# Interfacing Guide

Version 3.5

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# Interfacing Guide

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## Copyright Notice



## Trademarks

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# Conventions

The Interfacing Guide follows these typographic conventions

| This | Represents |
|---|---|
| **bold** | Anything you must type exactly as it appears |
| *italic* | Place holders for information you must provide. For example if you are asked to type *filename*, you would type the actual name for a file instead of the word shown in italic type. |
| ALL CAPITALS | Directory names, filenames and acronyms. |

**Keyboard Formats**

Key combinations and key sequences appear in the following formats.

| | |
|---|---|
| KEY1+KEY2 | A plus sign (+) between key names means to press and hold down the first key while you press the second key. For example, "press ALT+ESC" means to press and hold down the ALT key and press the ESC key. Then release both keys. |
| KEY1,KEY2 | A comma sign (,) between key names means to press and release the keys one after the other. For example, "press ALT,F" means to press and release the ALT key and then press the F key. |

# About This Manual

This manual is designed to explain how data can be imported into and exported from MassLynx for use in other applications. When you have read this manual you should be able to -

- Import data from Excel, Access and Notepad.
- Export quantify data to LIMS systems.
- Read ProteinLynx, OpenLynx and MetaboLynx report files.
- Read Chromatogram and Spectrum text files.

This manual assumes that you have no previous knowledge of MassLynx. However this manual does assume that you are familiar with using the Microsoft Windows NT Graphical Environment and have the basic skills required to work with Windows NT software.

If you have never used Microsoft Windows NT before we would suggest that you spend a short time reading **"Chapter 2 Learning the Basics"** in the **Microsoft Windows NT Workstation Start Here** guide supplied with your Windows NT software.

This manual also assumes knowledge of Access, Excel, Notepad and LIMS systems.

# Importing

There are several ways of importing data into a Sample List:

- Copying and pasting data from text editors, Access and Excel.
- Import Worksheet.
- Import Data.

## Copying Data

Data created in other Windows applications can be copied to the clipboard and pasted into the Sample List editor.

1. Press the  button or select **New** from the **File** menu. If the previous Sample List has not been saved you will be prompted to save it. A Sample List with one default row will be displayed.

2. Add rows and columns to the Sample List so that it matches the number of rows and columns as the other Windows application. Note if this is not done data may be lost.

3. Select the relevant area in the other Windows application and copy it.

4. In the Sample List editor, position the cursor on the cell at the top left corner of the paste area and select Paste.

Notes:

If copying from a text editor e.g. Notepad fields must be tab delimited.

When copying from an Access database the last record is not pasted and will have to be entered manually.

# Import Worksheet

Sample Lists can be created in a number of other packages and imported into MassLynx. MassLynx V3.0 and V3.1 allowed OpenLynx batch files and MassLynx V2.3 Sample List files to be imported. While these options are still supported, there are now several other file types that have been added.

- ACCESS 97
- Tab and Comma delimited text files
- Excel 97 and Excel 5.0, 6.0 and 7.0 files

## To Import a Worksheet

1. Choose **Import Worksheet** from the MassLynx **File** menu.

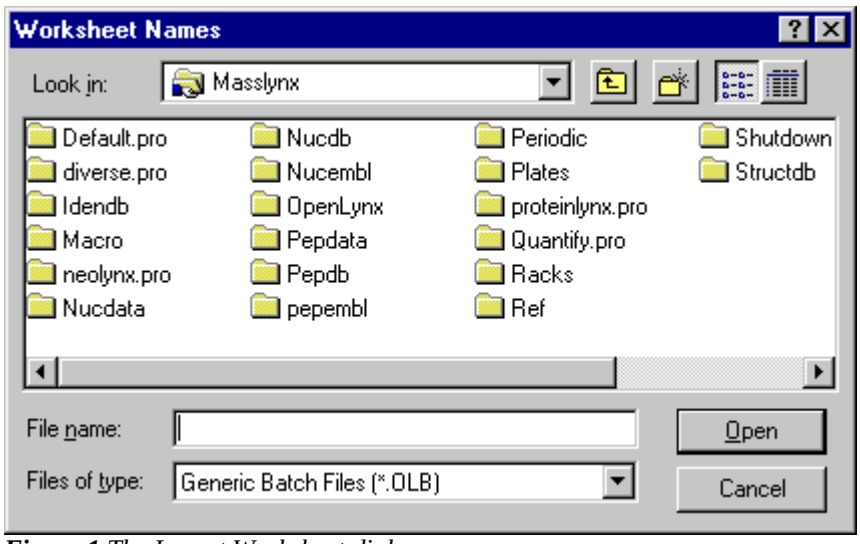



***Figure 1*** *The Import Worksheet dialog*

2. Locate the required file, or type in a file name, and press **Open**. Generic Batch files created in OpenLynx are the default file types. Click on the arrow, at the end of the **Files of type** box, to import a different file type.

# Creating Import Files

The following is a list of instructions on how to create files suitable for importing into MassLynx.

For all types of file fields must have the same name as in the Sample List (see Sample List on page 56) although they can be defined in any order. For Access 97 the data type must also match. The names correspond to the name in brackets on the **Customize Field Display** dialog.

# Access 97

When the table is created it must be called **ANALYSIS**.

It is recommended that the design view is used when creating a new table, this allows you to define the data type of the field.

You must have the first column called **Index** as the primary key. Column headings must match those shown on page 56. Other columns can be present but they will not be imported into the Sample List.

### To define the data type as a double

1. Select **Number** from the drop down list box in the **Data Type** column.

2. On the general page, at the bottom left of the screen, click on **Field Size** and select **Double** from the drop down list box.

### To save in access 97 format

The table can be saved as an access database by selecting **Save** from the **File** menu and can be imported into MassLynx in this format. Tables can also be saved as tab or comma delimited files for importing into MassLynx.

### To save in tab or comma delimited format

1. Select **Save As/Export** from the **File** menu, select the **To an External File or Database** option and press **OK**.

2. Select the required directory from the browser displayed, select **Text files (*.txt;*.csv;*.tab;*.asc)** from the **Save as type** drop down list box and then press the **Export** button.

3. Make sure the **Delimited** option is selected and press the **Next** button.

4. Check the **Include Field Names on First Row** option, select the type of delimiter to use and press the **Next** button.

5. Enter the name to save the file as and press the **Finish** button.

If files are saved as comma or tab delimited then they must be imported into MassLynx as comma or tab delimited files.

## Excel

You must have the first column called **Index**, other column headings must match those shown on page 56.

Select the area containing the data to be imported, including the column headings, and name the area ANALYSIS. To do this select **Define** from the **Name** option on the **Insert** menu, type ANALYSIS and press **OK**.

Leave all cells in General format

For a text field containing only numeric data an apostrophe ( ' ) must be inserted in front of the number.

If the file is to be saved as tab or comma delimited then Excel will only allow one sheet to be saved. If the current workbook contains more than one worksheet then each worksheet must be saved as a separate text file.

## Notepad

You must have the first column called **Index**, other column headings must match those shown on page 56.

Type in the field name/value and then a comma (or press tab for tab delimited files) and enter the next value. End each line with a carriage return.

Text fields should be enclosed in quotes.

# Import Data

Sample List data can be created in a number of other packages and imported into MassLynx. The file types supported are:

- ACCESS 97
- Tab and Comma delimited text files
- Excel 97 and Excel 5.0, 6.0 and 7.0 files

## To Import Data

1. In MassLynx ensure that the correct number of rows and columns is displayed. If this is not done then data will be lost.
2. Choose **Import Data** from the MassLynx **File** menu.
3. Locate the required file, or type in a file name, and press **Open**. Excel 5.0 files are the default file types. Click on the  arrow, at the end of the **Files of type** box, to import a different file type.

# Creating Import Files

The following is a list of instructions on how to create files suitable for importing into MassLynx.

For all types of file

- Fields must not have column headings.
- Fields must be in the same order as they are to appear in the MassLynx Sample List

## Access 97

When the table is created it must be called **ANALYSIS**.

For Access 97 the data type of the column must match.

It is recommended that the design view is used when creating a new table, this allows you to define the data type of the field.

To define the data type as a double see Import Worksheet above.

To save in tab or comma delimited format follow the instructions for Import Worksheet above, except for step 4 where the **Include Field Names on First Row** option should not be checked.

If files are saved as comma or tab delimited then they must be imported into MassLynx as comma or tab delimited files.

## Excel

Select the area containing the data to be imported, including the column headings, and name the area ANALYSIS. To do this select **Define** from the **Name** option on the **Insert** menu, type ANALYSIS and press **OK**.

Leave all cells in General format

For a text field containing only numeric data an apostrophe ( ‘ ) must be inserted in front of the number.

If the file is to be saved as tab or comma delimited then Excel will only allow one sheet to be saved. If the current workbook contains more than one worksheet then each worksheet must be saved as a separate text file.

## Notepad

Type in the field name/value and then a comma (or press tab for tab delimited files) and enter the next value. End each line with a carriage return.

Text fields should be enclosed in quotes.

# Exporting

There are several ways of exporting data from MassLynx:

- Export to LIMS.
- Copying Chromatogram and Spectrum peak lists.
- Export SEQUEST file.
- OpenLynx Batch files.
- OpenLynx Browser files.
- ProteinLynx Browser files.

## 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. 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. All fields are text.

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

e.g. LIMS EXPORT FILE:
C:\Masslynx\lims1
Tue Nov 10 11:33:10 1998

### Compound Section header fields

The compound section will include an entry for each sample in the current sample list. The header will contain the File Name, Sample ID and any text entered in the SPARE_1 to SPARE_5 fields in the sample list.

E.g. ASSAY01,ID,,,,,

### Samples Section

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 data type column shows what type of field the data was exported from.

| Field Description | Data Type |
|---|---|
| The compound number shown in the compound box in the quantification method. | int |
| The text name of this compound. | char |
| The scan at which the matching peak was found in the current sample datafile. | Int |
| The retention time of the matching peak. | Float |
| The relative retention time at which the matching peak was found. | Float |
| The area of the matching peak. | Float |
| The height of the matching peak. | Float |
| The response of the sample for this compound. | Float |
| The flags associated with the peak. | Text |
| The concentration of compound recorded for this sample. | Float |
| The blank subtracted concentration of the compound for this sample. | Float |
| The chromatogram trace used to locate peaks for this compound. | Char |
| The error between the expected concentration and the calculated concentration. | Float |
| The ordinal number of the compound in the quantification method that is used as the reference peak for this compound. | Int |
| The area of the reference peak used for this compound for this sample. | Float |
| The height of the reference peak | Float |
| The retention time of the reference peak. | float |
| The modification date of the peak used to quantify this compound for this sample. This refers manual modification of the peak. | Text |
| The modification time of the peak. | Text |
| The modification text (modification comment) of the peak. | Text |
| The MassLynx user who altered the peak. | Text |
| The mass of the peak. | Float |
| The retention time the peak was expected at for this compound. | Float |

| Field Description | Data Type |
|---|---|
| The relative retention time the peak was expected at for this compound. | Float |
| The user factor associated with this compound. | Float |
| The user RF factor associated with this compound. | Float |
| The start retention time of the detected peak | Float |
| The end retention time of the detected peak | Float |

### 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:

E.g.

Compound 1 name: I. Std

Response Factor: 846.154

Response type: External Std, Area

Curve type: RF

Compound 2 name: Parent

Coefficient of Determination: 1

Calibration curve: 0.568051 * x + 0.0010347

Response type: Internal Std ( Ref 1 ), Area * ( IS Conc. / IS Area )

Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

Compound 3 name: Metabolite

Coefficient of Determination: 1

Calibration curve: 0.336996 * x + -0.00516146

Response type: Internal Std ( Ref 1 ), Area * ( IS Conc. / IS Area )

Curve type: Linear, Origin: Exclude, Weighting: 1/x, Axis trans: None

All fields are text. It is possible to parse the correlation coefficients out, but their format will depend on how the quantify methods are set up, so this will have to be done on a per application basis.

# Copying to and from the Windows NT Clipboard

The Windows NT Clipboard provides temporary storage for information that is being transferred between application programs (word processors, spreadsheets, MassLynx etc.). You can use the Clipboard to move data out of the Chromatogram and Spectrum windows as a text list. This data can then be pasted into reports written with a Windows compatible word processor.

## To copy a chromatogram as a text list to the Clipboard

1. Display the required time range in a chromatogram window.

2. Press the  Toolbar button or choose **Copy Chromatogram List** from the **Chromatogram Edit** menu. The section of the chromatogram on display will be transferred to the Clipboard as (time, intensity) pairs or (scan, intensity) pairs depending on the horizontal axis setting.

3. To read the information into another application, choose **Paste** from the other application's **Edit** menu.

Copying the Chromatogram list to the clipboard gives the following format.

*Retention Time or Scan Number* *Intensity*
*Retention Time or Scan Number* *Intensity*
*Retention Time or Scan Number* *Intensity*
*Retention Time or Scan Number* *Intensity*

The retention time or scan/intensity pairs are separated by a tab.

## To copy integrated chromatogram peaks as a text list to the Clipboard

1. Display the required time range in a chromatogram window

2. Press the  Toolbar button or choose **Copy Detected Peaks** from the **Chromatogram Edit** menu. The chromatogram peaks on display will be transferred to the Clipboard. The information transferred for each peak is the peak top, height, area, start, end, start height and end height.

3. To read the information into another application, choose **Paste** from the other application's **Edit** menu.

Copying the Chromatogram list to the clipboard gives the following format.

| | | | | | | |
|---|---|---|---|---|---|---|
| *Retention Time* | *Peak Height* | *Peak Area* | *Peak Start RT* | *Peak End RT* | *Peak Start Intensity* | *Peak End Intensity* |
| *Retention Time* | *Peak Height* | *Peak Area* | *Peak Start RT* | *Peak End RT* | *Peak Start Intensity* | *Peak End Intensity* |

The fields are separated by a tab.

### To copy a spectrum as a text list to the Clipboard

1. Display the required mass range in a Spectrum window.

2. Press the  Toolbar button or choose **Copy Spectrum List** from the **Spectrum Edit** menu. The section of the spectrum on display will be transferred to the Clipboard as (mass, intensity) pairs.

3. To read the information into another application, choose **Paste** from the other application's **Edit** menu.

Copying the Spectrum list to the clipboard gives the following format.

*Mass* *Intensity*
*Mass* *Intensity*
*Mass* *Intensity*
*Mass* *Intensity*

The mass/intensity pairs are separated by a tab.

# Export SEQUEST file

MassLynx has a facility to convert files into a format which can be used by the "SEQUEST" program. The "SEQUEST" program correlates uninterpreted tandem mass spectra of peptides with amino acid sequences from protein and nucleotide databases. It is written by Jimmy Eng and John Yates (University of Washington). Further details can be obtained via the Internet at http://thompson.mbt.washington.edu/sequest.

## To Export a SEQUEST file

1. Display the relevant centered MS/MS data file select **Export SEQUEST file** from the **File** menu.

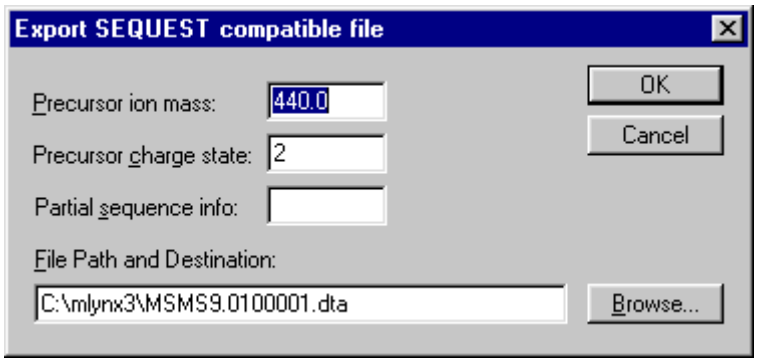



***Figure 2*** *Export SEQUEST dialog*

2. The **Precursor ion mass** is picked up from the data file, if it was entered in the Function Editor, otherwise type in a value.

3. The **Precursor charge state** defaults to 2, change this as required.

4. Enter any known sequence information in the **Partial sequence info** box.

5. **File Path and Destination** is the location and filename that the file will be saved to. The file name is the original file name with the scan and function numbers appended to it. To change the destination press the **Browse** button and select a new destination from the dialog displayed, or type a new one in.

6. Press the **OK** button.

**Note**: this option is only enabled if BioLynx is installed.

The file produced is an ASCII text file with the following format.

*Precursor mass Charge*
*Mass Intensity*
*Mass Intensity*
*Mass Intensity*
*Mass Intensity*

The mass/intensity pairs are separated by a space.

# OpenLynx Batch Files

OpenLynx Batch files ( *.olb) are produced when samples are submitted from the OpenLynx Login program. When created they are stored in the Masslynx\Openlynx\BatchDB folder. When they have been acquired and processed they are moved to the Masslynx\Openlynx\BatchDB\Processed folder.

## Paragraphs

The file will hold section blocks of data called paragraphs. A file will have a "Batch" paragraph and at least one "Plate" paragraph, followed by a paragraph for each sample to be analysed. Where there is more than one plate in an analysis, there will be a paragraph for each plate followed by sample paragraphs for each sample.

A paragraph will always start with the name of the section surrounded by square parentheses on a line by itself. i.e. [*SectionName*].

e.g. [*SectionName1*]
....Data Item 1...
....Data Item 2…
[*SectionName2*]
….Data Item 1…
….Data Item 2…

A typical multi-plate analysis file would be arranged as follows

[Batch]
….Data Item 1…
….Data Item 2…
[Plate:1]
....Data Item 1...
....Data Item 2…

[Sample:1.1]
....Data Item 1...
....Data Item 2…

[Sample:1.n]
....Data Item 1...
....Data Item 2…
[Plate:2]
....Data Item 1...
....Data Item 2…
[Sample:2.1]
....Data Item 1...
....Data Item 2…
[Sample:2.n]
....Data Item 1...
....Data Item 2…
[Plate:m]
....Data Item 1...
....Data Item 2…

[Sample:m.1]

....Data Item 1...
....Data Item 2…

[Sample:m.n]

....Data Item 1...
....Data Item 2…

## Batch Block

The first paragraph in the file will contain information that is pertinent to the whole batch.

MSMethod
MSTune
LCMethod
EconomyScheduling
PriorityScheduling
AnalysisTime
ProcessParameters
Process
UserName
BatchID
UserAddress
SampleReportEnable
NumberOfPlates

## Plate Block

A file will contain a plate block for each plate which will contain information that is pertinent to the whole plate rather than a specific well. Within this plate block will be information concerning the plate description, plate ID and wells used. Where samples are not being presented in a plate this block can be used to describe the batch of samples loaded into an autosampler carousel.

JobCode
UserName
Rows
Columns
Track
NumberOfWells

## Sample Block

For each sample to be analysed there will be a sample block that contains well position, and other information, specific to a certain sample.

Well
SampleDescription
Conditions
SampleID
MSDataName
SampleType
MSInjectionVolume
NumberOfMasses
Mass1
NumberOfFractions
NumberOfWaveLengths
NumberOfConcs
NumberOfFormulae
NumberOfFactors
NumberOfUserFields

## Fields

Sections will have a group of fields, each field will be on one line. The field name will be the first item on the line, followed by "=" and then the data item for that field. The type of data will depend on the field type.

i.e. [*SectionName*]
*FieldName1=Data1*
*FieldName2=Data2*
...

e.g. [Plate:3]
JobCode=JB123456
NumberOfWells=96

## Comments

A comment line is denoted by the first character being a semi-colon. A comment line can be any where in a section. Multiple line comments must have a semi-colon preceding each line.

# File Format

### [Batch]

When creating files manually the fields marked an (M) must be defined, all other fields are optional.

| Field/Section Name | Data Type | Description |
|---|---|---|
| NumberOfPlates (M) | Integer | Number of plates in analysis. |
| LabName | Text | Laboratory name. |
| MSMethod | Text | The name of the MS method to be used. |
| MSTune | Text | The name of the MS Tune file to be used. If not specified the current instrument tuning parameters will be used. |
| LCMethod | Text | The name of the acquisition Inlet method to be used. |
| InletPreRunMethod | Text | The name of the acquisition Inlet prerun method to be used. If not specified no prerun is performed. |
| InletPostRunMethod | Text | The name of the acquisition Inlet postrun method to be used. If not specified no postrun is performed. |
| InletSwitchMethod | Text | The name of the acquisition Inlet column switch method to be used. If not specified no switch method is performed. |
| Process | Text | Path of External Program to be executed for sample processing. Directory is not necessary if file exists in current directory. |
| ProcessParameters | Text | Path of Parameter File to be used by External Program. |
| EconomyScheduling | Integer | None zero if batch is to be run as a Night-Time task. Otherwise will be scheduled normally. |
| PriorityScheduling | Integer | None zero if batch is to be run as a Priority task. Otherwise will be scheduled normally. |
| AnalysisTime | Float | Time of analysis for each sample in the batch. Equals zero if no time is specified. |
| BatchID | Text | Name of batch. |
| UserName | Text | Name of user submitting batch. |
| UserAddress | Text | E-mail address to send batch results to. |
| ReportScheme | Text | Name of the OpenLynx Browser report scheme to use when formatting output results. |
| SampleReportEnable | Boolean | Indicates if per sample printing is required. 0 = False, 1 = True |
| HPLCMethod | Text | Path of HPLC method parameter override file if one exists. |

**[Plate:N]**

Where N = Plate Number

| Field/Section Name | Data Type | Description |
|---|---|---|
| PlateID | Text | Plate Identifier. A text description of the plate can be defined in files created externally. This is not generated in files created from the OpenLynx Login program. |
| PlatePosition | Text | The description of the plate position, as co-ordinates for plate position in the autosampler bed.<br><br>1. X,Y.<br><br>2. Not used for a linear autosampler e.g. HP GC type.<br><br>Where X and Y are integers. |
| Origin | Text | The description of the start well position, as a pair of co-ordinates for well position in plate, or an absolute position<br><br>WellAwellX(or wellXwellA ) e.g. A1<br><br>Where X is an integer and A is an alphabetical character.<br><br>Or<br><br>TL=Top Left, TR=Top Right, BL=Bottom Left, BR=Bottom Right |
| JobCode | Text | Job or Batch Identifier. |
| UserName | Text | Name of operator performing analysis. |
| Rows (M) | Integer | Number of rows on plate |
| Columns (M) | Integer | Number of columns on plate |
| Track (M) | Text | R=Rows, C=Columns, RS=Rows Snake, CS=Columns Snake |
| NumberOfWells (M) | Integer | Number of wells used in plate or vials in an autosampler tray |

**[Sample:N:M]**

Where N = Plate Number, M = Well Number

| Field/Section Name | Data Type | Description |
|---|---|---|
| Well (M) | Text | The description of the well position, as co-ordinates for well position in plate, or an absolute position. There are two formats for a Well. This field can be used to identify a vial position in a non XY autosampler.<br><br>1. wellAwellY (or wellYwellA ) e.g. B6, 6B or 2,6.<br><br>2. Absolute rack position. e.g. 18<br><br>Where X and Y are integers and A is an alphabetical character. |
| SampleType | Integer | Sample type<br><br>0 = Unknown, 1 = Standard, 2 = QC and 3 = Blank. |
| NumberOfMasses | Integer | The number of masses defined. |
| Mass1 | Float | 1st mass to be used for targeting. This could be the mono-isotopic mass or the mass with the greatest intensity, derived from the formula's isotope cluster. If the analysis being performed by the MS requires an expected molecular weight then this field is **Mandatory** unless a formula is supplied. |
| Mass2 | Float | 2nd Mass. |
| MassN | Float | Nth Mass. |
| NumberOfFraction Triggers | Integer | The number of fractions defined. Only one fraction mass is currently supported by MassLynx. |
| Fraction1 | Float | 1St Mass to be monitored by Fraction Collection system. |
| Fraction2 | Float | Second Fraction Mass. Not currently used. |
| FractionN | Float | Nth Fraction Mass |
| NumberOfFormulae | Integer | The number of formulae defined. |
| Formula1 | Text | The 1st chemical composition, if used. |
| Formula2 | Text | The 2nd chemical composition |
| FormulaN | Text | The Nth chemical composition |
| NumberOfWavelengths | Integer | The number of wavelengths defined. |
| Wavelength1 | Text | The 1st wavelength, if used. |
| Wavelength2 | Text | The 2nd wavelength |

| Field/Section Name | Data Type | Description |
|---|---|---|
| WavelengthN | Text | The $N^{th}$ wavelength |
| NumberOfConcs | Integer | The number of concentrations defined. |
| Conc1 | Text | The $1^{st}$ concentration, if used. |
| Conc2 | Text | The $2^{nd}$ concentration |
| ConcN | Text | The $N^{th}$ concentration |
| NumberOfFactors | Integer | The number of user factors defined. |
| Factor1 | Float | $1^{St}$ User Factor if required. MassLynx currently only supports 1 User Factor. |
| Factor2 | Float | The $2^{nd}$ User Factor. Not currently used. |
| FactorN | Float | $N^{th}$ User Factor. Not currently used. |
| SampleID | Text | Sample Identifier |
| SampleDescription | Text | Sample Description |
| Conditions | Test | Sample conditions |
| MSDataName | Text | The name of the MS data file to be processed and/or created. |
| MSInjectionVolume | Float | The amount of sample to inject, for an MS analysis. |
| NumberOfUserFields | Integer | The number of user fields defined. |
| User1 | Text | $1^{St}$ User Field, if required. |
| User2 | Text | The $2^{nd}$ User Field. |
| UserN | Text | $N^{th}$ User Field. |

# OpenLynx Browser

## Sections

The file will hold section blocks of data. The start of a section block will always start with the name of the section surrounded by square parentheses on a line by itself. i.e. [*SectionName*].

The main body of the data will be enclosed by a pair of braces, the opening and closing braces will be the only characters on their respective lines.

i.e. [*SectionName*]
{
....Data...
}

Section blocks can have section blocks embedded in them, in some cases multiple instances of sections with the same name can be allowed, depending on the type of data.

e.g. [*SectionName1*]
{
....Data...
[*SectionName2*]
{
....Data...
}
}

## Fields

Sections will have a group of fields, each field will be on one line. The field name will be the first item on the line, followed by a list of TAB separated data items for that field. The type of data will depend on the field type.

i.e. [*SectionName*]
{
*FieldName1* *Data1*
*FieldName2* *Data2_1Data2_2*
...
}

## Comments

A comment line is denoted by the first character being a semi-colon. A comment line can be any where in a section. Multiple line comments have a semi-colon preceding each line.

## Tabulated Sections

Some sections can be considered to be a table, or list, of fields of the same type. Tabulated sections do not have any field names to describe the data but will normally have a comment line describing the names of the fields.

e.g. [*TableSection*]
{
;*Field1 Field2*
*Data1_1Data1_2*
*Data2_1Data2_2*
...
}

## Free Format Text Sections

The information in these sections contains free format text which may stretch over several lines. A line will be terminated with a <carriage return><linefeed> pair.

# File Section Descriptions

### SAMPLE

| Field/Section Name | Data Type | Description |
|---|---|---|
| Sample | Integer | The number of the sample in the batch. |
| Well | Text | The description of the well position, as a pair of co-ordinates for plate position in rack and well position in plate, or an absolute position. There are three formats for Well.<br>1. plateX,plateY:wellX,wellY<br>2. plateX,plateY:wellAwell1 (or well1wellA )<br>3. Absolute rack position.<br>Where X and Y are integers and A is an alphabetical character. |
| FileName | Text | The MassLynx NT MS data file name. |
| SampleType | Integer | Sample type: Unknown = 0, Standard = 1, QC = 2 or Blank = 3. |
| SampleID | Text | MassLynx Sample List input field. |
| SampleDescription | Text | MassLynx Sample List input field. |
| Date | Text | Date that MS data file was acquired. |
| Time | Text | Time that MS data file was acquired. |
| JobCode | Text | MassLynx Sample List input field. |
| TaskCode | Text | MassLynx Sample List input field. |
| UserName | Text | Current MassLynx user name. |
| LabName | Text | Laboratory name. |
| Instrument | Text | Instrument name. |
| Conditions | Text | MassLynx Sample List input field. |
| Submitter | Text | MassLynx Sample List input field. |
| Plate | Text | Description of micro-titre plate, if applicable. See below for detailed description. |
| INLET PARAMETERS | Section | Description of compound for testing. |
| COMPOUND | Section | Description of compound for testing. |
| FRACTION | Section | Results of any FractionLynx fraction collection. |
| FUNCTION | Section | MS function data and test results. There will be one FUNCTION section per MassLynx MS and DAD data functions. |
| ANALOG | Section | Analogue chromatographic data. |

**PLATE FIELD**

For samples acquired using a Gilson or Waters 2700 autosampler the following information will be written to the file, otherwise this field will be blank.

Version Number ( two digits )

Origin Location ( TL - top left, TR - top right, BL - bottom left, BR - bottom right )

Priority ( XY - x coordinate before y coordinate, YX - y coordinate before x coordinate )

Reference scheme ( LN - letter number, NL - number letter, NN - number number, LL - letter letter, SC - sequential continuous, SD sequential discontinuous )

1:Number Of Rows

2:Number Of Columns

3:Row Spacing

4:Column Spacing

5:Row Offset

6:Column Offset

7:Which Rows Offset ( O or E )

8:Which Columns Offset ( O or E )

9:Plate Width

10:Plate Height

11:Vial/Well Depth

12:Vial/Well Diameter

13:Vial One X

14:Vial One Y

Note that all spacings, etc are given to 0.1 of a mm.

e.g.

01,TL,XY,LN,1:8,2:12,3:120.0,4:120.0,5:0.0,6:0.0,7:O,8:O,9:1250.0,10:870.0,11:400.0,12:90.0,13:80.0,14:130.0

Which means:

Version = 01.

Origin Location = top left.

Priority = x coordinate before y coordinate.

Reference scheme = Letter Number.

1:Number Of Rows = 8.

2:Number Of Columns = 12.

3:Row Spacing = 12mm.

4:Column Spacing = 12mm.

5:Row Offset = 0.0mm.

6:Column Offset = 0.0mm.

7:Which Rows Offset ( O or E ) = Odd numbers, but because Row Offset = 0, this has no effect .

8:Which Columns Offset ( O or E ) = Odd numbers, but because Column Offset = 0, this has no effect.

9:Plate Width = 125mm.

10:Plate Height = 87mm.

11:Vial/Well Depth = 40mm.

12:Vial/Well Diameter = 9mm.

13:Vial One X = 8.0mm.

14:Vial One Y = 13.0mm.

### COMPOUND

| Field Name | Data Type | Description |
|---|---|---|
| Mono Mass | Float | The mass used for targeting. This could be the mono-isotopic mass or the mass with the greatest intensity, derived from the formula's isotope cluster. |
| Formula | Text | The chemical composition, if entered. |
| Name | Text | The name of the compound. Unused at present. |

### FRACTION

| Field Name | Data Type | Description |
|---|---|---|
| Mass | Float | The mass collected. |
| Org. Target | Float | The original mass minus any adducts. |
| Ion Mode | Text | The ionisation mode used to collect the fraction. |
| Start Time | Float | The time at which the fraction collection started. |
| End Time | Float | The time at which the fraction collection ended. |
| Start Site | Text | The name of the site at which the fraction collection started. |
| No. Of Tubes | Integer | The number of tubes the fraction was collected in. |

### INLET PARAMETERS

This is a free format text section.

### FUNCTION

| Field/Section Name | Data Type | Description |
|---|---|---|
| Function | Integer | The MassLynx MS data function number. |
| IonMode | Text | The type of ionisation mode e.g. AP+. |
| Type | Text | The type of MS scan function e.g. MS for full scan. |
| Description | Text | A brief description of the MS scan function. |
| SPECTRUM | Section | MS data and results of testing. There can be more than one SPECTRUM section in a function. |
| CHROMATOGRAM | Section | Chromatographic data. There can be more than one CHROMATOGRAM section in a function. |

### SPECTRUM

| Field/Section Name | Data Type | Description |
|---|---|---|
| ProcDesc | Text | Description of processing performed on spectrum. E.g. Combine (54:56-(38:39+74:75)) |
| Process | Integer | The number of the MassLynx saved mass spectrum. Only present if the processed spectrum was saved with data file. |
| State | Text | The result of testing the quality of the mass spectral data. |
| Peak ID | Integer | Spectrum Peak Identification number. |
| Peak Ref | Integer | Peak Reference Number. |
| Time | Float | The retention time of the mass spectrum. |
| TIC | Float | Total Ion Current, the sum of all the peak intensities in the spectrum. |
| BPI | Float | The intensity of the base peak in the mass spectrum. |
| BPM | Float | The mass of the base peak in the mass spectrum. |
| Continuum | Text | TRUE if the spectrum is stored in continuum format. Otherwise FALSE. |
| Saved | Text | TRUE if the processed spectrum was saved with the data file. Otherwise FALSE. |
| MASSES | Section | Section describing the results of testing, and finding significant masses. This includes all adducts. |
| RESULTS | Section | Section describing the results of the targeting of the expected compound. Masses from the same compound are combined into one item. |
| MS | Section | Section that holds all the mass/intensity pairs, for this mass spectrum. |
| SEARCH | Section | Section holding the results of a library search on this spectrum. This section will not be created if no search exists. |

### MASSES

| Field Name | Data Type | Description |
|---|---|---|
| Mass | Float | The input mass. |
| Exp. Mass | Float | The expected mass due to adduction. |
| Obs. Mass | Float | The mass that was actually observed. |
| % BPI | Float | The intensity of the mass peak as a percentage of the base peak intensity. |
| Int. Abs | Float | The absolute intensity of the MS peak. |

### RESULTS

| Field Name | Data Type | Description |
|---|---|---|
| Mass | Float | The input mass. |
| Found | Boolean | 1 if any of the possible adduct ions have been found for this compound, otherwise 0 |
| % BPI | Float | The sum of the percentage intensities for the compound. |
| % Purity | Float | A measure of the contribution of this compound to the spectrum as percentage of the TIC. This includes all MS peaks associated with this compound. |
| Confirmed | Boolean | False if any of the confirmation tests made failed. If not specified regarded as being True. |
| Status | Text | Description of confirmation failure. Not present if confirmed = TRUE |

### MS

| Field Name | Data Type | Description |
|---|---|---|
| Mass | Float | Observed mass of peak. |
| % BPI | Float | Intensity of peak as a percentage of the base peak. |

### ELEMENTAL

Contains results of elemental calculations if defined, otherwise this section does not appear.

| Field Name | Data Type | Description |
|---|---|---|
| Mass | Float | Actual observed mass for which elemental composition was searched. |
| Calc. Mass | Float | Calculated mass of reported formula |
| mDa | Float | Difference between observed mass and calculated mass in milli-daltons |
| PPM | Float | Difference between observed mass and calculated mass in parts per million |
| DBE | Float | Double Bond Equivalence. |
| Formula | Text | Representation of calculated chemical formula. E.g. C19 H14 O2 |

### SEARCH

Contains Spectrum library search results if library search was defined, otherwise this section does not appear.

| Field Name | Data Type | Description |
|---|---|---|
| Library | Text | Name of library in which the search was made. |
| HIT | Section | Contains information about a library hit. There can be several or no hits for each search |

### HIT

| Field Name | Data Type | Description |
|---|---|---|
| Entry | Integer | Library entry number hit was made against. |
| For | Integer | Forward search match value. Value between 0 and 1000. |
| Rev | Integer | Reverse search match value. Value between 0 and 1000. |
| Name | Text | Library entry name |
| F1 | Float | Library entry general purpose filter 1 value. |
| F2 | Float | Library entry general purpose filter 2 value. |
| Mass | Float | Library entry mass value. |

### CHROMATOGRAM

| Field/Section Name | Data Type | Description |
|---|---|---|
| TraceNumber | Integer | Number of chromatogram trace. |
| Description | Text | The description of the chromatogram type. |
| ProcDesc | Text | Description of processing performed on chromatogram. E.g. Smooth (Mn, 2x2) |
| MaxIntensity | Float | The absolute intensity of the point with maximum intensity in the chromatographic data. |
| TRACE | Section | A section that holds the chromatographic data. |
| PEAK | Section | Section(s) that hold information about peak(s) detected in the chromatogram. |

### TRACE

| Field Name | Data Type | Description |
|---|---|---|
| Time | Float | The time of the chromatographic point. |
| Int. %Max | Float | Intensity of the chromatographic point as a percentage of the maximum intensity. |

**PEAK**

| Field Name | Data Type | Description |
|---|---|---|
| Peak ID | Integer | Peak Identification number. |
| Peak Ref | Integer | Peak Reference Number. |
| Time | Float | Peak retention time in decimal minutes. |
| Peak | Float + Float | Peak start and end retention times in decimal minutes. Two floats separated by a TAB character. |
| Intensity | Float + Float | Peak baseline start and end intensity. Two floats separated by a TAB character. |
| Height | Float | Detected peak height. |
| AreaAbs | Float | Detected peak area. |
| Area %BP | Float | Detected peak area as percentage of the largest peak in the chromatogram. |
| Area %Total | Float | Detected peak area as percentage of the sum of all the peak areas in the chromatogram. |
| Width | Float | Peak width in decimal minutes. |
| RT Index | Float | Retention time index for peak. Field only output if RT Index has been calculated. |
| RT LogP | Float | Retention time LogP for peak. Field only output if RT LogP has been calculated. |
| Calc Conc | Float | Calculated concentration for peak. Field only output if calculated. |
| Calc Amount | Float | Calculated amount for peak. Field only output if calculated. |

**ANALOG**

| Field/Section Name | Data Type | Description |
|---|---|---|
| Number | Integer | The number of the MassLynx analog channel. |
| Description | Text | The description of the analog data source. |
| MaxIntensity | Float | The absolute intensity of the point with maximum intensity in the analog channel data. |
| TRACE | Section | A section that holds the chromatographic data. See description above. |
| PEAK | Section | Section(s) that hold information about peak(s) detected in the chromatogram. See description above. |

# MetaboLynx Browser

## Sections

The file will hold section blocks of data. The start of a section block will always start with the name of the section surrounded by square parentheses on a line by itself. i.e. [*SectionName*].

The main body of the data will be enclosed by a pair of braces, the opening and closing braces will be the only characters on their respective lines.

i.e. [*SectionName*]
{
....Data...
}

Section blocks can have section blocks embedded in them, in some cases multiple instances of sections with the same name can be allowed, depending on the type of data.

e.g. [*SectionName1*]
{
....Data...
[*SectionName2*]
{
....Data...
}
}

## Fields

Sections will have a group of fields, each field will be on one line. The field name will be the first item on the line, followed by a list of TAB separated data items for that field. The type of data will depend on the field type.

i.e. [*SectionName*]
{
*FieldName1* *Data1*
*FieldName2* *Data2_1Data2_2*
...
}

## Comments

A comment line is denoted by the first character being a semi-colon. A comment line can be any where in a section. Multiple line comments have a semi-colon preceding each line.

## Tabulated Sections

Some sections can be considered to be a table, or list, of fields of the same type. Tabulated sections do not have any field names to describe the data but will normally have a comment line describing the names of the fields.

e.g. [*TableSection*]
{
;*Field1 Field2*
*Data1_1Data1_2*
*Data2_1Data2_2*
...
}

## Free Format Text Sections

The information in these sections contains free format text which may stretch over several lines. A line will be terminated with a <carriage return><linefeed> pair.

# File Section Descriptions

### SAMPLE

| Field/Section Name | Data Type | Description |
|---|---|---|
| Sample | Integer | The number of the sample in the batch. |
| ProcessParameters | Text | MassLynx Sample List input field. Name of the MEP file used to process the data. |
| InjectionVolume | Float | MassLynx Sample List input field. Volume of sample injected, in micro-litres. |
| InletFileName | Text | MassLynx Sample List input field. Name of the Inlet Parameters file used to acquire the data. |
| MSMethodFileName | Text | MassLynx Sample List input field. Name of the Method File used to acquire the data. |
| MSTuneFileName | Text | MassLynx Sample List input field. Name of the Instrument Tune File used for the data acquisition. |
| Well | Text | The description of the well position, as a pair of co-ordinates for plate position in rack and well position in plate, or an absolute position. There are three formats for Well.<br><br>1. plateX,plateY:wellX,wellY<br><br>2. plateX,plateY:wellAwell1 (or well1wellA )<br><br>3. Absolute rack position.<br><br>Where X and Y are integers and A is an alphabetical character. |
| FileName | Text | The MassLynx NT MS data file name. |
| SampleType | Text | QC = Control Sample, Analyte = metabolised sample. |
| SampleID | Text | MassLynx Sample List input field. |
| SampleDescription | Text | MassLynx Sample List input field. |
| Date | Text | Date that MS data file was acquired. |
| Time | Text | Time that MS data file was acquired. |
| JobCode | Text | MassLynx Sample List input field. |
| TaskCode | Text | MassLynx Sample List input field. |
| UserName | Text | Current MassLynx user name. |
| LabName | Text | Laboratory name. |

| Field/Section Name | Data Type | Description |
|---|---|---|
| Instrument | Text | Instrument name. |
| Conditions | Text | MassLynx Sample List input field. |
| Submitter | Text | MassLynx Sample List input field. |
| Plate | Text | Description of micro-titre plate, if applicable. See below for detailed description. |
| COMPOUND | Section | Description of parent drug(s); the masses taken from the MassLynx Sample List. |
| FUNCTION | Section | MS function data and test results. There will be one FUNCTION section per MassLynx MS and DAD data functions. |
| ANALOG | Section | Analogue chromatographic data. |
| EXPECTED METABOLITES | Section | Description of metabolites searched for. |
| UNEXPECTED METABOLITES | Section | Description of potential metabolites found as a result of comparing the sample with a control. |

**PLATE FIELD**

For samples acquired using a Gilson or Waters 2700 autosampler the following information will be written to the file, otherwise this field will be blank.

Version Number ( two digits )

Origin Location ( TL - top left, TR - top right, BL - bottom left, BR - bottom right )

Priority ( XY - x coordinate before y coordinate, YX - y coordinate before x coordinate )

Reference scheme ( LN - letter number, NL - number letter, NN - number number, LL - letter letter, SC - sequential continuous, SD sequential discontinuous )

1:Number Of Rows

2:Number Of Columns

3:Row Spacing

4:Column Spacing

5:Row Offset

6:Column Offset

7:Which Rows Offset ( O or E )

8:Which Columns Offset ( O or E )

9:Plate Width

10:Plate Height

11:Vial/Well Depth

12:Vial/Well Diameter

13:Vial One X

14:Vial One Y

Note that all spacings, etc are given to 0.1 of a mm.

e.g.

01,TL,XY,LN,1:8,2:12,3:120.0,4:120.0,5:0.0,6:0.0,7:O,8:O,9:1250.0,10:870.0,11:400.0,12:90.0,13:80.0,14:130.0

Which means:

Version = 01.

Origin Location = top left.

Priority = x coordinate before y coordinate.

Reference scheme = Letter Number.

1:Number Of Rows = 8.

2:Number Of Columns = 12.

3:Row Spacing = 12mm.

4:Column Spacing = 12mm.

5:Row Offset = 0.0mm.

6:Column Offset = 0.0mm.

7:Which Rows Offset ( O or E ) = Odd numbers, but because Row Offset = 0, this has no effect .

8:Which Columns Offset ( O or E ) = Odd numbers, but because Column Offset = 0, this has no effect.

9:Plate Width = 125mm.

10:Plate Height = 87mm.

11:Vial/Well Depth = 40mm.

12:Vial/Well Diameter = 9mm.

13:Vial One X = 8.0mm.

14:Vial One Y = 13.0mm.

### COMPOUND

| Field Name | Data Type | Description |
|---|---|---|
| Mono Mass | Float | The parent drug used for targeting. This could be the monoisotopic mass or the mass with the greatest intensity, derived from the formula's isotope cluster. |
| Formula | Text | The chemical composition, if entered. |

### FUNCTION

| Field/Section Name | Data Type | Description |
|---|---|---|
| Function | Integer | The MassLynx MS data function number. |
| IonMode | Text | The type of ionisation mode e.g. AP+. |
| Type | Text | The type of MS scan function e.g. MS for full scan. |
| Description | Text | A brief description of the MS scan function. |
| ScanCycleTime | Float | The scan cycle time in seconds i.e. the scan duration + the inter-scan delay time. |
| InterScanDelay | Float | The inter-scan delay in seconds. |
| SPECTRUM | Section | MS data and results of testing. There can be more than one SPECTRUM section in a function. |
| CHROMATOGRAM | Section | Chromatographic data. There can be more than one CHROMATOGRAM section in a function. |

### SPECTRUM

| Field/Section Name | Data Type | Description |
|---|---|---|
| ProcDesc | Text | Description of processing performed on spectrum. E.g. Combine (54:56-(38:39+74:75)) |
| Process | Integer | The number of the MassLynx saved mass spectrum. Only present if the processed spectrum was saved with data file. |
| State | Text | The result of testing the quality of the mass spectral data. |
| Peak ID | Integer | Spectrum Peak Identification number. |
| Peak Ref | Integer | Peak Reference Number. |
| Peak Cluster ID | Integer | If this peak is considered to be the same as another peak (according to Setup parameter Min Peak Separation) then this is the number of the cluster containing this and all other similar peaks. A value of –1 indicates that this peak is considered separate from all others. |
| Control Peak ID | Integer | If the sample is an analyte and this spectrum matches one in the control, then the Peak ID of the control spectrum is written to this field. Only present if this spectrum has a matching control spectrum. |
| Time | Float | The retention time of the mass spectrum. |
| TIC | Float | Total Ion Current, the sum of all the peak intensities in the spectrum. |
| BPI | Float | The intensity of the base peak in the mass spectrum. |
| BPM | Float | The mass of the base peak in the mass spectrum. |
| Continuum | Text | TRUE if the spectrum is stored in continuum format. Otherwise FALSE. |
| Saved | Text | TRUE if the processed spectrum was saved with the data file. Otherwise FALSE. |
| MASSES | Section | Section describing the results of testing, and finding significant masses. This includes all adducts. |
| RESULTS | Section | Section describing the results of the targeting of the expected compound. Masses from the same compound are combined into one item. |
| MS | Section | Section that holds all the mass/intensity pairs, for this mass spectrum. |

### MASSES

| Field Name | Data Type | Description |
|---|---|---|
| Mass | Float | The input mass. |
| Exp. Mass | Float | The expected mass due to adduction. |
| Obs. Mass | Float | The mass that was actually observed. |
| % BPI | Float | The intensity of the mass peak as a percentage of the base peak intensity. |
| Int. Abs | Float | The absolute intensity of the MS peak. |

### RESULTS

| Field Name | Data Type | Description |
|---|---|---|
| Mass | Float | The input mass. |
| Found | Boolean | 1 if any of the possible adduct ions have been found for this compound, otherwise 0. |
| % BPI | Float | The sum of the percentage intensities for the compound. |
| % Purity | Float | A measure of the contribution of this compound to the spectrum as percentage of the TIC. This includes all MS peaks associated with this compound. |
| Confirmed | Boolean | False if any of the confirmation tests made failed. If not specified regarded as being True. |
| Status | Text | Description of confirmation failure. Not present if confirmed = TRUE |

### MS

| Field Name | Data Type | Description |
|---|---|---|
| Mass | Float | Observed mass of peak. |
| % BPI | Float | Intensity of peak as a percentage of the base peak. |

### ELEMENTAL

Contains results of elemental calculations if defined, otherwise this section does not appear.

| Field Name | Data Type | Description |
|---|---|---|
| Mass | Float | Actual observed mass for which elemental composition was searched. |
| Calc. Mass | Float | Calculated mass of reported formula |
| Mda | Float | Difference between observed mass and calculated mass in milli-daltons |
| PPM | Float | Difference between observed mass and calculated mass in parts per million |
| DBE | Float | Double Bond Equivalence. |
| Formula | Text | Representation of calculated chemical formula. E.g. C19 H14 O2 |

### CHROMATOGRAM

| Field/Section Name | Data Type | Description |
|---|---|---|
| TraceNumber | Integer | Number of chromatogram trace. |
| Description | Text | The description of the chromatogram type. |
| ProcDesc | Text | Description of processing performed on chromatogram. E.g. Smooth (Mn, 2x2) |
| MaxIntensity | Float | The absolute intensity of the point with maximum intensity in the chromatographic data. |
| TraceNumberIn Function | Integer | The number of the chromatogram trace relative to the start of the function. |
| TRACE | Section | A section that holds the chromatographic data. |
| PEAK | Section | Section(s) that hold information about peak(s) detected in the chromatogram. |

### TRACE

| Field Name | Data Type | Description |
|---|---|---|
| Time | Float | The time of the chromatographic point. |
| Int. %Max | Float | Intensity of the chromatographic point as a percentage of the maximum intensity. |

### PEAK

| Field Name | Data Type | Description |
|---|---|---|
| Peak ID | Integer | Peak Identification number. |
| Peak Ref | Integer | Peak Reference Number. |
| Peak Cluster ID | Integer | If this peak is considered to be the same as another peak (according to Setup parameter Min Peak Separation) then this is the number of the cluster containing this and all other similar peaks. A value of –1 indicates that this peak is considered separate from all others. |
| Time | Float | Peak retention time in decimal minutes. |
| Peak | Float + Float | Peak start and end retention times in decimal minutes. Two floats separated by a TAB character. |
| Intensity | Float + Float | Peak baseline start and end intensity. Two floats separated by a TAB character. |
| Height | Float | Detected peak height. |
| AreaAbs | Float | Detected peak area. |
| Area %BP | Float | The peak area as a percentage of the largest peak in the sample in which a metabolite was detected. If no metabolite found = 0. |
| Area %Total | Float | The peak area as a percentage of the total area of all peaks in the sample in which a metabolite was detected. If no metabolite found = 0. |
| Width | Float | Peak width in decimal minutes. |

### ANALOG

| Field/Section Name | Data Type | Description |
|---|---|---|
| Number | Integer | The number of the MassLynx analog channel. |
| Description | Text | The description of the analog data source. |
| MaxIntensity | Float | The absolute intensity of the point with maximum intensity in the analog channel data. |
| TRACE | Section | A section that holds the chromatographic data. See above. |
| PEAK | Section | Section(s) that hold information about peak(s) detected in the chromatogram. See above. |

### EXPECTED METABOLITES

This is a tabulated section.

| Field Name | Data Type | Description |
|---|---|---|
| Compound | Float | The number of the compound that this metabolite is associated with, starting from zero. |
| Precursor | Float | Mass to be searched for, the sum of the compound and metabolite. |
| Metabolite | Float | Mass of the metabolite, as specified on the MetaboLynx Setup Metabolites page. It is the mass difference between the Compound Mass and the Precursor. |
| Found | Boolean | 1 indicates mass was found, 0 not found. |
| Formula | Text | The formula of the metabolite if known. Absolute formula if the parent mass was specified as a formula (e.g. C18H24O2) or relative formula if parent mass was specified as a mass (e.g. +CO2). If the metabolite is not recognised the formula is 0. |
| ChroTrace | Integer list | This field is a comma-separated list of chromatogram traces searched when looking for this mass; the trace numbers start from 1. |
| Peak | Text list | If the mass was found, this field is a comma-separated list of chromatogram peak numbers in which the mass was found. Each peak is identified by a string of text containing four forward slash separated numbers in the following format:<br><br>*peak-number*/*function-number*/*trace-number*/*mass-found*<br><br>where the first 3 numbers are integers, the fourth a float.<br><br>If the mass was not found, this field is 0. |
| MetName | Text | Descriptive name of the metabolite |

### UNEXPECTED METABOLITES

This is a tabulated section.

| Field Name | Data Type | Description |
|---|---|---|
| Compound | Float | The number of the compound that this metabolite is associated with, starting from zero. |
| Precursor | Float | Mass to be searched for, the sum of the compound and metabolite. |
| Metabolite | Float | Mass of the metabolite, as specified on the MetaboLynx Setup Metabolites page. It is the mass difference between the Compound Mass and the Precursor. |
| Found | Boolean | 1 indicates mass was found, 0 not found. |
| Formula | Text | The formula of the metabolite if known. Absolute formula if the parent mass was specified as a formula (e.g. C18H24O2) or relative formula if parent mass was specified as a mass (e.g. +CO2). If the metabolite is not recognised the formula is 0. |
| ChroTrace | Integer list | This field is a comma-separated list of chromatogram traces searched when looking for this mass; the trace numbers start from 1. |
| Peak | Text list | If the mass was found, this field is a comma-separated list of chromatogram peak numbers in which the mass was found. Each peak is identified by a string of text containing four forward slash separated numbers in the following format:<br><br>*peak-number*/*function-number*/*trace-number*/*mass-found*<br><br>where the first 3 numbers are integers, the fourth a float.<br><br>If the mass was not found, this field is 0. |
| MetName | Text | Descriptive name of the metabolite |

# ProteinLynx Browser

## Sections

The file will hold section blocks of data. The start of a section block will always start with the name of the section surrounded by square parentheses on a line by itself. i.e. [*SectionName*].

The main body of the data will be enclosed by a pair of braces, the opening and closing braces will be the only characters on their respective lines.

e.g. [*SectionName*]
{
....Data...
}

Section blocks can have section blocks embedded in them, in some cases multiple instances of sections with the same name can be allowed, depending on the type of data.

e.g. [*SectionName1*]
{
....Data...
[*SectionName2*]
{
....Data...
}
}

## Fields

Sections will have a group of fields, each field will be on one line. The field name will be the first item on the line, followed by a list of TAB separated data items for that field. The type of data will depend on the field type.

i.e. [*SectionName*]
{
*FieldName1* *Data1*
*FieldName2* *Data2_1Data2_2*
...
}

## Tabulated Sections

Some sections can be considered to be a table, or list, of fields of the same type. Tabulated sections do not require any field names to describe the data.

e.g. [*TableSection*]
{
;*Field1 Field2*
*Data1_1Data1_2*
*Data2_1Data2_2*
...
}

# File Section Descriptions

### SAMPLE

**Note**: The fields may not appear in the same order as the table below and some empty fields will not appear at all.

| Field/Section Name | Data Type | Description |
|---|---|---|
| Sample | Integer | The number of the sample in the batch. |
| Well | Text | The description of the well position, as a pair of co-ordinates for plate position in rack and well position in plate, or an absolute position. There are three formats for Well.<br><br>1. wellX,wellY<br>2. wellAwell1 (or well1wellA )<br>3. Absolute rack position.<br><br>Where X and Y are integers and A is an alphabetical character. |
| Data_File_Name | Text | The MassLynx NT MS data file name. |
| Sample_ID | Text | MassLynx Sample ID. |
| Sample_Description | Text | MassLynx Sample description. |
| Spare1 | Text | User definable spare. |
| Spare2 | Text | User definable spare. |
| Spare3 | Text | User definable spare. |
| Spare4 | Text | User definable spare. |
| Spare5 | Text | User definable spare. |
| Date | Text | Date that MS data file was acquired. |
| Time | Text | Time that MS data file was acquired. |
| Job_Code | Text | MassLynx Sample List Jobcode field. |
| Task_Code | Text | MassLynx Sample List Taskcode field. |
| User_Name | Text | Current MassLynx user name. |
| Instrument | Text | Instrument name. |
| Plate | Text | Description of micro-titre plate, if applicable. |
| MS_File | Text | The MassLynx MS data file name. |
| Process_Parameters | Text | The MassLynx process parameter file name. |

| Field/Section Name | Data Type | Description |
|---|---|---|
| FUNCTION | Section | MS function data and results. There will be one FUNCTION section per MassLynx MS data functions. |

**FUNCTION**

| Field/Section Name | Data Type | Description |
|---|---|---|
| Function | Integer | The MassLynx MS data function number. |
| IonMode | Text | The type of ionisation mode e.g. AP+. |
| Type | Text | The type of MS scan function e.g. MS for full scan. |
| Description | Text | A brief description of the MS scan function. |
| PROCESS_PARAMETERS | Section | MS process parameter data and results. There will only be one PROCESS_PARAMETERS section in a FUNCTION. |
| SEARCH_PARAMETERS | Section | MS search parameter data. There will only be one SEARCH_PARAMETERS section in a FUNCTION. |
| SEARCH_RESULTS | Section | MS search results. There will only be one SEARCH_RESULTS section in a FUNCTION. |
| SPECTRUM | Section | MS raw spectrum data. There will only be one SPECTRUM in a function. **Note**: Only present for Maldi data. |
| PEAKLIST | Section | MSMS raw spectrum data. There will only be one PEAKLIST in a function. **Note**: Only present for MSMS data. |

### PROCESS_PARAMETERS

| Field Name | Data Type | Description |
|---|---|---|
| Do_Process | Boolean | 1 if processing has been performed, otherwise 0. |
| Combine_Mode | Text | Spectrum combine mode. |
| DoBackgroundSubtract | Boolean | 1 if background subtraction has been performed, otherwise 0. |
| PolynomialOrder | Int | Number indicating the polynomial order used in background subtraction. |
| BelowCurve | Int | Number indicating the below curve % used in background subtraction. |
| DoSmooth | Boolean | 1 if smoothing has been performed, otherwise 0. |
| SmoothChannels | Float | Number of channels smoothed. |
| NumberOfSmooths | Int | Number of smooths performed. |
| Smooth_Mode | Text | The smoothing method used. E.g. Savitzky-Golay |
| Min_Peak_Width | Int | Minimum spectral peak width. |
| Centroid_Percent | Float | Intensity of peak as a percentage of the base peak. |
| Centroid_Mode | Text | Spectrum centroid mode used. |
| PreCharge | Int | Pre charge state. |
| Min_Mass_To_Start | Float | Minimum start search mass. |
| Isotope_Factor | Float | Minimum isotopic factor value. |
| Relative_Deiso_Intensity | Int | The relative deiso intensity. |
| LockMassPeak_1 | Int | First lock mass value. |
| LockMassPeak_2 | Int | Second lock mass value.. |
| LockMassPeak_3 | Int | Third lock mass value. |

### SEARCH_PARAMETERS

| Field Name | Data Type | Description |
|---|---|---|
| Do_Search | Boolean | 1 if search performed, otherwise 0. |
| Database_Type | Text | Type of database searched. |
| Index_Path | Text | Path of database index. |
| Sequence_File | Text | Database sequence file name. |
| Trembl_Path | Text | Path of Trembl database |
| SearchServer | Text | Name of search server |
| Output_Type | Text | Type of output file. |
| PEAKLIST_location | Text | Location of Sequest output file. |
| MASS | Text | Location of mascot output file. |
| PepSea_location | Text | Location of PepSea output file. |
| MOWSE_location | Text | Location of mass intensity output file. |
| Organism | Text | Search organism. |
| Freetext | Text | Search free text. |
| Keyword | Text | Search key word. |
| Author | Text | Search author. |
| Accession | Text | The database accession code. |
| Subsequence | Text | Search sub sequence. |
| BileEqual | Boolean | 1 if treat I/L and Q/K as equivalent box checked, otherwise 0 |
| Do_Monoiso | Boolean | 1 if search monoisotopic peaks box checked, otherwise 0. |
| MAX_HITS | Integer | Maximum number of hits to return from the search. 0 if All selected. |
| SORT_TYPE | Text | BIO_SORT_PROB, BIO_SORT_LIKELIHOOD, BIO_SORT_ENTRY, BIO_SORT_COVERAGE or BIO_SORT_MATCH depending on the sort method. |
| Exclude_Lockmass | Boolean | 1 if lockmass excluded, otherwise 0. |
| Tolerance | Float | Peptide tolerance value. |
| Tolerance_Units | Text | Peptide tolerance units. |

| Field Name | Data Type | Description |
|---|---|---|
| Charge | Float | Peptide charge state. |
| MinToMatch | Int | Number of required matches. |
| Do_Digest | Boolean | 1 if digest simulation was performed, otherwise 0. |
| Fast_Digest_Reagent | Text | Name of digest reagent when using and index. |
| Digest_Index | Text | Digest index's file path and name. |
| Simulated_Digest_Reagent | Text | Name of primary digest reagent. |
| Secondary_Digest_Reagent | Text | Name of secondary digest reagent. |
| pFactor | Float | The pFactor value entered. |
| Missed_cleavages | Integer | Number of missed cleavage sites. |
| Do_Incomplete | Boolean | 1 if incomplete cleavage processing performed, otherwise 0. |
| Do_MW | Boolean | 1 if molecular weight restriction was specified, otherwise 0. |
| MW_from | Float | Molecular weight range minimum. |
| MW_to | Float | Molecular weight range maximum. |
| Do_PI | Boolean | 1 if isoelectric point restriction was specified, otherwise 0. |
| PI_from | Float | Isoelectric point range minimum. |
| PI_to | Float | Isoelectric point range maximum. |
| Do_Modifiers | Boolean | 1 if modification was specified, otherwise 0. |
| Reduced_cysteine | Boolean | 1 if reduced cysteine was specified, otherwise 0. |
| MODIFIERS | Section | Description of the modifiers used during processing. |

**MODIFIERS**

| Field Name | Data Type | Description |
|---|---|---|
| *Name of modifier* | Boolean | 1 if always use this modifier box checked, 0 if use when needed to match peptide box checked. |

### SEARCH_RESULTS

| Field Name | Data Type | Description |
|---|---|---|
| File_Name | Text | Search result file name with its full path |
| PRP_File_Name | Text | The hit section does not appear in this file but in the file named above. One HIT section defines one database Hit. There can be more than one HIT sections. |

### SPECTRUM

| Field/Section Name | Data Type | Description |
|---|---|---|
| LockMassUsed | Float | The lock mass value used |
| MONOISOMASSES | Section | MS monoisomasses data. There will only be one MONOISOMASSES in a SPECTRUM. |
| CORRECTION_FACTOR | Section | MS raw spectrum data. There will only be one CORRECTION_FACTOR in a SPECTRUM. |

### MONOISOMASSES

| Field Name | Data Type | Description |
|---|---|---|
| | Float | One monoisomass value per line. There can be more than one line |

### CORRECTION_FACTOR

| Field Name | Data Type | Description |
|---|---|---|
| Correction_Factor | Float | Correction factor applied to the whole spectrum. Calculated from the lock mass. |
| Offset_Factor | Float | Correction factor applied to the whole spectrum. Calculated from the lock mass. |
| ProcessHistory | Text | Process history information text string |

**PEAK_LIST**

| Field Name | Data Type | Description |
|---|---|---|
| Output_Filename | Text | The name of the Mascot or Sequest compatible peak information file.<br><br>e.g.<br><br>Mascot file<br><br>C:\TEMP\hilo07.004.2.1.pkl<br><br>where 004 = the scan number<br>2 = the function number<br>1 = the charge state<br><br>Sequest file<br><br>C:\MASSLYNX\hilo07.0100001.dta<br><br>where 0001 = the scan number<br>01 = the function number. |

## Bio-Rad File Descriptions

If the Bio-Rad box was checked then a SampleID.txt file is produced with the following format.

| Field Name | Data Type | Description |
|---|---|---|
| VIEW_ONE | Section | Database protein entry information. There will only be one VIEW_ONE section per HIT. |
| VIEW_TWO | Section | Database match information There will only be one VIEW_TWO section per HIT. |
| VIEW_THREE | Section | Database protein sequence There will only be one VIEW_THREE section per HIT. |

### VIEW_ONE

Some entries do not contain data on all the line types, and some line types occur many times in a single entry.

| Field Name | Description |
|---|---|
| ID | Identification line showing the entry name of the sequence. |
| AC | The accession number, a unique number used to identify entries. |
| DT | Date of entry or last modification. |
| DE | Description line containing general descriptive information. |
| GN | Gene name. |
| OS | The organism species line specifies the organism which was the source of the sequence. In most cases this is the Latin name followed by the English name (in parentheses). For viruses only the common English name is given. If the sequence is identical for more than one species the OS lines will list the names of all those species. |
| OG | The Organelle lines indicate if the gene coding for a protein originates from the mitochondria, the chloroplast, a cyanelle or a plasmid. |
| OC | The organism classification lines contain the taxonomic classification of the source organism. |
| RN | Reference number |
| RP | Reference position |
| RC | Reference comment |
| RX | Reference cross-reference |
| RA | Reference authors |
| RL | Reference location (Journal information) |
| CC | Comments or notes used to convey useful information. |
| DR | The database cross-reference lines are used as pointers to related information in other data collections. E.g. Protein Data Bank (PDB). |
| KW | Keyword lines provide information which can be used to generate cross-references to other entries. |
| FT | Feature table data lists regions of interest in the sequence - post-transitional modifications, binding sites, enzyme active sites etc. |
| SQ | Sequence header followed by sequence data . |

### VIEW_TWO

Some entries do not contain data on all the line types, and some line types occur many times in a single entry.

| Field Name | Description |
|---|---|
| ID | Identification line showing the entry name of the sequence. |
| Accession number | The accession number, a unique number used to identify entries. |
| Description | Description line containing general descriptive information. |
| Species | The organism species line specifies the organism which was the source of the sequence. |
| Number of matched peptides | The number of matched peptides |
| Probability score | MOWSE type score. |
| Percent coverage | % sequence coverage. |
| Isoelectric point | The isoelectric point of the entry. |
| Molecular weight | The molecular weight of the entry. |
| Matching peptides | A list of matching fragment masses with their molecular weight (**MW**), mass error (**Delta**), the position of the peptide in the sequence (**start** and **end**) and the **sequence**. If a * appears to the left of one of these entries then it is a single partial fragment (i.e. one missed cleavage site), if ** appears it is a double partial fragment (i.e. two missed cleavage sites). |
| Unmatched masses | A list of unmatched masses showing the Searched mass, the Query mass and the Charge State. |

### VIEW_THREE

This view displays the sequence specific to the entry as a text string.

# File Formats

## Sample List

The Sample Lists are held in Microsoft Access which mean their contents are readily available to numerous other windows programs. Sample Lists created by the MassLynx system have the .SPL extension.

| Label | Format | Description |
|---|---|---|
| VERSION | Double | Database version number. |
| Index | Double | Used internally to keep samples sequenced when editing. |
| FILE_NAME | Char (255) | Raw data file name for this sample. Can be name or full path. |
| MS_FILE | Char (255) | MS method parameter file to use when acquiring this sample. Can be name or full path. |
| MS_TUNE_FILE | Char (255) | MS tuning parameter file to use when acquiring this sample. Can be name or full path. If empty the current tune settings will be used. |
| INLET_FILE | Char (255) | Inlet method parameter file to use when acquiring this sample. Can be name or full path. Only required if a programmable inlet acquisition system is being used to acquire sample. |
| INLET_PRERUN | Char (255) | Inlet pre-run method parameter file to use prior to acquiring this sample. Can be name or full path. If empty no pre-run is performed. Only required if a programmable inlet acquisition system is being used to acquire sample. |
| INLET_POSTRUN | Char (255) | Inlet postrun method parameter file to use subsequent to acquiring this sample. Can be name or full path. If empty no post-run is performed. Only required if a programmable inlet acquisition system is being used to acquire sample. |
| INLET_SWITCH | Char (255) | Inlet pre-run method parameter file to use prior to acquiring this sample if inlet system has had to make a column switch, this will be used in preference to INLET_PRERUN. Can be name or full path. If empty no column switch pre-run is performed. Only required if a programmable inlet acquisition system is being used to acquire sample. |
| AUTO_FILE | Char (255) | Autosampler method parameter file to use when acquiring this sample. Can be name or full path. Only required if a programmable autosampler system is being used to acquire sample. |
| SAMPLE_LOCATION | Char (255) | Defines location of sample to be acquired on autosampler bed. Format will depend on type of autosampler being used. |
| INJ_VOL | Double | Volume of sample to inject when acquiring with programmable autosampler |

| Label | Format | Description |
|---|---|---|
| PROCESS | Char (255) | External process to run to perform processing of sample. Can be name or full path. Only required if external processes are being run, if empty no process will be run for this sample. |
| PROCESS_PARAMS | Char (255) | Name of external process parameter file to use when processing samples. Available to external process via MLCURSMP.TXT file. |
| PROCESS_OPTIONS | Char (255) | Options to specify on command line of external process when it is executed |
| FILE_TEXT | Char (255) | Sample text description to be used for sample. Will be recorded in data file header. |
| JOB | Char(255) | Job description for sample. Will be recorded in data file header. |
| TASK | Char(255) | Task description for sample. Will be recorded in data file header. |
| USER | Char(255) | User name for sample. Will be recorded in data file header. |
| SUBMITTER | Char(255) | Submitter for sample. Will be recorded in data file header. |
| CONDITIONS | Char(255) | Condition information for sample. Will be recorded in data file header. |
| TYPE | Char (255) | Sample type to use during Quantify. Currently can be one of ANALYTE, BLANK, QC or STANDARD |
| ID | Char(255) | The sample ID from OpenLynx. |
| CONC_A … CONC_T | Char (255) | 20 fields used to specify the concentration levels of compounds within this sample. Used during the quantify process. |
| WAVELENGTH_A… WAVELENGTH_J | Double | 10 fields used to specify wavelengths to analyse for this sample. Used during OpenLynx processing. |
| MASS_A … MASS_T | Char (255) | 20 fields used to specify masses to analyse for this sample. Used during the OpenLynx process. Masses can be real numbers or chemical formulae |
| STOCK_DIL | Double | Not currently used reserved for future use |
| USER_DIVISOR_1 | Double | Divisor used during concentration calculation stage of Quantify. Defaults to 1 if not specified. |
| USER_FACTOR_1 … USER_FACTOR_3 | Double | Multipliers used during concentration calculation stage of Quantify. Defaults to 1 if not specified. |
| HPLC_FILE | Char(255) | The additional LC information for this sample (used by OpenLynx) |
| SPARE_1 … SPARE_5 | Char (255) | General purpose fields available to the User to store extra information about the sample. |
| ACQU_PROCESS | Char (255) | External process to run when acquiring data. Can be name or full path. Only required if external processes are being run, if empty no process will be run for this sample. |

| Label | Format | Description |
|---|---|---|
| ACQU_PROCESS_ PARAMS | Char (255) | Name of external process parameter file to use when acquiring samples. Available to external process via MLCURSMP.TXT file. |
| ACQU_PROCESS_ OPTIONS | Char (255) | Options to specify on command line of external process when it is executed |
| SAMPLE_GROUP | Char (255) | Used too inform QuanLynx that the optimisation file for an Analysis sample should combine the optimisations for a number of compounds sample groups are used. Each sample group item is a unique one or two letter code in upper case. Thus 'A:B:C', 'AA BB CC', 'A….ZZ….QP' are all valid three item groups.<br><br>If the sample group field is empty then all the compounds will be optimised; one method file will be created and used for all the analysis samples.<br><br>If a sample group in the analysis sample list does not have a corresponding entry in the compound list, then that group will not be run. |
| FRACTION_FILE | Char (255) | Raw data file name for this sample. Can be name or full path. |
| FRACTION_1 to FRACTION_4 | Char (255) | References to the masses (MASS_A to MASS_T) to be monitored when performing fraction collection acquisition. |
| QUAN_REF | Char (255) | This field specifies which sample (if any) is to be used to adjust the retention time window of the quantification method created for the analysis. The first sample in the current group that has this field set to anything other than blank will be used. |
| AUTO_ADDITION | Char (255) | The Waters 2790 autosampler can take samples from up to 15 vials and inject them sequentially. This field contains a list of the sample locations separated by a semi-colon (;) e.g. A:1;A:2;A:3. The volume specified in the INJ_VOL field is drawn from each vial. |
| METH_DB | Char (255) | The full path to the quantify method file used for this sample group in QuanLynx. |
| CURVE_DB | Char (255) | The full path to the calibration curve file used for this sample group in QuanLynx. |
| DUMP_FILE | Char (255) | The full path to the text export file used for this sample group in QuanLynx. |
| PROCESS_ACTION | Char (255) | The Action that the process manager is to perform should the external application return an error |

## An Example Generic Sample List File

Below is an example of a small single sample generic sample list file.

[Batch]

MSMethod=DEFAULT.MDB
MSTune=DEFAULT.DBF
LCMethod=DEFAULT
ProcessParameters=C:\MASSLYNX\LC1.olp
Process=C:\MASSLYNX\OPENLYNX.EXE
UserName=john doe
BatchID=13
NumberOfPlates=1

[Plate:1]

JobCode=13
UserName=john doe
Rows=0
Columns=0
Track=R
NumberOfWells=1

[Sample:1:1]

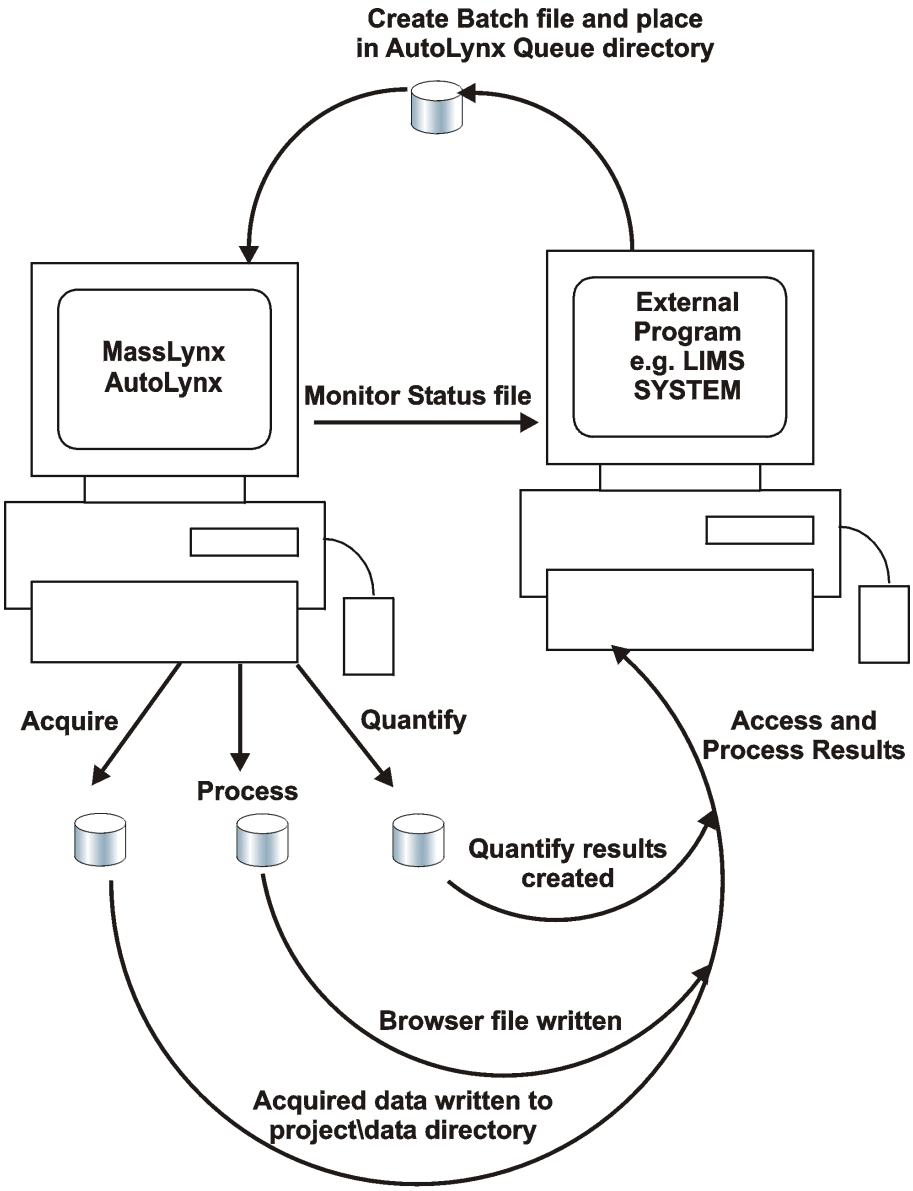
Well=25
SampleDescription=testsample
SampleID=tst11
MSDataName=test1
SampleType=0
MSInjectionVolume=15.0000
NumberOfMasses=1
Mass1=504.00
NumberOfWaveLengths=1
Wavelength1=254.0
NumberOfConcs=2
Conc1=50.000
Conc2=100.000
NumberOfFormulae=1
Formula1=CH3CH2Cl

# AutoLynx

AutoLynx is an application that enables batches to be submitted to the MassLynx queue for automatic acquisition, processing and report generation.

Applications can be written (e.g. in Visual Basic) to:

- Take information from other software packages (e.g. LIMS systems) and automatically create batch files.
- Add these batch files to the AutoLynx queue. (AutoLynx will then add them to the MassLynx queue and perform the processing defined on the AutoLynx settings dialog).
- Monitor the progress of the batch file.
- Automatically read the acquired data, or processed results, for further processing and/or exporting into other software packages.




**Where Process can be OpenLynx, ProteinLynx, MetaboLynx or a user written process**

To produce the required Browser file the Process column in the Sample List must be defined as:

- OpenLynx to produce an OpenLynx Browser file.
- PeptideAuto to produce an ProteinLynx Browser file.
- MetaboLynx to produce an MetaboLynx Browser file.

For more information on AutoLynx see the MassLynx NT Users Guide.

# Status.ini

The Status.ini file contains details of the current status of the Mass Spectrometer, LC system and the MassLynx Queue.

To create a Status.ini file select **Options** from the **MassLynx Tools** menu to display the options dialog.

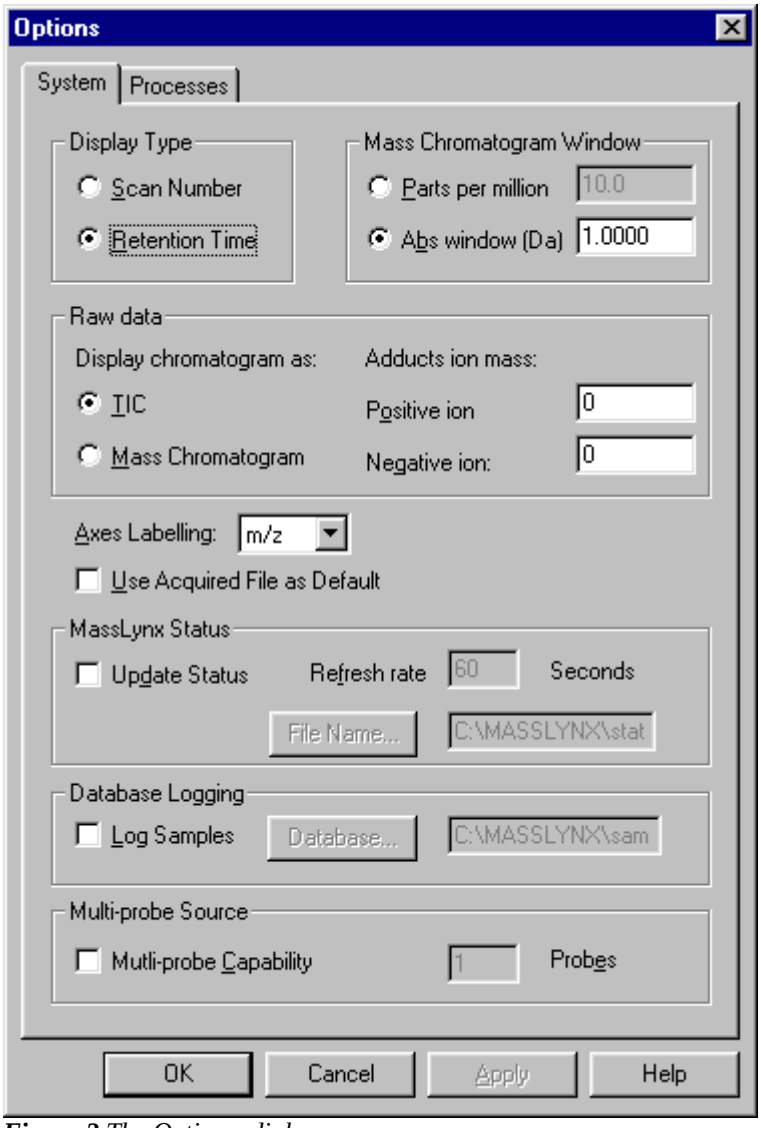



***Figure 3*** *The Options dialog*

On the **Status** page check the **Update Status** box to write details to a status file.

By default the details in this file are updated every 60 seconds, to change this enter a new time in the **Refresh rate** box.

The default filename and location is C:\MASSLYNX\status.ini. To change this press the **File Name** button, select a directory using the browser displayed, enter a new file name and press **Open**. **Note**: do not use the name of an existing *.ini file in the current directory as this will cause problems with other software.

If any of these fields are changed MassLynx must be closed down and restarted for the changes to take effect.

These files can be viewed in Notepad or by third party software across a network. This allows users to detect software or hardware errors, to decide which instrument should be used to acquire samples or when data has been acquired and is ready for further processing.

# File Format

The format of the Status.ini file is as follows:

[MS Status]

Operate=2
Status=Scanning

[LC Status]

Status=0
Ready=0
%A=100.0
%B=0.0
%C=0.0
%D=0.0
Flow Rate=0.000

[Queue Status]

Queue Paused=0
Process Running=1
1=test  Samples 1 to 5: Sample 1 Acquiring  Running
2=test1  Samples 1 to 5:  Waiting
3=test2  Samples 1 to 2:  Waiting
Total samples=12

[Time Stamp]

Time=06-002-1999,10:37:59

### MS Status

The MS Status section shows mass spectrometer information.

**Operate** Shows the state of the mass spectrometers high voltage electronics. It has two values:

| | |
|---|---|
| 1 | The mass spectrometer is in standby |
| 2 | The mass spectrometer is in operate |

**Status** Shows the status of the mass spectrometer. It can have one of the following values:

| | |
|---|---|
| No Instrument | There is no mass spectrometer attached to the PC. |
| Not Scanning | The mass spectrometer is idle. |
| Solvent Delay | The mass spectrometer has started acquiring data and is in solvent delay. |
| Scanning | The mass spectrometer is acquiring sample data. |
| Waiting for Injection | The mass spectrometer is waiting for the autosampler to inject the sample. |

This information is useful during automation of a list of samples. For example the inlet system will continually poll this parameter while the mass spectrometer is acquiring in order to determine when it has reached a suitable status (Waiting for injection) for the next sample to be injected and a new data file to be acquired.

### LC Status

This section shows inlet system information.

**Status** Shows whether there is an error with the inlet system. If an error occurs then the appropriate action can be taken by the software to stop the automation. It has two values:

| | |
|---|---|
| 0 | There is no error in the inlet system |
| 1 | Inlet system has an error |

**Ready** Shows whether the inlet system is ready to inject a new sample. It has two values:

| | |
|---|---|
| 0 | Inlet system is not ready to inject the next sample |
| 1 | The inlet system is ready to inject the next sample |

**%A, %B, %C and %D** These parameters detail what percentage of the four possible reservoirs will be used for the mobile phase.

**Flow Rate** This gives the flow rate of the HPLC (ml/min).

### Queue Status

This section shows sample list queue information.

**Queue Paused** This shows whether the process queue is paused. It has two states:

| | |
|---|---|
| 0 | The process queue is not paused |
| 1 | The process queue is paused |

**Process Running** This shows whether the sample list is running a process. It has two states:

| | |
|---|---|
| 0 | MassLynx is not running a process |
| 1 | MassLynx is running a process |

**1, 2, …. N** These lines refer to the queue of batches waiting to be processed. The format of the lines is as follows, from left to right:

"Batch No." "MassLynx Batch ID" "Samples range" "Sample status" "Batch status"

Batch No. is an index of the batches in the queue.

MassLynx Batch ID is the identifier of the batch (e.g. sample list name).

Samples range indicates the range of samples in the batch.

Sample status has the form "Sample n Acquiring" to indicate which sample is running.

Batch status is "Running" if a sample from that batch is being processed, or "Waiting" if the batch is in the queue.

**Total Samples**

This parameter gives the total number of samples in all the batches in the queue

### Time Stamp

This shows the time the data system last updated a data file. If this value does not increase as often as its refresh rate assume the data system is no longer responding.

# Notes

# Notes

# Index