details). If the Chromatogram window is already on display it becomes the current window.



- **To select Chromatograms using the Sample List**

If whole rows are selected in the Sample List editor, Chromatograms from the data files represented by these rows will be displayed.

- **To select a Chromatogram from Spectrum**


Double click on the spectrum at the mass of interest. The chromatogram displayed will be the mass chromatogram of the mass indicated by the click.

If the Chromatogram window is already on display, the selected chromatogram will either

- Be added to the one currently on display.
- Replace the one currently on display if the  Chromatogram Toolbar button is activated.
- Be displayed in a new document window of its own if the  Chromatogram Toolbar button is activated.

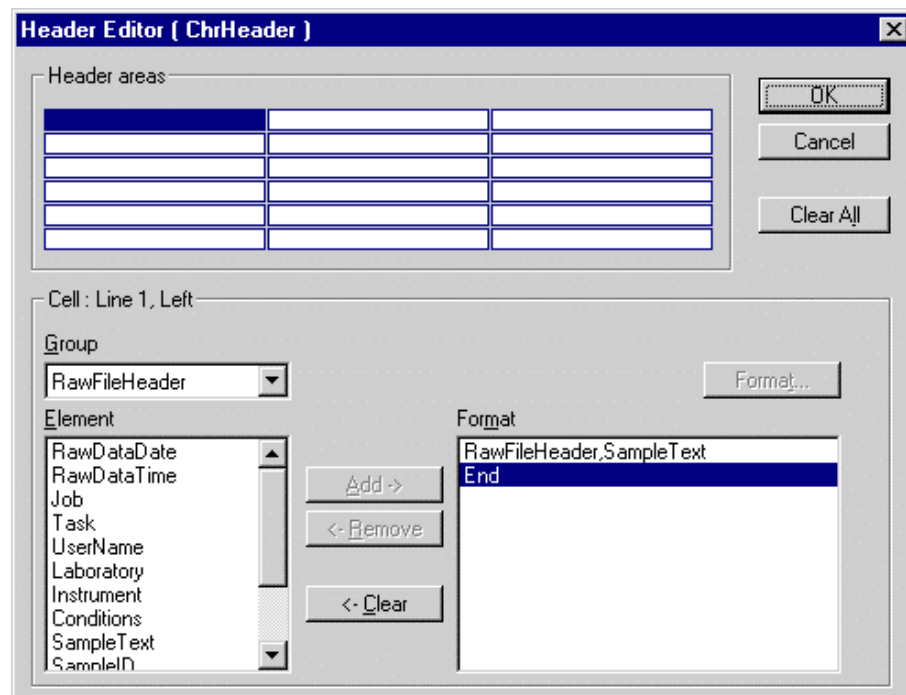
- **To Remove Chromatogram traces and document windows**

To remove a particular chromatogram trace, click on the trace with the mouse to make it the currently selected trace and then press the **DELETE** key. You will be prompted to confirm the deletion, press **OK** to confirm the delete.

To close a particular chromatogram document window press the Windows close button  at the top right hand corner of the document window.

## The Header Editor

The Header Editor is used to determine what information is displayed in the header for each of the MassLynx program windows. The Header Editor can be accessed from most of the MassLynx program windows by double clicking on the Window header with the left mouse button or via the **Header** button in the **Display View** dialog box.



*Figure 1.25 The Header Editor*

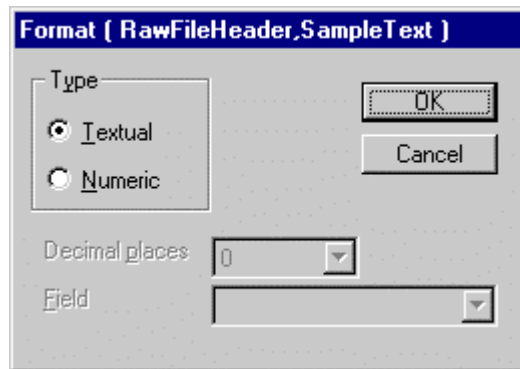
The MassLynx Window Header can be thought of as a table that has 6 rows and 3 columns. Various pieces of information can be displayed in the header including your own text. Information can be displayed on lines 1 to 6. On each line information can be displayed in three positions, left, center or right.

At the top of the Header Editor dialog there is a graphical representation of the current header. The Header Editor areas that are currently displaying information are shaded in gray. A maximum of eight areas can be used at one time to display header information.

### ■ To add information to the displayed header

1. Select the **Header Area** in which you wish to display information by clicking on the area with the left mouse button.
2. Select the **Group**, from the drop down list, that contains the information you wish to append to the displayed header.
3. Highlight the information required in the **Element** list box. Highlight the field before which you wish to insert the information in the **Format** box and choose the **Add** button. To add information at the end of the currently displayed information, highlight **End** and choose the **Add** button.

4. To add your own text to the header select [**T**ext] in the **Element** list box and choose the **Add** button. The **User Text** dialog will appear, type your text and choose the **OK** button. Your user text will be shown in the **Format** list box and will be displayed in the header when you leave the Header Editor dialog.
5. If you wish to format the information in the header, highlight the relevant field in the **Format** box and choose the **Format** button. For numeric information you can select the number of decimal places displayed in the range 0 to 6.



*Figure 1.26 The Header Editor Format dialog*

6. Repeat steps 1 to 5 as required. A maximum of eight areas can be used at one time to display header information.
7. Choose the **OK** button to exit and save the changes.

**Note:** If the information in one of the Header Editor areas overlaps another area, the overlapped area will not be displayed.

#### ■ To remove information from the displayed header

1. Select the **Header Area** from which you wish to remove information by clicking on the area with the left mouse button.
2. To remove a single field, highlight the information you wish to remove in the **Format** list box and press the **Remove** button. To remove all the information from one Header Editor area, select the area and press the **Clear** button. To remove all information from all Header Editor areas choose the **Clear All** button.
3. Repeat steps 1 and 2 as required.
4. Choose the **OK** button to exit and save the changes.

## Printing Data

MassLynx prints data using the Windows NT Print Manager so any printing device supported by Microsoft Windows NT can be used with MassLynx.

All of the operations involved in setting up your printer are controlled by Windows NT and are fully covered in the *Microsoft Windows NT System Guide*. The only MassLynx specific procedures to learn are those involved in selecting what to print.

The printer can be set up either using the **Printer Setup** command found in each **MassLynx File** menu, or by using the Windows NT Print Manager.

### ■ Printing a specific MassLynx window using the Toolbar

Many of the MassLynx Windows have Print buttons on the Toolbar.



Press to print current window in portrait format.



Press to print current window in landscape format.

### ■ Printing a specific MassLynx window using the menu

To print a specific MassLynx window using the menu commands, select the Window you wish to print and choose **Print** from the window's **File** menu.

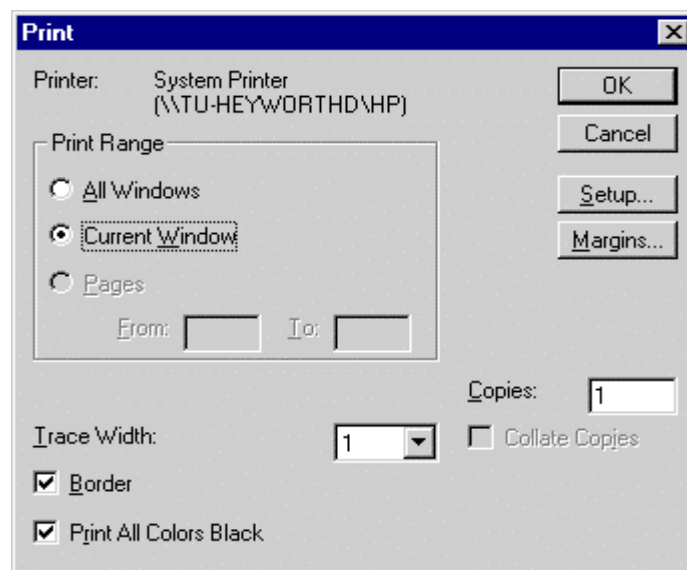


Figure 1.27 File Print dialog

**All Windows** Select this radio button to print all document windows on display.






**Current Window** Select this radio button to print only the currently selected document window.

**Trace Width** From the drop down list box, select the thickness of the line used to print chromatogram traces or spectral peaks. Trace Width can be set to values between 1 and 5, a higher value will give a thicker line.

**Print All Colors Black** Check this box to map all the colors in the MassLynx display to black. This option is useful when using black and white printers.

## Window Commands

Most of the MassLynx program windows have a top level menu command called **Window**. The subcommands of **Window** help you to organise the document windows of that program so that they fit conveniently into the main service window. The **Window** commands are also available on many of the MassLynx Toolbars.

Toolbar Button	Menu Command	Function
	<b>Tile</b>	<p>Arranges open windows side by side on the screen, dividing the available space equally between the open windows so that all of them are visible.</p> <p>To arrange the windows in a particular order, click on the title bar of each window in turn to make it the active window before selecting the Tile command. The windows will be tiled in the order in which they were selected with the most recently selected window first.</p>
	<b>Cascade</b>	Arranges document windows so that the title bar of each window is visible.
	<b>Stack</b>	Arranges documents vertically above each other.
	<b>Arrange icons</b>	Arranges all iconised windows into rows.
	<b>Window list</b>	<p>Gives a list of available windows. The currently active window has a tick next to its name. Clicking on another window will make that the currently active window. In the case of <b>Spectrum</b> and <b>Chromatogram</b> this becomes a list of the traces displayed in each window.</p>
	<b>Window New Trace Replace Trace</b>	Choosing this option causes each subsequent trace to replace the currently selected trace.
	<b>Window New Trace New Window</b>	Choosing this option causes each subsequent trace to be displayed in a new window.
	<b>Window New Trace Add Trace</b>	Choosing this option causes each subsequent trace to be added to those displayed in the current window.

## Getting Help

The MassLynx Help system contains detailed information on how to use MassLynx. Most of the information in this manual is available on-line while you are using MassLynx by accessing the Help system.

MassLynx Help can be accessed either from the MassLynx top level menu or from any of the MassLynx program windows. It can also be accessed by selecting the **MassLynx NT User Guide** icon in the MassLynx group.

If you enter Help from the MassLynx top level menu you will be given a general index of topics covering the whole of MassLynx. If you enter MassLynx Help from one of program windows you will be given help on that particular topic. For example if you choose Help from Spectrum you will be given Help on Spectrum. MassLynx Help also allows you to search for Help on a specific topic or keyword.

For more information on using Windows Help systems you can choose **Using Help** from the **Help** menu on the MassLynx window. This topic gives detailed instructions on how to use Windows Help systems. Alternatively you can refer to the *Microsoft Windows NT System Guide*.

## The About Box

The About box gives you information about MassLynx, including the version number.



Figure 1.28 The About Box

## Micromass on the Web

The Micromass Web site address is <http://www.micromass.co.uk> it can be accessed as normal through your internet browser or by selecting **Micromass Home Page** from the **Micromass on the Web** option on the top level **Help** menu.