Manipulating the display

Formatting the Sample List

Column widths can be changed, in the same way as any Windows spreadsheet. Position the mouse pointer on the line between two column headings, until a double headed arrow appears, click the left mouse button and drag until the column is the required width.

There are many different columns of information that can be displayed in the Sample List; the user can select which columns are currently displayed. Press the  Toolbar button or select **Customize Display** from the **Field** option on the **Samples** menu to invoke the Customize Field Display dialog.

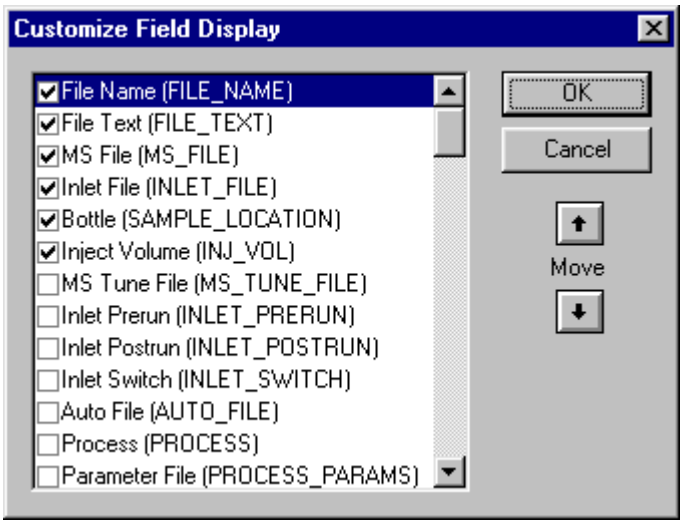


Figure 2.9 *The Customize Field Display dialog*

Check the box next to a field to include it in the Sample List. To change the order in which the fields are displayed click with the left mouse button on the name of the field in the list and press the  or  **Move** buttons until the field is in the required position.

To view field properties click on a column heading and press the  Toolbar button or select **Properties** from the **Field** option on the **Samples** menu, the **Field Properties** dialog will be displayed.

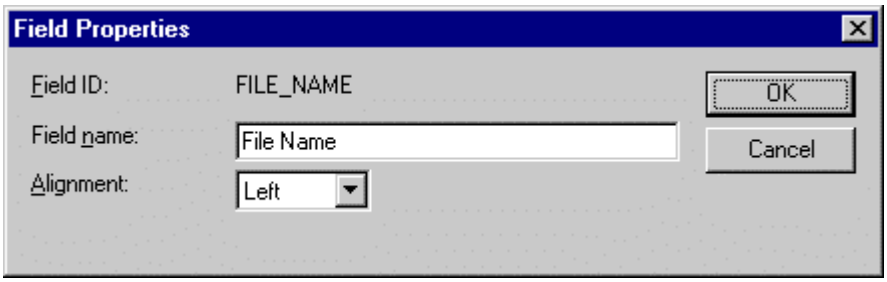


Figure 2.10 *The Field Properties dialog*

To change the name displayed at top of the column type a new name into the **Field Name** box. To change the alignment of text in the column, choose Left, Right or Center from the **Alignment** list.

The alignment of text in a cell, column or row can also be changed by selecting the area, and pressing one of the  ,  or  Toolbar buttons or selecting **Left**, **Center** or **Right** from the **Align** option on the **Field** option on the **Samples** menu.

A customized Sample List format can be saved by selecting **Save Format** from the **Samples** menu and entering a name in the dialog displayed. To retrieve a previously saved format, select **Load Format** from the **Samples** menu and select the required format from the list.

Selecting areas

Areas may be selected with the mouse, the keyboard or a combination of both of these methods.

With the Mouse

To select	Click with the left mouse button on
A single cell	The required cell
A block of cells	The first cell in the block, hold down the left mouse button and drag until the required cells are highlighted.
A row	The row number
A column	The column heading
The whole Sample List	The box at the top left corner of the Sample List

	ID	File Name
1	ID	Default
2	ID	Default

With the keyboard

Position the cursor at the top left corner of the area to be selected, hold down the shift key and use the arrow keys to select an area.

Inserting Rows

To insert a single row position the cursor on the row where the sample is to be inserted. Note the sample will be inserted above the row selected.

- Press the  Toolbar button.

-or-

- Select **Insert** from the **Samples** menu.

-or-

- Press the **Insert** keyboard key.

To insert multiple rows highlight the number of rows required and continue as for a single row.

Editing Data in a Cell

Data can be changed in various ways, the following is a description of the most common ways of editing data.

For the following field types files created and saved in the appropriate directories of the current project can be included in the sample list by double clicking on a cell, with the left mouse button, and selecting the file from the drop down list displayed.

If the file required is in another project then click on a cell, with the left mouse button, and enter the full path name.

Field	File Type	Directory
MS File	*.dbf	Acqudb
Inlet File	*.wat (Waters 2690), *.w60 (Waters 600), *.w27 (Waters 2700), *.w29 (Waters 2790), *.clc (Waters Cap LC), *.gil (Gilson), *.h11 (HP 1100), *.h50(HP 1050), *.h68 (HP 6890), *.h90 (HP 1090), *.szu (Shimadzu), *.jas (Jasco 900), *j15 (Jasco 1500), *.asx (Cetac ASX500), *.as1 (Cetac ASX100), *.ct2 (CTC A200S)	Acqudb
Process	*.exe	MassLynx
MS Tune File	*.dbf	Acqudb
Inlet Prerun	See Inlet File	Acqudb
Inlet Postrun	See Inlet File	Acqudb
Inlet Switch	See Inlet File	Acqudb
Autofile	See Inlet File	Acqudb
Parameter File	*.olp (OpenLynx), *.mlp (ProteinLynx), *.mep (MetaboLynx), *.rle (NeoLynx)	Methdb
Process Options		
Acqu Process	*.exe	MassLynx
Fraction File	*.frc	Acqudb
HPLC File	*.wat, *.h11	Acqudb

For the following fields you must select one of the displayed values from the drop down list box.

Field	Values
Sample Type	Analyte, Blank, QC or Standard
Action on Error	Ignore Error, Suspend this Batch, Suspend All batches or Delete this Batch
Fraction Trigger	Mass A to T, TIC, Analog or No Trigger

For all other fields to overwrite data in a cell click on the cell, with the left mouse button, and type in a new value. When replacing data in a single cell cut, copy, paste etc. can be performed on the usual manner or a single right mouse click will display the following pop up menu.

Figure 2.11 *The Edit Area pop up menu*

To edit data within a cell double click, with the left mouse button, on the cell. All data in the cell is highlighted. Use the left mouse button or the keyboard arrow keys to position the cursor within the cell and add, delete, copy or paste data as normal or click with the right mouse button to display the following pop up menu.

Figure 2.12 *The Edit Cell pop up menu*

Editing Data in a Column

Selecting an area and pressing the  Toolbar button, or selecting **Down** from the **Fill** option on the **Samples** menu, will fill the selected range with the first element in each column.

Selecting an area and pressing the  Toolbar button, or selecting **Series** from the **Fill** option on the **Samples** menu, will fill the selected range with series data, e.g. if the first cell in a column is bottle1 the next will be bottle2, bottle3 etc.

Pressing the  Toolbar button or selecting **Insert** from the **Samples** menu inserts samples into the Sample List. If a row has been selected, a new row is inserted above the current one. If more than one row is selected this inserts the same number of rows above the first row of selection. If a column has been selected, the same number of rows as there were originally in the column are inserted before the first row. The data inserted into these new rows will continue the series from the row above selection.

E.g. in the following example, selecting the two rows highlighted in the first picture and pressing insert will give the second picture.

	ID	Bottle
1	ID	Bottle
2	ID1	Bottle1
3	ID10	Bottle3
4	ID11	Bottle4

	ID	Bottle
1	ID	Bottle
2	ID1	Bottle1
3	ID2	Bottle2
4	ID3	Bottle3
5	ID10	Bottle3
6	ID11	Bottle4

If there is more than one number in a field then only the last number is incremented when Fill Series is selected. E.g. Sample1run1, when Fill Series is selected the next field will be Sample1run2 etc.

Cut, **Copy** and **Paste** can also be used to enter data. Select an area, Cut or Copy the data and Paste to a new area. Note the Paste area must be same size as the Cut or Copy area.

Deleting Rows and Columns

Press the delete row button  to delete the selected rows. If the whole table is selected then the cells are cleared not deleted.

To remove a column from the display, select the column and press the  toolbar button. This will remove the whole column.

Starting an Acquisition

Press the  Toolbar button or select **Start** from the **Run** menu to start the acquisition.

Number of Injections

Select **Number of Injections** from the **Samples** menu to display the Number Of Injections dialog.

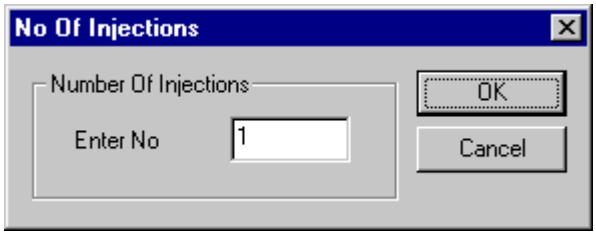


Figure 2.13 *The Number of Injection dialog*

Enter the number of injections and press **OK**.

This controls the number of injections taken from one bottle. E.g. for the following Sample List:

	File Text	MS File	Inlet File	Bottle	Inject Volume	File Name
1	Default file	DEFAULT	DEFAULT	1	10	DEFAULT01
2	Default file	DEFAULT	DEFAULT	2	10	DEFAULT02
3	Default file	DEFAULT	DEFAULT	3	10	DEFAULT03
4	Default file	DEFAULT	DEFAULT	4	10	DEFAULT04
5	Default file	DEFAULT	DEFAULT	5	10	DEFAULT05
6	Default file	DEFAULT	DEFAULT	6	10	DEFAULT06

If Number of Injections is changed to 2, the bottle column selected and Fill Series is selected then the Sample List changes to:

	File Text	MS File	Inlet File	Bottle	Inject Volume	File Name
1	Default file	DEFAULT	DEFAULT	1	10	DEFAULT01
2	Default file	DEFAULT	DEFAULT	1	10	DEFAULT02
3	Default file	DEFAULT	DEFAULT	2	10	DEFAULT03
4	Default file	DEFAULT	DEFAULT	2	10	DEFAULT04
5	Default file	DEFAULT	DEFAULT	3	10	DEFAULT05
6	Default file	DEFAULT	DEFAULT	3	10	DEFAULT06

Indicating that injections 1 and 2 are taken from bottle 1, injections 2 and 3 are taken from bottle 2 etc.

Action On Error

The Action on error field allows the users to define what happens to a batch if an error occurs. Select **Action on error** from the **Customize Field Display** dialog to display the column on the sample list. Double click on a cell to display a dropdown list box and select one of the options.

Figure 2.14 *The Action on error options*

Ignore Error Ignore the error and continue with the acquisition.

Suspend This Batch Pauses the current batch and continues with the next batch in the MassLynx Queue.

Suspend All Batches Pauses all batches.

Delete This Batch Deletes the current batch from the queue and continues with the next one.

If no action is chosen then Ignore Error is used.

Updating the Sample List from the Plate Layout

As mention earlier if a Waters 2700, Waters 2790 or Gilson autosampler is installed, and controlled via MassLynx, then the Bed Layout and Plate Layout is shown on the MassLynx screen next to the Sample List.

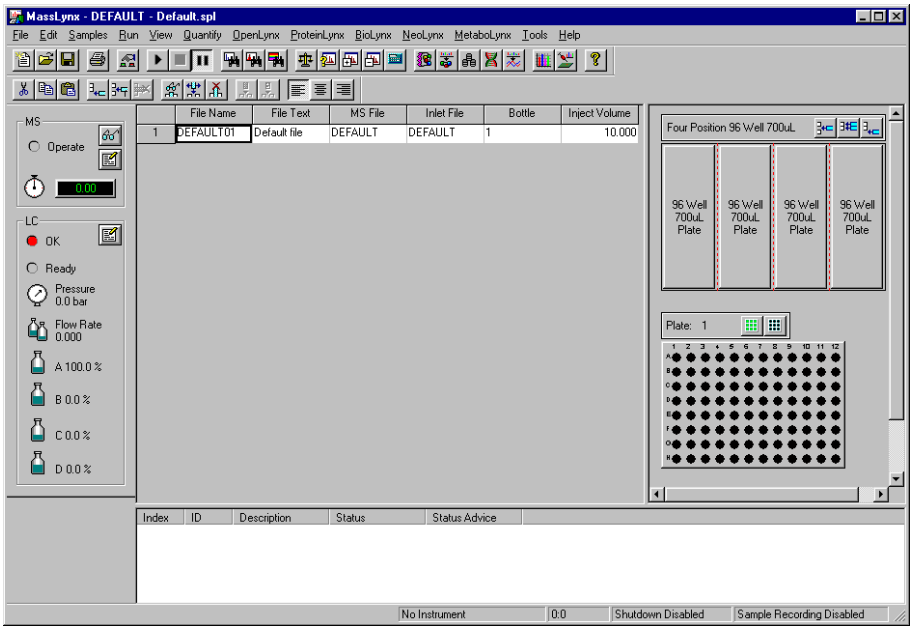


Figure 2.15 *The MassLynx Screen with Plate and Bed Layout*

If this pane is not visible position the cursor on the right of the screen until ✣ is displayed, click with the left mouse button and drag to the right, until the pane is the required size. The height of the pane can also be altered the same way.

The Bed and Plate Layout Pane

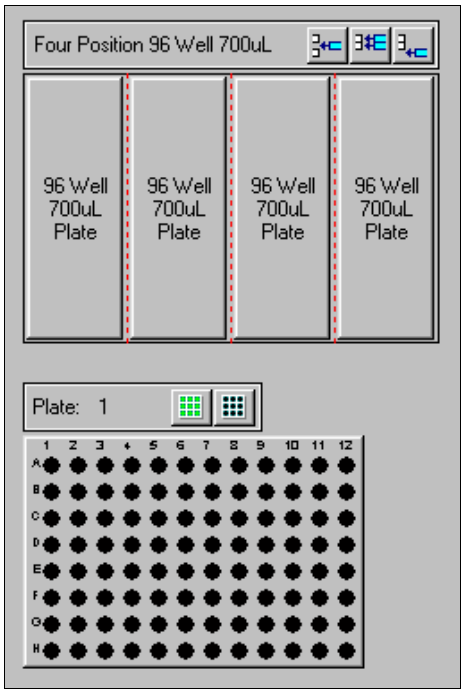


Figure 2.16 *Plate and Bed Layout*

This pane shows the name of the currently selected Bed Layout and a picture of the layout. Below this is the Plate number and a picture of the plate.

Note: The toolbar buttons used in the descriptions below are those on the Plate Layout pane, not those on the Sample List toolbar.

To Select the Bed Layout

For the Waters 2790 autosampler there is only one Bed Layout shown above (**Figure 2.16**).

For the Waters 2700 and Gilson autosamplers the Bed Layout selected on the Autosampler parameters, Sampler Configuration page is displayed. See the relevant Data Acquisition Guide for details.

To Select the Plate

Click on a plate in the Bed Layout area, the plate number will be updated and if the plate is different from the previous one the picture will be updated.

To Select Vials

Selected vials are shown in green unselected ones in black.

To select a vial click on a black vial with the left mouse button. To select all vials on the plate press the  button or click, with the right mouse button, on the plate and choose **Select all Vials** from the pop up menu displayed.

To Deselect Vials

To deselect a vial click on a green vial with the left mouse button. To deselect all vials on the plate press the  button or click, with the right mouse button, on the plate and choose **Un-select all Vials** from the pop up menu displayed.

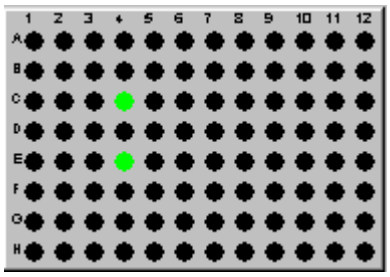
To Add Samples to the Sample List

Select the required vials and press the  button (on the Plate Layout pane) or click, with the right mouse button, on the plate and choose **Add** from the pop up menu displayed.

The vials selected on each plate will be appended to the sample list. The fields will be filled as though a Fill Series has been performed (see page 99). E.g. if the last row in sample list was

39	ASSAY39	15pg/ml std	DEFAULT	DEFAULT	69	10.000

and the following vials from plate 1 were added



then the sample list will be updated as follows.

39	ASSAY39	15pg/ml std	DEFAULT	DEFAULT	69	10.000
40	ASSAY40	15pg/ml std	DEFAULT	DEFAULT	1:4,C	10.000
41	ASSAY41	15pg/ml std	DEFAULT	DEFAULT	1:4,E	10.000

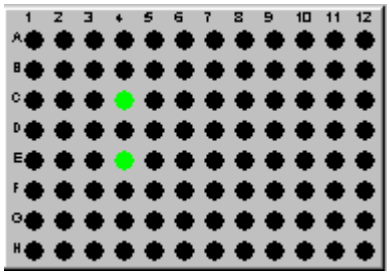
To Insert Samples into the Sample List

Select the required vials and click on the row where the samples are to be inserted. Note the samples will be inserted above the row selected. Press the  button (on the Plate Layout pane) or click, with the right mouse button, on the plate and choose **Insert** from the pop up menu displayed.

The vials selected on each plate will be inserted into the sample list. The fields will be filled as though a Fill Series has been performed (see page 99). E.g. if the following row is selected in the sample list

33	ASSAY33	0.5pg/ml std	DEFAULT	DEFAULT	63	10.000
34	ASSAY34	0.75pg/ml std	DEFAULT	DEFAULT	64	10.000

and the following vials from plate 1 were inserted



then the sample list will be updated as follows.

33	ASSAY33	0.5pg/ml std	DEFAULT	DEFAULT	63	10.000
34	ASSAY34	0.5pg/ml std	DEFAULT	DEFAULT	1:4,C	10.000
35	ASSAY35	0.5pg/ml std	DEFAULT	DEFAULT	1:4,E	10.000
36	ASSAY34	0.75pg/ml std	DEFAULT	DEFAULT	64	10.000

Note: File Names may need to be updated as this operation may cause names to be duplicated.

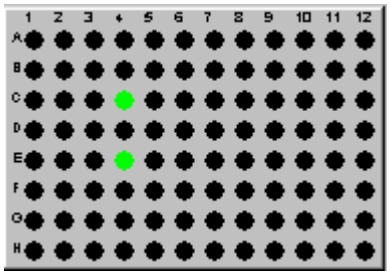
■ To Replace Samples in the Sample List

Select the required vials and the rows to be replaced. Note the rows to be replaced must be next to each other and must match the number of samples selected. Press the  button (on the Plate Layout pane) or click, with the right mouse button, on the plate and choose **Replace** from the pop up menu displayed.

The SAMPLE_LOCATION field for the selected samples will be replaced by location of the vials selected from the plate(s). E.g. if the following rows are selected in the sample list

32	ASSAY32	0.2pg/ml std	DEFAULT	DEFAULT	62	10.000
33	ASSAY33	0.5pg/ml std	DEFAULT	DEFAULT	63	10.000
34	ASSAY34	0.75pg/ml std	DEFAULT	DEFAULT	64	10.000
35	ASSAY35	1pg/ml std	DEFAULT	DEFAULT	65	10.000
36	ASSAY36	2pg/ml std	DEFAULT	DEFAULT	66	10.000

and replaced with the following vials from plate 1



then the sample list will be updated as follows.

32	ASSAY32	0.2pg/ml std	DEFAULT	DEFAULT	62	10.000
33	ASSAY33	0.5pg/ml std	DEFAULT	DEFAULT	1,1:C,4	10.000
34	ASSAY34	0.75pg/ml std	DEFAULT	DEFAULT	1,1:E,4	10.000
35	ASSAY35	1pg/ml std	DEFAULT	DEFAULT	65	10.000
36	ASSAY36	2pg/ml std	DEFAULT	DEFAULT	66	10.000