

## 7. Controlling Quantify Reports

Four printed reports of quantification results are available:

**Quantify Compound Summary Report** Displays quantification results for each of the Quantify compounds ordered by compound.

**Quantify Sample Summary Report** Displays quantification results for each of the Quantify compounds ordered by sample.

**Quantify Calibration Report** Gives calibration curve graph for each Quantify compound.

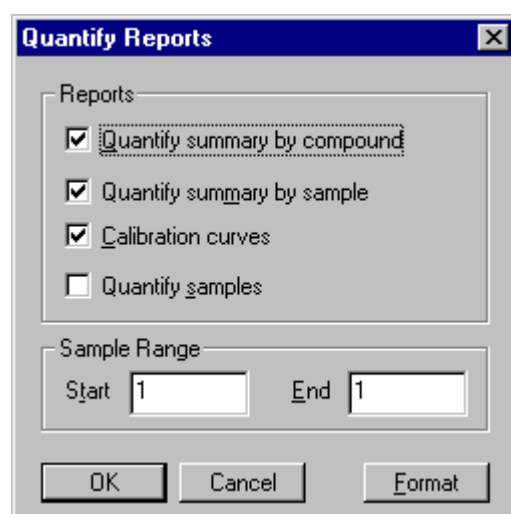
**Quantify Sample Report** Graphically displays all located chromatogram peaks and tables quantification results. Report is grouped by sample. Note: Chromatogram is invoked when producing the report.

### ■ To print Quantify Reports

1. Quantify Reports will be automatically printed at the end of a sample list analysis when the **Print Quantify Reports** field is selected when a sample list analysis is started.

-or-

Choose **Print Report** from the Quantify **File** menu.



*Figure 7.29 Quantify Reports dialog*

2. Choose which reports you wish to print by selecting the relevant check boxes.
3. In the **Start** and **End** fields, enter the range of samples that you want the report to include.
4. Choose **OK** to save changes.

The **Print Report** dialog will be displayed.

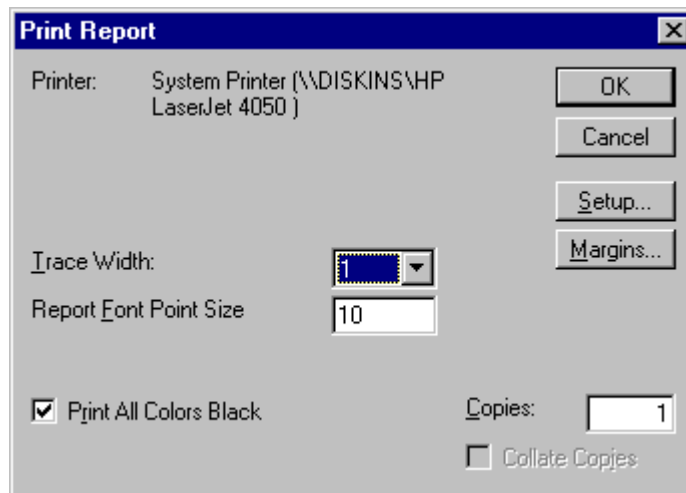


Figure 7.30 Quantify Print Report dialog

5. Set the printing parameters as required. The Quantify Report margins can be altered by selecting the **Margins** button.
6. Choose the **OK** button to print the Reports.

■ **To change the format of the Quantify Reports**

1. Select **Report Format** from the Quantify **File** menu, or select **Print Report** from the Quantify **File** menu and choose the **Format** button.

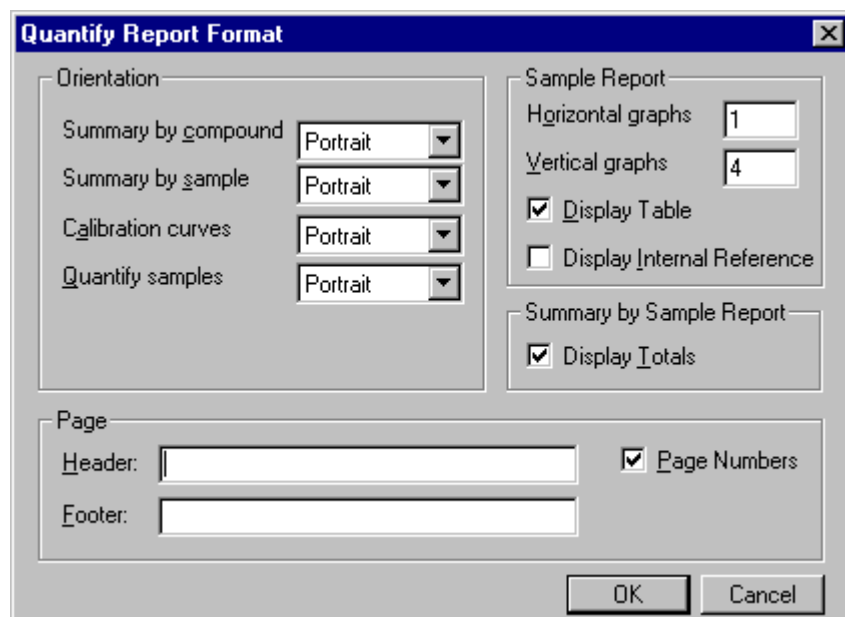


Figure 7.31 Quantify Report Format dialog

2. From the **Orientation** drop down list boxes, set the orientation of each report to Portrait or Landscape.
3. In the **Page Header** and **Footer** fields, enter the header and footer that you want to appear on each page.
4. Check the **Page Numbers** box to insert page numbers on each page of the reports.

5. In the **Horizontal graphs** and **Vertical graphs** fields specify the number of Horizontal or Vertical graphs that you want each sample report to display.
6. Check the **Display Table** box to print a Summary Table of the sample results as well as the graphs.
7. Check the **Display Internal Reference** box to print the Internal Standard Chromatogram with the Analyte Chromatogram. The Internal Standard for a compound is specified in the Internal Ref field in the Method Editor.
8. In the **Summary by Sample Report** area, check the **Display Totals** box to display the breakdown of total compounds for each sample report.
9. To accept the amendments to the layout of the printed reports, press **OK**.

Report formats and Quantify Summary formats can be saved and retrieved from the Quantify window. This enables you to create specific summary and report formats to display different types of data.

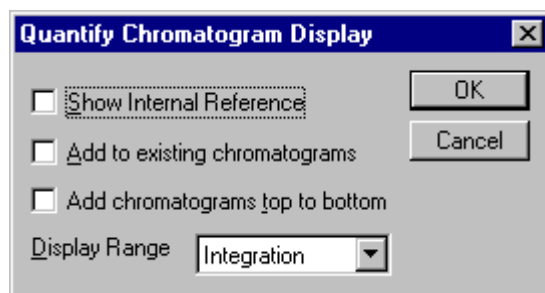
#### ■ To select which fields are displayed in the Quantify Summary Reports

Select **Output Compound Format** or **Output Sample Format** from the Quantify **Edit** menu.

For more information about formatting Summary Reports see "To select which fields will be displayed in the Summary window and Summary Reports" on page 313.

#### ■ To select the Chromatogram display range for the Quantify Sample Report

The Quantify Sample Report uses the Chromatogram display parameters, which can be controlled by selecting **Chromatogram** from the Quantify **Display** menu.



*Figure 7.32 Quantify Chromatogram Display dialog*

**Show Internal Reference** Check this box to display the internal reference with the current peak.

**Add to existing chromatograms** Check this box to add each new chromatogram trace to those already displayed.

**Add chromatograms top to bottom** Check this box to add each new chromatogram trace to the bottom of the previous trace.

**Display Range** From the drop down list box, select **Integration** to use the range which was integrated over, **Acquisition** to use the range acquired over. If the **Display Range** is set to **Keep Current** the system will use the range acquired over.

### ■ To Print Quantify windows

1. Choose **Print** from the **Quantify File** menu.
2. Select to print **All Windows** or **Current Window** and choose the **OK** button to print the Quantify windows.

### ■ To print Quantify windows using the Quantify Toolbar



Press to print the current Quantify window display in portrait format.



Press to print the current Quantify window display in landscape format.

### ■ Writing Quantify Summary to the Clipboard

Quantify allows the equivalent of the Quantify Summary Report to be written to the Clipboard. From here the information can be pasted into other applications such as a spreadsheet. Quantify uses the currently selected Sample List, Method and Peak List files.

Two options are available, the Quantify Summary Report can either be ordered by compound or by sample.

To write the Quantify summary information to the clipboard select **Copy Summary By Compound** or **Copy Summary By Sample** from the **Quantify Edit** menu.

## Export to LIMS File

Quantification results can be written to a text file for use with LIMS systems. This can be performed automatically by selecting the Export Results to LIMS option on the Quantify Samples dialog ( see page 308 ). The results can also be exported from the Quantify window. Select **Export to LIMS File** from the **File** menu, select a file from the browser displayed or enter the name of a new one and press **Save**. If the selected file already exists, the user will be prompted to overwrite the existing file.

The file generated will consist of three areas; the Header Section , the Samples Section and the Calibration section.

### The Header Section

The header section contains the following four sections. Each shows the full path name of the file generated by or used to create the report and the date and time that the file was last modified.

- LIMS EXPORT FILE            The LIMS file generated
- SAMPLELIST                 The Sample List file.
- QUANMETHOD                The quantification method file.
- QUANCALIBRATION         The quantify curve file.

### The Samples Section

The samples section will include an entry for each sample in the current sample list. For each sample there will be one entry for each compound named in the compound box in the quantify method. Each entry will have the following fields, separated by a comma.

- The compound number shown in the compound box in the quantification method.
- The text name of this compound.
- The scan at which the matching peak was found in the current sample datafile.
- The retention time of the matching peak.
- The relative retention time to the referenced peak at which the matching peak was found.
- The area of the matching peak.
- The height of the matching peak.
- The response of the sample for this compound.
- The flags associated with the peak.
- The concentration of compound recorded for this sample.
- The blank subtracted concentration of the compound for this sample.
- The chromatogram trace used to locate peaks for this compound.
- The error between the expected concentration and the calculated concentration for this sample for a fixed concentration compound.
- The ordinal number of the compound in the quantification method that is used as the reference peak for this compound.
- The area of the reference peak.
- The height of the reference peak

- The retention time of the reference peak.
- The modification date of the peak used to quantify this compound for this sample. This refers to manually modifying the peak, for example by double clicking on the entry in the peak display in the quantification window.
- The modification time of the peak.
- The modification text (modification comment) of the peak.
- The MassLynx user who altered the peak.
- The mass of the peak.
- The retention time the peak was expected at for this compound.
- The relative retention time the peak was expected at for this compound.
- The user factor associated with this compound.
- The user RF factor associated with this compound.
- Start retention time of the detected peak.
- End retention time of the detected peak.

### **The Calibration Section**

The calibration section will have a subsection for each calibration curve calculated for the current quantification calibration.

Each subsection will contain information as displayed on the calibration graphs window. Where a line entry is inappropriate it will not be entered in the report file.

- Correlation coefficient: or Coefficient of Determination:
- Response Factor: or Calibration Curve:
- Response Type:
- Curve Type:, Origin:, and Weighting:

## Files Used During Quantify

Four types of files are used by the Quantify program these are Sample List, Method, Peak List and Calibration Curve. The current file of each type can be selected from the **Quantify File** menu. It is recommended that you use the **Projects** option when doing quantification as this allows you to organise and access your data more easily. For more information see "Projects" on page 295.

### The Sample List (.SPL) File

Three items in the Sample List are required for quantification.

**File Name** Specifies the sample data file name, which will be the same name as the corresponding Peak List file.

**Type** Specifies the type of sample. This should be set to **Standard** if the sample is to be used to form a calibration curve, **Analyte** if the concentration of the compounds within the samples is to be calculated, **QC** if it is a quality control sample or **Blank** if the sample doesn't contain any analyte compounds.

**Concentration** Only required if the sample is a standard and is optional for QC samples. Specifies the known concentrations of the compounds within the standard. This does not apply to compounds whose concentration has been specified as being constant, (fixed), within all samples.

The Sample List files are normally stored in the \SAMPLEDB directory.

### The Quantify Method (.MDB) File

The Quantify Method contains an entry for each of the compounds being analysed determining how the data is to be processed. The same method is applied to all the samples in the analysis. For more information see "Create a Quantify Method" on page 296. The Method files are normally stored in the \METHDB directory.

### Peak Lists (.PDB) File

A Peak List contains peaks that were detected when integrating chromatograms. Further information gathered as a result of running Quantify, such as compound name and concentration, are also saved in the peak list.

Peak Lists are produced as a result of running the MassLynx automated Quantify software or by the Chromatogram service. One Peak List should be formed for each of the samples in the analysis, the Peak List will have the same name as the sample from which it was formed.

For more information on examining, modifying and creating Peak Lists see the Chromatogram section of the MassLynx Users Guide.

The Peak List files are normally stored in the \PEAKDB directory.

### Calibration Curves (.CDB) File

Stores the Quantify Calibration Curves which are produced for each of the compounds within the method. The Calibration Curve file has the same name as the method used to create it. The Calibration files are normally stored in the \CURVEDB directory.