

MassLynx 4.1

Getting Started Guide

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USA

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Customer comments

Please contact us if you have questions, suggestions for improvements, or find errors in this document. Your comments will help us improve the quality, accuracy, and organization of our documentation.

You can reach us at tech_comm@waters.com.

Contacting Waters

You will be able to resolve most MassLynx issues yourself. However, if this is not the case, you must contact Waters.

Customers in the USA and Canada should report maintenance problems they cannot resolve to Waters Technical Service (800 252 4572). All others should visit <http://www.waters.com> and click Offices, or phone their local Waters subsidiary or Water corporate headquarters at 34 Maple Street, Milford, MA 01757, USA.

When contacting Waters, have the following information available:

- The nature of the problem
- Your instrument serial number(s)
- Your software version (click Help > About in the main MassLynx window)
- Any error messages received



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1

Before you start

This chapter will introduce MassLynx, explain installation, and describe what you need to have ready before starting to use the software.

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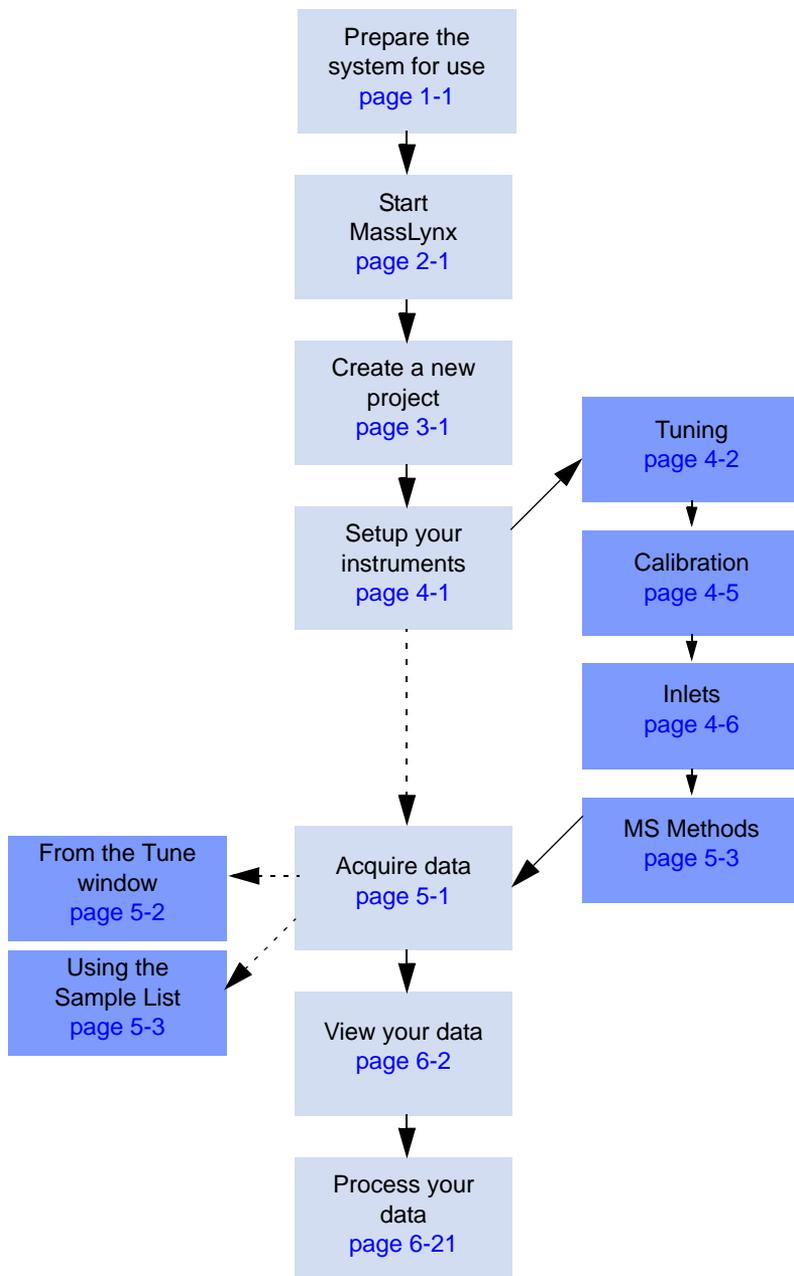
Introduction

MassLynx™ is a powerful software application that configures and controls your Waters mass spectrometer, and provides many features to analyze and process the data acquired.

This guide will lead you through the steps you need to take to get started with MassLynx and be quickly on the way to real, valuable results.

The following diagram shows the tasks that need to be performed to get up and running with MassLynx; they will be outlined in more detail, step by step, later in the guide.

Steps to get started with MassLynx:



Installing MassLynx

In most cases MassLynx will be installed for you by a Waters engineer. If you already have MassLynx installed, skip this section.

Requirements:

- Before installing MassLynx, refer to the Release Notes for detailed information relating to the release. You should also consult this documentation if upgrading MassLynx, or if applying Software Change notes (SCNs). If you are in any doubt about how to proceed, contact your Waters support representative.
- You may be asked for information about your mass spectrometer and PC during installation. If you are unsure of any details, cancel the installation wizard, confirm the information required, then begin the installation procedure again.
- You must be logged on to the PC using a user account that has administrative privileges.
- The PC you are installing MassLynx on must be running Windows® XP Professional SP2 or Windows 2000 SP4.

Prerequisites:

- If you have previously installed Waters Instruments Component Software, uninstall it using Windows Add or Remove Programs.
- Close all running programs.

Installation tips:

- QuanLynx, OpenLynx, and SDMS support are discussed in this document. You may wish to review the information on those features before deciding whether to install them. See [Quantitation using QuanLynx on page 6-21](#), [Providing access and distributing results using OpenLynx on page 6-21](#), and [Storing results in SDMS on page 6-23](#) for more information.
- If you want to install OALogin, OAToolkit, or the Diversity browser, refer to [Additional OpenLynx installation instructions on page A-1](#).

To install MassLynx:

1. If MassLynx has been supplied on a CD, or other removable media, insert it into the appropriate drive.

2. After a few moments the installer should appear automatically. If it does not, use Windows Explorer to navigate to the directory containing the file setup.exe, and double-click the file; the MassLynx installer is displayed.
3. If the InstallShield Wizard informs you of required software to install before the MassLynx can proceed (for example, JRE 1_5_0_3 and Java3D 1_3_1), click Next to install it.
4. Follow the on-screen instructions, choosing the features you wish to install, referring to these guidelines:
 - Install MassLynx into the folder suggested – C:\MassLynx – and do not move it after installation has completed.
Rule: Do not change the folder. MassLynx must reside on the C: drive.
 - You will be given the option to install MassLynx with no security, Basic Security, or Full Security. Many systems are installed with no security, but if you need to restrict access to MassLynx or ensure that files cannot be tampered with, select Basic or Full security. For an explanation of these options, please see the *MassLynx Security Guide*.
 - Key disks are required to install most Application Managers. You will be asked to enter the location of the key disk during the installation process. If you do not have an appropriate key disk – and believe you should – contact your MassLynx system administrator.

Tasks to complete after installing MassLynx:

1. Remove the CD and store the key disks and the installation CD in a safe place.
2. Shut down the PC you have installed MassLynx on, restart it, and then wait for the desktop to appear.
3. Reboot your mass spectrometer's embedded PC. For information on how to do this, refer to the *Operator's Guide* for your instrument.
4. Wait at least 4 minutes before starting MassLynx.

Installing additional Application Managers

Unless you have installed MassLynx with Full Security, it is possible to install additional Application Managers at any time.

To install additional Application Managers:

1. In Windows, open the Add or Remove Programs window from the Control Panel.
2. Click Micromass MassLynx V4.1.
3. Click Change.
4. Follow the on-screen instructions, selecting Modify – Add Application Managers to existing MassLynx V4.1 Installation when that option is presented.

Tip: If you want to install OALogin, OAToolkit, or the Diversity browser, refer to [Additional OpenLynx installation instructions on page A-1](#).

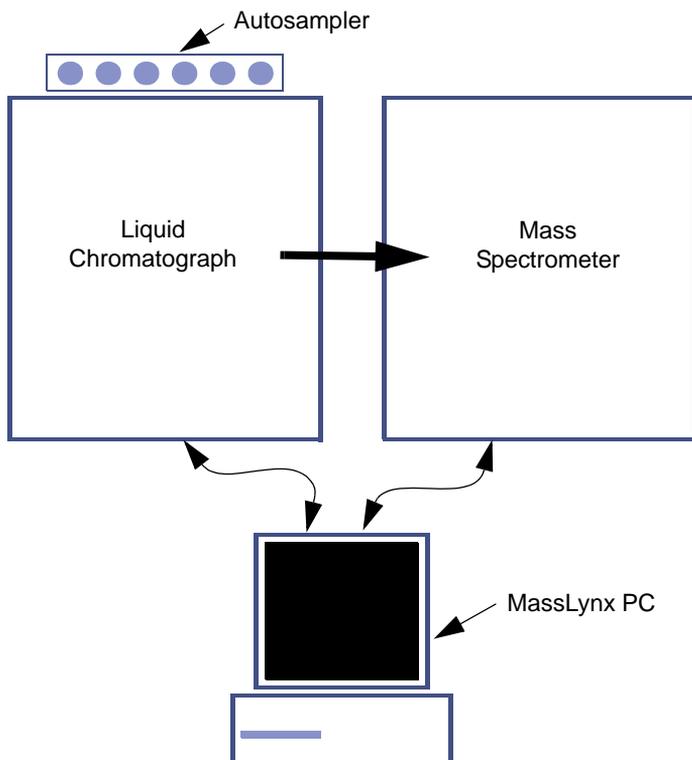
Preparing the system for use

Before starting to use MassLynx to acquire and process data, you need to make sure that your system is ready for use.

If you have an LC/MS system, it will contain some of these components:

- Pump (also known as a Solvent Delivery System). This will be a Liquid Chromatograph (LC/HPLC/UPLC).
- Autosampler.
- Detector (usually PDA or UV).
- Mass Spectrometer.
- MassLynx PC.

Example LC/MS system layout:



If you have a GC/MS system, it will contain some of the these components:

- Gas Chromatograph (GC).
- Autosampler.
- Mass Spectrometer.
- MassLynx PC.

Before starting to use MassLynx, you will need to make sure that the instruments are:

- Properly installed
- Properly connected
- Switched on and ready

In many cases a Waters engineer will have installed and connected the instruments for you. If you are not sure that the instruments are properly installed and connected, refer to the instrument documentation or contact your Waters support representative.

In addition to making sure that the instruments are ready, you should ensure that the PC is turned on and that MassLynx has been successfully installed.

Once you have confirmed that the system is ready for use, move on to the next section – Starting MassLynx.

2 Starting MassLynx

This chapter will tell you how to open the MassLynx application and explain the main features of the MassLynx window.

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Opening MassLynx

To open MassLynx:

1. Click Start > All Programs (or Programs) > MassLynx > MassLynx V4.1.

Alternative: Double-click the MassLynx V4.1 icon on the Desktop.

2. If you have a security-enabled system, type your logon name and password in the MassLynx Login dialog box. Check that the domain is set correctly, then click OK.

Tip: If the MassLynx Login dialog box appears and you do not know a logon name and password to access MassLynx, contact your MassLynx System Administrator. If you have just installed a security-enabled system and need assistance, refer to the *MassLynx Security Guide*.

The MassLynx window

When MassLynx has opened you will see the main MassLynx window, similar to the one shown below.

Typical MassLynx window:

Banner Menu bar Tool bar Sample List menu bar Information bar

The screenshot shows the MassLynx software interface. At the top is a blue banner displaying the project name 'MassLynx - Quantify - Quantify.spl'. Below the banner is a menu bar with options: File, View, Run, Security, Help. A tool bar follows, containing icons for file operations, a 'Shortcuts' button, and 'Queue' and 'Status' buttons. Below the tool bar is an information bar showing 'Queue Is Empty'. The main area is divided into a left sidebar and a central table. The sidebar contains icons for 'Instrument', 'Inlet Method', 'MS Method', 'MS Tune', 'Edit Shutdown or Startup', 'Shutdown', 'Startup', and 'Options'. The central table is the 'Sample List editor' with columns: File Name, Mass A, Control, Process, Parameter File, Structure, Subject Time, and Subject Text. The table contains 30 rows of data, with the first row highlighted. At the bottom is a status bar showing 'Ready', 'Instrument Not Present', '0:0', and 'Only Error Shutdown Enabled'.

	File Name	Mass A	Control	Process	Parameter File	Structure	Subject Time	Subject Text
1	ASSAY01	0.000					0.000	
2	ASSAY02	0.200					0.000	
3	ASSAY03	0.500					0.000	
4	ASSAY04	0.750					0.000	
5	ASSAY05	1.000					0.000	
6	ASSAY06	2.000					0.000	
7	ASSAY07	5.000					0.000	
8	ASSAY08	10.000					0.000	
9	ASSAY09	15.000					0.000	
10	ASSAY10	0.300					0.000	
11	ASSAY11	2.000					0.000	
12	ASSAY12	12.000					0.000	
13	ASSAY13	0.000					0.000	
14	ASSAY14	0.000					0.000	
15	ASSAY15	0.000					0.000	
16	ASSAY16	0.000					0.000	
17	ASSAY17	0.000					0.000	
18	ASSAY18	0.000					0.000	
19	ASSAY19	0.000					0.000	
20	ASSAY20	0.000					0.000	
21	ASSAY21	0.000					0.000	
22	ASSAY22	0.000					0.000	
23	ASSAY23	0.000					0.000	
24	ASSAY24	0.000					0.000	
25	ASSAY25	0.000					0.000	
26	ASSAY26	0.000					0.000	
27	ASSAY27	0.000					0.000	
28	ASSAY28	0.000					0.000	
29	ASSAY29	0.000					0.000	
30	ASSAY30	12.000					0.000	

Status bar MassLynx bar Sample List editor

The window contains:

- A banner, which displays the names of the current project and Sample List.
- A top-level menu bar, providing access to some of the main features.
- A tool bar, providing one-click access to different view modes and some common features.
- An information bar (below the tool bar), usually showing the status of the sample currently being acquired or processed.

- The MassLynx bar, with various tabs, at the left-hand-side of the window. The contents of the MassLynx bar varies between Shortcut, Queue and Status views, and as different tabs are selected.
- The Sample List editor, where Sample Lists can be created, viewed and edited.
- A Sample List menu bar (above the Sample List editor), providing access to commands associated with the Sample List.
- A status bar, at the bottom of the window, giving information on MassLynx's current status.

The icons in the MassLynx bar provide access to most of the features available in MassLynx, through a range of windows and dialog boxes. The tabs on the left of the MassLynx bar control which icons are shown.

Example: To access instrument control features, click the Instrument tab on the left of the MassLynx bar. The features available are shown in the MassLynx bar, with an icon for each feature.

To open the Inlet Method editor, click Inlet Method (or the icon above the text).

3

Creating a project

Projects contain both the configuration files necessary to perform an acquisition and the data that is acquired. This chapter will explain how to create a project, and will describe the project structure so that you find it easy to manage information later on.

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Creating a new project

A project contains the configuration information for your instruments and stores the data that will be acquired. MassLynx will initially open with an example project, but you should create your own project to store settings and data.

Tip: Projects are flexible, and can hold a variety of settings that apply to a range of requirements in one work area. Separate projects might be appropriate for different work areas or users.

To create a new project:

1. Click File > Project Wizard.
2. Click Yes on the message warning that some services will be closed down.
3. In the Create Project dialog box, type a name for your project and, optionally, a description.
4. Enter the directory you want to create your project in.

Recommendation: Do not create projects in the directory in which MassLynx was installed (usually C:\MassLynx) or any of its subdirectories.

5. Click Next, then select one of the three options for creating a project:
 - Create a completely new project
 - Create using current project as template – the method and metadata files (such as tuning and calibration files) will be copied into the new project. Select the box if you want to copy the sample lists as well.
 - Create using existing project as template – the method and metadata files (such as tuning and calibration files) will be copied from the specified project into the new project created.

Tip: Unless you will be doing very similar work to someone who has already been using the system, select Create new project.

6. Click Finish.

Result: The new project has been created.

Take a few moments to read the next section, so that you can achieve your goals more quickly by understanding projects.

Understanding project structure

Understanding the structure of a MassLynx project helps you find the files you need more quickly, and makes complicated tasks easier to perform. The terms used might not be familiar at first, but you will come to understand them as you work with MassLynx.

A directory, called *<project name>.pro*, will be created for each project. If a new project is called MyProject, for example, a folder called MyProject.pro would be created. Within this directory, a number of sub-directories are created.

Project sub-directories:

Directory name	Contents
Acqudb	Acquisition information such as tuning parameters, calibration settings, and inlet methods.
Curvedb	Quantitation calibration curve information.
Data	Raw data files.
Methdb	Method files for some Application Managers.
Peakdb	Peak list files.
Sampledb	Sample lists.

When data files are acquired they may contain more than one acquisition function and may also contain processed data derived from the original raw data – refined spectra, for example.

The data from each sample is placed into its own sub-directory within the data directory. This sub-directory is called *<file name>.raw*, where the file name has been specified by you – either in the Tune window or the sample list. Details on the types of file created in these individual sub-directories can be found in the MassLynx help.

4 Instrument setup

This chapter will outline the steps that need to be taken to set up your system before data can be acquired.

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Mass calibrating your mass spectrometer	4-5
Setting up an inlet method	4-6

Tuning your mass spectrometer

What is tuning?

To obtain the most useful results from your mass spectrometry system, the controls of the instrument need to be adjusted to achieve the best resolution (narrowest peak) and highest sensitivity (tallest peak) possible.

You can make these adjustments through MassLynx and, on some instruments, MassLynx can even tune the instrument automatically.

If the instrument is not tuned properly, the results you obtain will be less useful, and possibly even misleading.

Tuning your instrument

The instrument is tuned from the Tune window. To open the Tune window, click MS Tune on the MassLynx bar, Instrument tab; the Tune window for your instrument will appear.

MassLynx is capable of controlling many different types of mass spectrometer, so the exact display of the Tune window will vary substantially from instrument to instrument. The Tune window for each instrument provides access to instrument controls on the left hand side and a peak display on the right hand side.

Warning: Consult the safety information in the *Operator's Guide* for your mass spectrometer before commencing the tuning process.

To tune the instrument:

1. Supply a known sample to the mass spectrometer.
2. Adjust the instrument controls to achieve the best peak shape possible.
3. Save the tuning settings by clicking File > Save As in the tune window.

Detailed instructions on how to do this are supplied in the *Operator's Guide* for your mass spectrometer.

The AutoTune Wizard

For ZQ, Quattro Micro API, and Quattro Premier instruments, the AutoTune Wizard helps tune your instrument by automatically adjusting the instrument controls until the best peak shape is achieved.

The AutoTune Wizard also provides the ability to automatically mass calibrate the instrument, and to setup MS methods. Information on mass calibration and setting up MS methods is given later in this document (see [Mass calibrating your mass spectrometer on page 4-5](#) and [Setting up an MS method on page 5-3](#)).

Rule: AutoTune can only be used for samples that are supplied to the mass spectrometer by infusion.

Recommendations:

- AutoTune is only suitable if you have a small number of compounds to tune.
- It is recommended that a calibration (see [Mass calibrating your mass spectrometer on page 4-5](#)) is performed at the same time as a full Autotune.

To run the AutoTune Wizard:

1. Infuse a suitable tuning and calibration solution to the instrument for use during the process. The sample should be as pure as possible, and you should know the masses of the compounds it contains.
If you are in doubt about how to infuse a sample, consult the *Operator's Guide* for your instrument.
2. In the tune window, click Options > AutoTune; the AutoTune Wizard appears.
3. Select AutoTune - Full, and Calibrate Instrument.
4. Click Next, then enter the file names you wish to use to save your tune settings.
5. Check that the temperatures to be used are appropriate.

Tip: The default temperatures are likely to be appropriate if you are infusing the sample in combination with a mobile phase at high flow rate.

If you are infusing at a low flow rate, select the Adjust Default Temperatures box. The temperatures that are then displayed (which can be adjusted if required) are likely to be appropriate for low flow rate infusions.

To revert to temperatures appropriate for a high flow rate, clear the Adjust Default Temperatures box.

If you are in doubt, consult the *Operator's Guide* for your instrument.

6. Click Next, then enter an appropriate calibration reference file for the sample you are infusing, and the file name you wish to use to save your calibration settings.
7. Check that the calibration range settings are appropriate – their default values are likely to be sensible in most situations.
8. Select whether a printed calibration report should be generated.
9. Click Next, then enter the masses for the sample you are going to use during the tuning process. You can choose to fill these values automatically from the Tune window or calibration file, if required.
10. Set the Span for each mass to 5.
11. Check that the setting for desired peak width is appropriate: the default values will be sensible in most situations.
12. Click Next.

Result: The AutoTune process will begin.

13. When you are shown the results at the end of the AutoTune, you can choose to Finish and save the tuning and calibration settings, or to go Back and repeat the process with different settings or a different sample.

Mass calibrating your mass spectrometer

What is mass calibration?

Once the best peak shape possible has been achieved through tuning, the instrument needs to be calibrated so that the peak is recorded at the correct mass.

MassLynx provides an automated method to do this. A reference file, containing the expected masses of the peaks for a known sample, is compared against the peaks obtained when an acquisition is performed on the known sample.

At the end of the process, the instrument will be calibrated to provide accurate results. You must re-calibrate the instrument from time to time, as detailed in the *Operator's Guide* for your mass spectrometer.

Calibrating your instrument

The particular method of calibration will vary between instruments, but it is normally performed through the calibration window. To open the calibration window, click MS Tune on the Instrument tab of the MassLynx bar, then click Calibration > Calibrate Instrument.

Detailed instructions on how perform calibration are supplied in the *Operator's Guide* for your mass spectrometer.

The AutoTune Wizard

If you have a ZQ, Quattro Micro API, or Quattro Premier instrument, you can calibrate using the AutoTune Wizard. For details on how to do this, see [The AutoTune Wizard on page 4-3](#).

ToF calibration

For some time-of-flight (ToF) and quadrupole time-of-flight (Q-ToF) instruments, a wizard is provided to help you calibrate the instrument. The wizard assists you in preparing the mass spectrometer for the acquisition of accurate mass data.

For details on calibrating your ToF instrument, refer to the online Help for your instrument.

Setting up an inlet method

What is an inlet method?

Mass spectrometers are often used in conjunction with an inlet system such as a liquid chromatograph (LC) or a gas chromatograph (GC). MassLynx can control this equipment during data acquisition to provide complete control of an experiment. Autosamplers will often be used to automate the running of samples.

An inlet method is a group of settings for the inlet system. An inlet method can be created and then specified for use during an experiment, and those settings will be applied during the data acquisition. A number of different inlet methods can be created, saved, and used for different types of experiment.

Choosing your pump, autosampler, and detector

Inlets are configured through the Inlet Method window. To open this window, click Inlet Method on the MassLynx bar, Instrument tab; the Inlet Method window will appear.

To select the inlet modules you are using:

1. Click Tools > Instrument Configuration; the Inlet Configuration dialog box is displayed.
2. Click Configure; the Inlet Configuration Wizard is displayed.
3. Select the required pump (often a liquid chromatograph or gas chromatograph), and click Next.
4. Select the required autosampler, and click Next.

Restriction: Only the autosamplers that are compatible with the chosen pump will be displayed.

5. Select the required detector, and click Next.

Restriction: Only the detectors that are compatible with the chosen pump and autosampler will be displayed.

6. Depending on the configuration selected, the HPIB Communication or GPIB Communication settings may be displayed. If they are, enter appropriate values and click Next.
7. The Configuration Successful message is displayed. Click Finish to return to the Inlet Configuration dialog box, then Finish again to return to the main Inlet Method window.

Depending on the inlet modules selected, installation wizards may appear to guide you through the installation of specific software relating to those modules. If so, follow the on-screen instructions, selecting the options appropriate for your system.

Specifying your inlet settings

The configuration options available vary substantially between different inlets. In all cases, however, you access the options by clicking the icons in the Inlet Method window bar on the left side of the screen.

In the Inlet Method window bar there will be a Status icon – providing access to information on the current inlet status – and one or more of the following icons, depending on the inlet equipment you have specified:

- Inlet
- Autosampler
- Detector

You can also specify the way in which inlet or detector runs should be triggered, that data acquisition should only commence when certain events are detected, and that events should be sent to the inlet system at the end of acquisition. These features are configured using the Events and Triggering Wizard, accessed from the Inlet Configuration dialog box.

Detailed instructions on how to configure the options available for your inlet are available by clicking Help > Help On Inlet, Help > Help On AutoSampler, and Help > Help On Detector, respectively. Help for the Inlet Method window, including how to use the wizards, is available by clicking Help > Help On Editor.

Recommendation: To obtain the best results, refer to the documentation supplied with your inlet equipment as well as the MassLynx documentation.

5 Acquiring data

This chapter will explain how you acquire data using MassLynx. It will cover how to:

- Acquire data for a single sample through the Tune window.
- Create MS methods and Sample Lists for automated data acquisition.

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Acquiring data from the tune window

The easiest way to acquire data is directly from the Tune window. When using this method you can:

- Start and stop acquisitions
- Control most of the scanning parameters

The disadvantages of this method are that you cannot:

- Use inlet methods
- Acquire SIR (Selected Ion Recording) or MRM (Multiple Reaction Monitoring) data
- Acquire analog data
- Acquire data from multiple samples unattended

If you need to use any of these features, acquire data using the Sample List.

To acquire data from the Tune window:

1. Click MS Tune on the Instrument tab of the MassLynx bar to open the Tune window.
2. Ensure the instrument is in Operate mode. If the indicator in the bottom right of the Tune window is not green, click the adjacent Operate button.
3. Click the Acquire button; the Acquisition Setup dialog box is displayed.
4. Enter the settings you wish to use for the acquisition.
5. Click Start.

Caution: MS instruments require the Tune window to be open to acquire data, whether the acquisition is done directly from the Tune window or by using the Sample List. If you try to close the Tune window, a warning message will be displayed to this effect; if you choose to close the window anyway then acquisition will stop.

Acquiring data from the sample list

Setting up an MS method

What is an MS method?

Mass spectrometers can acquire a number of different types of data from the samples supplied. While these will vary depending of the capabilities of the instrument they may include, for example:

- a scan over a specified range of masses
- a scan of a single targeted mass
- the results of scanning the fragments of particular target ions

Different data types can be acquired from a sample in a single experiment.

An MS method is a group of settings defining the scans that the mass spectrometer should perform. Once an MS method has been saved, these settings can be used when acquiring data from samples.

Setting up MS methods

Detailed instructions on the options available when setting up MS methods are supplied in the *Operator's Guide* for your instrument. If you have a ZQ, Quattro Micro API, or Quattro Premier instrument, you may be able to set up SIR and MRM methods using the AutoTune wizard – refer to the online Help supplied with the instrument for more information.

MS methods are set up using the Experiment Setup window. To open this window, click MS Method on the Instrument tab of the MassLynx bar.

The window contains the current list of functions – types of scan – that have been defined for the MS method. The buttons on the tool bar indicate the different types of function available for your instrument. Click these buttons to add a function of that type to the MS method.

To the right of the description for each function is a colored bar showing the time period over which the function will be used. The total time for the MS method is displayed between the tool bar and the function list: this can be modified by typing a new value in the Total Run Time box.

Save the MS method when you have finished setting it up, so that it can be used when data is acquired.

Tip: Unless you wish to overwrite the existing MS method, save the file with a new name.

Creating a Sample List

What is a Sample List?

A MassLynx Sample List is a list of the samples available for analysis by the mass spectrometer. Among other things, it can include:

- Information on the name to be given to the data acquired
- Inlet methods to use
- MS methods to use
- Tune settings to apply

A Sample List can be set up for each different set of samples you wish to run, then saved and loaded as it is needed. You can create as many Sample Lists as you like for each project. The Sample List that was open last will be automatically loaded when MassLynx starts.

Sample Lists are also utilized by the Application Managers – such as QuanLynx – that can be used to process your data.

Tips:

- The Sample List display can be customized to hide some of the columns shown by default, and to add many more. Choosing the right columns for the work you are doing can help improve your efficiency when working with MassLynx. For more details, see [Customizing the Sample List display on page 5-8](#).
- Information in hidden columns can influence the way the system operates. If you experience unexpected behavior when running a sample list you have not created yourself, temporarily display the hidden columns to check the contents. For more details, see [Customizing the Sample List display on page 5-8](#).

Minimum requirements for the Sample List

If there is an inlet connected, your sample list must contain – as a minimum – the columns indicated in the table below.

Required sample list columns:

Column name	Field ID
File Name	FILE_NAME
Inlet File	INLET_FILE
MS File	MS_FILE
Bottle	SAMPLE_LOCATION
Inject Volume	INJ_VOL

Tip: As column names are configurable, they may differ from those given above. The field IDs will remain the same whatever the name of the column.

With these columns displayed, the Sample List will look similar to this:

Example Sample List:

	File Name	Inlet File	MS File	Bottle	Inject Volume
1	ExampleAnalyte	Default	DEFAULT	1.1	1.000

Using a sample list with these columns will enable you to acquire a basic raw data file. When using an Application Manager to process data, more columns will normally be required – refer to the Application Manager’s help for details.

Creating or editing a Sample List

The Sample List, displayed in the main MassLynx window, is similar to a spreadsheet. You can type values directly into the highlighted cell or, depending on the type, right-click or double-click in a cell to choose a file or from a list of options. You can also copy, cut, and paste cells, rows, and columns.

To add another sample (row):

1. On the Sample List menu bar, click Samples > Add.
2. Enter the number of samples you wish to add.

3. Click OK; the new samples will be added to the bottom of the Sample List.

You can also insert rows for additional samples by clicking Samples > Insert; the new sample row is inserted above the current selection.

Filling cells automatically

Rather than entering values individually into every cell in the Sample List, it is possible to automatically fill cells, saving on time and replicated effort. There are a number of different features available to help you:

Adding new sample rows

When you add or insert new rows, the values from the row above are automatically inserted into the new row.

Entering appropriate values for one row and then creating a number of new rows is much quicker than creating empty rows first and then entering appropriate values manually.

Fill down

The fill down feature enables the contents of one cell to be inserted into multiple cells on subsequent rows.

To use this feature, select an area more than one row in depth and, on the Sample List menu bar, click Samples > Fill > Down. The contents of the first selected cells will be inserted into the cells below.

Fill series

The fill series feature will insert the contents of one cell into multiple cells on subsequent rows, incrementing the numerical values for each cell. If the first cell contains 1:20, for example, the next cell would have 1:21 inserted, the next 1:22, and so on.

To use this feature, select an area more than one row in depth and, on the Sample List menu bar, click Samples > Fill > Series.

The autosampler bed layout

If you have a Waters or Gilson autosampler installed, you can use the autosampler bed layout display to insert information directly into the Sample List.

To insert information from the autosampler bed layout:

1. Click Samples > AutoSampler Bed Layout.
Result: The AutoSampler Bed Layout dialog box is displayed.
2. Select the samples you wish to add to the Sample List.
3. Use the buttons at the top of the dialog to add samples to the list, replace the selected sample, or insert the sample at the selected line. More than one sample can be added at once.

Copying data from a spreadsheet

Spreadsheets created in other Windows applications can be copied into the Sample List.

To copy data from a spreadsheet:

1. Add rows and columns to the Sample List so that it matches the number of rows and columns in the data you want to copy.
2. Select the relevant area in the other Windows application, then copy it.
3. Click Edit > Paste on the Sample List menu bar.

Caution: Data will be lost if the Sample List does not have the same rows and columns as the spreadsheet information being copied.

Specifying the inlet and MS method

If you have worked through [What is an inlet method? on page 4-6](#) and [Setting up MS methods on page 5-3](#), one or more inlet method and MS method files will have been created. These files will be used during data acquisition.

To specify which inlet method to use:

1. Double-click in the Inlet File column for the sample.
Alternative: In the Inlet File column for the sample, right-click, then click Browse.
2. Click the inlet method you want to use; click OK.

To specify with MS method to use:

1. Double-click in the MS File column for the sample.

Alternative: In the MS File column for the sample, right-click, then click Browse.

2. Click the MS method file you want to use; click Open.

Tip: If you cannot see these columns, customize the display so that they are visible. See [Customizing the Sample List display on page 5-8](#) for details.

Importing Sample Lists and data

MassLynx allows you to import complete Sample Lists from other software applications, and also provides a feature for you to import data into Sample Lists you have created. OpenLynx batch files, (*.olb) containing lists of samples that failed to run, can also be imported directly into the Sample List.

For detailed information on how to import Sample Lists and data, refer to the main online *MassLynx Help*.

Customizing the Sample List display

Many different columns of information can be displayed in the Sample List. The display you choose will be saved when you save the Sample List, although the display format can also be saved separately if you wish.

Tip: Displaying the most appropriate columns, and hiding those that are not needed, will help you to quickly see everything you need without being distracted by unnecessary information.

To customize visible columns and column order:

1. On the Sample List menu bar, click Samples > Format > Customize.

Alternative: Right-click on the Sample List and click Customize Display.

2. In the Customize Field Display dialog box, select the boxes next to columns you want to be visible, and clear the boxes next to columns you want to hide.
3. To change the order of columns, select a column in the list and click the Move up or down arrows until the column is in the required position. Repeat this for other columns if necessary.
4. When you have finished making changes, click OK.

To customize column titles, decimal places, and alignment:

1. Click a cell in the column you want to modify, then – on the Sample List menu bar – click Samples > Column > Properties.

Alternative: Right-click on the column heading and click Properties.

2. Modify the column title, alignment, and (for numeric columns only) the number of decimal places displayed.
3. Click OK.

Starting data acquisition

The process of acquiring data is simple and straightforward: all the work you have already done in tuning and calibrating the instrument, and configuring the inlet and MS methods, is utilized at this stage.

To start data acquisition:

1. Click MS Tune on the Instrument tab of the MassLynx bar to open the Tune window.

Caution: MS instruments require the Tune window to be open to acquire data, whether the acquisition is done directly from the Tune window or by using the Sample List. If you try to close the Tune window a warning message will be displayed to this effect: if you choose to close the window anyway then acquisition will not proceed.

2. Ensure the instrument is in Operate mode. If the indicator in the bottom right of the Tune window is not green, click the adjacent Operate button.

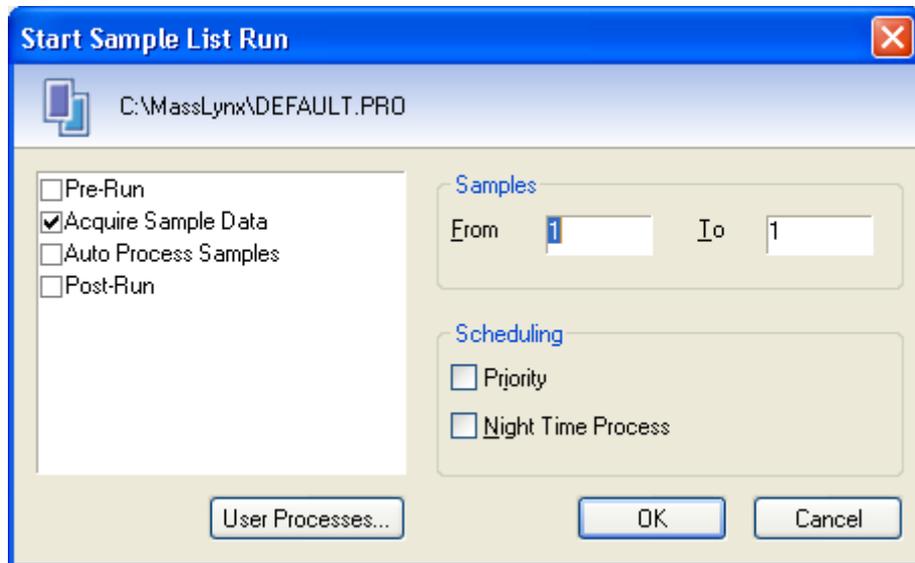
Tip: Instruments must be in Operate mode to acquire data. The current status of the instrument can be checked either in the Tune window – the indicator at the bottom right of the window will be colored green if the instrument is in Operate – or by clicking the Status button on the MassLynx tool bar.

3. In the main MassLynx window, click .

Alternative: Click Run > Start.

Result: The Start Sample List Run dialog box is displayed.

Start Sample List Run dialog box:



4. Make sure that the Acquire Sample Data box is selected, and that the samples to be run are correctly indicated. The other options (to perform Pre-Run and Post-Run processes, and to Auto Process Samples) should be left unselected unless you know that you want to perform these actions.
5. Click OK.

Result: MassLynx checks the Sample List to validate the entries and methods specified, then begins data acquisition. If any problems are found, explanatory messages will be displayed, and acquisition will not begin.

Tip: If data acquisition does not begin, check that the inlet is connected and not in error, and that you have not accidentally clicked the Pause button on the MassLynx tool bar.

Viewing the data acquisition progress

During acquisition, the Information bar above the Sample List will provide information on the progress of the acquisition. You can see all the jobs currently running, waiting, or paused by clicking the Queue button on the MassLynx tool bar. The status of individual jobs can then be viewed by clicking on the job in the MassLynx bar.

Viewing the chromatogram and spectrum during data acquisition

To view the chromatogram for the data currently being acquired:

1. On the Sample List menu bar, click Chromatogram to open the Chromatogram window.
2. Click . The chromatogram display is updated as the acquisition proceeds.

Alternative: Click Display > Real-Time Update.

To view the spectrum for the data currently being acquired:

1. On the Sample List menu bar, click Spectrum to open the Spectrum window.
2. Click Display > Real-Time Update; the Spectrum Real-Time Update dialog box is displayed.
3. Select Enable Real-Time Update.
4. Select the type of data you want to display; click OK.

6 Viewing, processing and storing results

This chapter will explain how you can:

- View the data you have acquired
- Manipulate the display to get the most useful results
- Move on to more advanced processing of your data
- Store your results

Contents:

Topic	Page
How to view, process, and store results	6-2
Viewing and manipulating chromatograms	6-3
Viewing and manipulating spectra	6-13
Processing and interpreting data	6-21
Storing results in SDMS	6-23

How to view, process, and store results

Acquiring data by running samples is usually just the beginning – you want to view the results obtained, store them for future reference, and, perhaps, process them to gain further understanding or enhance clarity.

The steps that need to be taken will depend on what you are trying to achieve with your work. MassLynx and the Application Managers provide a great many options to help you, but it is usual to begin by viewing the chromatograms and spectra obtained from the samples.

You can concentrate on certain parts of the chromatogram or spectra, and manipulate them to improve the clarity of the results – to remove background noise, for example. You can also display spectra related to specific chromatogram points, and the chromatograms associated with individual spectra.

You can then process the results by using the Application Managers included with MassLynx (QuanLynx and OpenLynx) to gain more value from the data acquired, and access other optional Application Managers that provide features specific to the type of work being done.

The results will be saved within the project you created. If you have Waters NuGenesis SDMS (Scientific Data Management System), the results can be stored there for sharing and review across your enterprise.

Viewing and manipulating chromatograms

There are a number of different types of chromatogram that can be displayed by MassLynx. It is helpful to have a concept of what each one means so that you can choose the most appropriate type for your needs.

Types of chromatogram:

Chromatogram type	Description
Total Ion Current (TIC)	Usually the default type of chromatogram opened in MassLynx, a TIC chromatogram can be thought of as a summed spectrum plotted over time. It shows the total current resulting from the detection of ions (of whatever mass) over the period of the MS scan.
Base Peak Intensity (BPI)	<p>A BPI chromatogram is a variant of a TIC chromatogram. It plots, for each scan throughout the period of the MS scan, the intensity of only the most abundant ion at the time of that scan. It ignores all the other, less abundant, ions detected at the same time.</p> <p>The BPI chromatogram exhibits a greater apparent resolution and signal-to-noise but will only contain contributions from the most intense components. Therefore, it is possible that some peaks in the TIC chromatogram may not be visible in the BPI chromatogram.</p>
Mass	<p>A mass chromatogram shows the ion current resulting from a specified mass only.</p> <p>The mass chromatogram can reduce complexity and make it easier to identify a known component.</p>
Analog	During an acquisition, MassLynx can store analog information obtained from an auxiliary source such as a UV detector. If analog data has been acquired it can be displayed using an analog chromatogram.

Opening the Chromatogram window

Chromatograms acquired in your data files are viewed using the Chromatogram window.

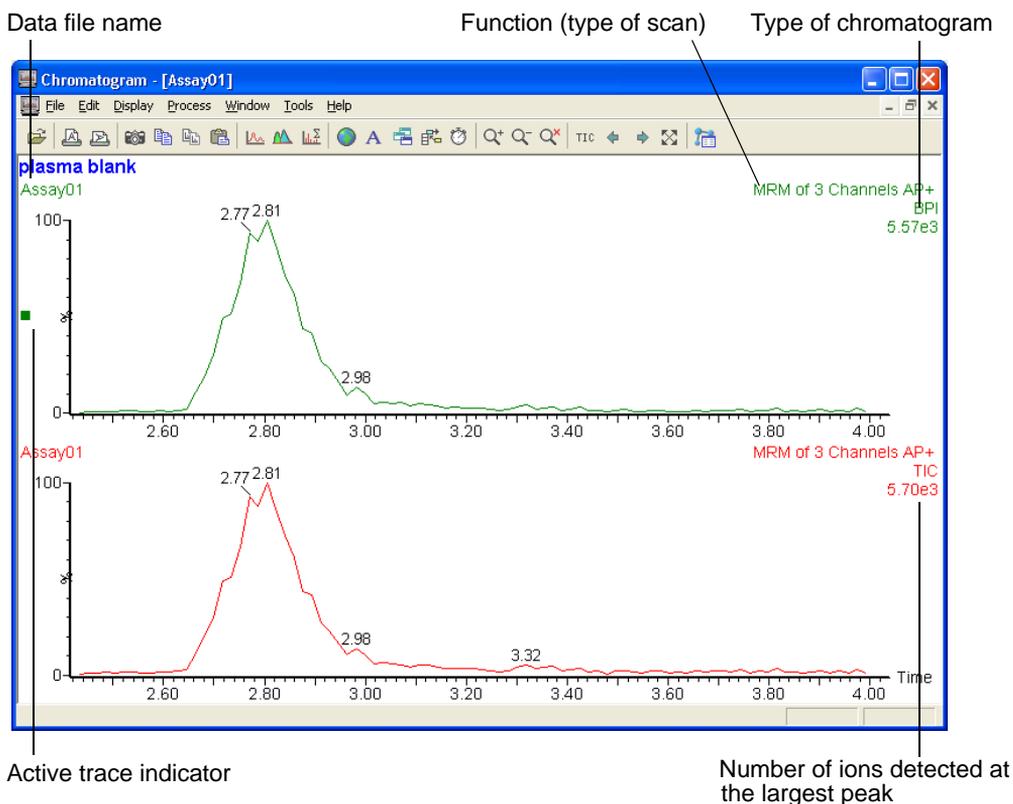
To open the Chromatogram window:

1. In the Sample List, click the number to the left of the sample you wish to view, so that the whole row is highlighted. You can choose more than one sample by clicking to the left of the first sample and dragging to the last.
2. On the Sample List menu bar, click Chromatogram.

You will now see the chromatogram of the data acquired from running the selected sample. Time is shown along the x axis (horizontal) and intensity is shown along the y axis (vertical).

There are several important areas on the screen to note:

Typical Chromatogram window:



Tips:

- The information displayed in the Chromatogram window can be configured by clicking **Display > View > Header**. For information on how to use this feature, refer to the *MassLynx Help*.
- You can also open the chromatogram for a data file from the Spectrum window. For details, see [Using the Spectrum on page 6-14](#).

Using the Chromatogram

To focus on the most important areas of the results, the Chromatogram display can be changed in a number of ways. Some of the most commonly used are:

- Showing only part of the chromatogram
- Magnifying the chromatogram, or part of the chromatogram
- Opening the spectrum relating to a point, or range, on the chromatogram

Showing part of the chromatogram

To show part of the chromatogram:

1. Click on the furthest left part of the chromatogram you wish to see.
2. Drag to the furthest right part of the chromatogram you wish to see; a line will be drawn to show how much of the chromatogram will be displayed.
3. Release the mouse button; the chromatogram display will be updated.

Alternatives:

- Click **Display > Range > From** to set the beginning and end time values manually.
- Click **Display > Range > Center > On time** to center the display on a specified time value.

To revert to seeing all of the chromatogram, click the  tool bar button, or click **Display > Range > Default**, and click **OK**.

Magnifying the chromatogram

To magnify the chromatogram:

1. Activate the chromatogram you want to magnify by clicking on it; the active trace indicator should appear beside it at the left of the window.
2. Click the  tool bar button; the chromatogram trace will be magnified, with the degree of magnification indicated at the top left of the trace.
3. To magnify the chromatogram further, click the button again.

To reduce the degree of magnification, click the  tool bar button.

To magnify part of the chromatogram:

1. Activate the chromatogram you want to magnify by clicking on it; the active trace indicator should appear beside it at the left of the window.
2. Click Display > Range > Magnify.
3. In the Chromatogram Magnify dialog box, type a custom magnification in the By box.
4. In the From and To boxes, type the times to which you would like to apply the magnification.
5. To specify a different magnification for another time range, select another number from the Range list, then repeat steps 3 and 4.
6. Click OK.

To revert to seeing the chromatogram without magnification, click the  tool bar button.

Opening a spectrum from the chromatogram trace

Opening the spectrum for a single point on the chromatogram

To open the spectrum for a single point on a chromatogram trace, right-click on the point of the chromatogram for which you want to see the spectrum. The Spectrum window will appear, showing the relevant spectrum.

A 'pointer', made up of a triangle  and a line running through the chromatogram trace, should appear at the point you clicked in the Chromatogram window. If it does not, make it visible by clicking Display >

Pointer. You can display the spectrum for different points on the chromatogram by dragging this pointer left and right along the trace.

You can open further spectra in the Spectrum window by right-clicking on other points on the chromatogram trace.

Opening the spectrum for a chromatogram range

You can also display a combined spectrum relating to a range of points along a chromatogram trace.

Tip: This feature is often used to produce a combined spectrum for a peak in the chromatogram.

To display a combined spectrum for a chromatogram range:

1. Right-click on the furthest left point you wish to include.
2. Drag to the furthest right point you wish to include; a line will be drawn to show how much of the chromatogram will be included.
3. Release the mouse button; the Spectrum window will display the combined spectrum.

Displaying chromatograms

You can display various types of chromatogram, as outlined in [Viewing and manipulating chromatograms on page 6-3](#), depending on the type of data acquired. You can also remove existing spectra and control how new spectra are created.

Tip: The types of chromatogram you use – and the ways in which they are processed – will depend on your particular situation. Consider your needs and objectives before deciding which features are going to be most helpful.

How to display the different types of chromatogram

Displaying different types of chromatogram:

To display this type of chromatogram	Do this
TIC	<ol style="list-style-type: none">1. Click Display > Tic.2. Click the function for which you wish to display the chromatogram.3. Click OK.
BPI	<ol style="list-style-type: none">1. Click Display > Tic.2. Click the function for which you wish to display the chromatogram.3. Select BPI Chromatogram.4. Click OK.
Mass	<ol style="list-style-type: none">1. Click Display > Mass.2. Type the mass (m/z) you are interest in into the Description box.3. Click the function for which you wish to display the chromatogram.4. Click OK.
Analog	<ol style="list-style-type: none">1. Click Display > Analog.2. Click the channel for which you wish to display the chromatogram.3. Click OK.

Tips:

- In the Options dialog box, you can specify the types of chromatogram that should appear by default. Open this dialog box by clicking on the Tools tab of the MassLynx bar, then clicking Options.
- You can apply advanced chromatogram display settings automatically to the Chromatogram window by using Chrotool. See [Automating chromatogram display with Chrotool on page 6-11](#) for further details.

Choosing whether to add traces, replace traces, or create a new window

Many of the operations you perform in the Chromatogram window – including displaying different types of chromatogram – will create a new chromatogram trace.

You can choose whether to add the new trace to the current window (the default setting), replace the current trace with the new one, or create the new trace in another window within the Chromatogram window.

Setting new traces display options:

To	Do this
Add the trace	Make sure neither the  nor  tool bar buttons are selected.
Replace the current trace	Select the  tool bar button
Create the trace in a new window	Select the  tool bar button

Removing chromatograms from the display

Removing chromatograms from the display does not alter the saved data – you are always able to recreate the removed chromatogram.

To remove a single chromatogram from the display:

1. Activate the chromatogram you want to remove by clicking on it.
Result: The active trace indicator should appear beside it at the left of the window.
2. Press the Delete key on the keyboard.
3. Click OK to confirm that you want to remove the chromatogram.

To remove multiple chromatograms from the display:

1. Click Display > Remove.
2. In the Remove Chromatogram dialog box, click the chromatograms you want to remove.
3. Click OK.

Processing your chromatograms

You can manipulate your chromatograms to highlight the areas of most interest, reduce background noise, and improve presentation.

Three processes are available for use on chromatograms:

- Background Subtract (polynomial background subtraction)
- Smoothing
- Integration

Background subtraction and smoothing help to improve the presentation of the data. Integration locates peaks, positions baselines and calculates peak statistics for quantitative work.

A short overview of each of these is given below. For detailed information on all the settings available, refer to the main online *MassLynx Help*.

Background subtraction

Background Subtract fits a smooth curve through the noise in the chromatogram trace then subtracts this curve from the chromatogram, leaving the peaks on a flat baseline.

To perform a background subtract:

1. In the Chromatogram window, click Process > Subtract.
2. Set the options required. The main MassLynx Help provides detailed information on the meaning of each option.
3. Click OK.

Smoothing

Smoothing improves presentation and aids interpretation of a chromatogram by increasing the apparent signal-to-noise ratio.

Two types of smoothing are available for chromatograms: Moving Mean and Savitzky Golay. Both methods slide a 'window' along the chromatogram, averaging the data points in the window to produce a point in the smoothed chromatogram.

Moving Mean takes the arithmetical mean of the intensities of the data points in the window.

Savitzky Golay takes an average of the intensities weighted by a quadratic curve. This tends to enhance peak and valley shapes, as well as preserving the height of the peaks better than the Moving Mean. However, Savitzky Golay does tend to produce small artifacts on either side of the real peaks.

To perform smoothing:

1. In the Chromatogram window, click Process > Smooth.
2. Set the size of the window, the number of smooths, and the smoothing method.
3. Click OK.

Integration

The integrate process locates peaks, positions baselines and calculates both the heights and areas of the peaks above their baselines. There are two possible integration methods available – the normal algorithm and the Apex peak integration algorithm.

Both methods can be preceded by smoothing, and a thresholding process can be applied after integration. The thresholding process can reject peaks, based on whether their height (or area) is less than an absolute value, or less than a specified fraction of the height (or area) of the largest peak.

To perform integration:

1. In the Chromatogram window, click Process > Integrate.
2. Set the options required. The main MassLynx Help provides detailed information on the meaning of each option.
3. Click OK.

Tip: To integrate multiple chromatograms at once – on data already acquired or as part of the acquisition process – you should use QuanLynx.

Automating chromatogram display with Chrotool

You can save display options and apply them to the Chromatogram window, either manually or automatically, by using Chrotool. This is particularly useful if you often want to show a certain type of chromatogram – the chromatogram for a certain mass, for instance. It may also be useful if the

chromatogram displayed by default when the Chromatogram window opens is not the most appropriate for your needs.

Open Chrotool from the Chromatogram window by clicking Display > ChroTool.

Chrotool allows you to save and apply all of the options that can be set when creating a TIC, BPI, Mass, or Analog chromatogram. These options can then be applied to the Chromatogram window either manually – by clicking the saved settings in Chrotool – or automatically when the Chromatogram window is opened.

Detailed information on using Chrotool is available in the main online *MassLynx Help*.

Viewing and manipulating spectra

You can view the spectra of the data acquired from running samples. The Spectrum window shows the mass of ions (or, to be more exact, the mass-to-charge ratio of those ions) detected during data acquisition.

The data acquired will usually be made up of a number of scans performed in very rapid succession. Each scan produces a spectrum: you can use the Spectrum window to step through the data obtained during the scans, or see the results of a number of scans on screen at one time.

Opening the Spectrum

Spectra acquired and saved in your data files are viewed using the Spectrum window.

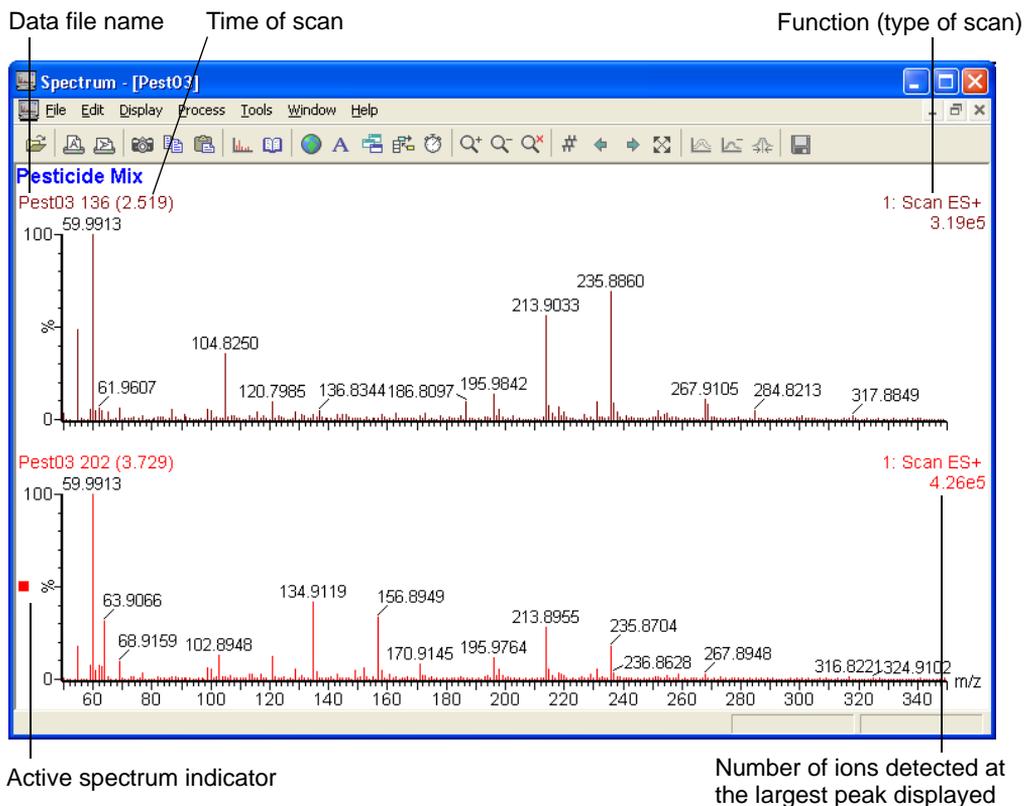
To open the Spectrum window:

1. In the Sample List, click the number to the left of the sample you wish to view, so that the whole row is highlighted. You can choose more than one sample by clicking to the left of the first sample and dragging to the last.
2. On the Sample List menu bar, click Spectrum.

You will now see the spectrum acquired for the first scan of the selected sample. The mass-to-charge ratio (m/z) is shown along the x axis (horizontal) and intensity is shown along the y axis (vertical).

There are several important areas on the screen to note:

The Spectrum window:



Tips:

- The information displayed in the Spectrum window can be configured by clicking Display > View > Header. For information on how to use this feature, refer to the *MassLynx Help*.
- You can also open the spectrum from the Chromatogram window. For details, see [Using the Chromatogram on page 6-5](#).

Using the Spectrum

To enable you to focus on the most important areas of the results, the Spectrum display can be changed in a number of ways. Some of the most commonly used are:

- Showing only part of the spectrum

- Magnifying the spectrum
- Opening the chromatogram relating to a single mass, or range of masses, shown on the spectrum

Showing part of the spectrum

To show part of the spectrum:

1. Click on the furthest left part of the spectrum you wish to see.
2. Drag to the furthest right part of the spectrum you wish to see; a line will be drawn to show how much of the spectrum will be displayed.
3. Release the mouse button; the spectrum display will be updated.

Alternative: Click Display > Range > From to set the beginning and end mass values manually.

To revert to seeing all of the spectrum, click the  tool bar button, or click Display > Range > Default, and click OK.

Magnifying the spectrum

To magnify the spectrum:

1. Activate the spectrum you want to magnify by clicking on it; the active spectrum indicator should appear beside it at the left of the window.
2. Click the  tool bar button; the spectrum will be magnified, with the degree of magnification indicated at the top left of the spectrum.
3. To magnify the spectrum further, click the button again.

To reduce the degree of magnification, click the  tool bar button.

To magnify part of the spectrum:

1. Activate the spectrum you want to magnify by clicking on it; the active spectrum indicator should appear beside it at the left of the window.
2. Click Display > Range > Magnify.
3. In the Spectrum Magnify dialog box, type a custom magnification in the By box.
4. In the From and To boxes, type the masses to which you would like to apply the magnification.

5. To specify a different magnification for another mass range, select another number from the Range list, then repeat steps 3 and 4.
6. Click OK.

To revert to seeing the spectrum without magnification, click the  tool bar button.

Opening a chromatogram from the spectrum

Opening the chromatogram for a single mass

To open the chromatogram for a single mass shown on the spectrum, right-click on the point of the spectrum you want to see the chromatogram for. The Chromatogram window will appear, showing the relevant chromatogram.

You can open further chromatograms in the Chromatogram window by right-clicking on other points on the spectrum.

Opening the chromatogram for a range of masses

You can also display a chromatogram relating to a range of masses displayed on your spectrum.

To display a chromatogram for a range of masses:

1. Right-click on the smallest mass you wish to include.
2. Drag to the largest mass you wish to include; a line will be drawn to show the extent of the masses that will be included. The mass range will also be indicated in the status bar at the bottom left of the Spectrum window.
3. Release the mouse button; the Chromatogram window will display the chromatogram for the mass range.

Displaying spectra

You can choose to display the spectrum for a specific time, remove existing spectra, and control how new spectra are created.

Tips:

- The ways in which you display and process the spectra will depend on your particular situation: consider your needs and objectives before deciding which features are going to be most helpful.

- Some of the processing options outlined below will only appear if the operation can be performed on the type of data you have acquired.

How to display the spectrum for a specific retention time

When you open the Spectrum window from the Sample List, the spectrum for the first scan of the data acquisition is displayed.

To display the spectrum for a specific retention time:

1. Click Display > Spectrum > At.
2. In the Display RAW Spectrum dialog box, type the time for which you want to display the spectrum, and select the desired function.
3. Click OK; the spectrum acquired at the time nearest to the time specified is displayed.

Tip: You can also display the spectrum for a specific retention time by right-clicking on that time on the chromatogram trace for the data. For details on how to do this, see [Opening a spectrum from the chromatogram trace on page 6-6](#).

Choosing whether to add spectra, replace spectra, or create a new window

Many of the operations you perform in the Spectrum window – including displaying different spectra for different times – will create a new spectrum on the screen.

You can choose whether to add the new spectrum to the current window (the default setting), replace the current spectrum with the new one, or create the new spectrum in another window within the Spectrum window.

Setting new spectra display options:

To	Do this
Add the spectrum	Make sure neither the  nor  tool bar buttons are selected.
Replace the current spectrum	Select the  tool bar button
Create the spectrum in a new window	Select the  tool bar button

Removing spectra from the display

Removing spectra from the display does not alter the saved data – you are always able recreate the removed spectrum.

To remove a single spectrum from the display:

1. Activate the spectrum you want to remove by clicking on it; the active spectrum indicator should appear beside it at the left of the window.
2. Press the Delete key on the keyboard.
3. Click OK to confirm that you want to remove the spectrum.

To remove multiple spectra from the display:

1. Click Display > Remove.
2. In the Remove Spectra dialog box, click the spectra you want to remove.
3. Click OK.

Processing your spectra

A number of features are available to enhance the clarity of your spectra, helping you to analyze and share your results more effectively.

Spectrum processing features:

Process	Description	How to
Refine	Automatically removes background ions from a spectrum, thereby allowing it to be more easily identified – by library search, for example. The Refine process operates on centroid-mode data only.	Click Process > Refine

Spectrum processing features:

Process	Description	How to
Combine	<p>Produces a single spectrum by subtracting averaged background spectra from the average of the spectra from a TIC peak. The combined scan exhibits enhanced signal-to-noise and improved mass accuracy.</p> <p>The Combine spectra process operates on centroid-mode or continuum data.</p>	Click Process > Combine
Background subtract	<p>Adjusts the zero level in a continuum spectrum to lessen the effect of chemical noise, Chemical noise can be caused by occurrences such as column bleed.</p> <p>Background subtract improves presentation and aids interpretation.</p>	Click Process > Subtract
Smooth	<p>Reduces the high-frequency noise present in a spectrum, thus aiding interpretation.</p> <p>Data should be smoothed before mass measurement is attempted with the Center process, otherwise peaks may be created from the noise spikes.</p>	Click Process > Smooth

Spectrum processing features:

Process	Description	How to
Center	Uses all the points across a peak in a continuum trace to calculate the mass of the peak center. The centering process can be used either to label each peak with the calculated mass, or to produce a single bar from each peak in a continuum spectrum.	Click Process > Center
Mass measure	Performs a combination of background subtraction, smoothing, and centering in one command.	Click Process > Mass Measure
Integrate	Locates spectral peaks, draws baselines and calculates peak areas. Spectrum integration works over the full mass range of the spectrum.	Click Process > Integrate
Transform	Uses charge states assigned to each peak to display the m/z spectrum on a true molecular mass axis. Rule: Transform will only be available if it was selected during installation.	Click Process > Transform
MaxEnt	Uses the maximum entropy method to produce true molecular mass spectra from multiply-charged ElectroSpray spectra. Rule: MaxEnt will only be available if it was selected during installation.	Click Process > MaxEnt

Detailed information on the settings that apply to each of these processing features is supplied in the main MassLynx Help.

Processing and interpreting data

The data acquired from your instruments can be processed and distributed in many different ways to provide the information you need. As there are many different uses for mass spectrometry, MassLynx provides a range of utilities that assist with these various needs: these utilities are known as Application Managers.

The Application Managers available will depend on your organization's priorities. Data processing with two Application Managers – QuanLynx and OpenLynx – is available to all users, and will be accessible so long as these Application Managers were selected at installation time.

Tip: If QuanLynx and OpenLynx were not installed during the initial MassLynx installation, they can be added to the system at any time. For details, see [Installing additional Application Managers on page 1-6](#).

Quantitation using QuanLynx

QuanLynx is used to quantify samples – to determine how much of a known compound is in a sample.

To do this, QuanLynx compares the data acquired with a calibration curve – representing the known values for different amounts of the compound – and then calculates the quantity of the compound found in the sample.

To access QuanLynx, click the QuanLynx tab on the left of the MassLynx Shortcut bar.

For a quick start guide to QuanLynx, see the online *QuanLynx Help*.

Providing access and distributing results using OpenLynx

OpenLynx is a versatile Application Manager providing report generation and distribution features, alongside capabilities for walk-up access and submission of samples using the optional OALogin module.

To access OpenLynx, click the OpenLynx tab on the left of the MassLynx Shortcut bar.

For a quick start guide to OpenLynx, see the online *OpenLynx Help*.

Processing data using other Application Managers

One or more other Application Managers may be installed on your system. Each Application Manager will appear as another tab on the left of the MassLynx shortcut bar. To access an Application Manager, click the tab; the MassLynx bar will show icons linking you to the features available.

Assistance is available for each Application Manager by clicking the question mark  to the right of the Application Manager's name in the MassLynx bar.

Storing results in SDMS

The results you obtain will be stored in the project that was used to acquire them. They can be opened from within the project, and you can also view data from other projects in the Chromatogram and Spectrum windows by browsing to the data files of interest.

If you have Waters NuGenesis SDMS (Scientific Data Management System) the data acquired through MassLynx can be shared by sending it to SDMS. Data can also be retrieved from SDMS for viewing and processing in MassLynx.

Configuring MassLynx SDMS settings

MassLynx SDMS settings need to be configured before you can start sending and retrieving data.

To configure SDMS settings:

1. Click the SDMS tab on the left of the MassLynx Shortcut bar.
2. Click Configure.
3. Enter the location of the archive folder.
Tip: Your SDMS system will need to be configured to monitor the directory specified here.
4. Select the file types that you want to be available for sending to SDMS.
Tip: While selecting View All Files will allow all file types to be seen in the Send dialog box, it will only be possible to send the specific file types selected.
5. Type the URL of the NuGenesis Vision Browser, used to retrieve information.
Tip: Check that you have entered the URL correctly by clicking the Launch button.
6. Click OK.

Sending data to SDMS

When you are ready to send data to SDMS, it is possible to choose which files should be sent and whether the originals should be removed.

To send data to SDMS:

1. Click the SDMS tab on the left of the MassLynx Shortcut bar.
2. Click Send.
3. Browse to the location of the data you wish to send.
4. In the drop-down list on the right of the dialog box, click the type of file you want to send.

Tip: Only the types of file specified in the Configure dialog box will be available.

5. In the list of available files at the top right of the dialog box, click the files you wish to send, then click Add to Archive. Alternatively, click Add All to add all of the files in the available files list.

Result: The files you have specified are shown in the Archive File List at the bottom of the dialog box. These are the files that will be made available to SDMS when you click Send.

6. Repeat steps 3 to 5 for additional files you wish to send.
7. If you want to remove the original files from disk, select Remove Original.
8. Click Send.

Requirement: For the data to be successfully archived, SDMS will need to be correctly set up to monitor the configured archive folder.

Retrieving data from SDMS

You retrieve data using the NuGenesis Vision Browser. If it has been configured, you can access the Browser by clicking the SDMS tab on the left of the MassLynx Shortcut bar, then clicking Retrieve.

Help on locating, viewing, and restoring your data can be available by clicking the question mark button in the Vision Browser.

A Additional OpenLynx installation instructions

This appendix provides installation instructions for OpenLynx Login, OpenLynx Toolkit, and the Diversity browser.

Key disks are required to install these components. You will be asked to enter the location of the key disk during the installation process. If you do not have an appropriate key disk – and believe you should – contact your MassLynx system administrator.

Contents:

Topic	Page
Installing OpenLynx Login	A-2
Installing OpenLynx Toolkit	A-5
Installing Diversity browser	A-22

Installing OpenLynx Login

Requirements:

- Before installing OpenLynx Login, you must install MassLynx on the PC controlling the mass spectrometer. Refer to [Installing MassLynx on page 1-4](#) for details.
- The OpenLynx Login PC must be able to communicate with the MassLynx PC. If OpenLynx Login is installed on a different PC to MassLynx, a network connection is required.

There are three steps to installing OpenLynx Login:

1. Sharing the installation directory on the MassLynx PC.
2. Mapping a drive on the OpenLynx Login PC to the MassLynx PC.
3. Installing OpenLynx Login on the OpenLynx Login PC.

Sharing the installation directory on the MassLynx PC

To share the installation directory on the MassLynx PC:

1. Open Windows[®] Explorer, right-click the directory that MassLynx was installed into (usually C:\MassLynx), then click Properties.
2. Click the Sharing tab.

Tip: If a warning message is displayed, click If you understand the risk but still want to share the root of the drive, click here to open the Sharing page.

3. Select Share this folder.
4. Enter a name in the Share name box.
5. Click Apply.

Tip: If a warning message is displayed because the share name is too long, select the appropriate response and amend the share name.

6. Click OK.

Result: The directory is shared. In Windows Explorer, the directory now shows a hand under the folder icon.

Mapping a drive on the OpenLynx Login PC to the MassLynx PC

To map the drive:

1. On the PC on which you wish to install OpenLynx Login, open Windows Explorer, then click Tools > Map Network Drive.
2. In the Drive box, click a drive letter without a folder currently mapped to it (an available drive).
3. Click Browse, then browse to the MassLynx PC and select the shared directory created during [Sharing the installation directory on the MassLynx PC on page A-2](#).
4. Click Finish.

Result: The shared directory is mapped to the drive letter selected.

Installing OpenLynx Login

To install the OpenLynx Login program on the login PC:

1. Log on to the PC using a user account with permission to install software – usually an administrator account.
2. Insert MassLynx 4.1 CD 2 into the appropriate drive.
3. Use Windows Explorer to navigate to the OALogin directory, then double-click setup.exe; the OALogin installer is displayed.
4. Click Next, confirm that you accept the license agreement, then click Next again to accept the installation directory for OALogin.
5. On the MassLynx Folder page, click Change, then Browse to the MassLynx installation directory. If you are installing on a PC other than the MassLynx PC, this will be the drive that was mapped during [Mapping a drive on the OpenLynx Login PC to the MassLynx PC on page A-3](#).
6. Click Next, then click Install to begin the installation process.

Tip: If an OALogin - Wizard error message is displayed, stating that the selected directory does not contain a valid MassLynx installation, click OK, then repeat step 7.

7. When prompted, browse to the location of the key disk that has been supplied. If you do not have the appropriate key disk, contact your MassLynx system administrator.

Result: OpenLynx Login is installed.

Installing OpenLynx Toolkit

OAToolkit enables administrators to manage OALogin users from a single PC, and monitor the status of Acquisition PCs.

The OAToolkit software comprises:

- Administration Tool — Enables an administrator to create and manage all OALogin users from a single PC, and to replicate that information to multiple OALogin PCs and Acquisition PCs.
 - OAToolkit Service — Runs in the background on one or more Acquisition PCs, monitors sample batches submitted by OALogin users that were uploaded from the Administration Tool, and automatically:
 - relocates data produced during the processing of an OALogin user's batch of samples.
 - creates new project folders in which to store the processing data on a timed basis.
 - converts report files to different formats (XML and HTML, for example).
- Tip:** Settings that you can customize in the Administration Tool enable the service to perform these automatic actions.
- Remote Status Monitor — Enables any user to monitor the status of multiple instruments and their batch queues from a single PC.

This section describes a typical hardware setup and how to install and set up the software.

Contents:

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Typical hardware setup for OAToolkit	A-6
Installing the software	A-6
Setting up the OAToolkit Service	A-7
Remote Status Monitor	A-13

Typical hardware setup for OAToolkit

This section describes the typical hardware setup. Logically, there are four PCs:

- Acquisition PC — a PC that has MassLynx and the OAToolkit Service running, and is attached to an instrument.
- OALogin PC — any regular OALogin Terminal which is normally used to log samples on the Acquisition PC.
- File Storage PC — a PC on the same network domain as the Acquisition PC that will be used to store files moved from the Acquisition PC by the OAToolkit Service.
- Administration PC — a PC that has the OAToolkit Administration Tool installed.

It is not necessary to have four separate PCs to run the OAToolkit. You can, for example, use the same PC to run the OAToolkit Administration Tool and to store the files sent from the OAToolkit service. However, for the scope of this discussion, each PC is treated as a separate entity.

Installing the software

To run OAToolkit, you need to install the Administration Tool on the Administration PC, and the OAToolkit Service on the Acquisition PC.

Installing the OAToolkit Administration Tool on the Administration PC

To install the OAToolkit Administration Tool:

1. At the Administration PC, insert MassLynx 4.1 CD 2.
2. Browse to the OAToolkit directory, then double-click setup.exe.
3. In the dialog, select the check box OAToolkit Administration Tool.
4. In the dialog, select the default installation directory of C:\OAToolkit.
5. When prompted, browse to the location of the key disk that has been supplied. If you do not have the appropriate key disk, contact your MassLynx system administrator.

When the installation has finished, there is a directory C:\OAToolkit on the Administration PC.

Installing the OAToolkit Service on the Acquisition PC

To install the OAToolkit Service:

1. At the Administration PC, insert MassLynx 4.1 CD 2.
2. Browse to the OAToolkit directory, then double-click setup.exe.
3. In the dialog, select the check box OAToolkit Service.
4. In the dialog, select the default installation directory of C:\OAToolkit.
5. When prompted, browse to the location of the key disk that has been supplied. If you do not have the appropriate key disk, contact your MassLynx system administrator.

When the installation has finished, there is a directory C:\OAToolkit on the Acquisition PC, and the OAToolkit Service is running.

Setting up the OAToolkit Service

The OAToolkit Service monitors batch files that have been processed on the Acquisition PC. When the service locates a batch file that belongs to a recognized OALogin user, it transfers the raw data files, report files, batch files, and so on, that are associated with that sample. Typically, most OAToolkit administrators would want these files moved to a separate File Storage PC, not the Acquisition PC.

This section details how to set up one Acquisition PC and one File Storage PC to which the OAToolkit will transfer files.

Requirement: Both PCs must be on the same network domain.

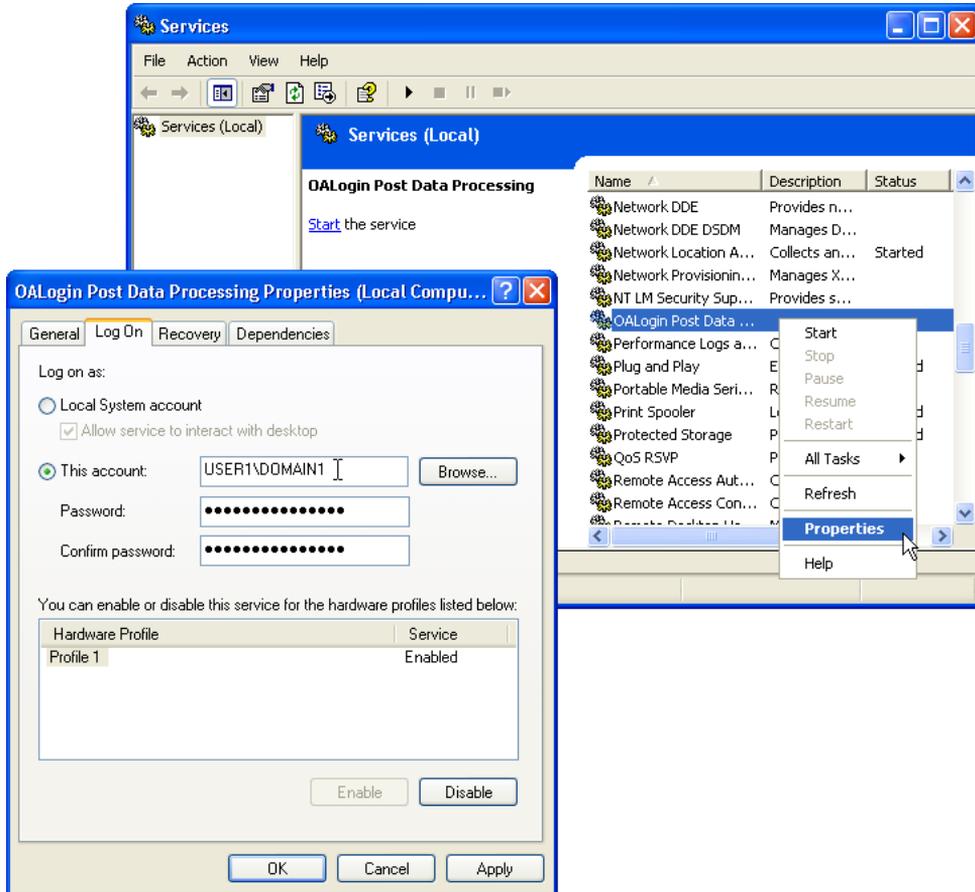
Setting Up the OAToolkit Service on the Acquisition PC

To enable the service to transfer data to File Storage PCs on the same network, the OAToolkit service must be logged in as a domain user.

To log in the service:

1. Log in to the Acquisition PC as a local Windows administrator.
2. On the Windows desktop, select Start > Run. The Run dialog opens.
3. In the Run dialog, type Services.msc, and then click OK. The Services dialog opens.

Setting up the Acquisition PC - OALogin Post Data Processing Properties (Local Computer) dialog:



4. In the Services (Local) list, locate the service OALogin Post Data Processing, and then stop the service.
5. In the service list, right-click the OALogin Post Data Processing service and select Properties.
6. Select the Log On tab.
7. Select the option This account:, and then type the fully-qualified user account name and password.

In the example graphic above, the service is being started using the domain user DOMAIN1\USER1.

8. Click Apply, and then click OK.

9. Start the service.

In the example, the service now has all the permissions and the privileges of the domain user USER1.

10. Log out as the local administrator, and log back in as the normal Acquisition PC user.

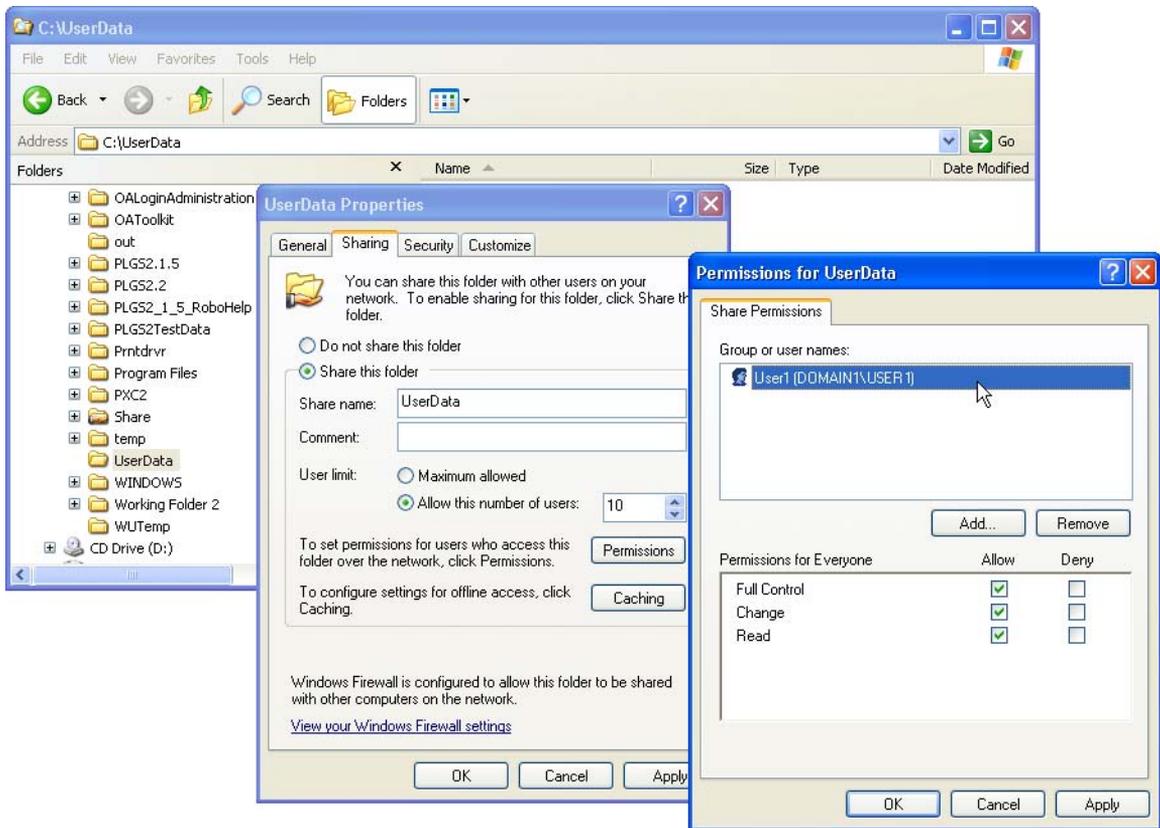
You now need to set up a folder on the File Storage PC so that it is ready to accept files from the service.

Setting Up the File Storage PC

To set up the File Storage PC:

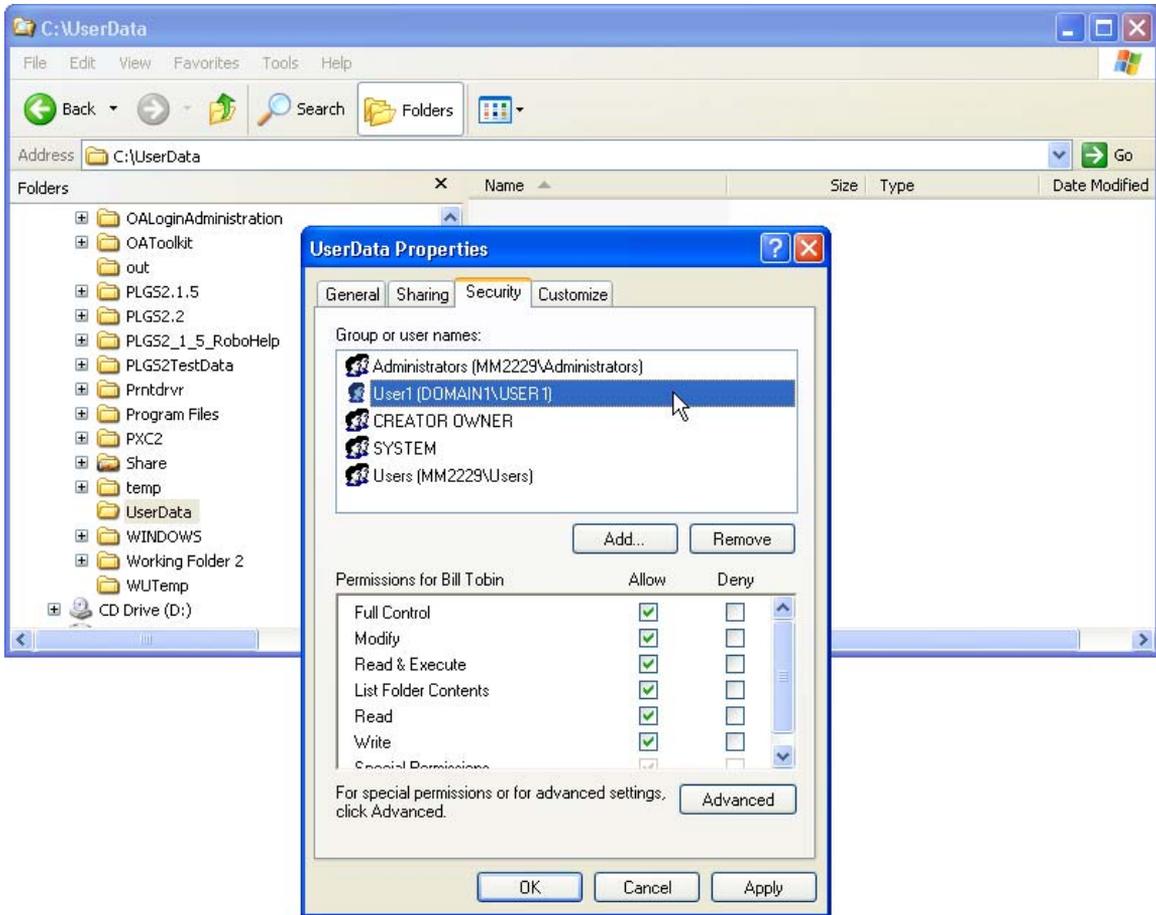
1. Log in to the File Storage PC. Ensure that you are logged in as a user who has rights to create and share directories locally.
2. Create a directory, for example C:\UserData.
3. Set up the share permissions on this directory to enable the service user on the Acquisition PC to have full privileges.

Setting up the File Storage PC - Permissions dialog - Sharing page:



4. Click the Security tab, add the user, and then set full NTFS permissions for the user.

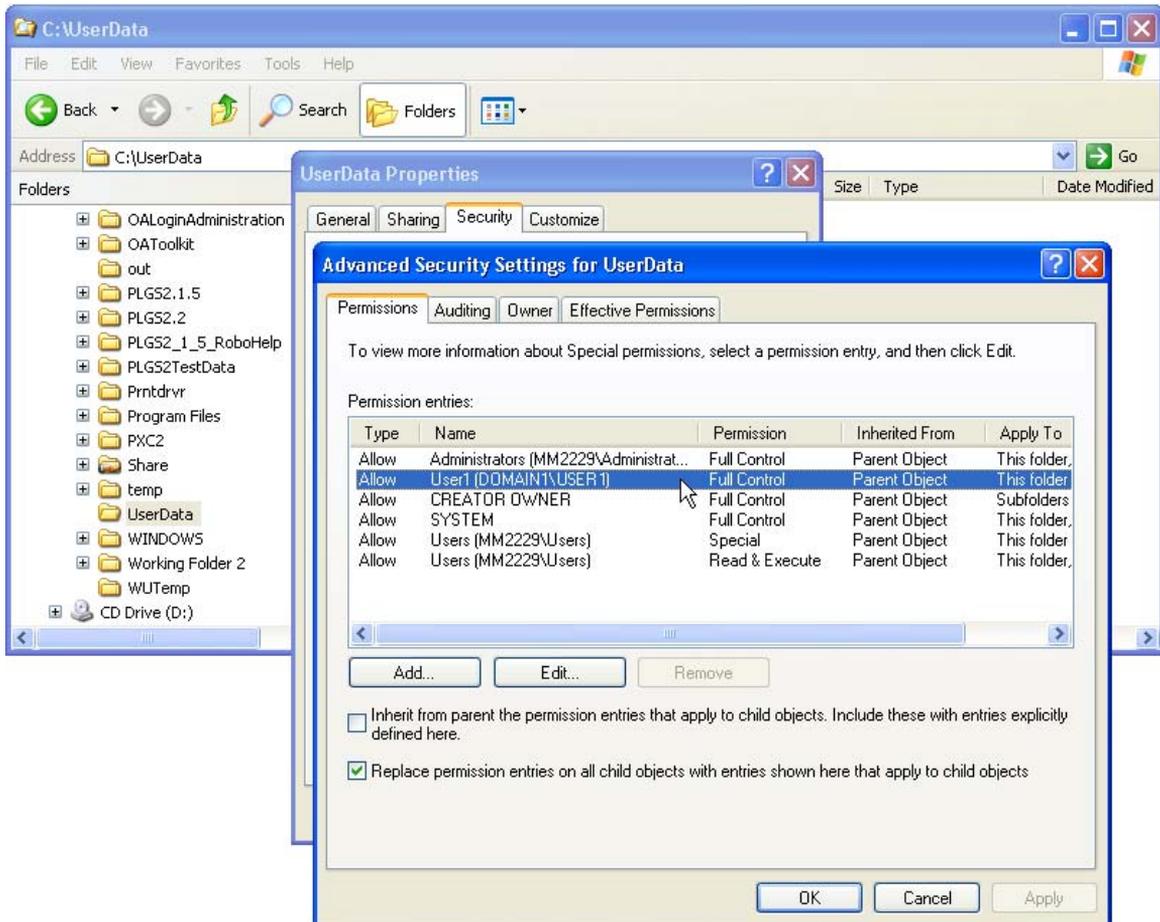
Setting up the File Storage PC - Permissions dialog - Security page:



5. On the Security page, click Advanced.

The OAToolkit Service user must have the ability to create directories underneath the shared directory. For example, the OAToolkit administrator might need the system to create directories for specific users such as `UserData\User1` and `UserData\User2`. To enable this, you use the advanced security settings.

Setting up the File Storage PC - Permissions dialog - Advanced Security - Permissions page:



6. On the Advanced Security Settings - Permissions page, select the user in the list.
7. Clear the check box Inherit from parent the..., and select the check box Replace permission entries on all child objects...
This gives the OAToolkit Service user full control over sub-folders.
8. Click OK in all dialogs to exit.

Remote Status Monitor

The Remote Status Monitor (RSM):

- Monitors the state of one or more Acquisition PCs.
- Writes monitoring information to an XML file, which is then read by an HTML page. The information can then be viewed in a Web browser.

This section refers to two different computers:

- Administration PC — a PC that has the Remote Status Monitor software installed.

Requirement: This PC must be powered up at all times and be available to monitor instruments.

- Acquisition PC — any MassLynx PC which is being monitored.

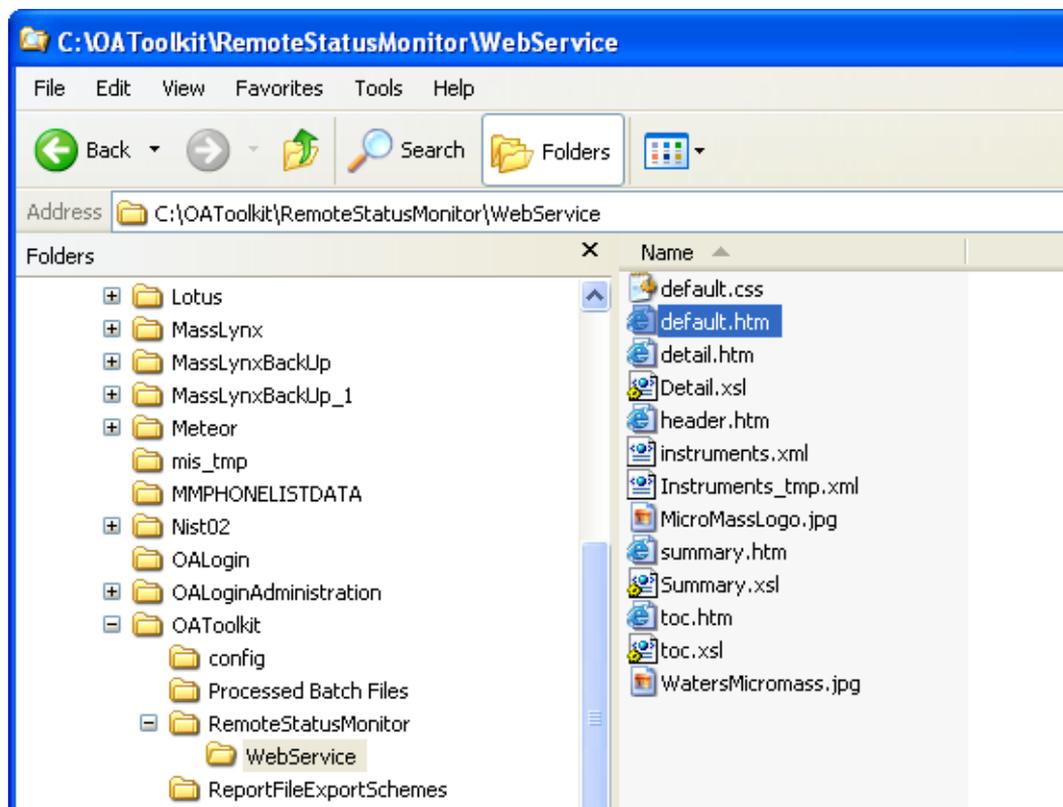
Installing Remote Status Monitor

To install Remote System Monitor:

1. At the Administration PC, insert MassLynx 4.1 CD 2.
2. Browse to the OAToolkit directory, then double-click setup.exe.
3. In the OAToolkit wizard:
 - Accept the terms of the license agreement.
 - Select to install the OAToolkit Remote Status Monitor.
 - Install the application in the folder C:\OAToolkit.
4. When prompted, browse to the location of the key disk that has been supplied. If you do not have the appropriate key disk, contact your MassLynx system administrator.

When the installation has completed, there is a directory C:\OAToolkit\Remote Status Monitor\WebService on the Administration PC. Within this directory, there is a file named default.htm; this is the file that is used to monitor the instruments through a Web browser.

Location of default.htm in OAToolkit:



Setting up, registering and monitoring instruments

Requirement: Your company network administrator should be present when these procedures are being performed.

To have a configuration that proves that the RSM is running correctly, there should be at least one Administration PC, and one Acquisition PC.

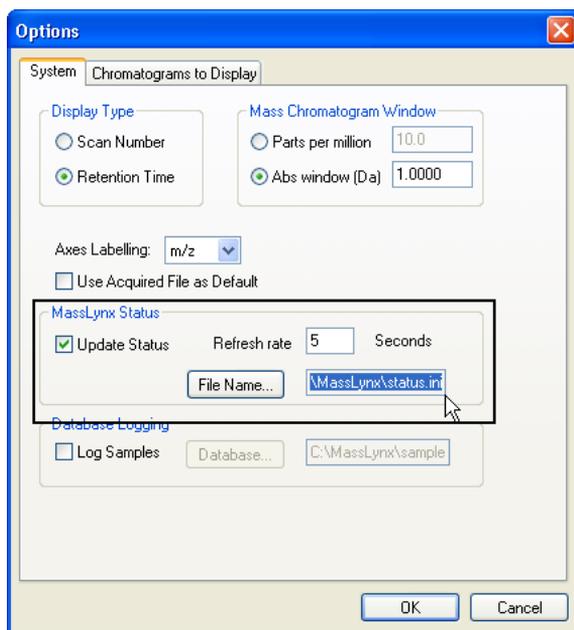
Any Acquisition PC that is to be monitored must be set up so that MassLynx writes to its status file. This is not a default option on installation of MassLynx.

To set up the Acquisition PC for monitoring:

1. On the Acquisition PC, start MassLynx.
2. From the MassLynx Shortcut Bar Menu, click Tools, and then from the Shortcut Bar, click Options.

3. In the Options dialog, click the System tab.
4. On the System page MassLynx Status options, ensure that the following are set:
 - Update Status is selected.
 - Refresh Rate = 5 seconds
 - File Name is C:\MassLynx\status.ini

MassLynx Status options:



5. Click OK, and then restart MassLynx.
This Acquisition PC is now ready to be monitored.

Registering and monitoring instruments

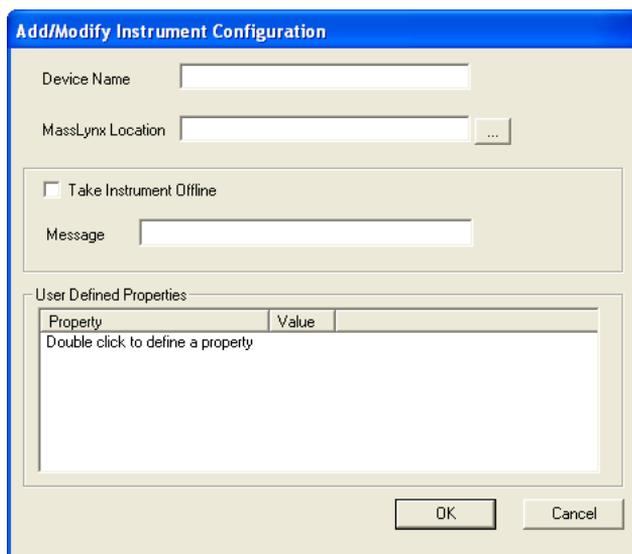
To monitor the instrument, you must register the instrument with Remote Status Monitor (RSM). This enables you to run RSM and view the results.

Requirement: The user on the Administration PC must have read privileges to the directory C:\MassLynx on the Acquisition PC. This enables RSM on the Administration PC to read the Status.ini file.

To register and monitor instruments:

1. On the Administration PC, select:
Start > All Programs > OAToolkit Remote Status Monitor
The main Remote Status Monitor screen opens.
2. To register the instrument, click . The Add/Modify Instrument Configuration dialog opens.

Remote Status Monitor - Add/Modify Instrument Configuration dialog:

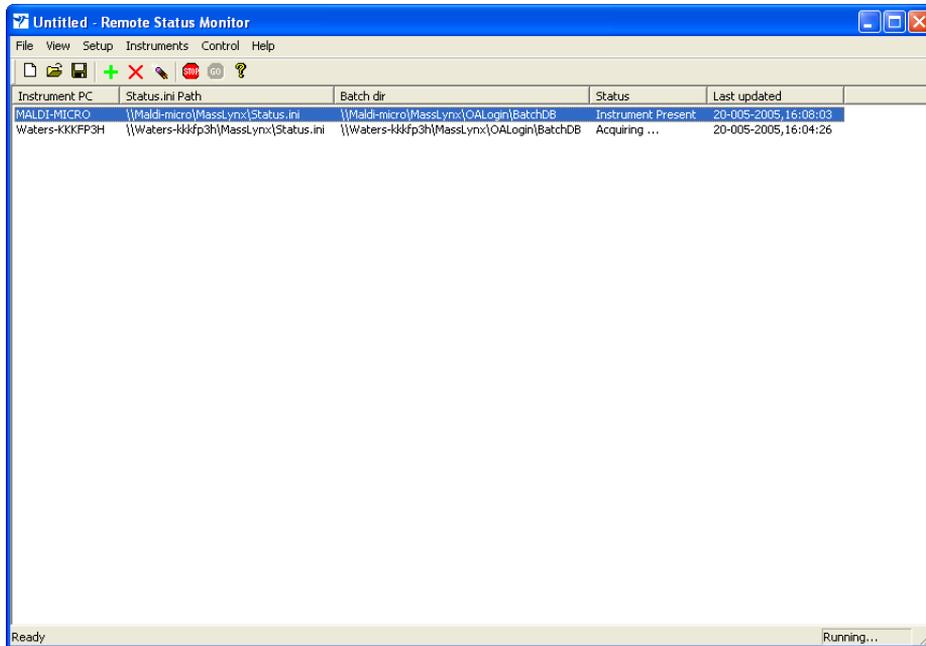


The screenshot shows the 'Add/Modify Instrument Configuration' dialog box. It features a blue title bar and a light beige background. The dialog contains the following elements:

- Device Name:** A text input field.
- MassLynx Location:** A text input field with a browse button (three dots) to its right.
- Take Instrument Offline:** A checkbox.
- Message:** A text input field.
- User Defined Properties:** A section containing a table with two columns: 'Property' and 'Value'. The table has one row with the text 'Double click to define a property'.
- Buttons:** 'OK' and 'Cancel' buttons at the bottom right.

3. In the Device Name text box, type a unique ID.
This name will be displayed in all pages of the RSM to identify the instrument.
4. In the MassLynx Location text box, type the path, or browse to the location of MassLynx on the Acquisition PC.
5. Click OK.
The instrument details are displayed in the list on the main RSM screen.
6. To start monitoring, click . If the instrument is on-line, functioning but not acquiring, the status is Idle.

Remote Status Monitor - instrument registered and monitored:



The screenshot shows a Windows application window titled "Untitled - Remote Status Monitor". The window has a menu bar with "File", "View", "Setup", "Instruments", "Control", and "Help". Below the menu bar is a toolbar with icons for file operations and a help icon. The main area contains a table with the following data:

Instrument PC	Status.ini Path	Batch dir	Status	Last updated
MALDI-MICRO	\\Maldi-micro\MassLynx>Status.ini	\\Maldi-micro\MassLynx\OALogin\BatchDB	Instrument Present	20-005-2005, 16:08:03
Waters-KXKFP3H	\\Waters-k44fp3h\MassLynx>Status.ini	\\Waters-k44fp3h\MassLynx\OALogin\BatchDB	Acquiring ...	20-005-2005, 16:04:26

The status bar at the bottom of the window shows "Ready" on the left and "Running..." on the right.

Viewing instrument details in a Web browser

To view the default.htm file, which shows instrument details in a Web browser, you must create a virtual directory on the Windows Internet Information Services (IIS) on the Administration PC.

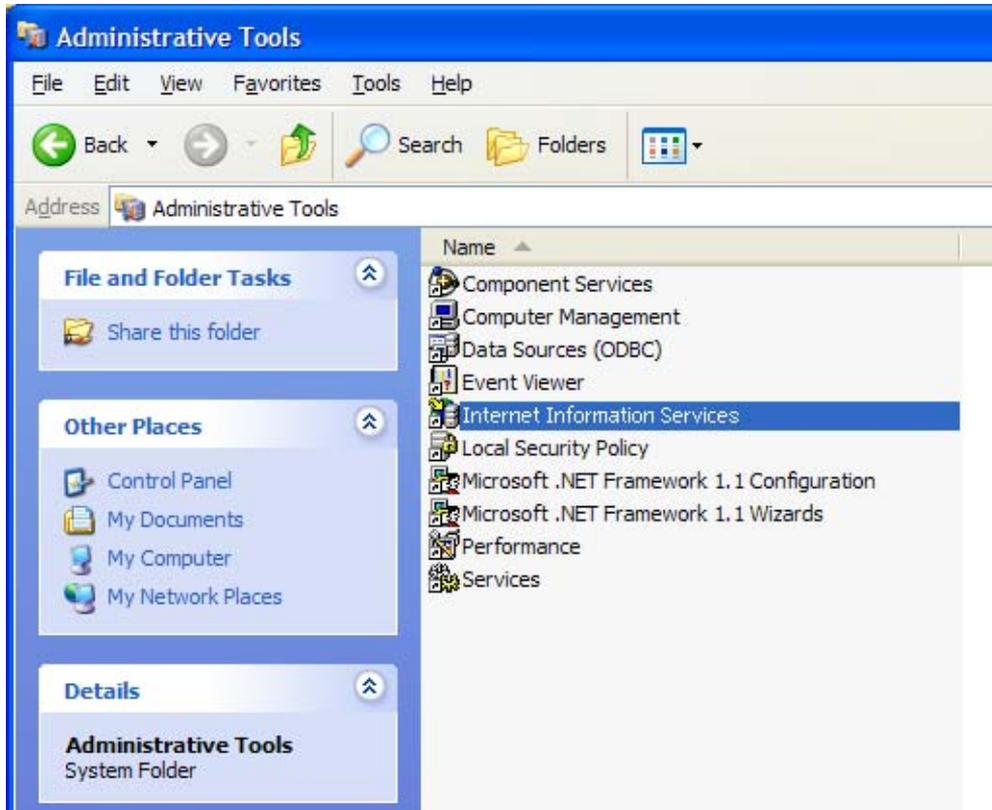
Tip: If IIS is not installed on the Administration PC, please refer to the Windows documentation.

The RSM writes status and batch information for the instrument(s) to its internal XML files, which are read by the default.htm file.

To create a virtual directory on IIS:

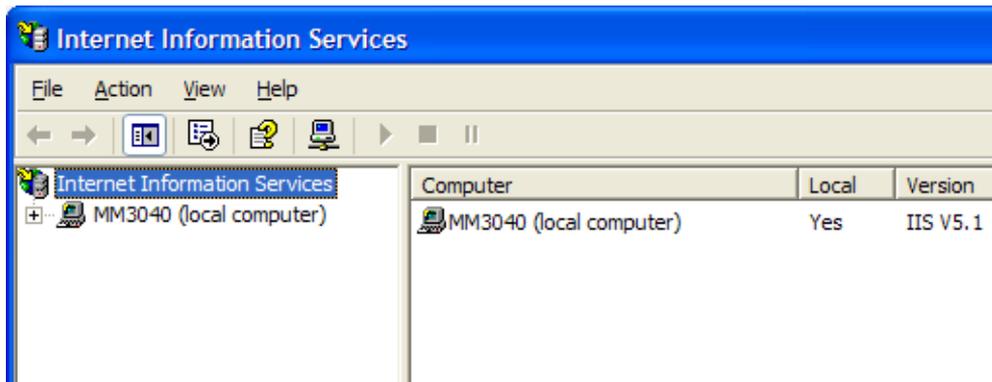
1. In the Windows operating system, select Start > Control Panel > Administrative Tools.

Windows Administrative Tools list:



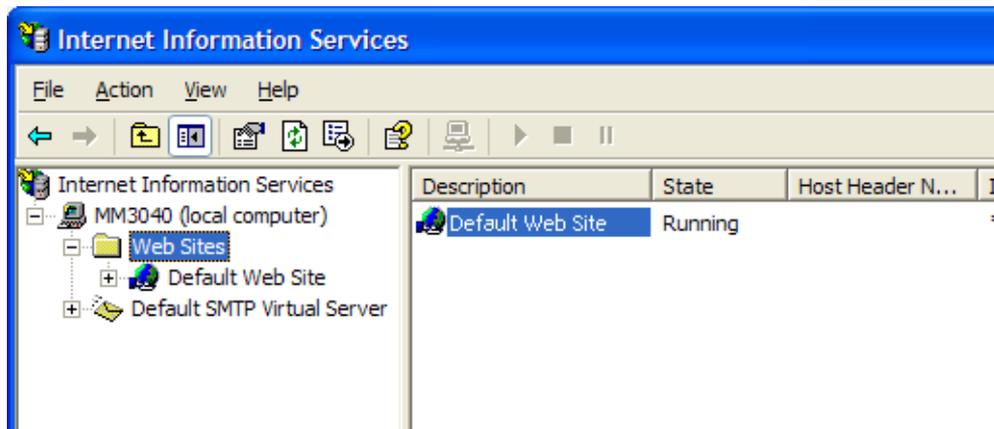
2. Click Internet Information Services.
The Internet Information Services window opens.

Windows Internet Information Services window:



- Expand the local computer tree, and then click Web Sites.

Windows Internet Information Services - Web sites list:



- In the table, right-click Default Web Site, and then select New > Virtual Directory...

The Virtual Directory Creation wizard opens.

- In the wizard:

- Type a name for the virtual directory, such as InstrumentInfo.
- Browse to the directory that contains the default.htm file
C:\OAToolkit\RemoteStatusMonitor\WebService
- Select the check boxes for the access permissions Read, Run scripts (such as ASP), and Browse.

To view instrument details in Web browser

- In a Web browser, type the URL

http:\\<Administration PC name>\\<virtual directory alias>\default.htm

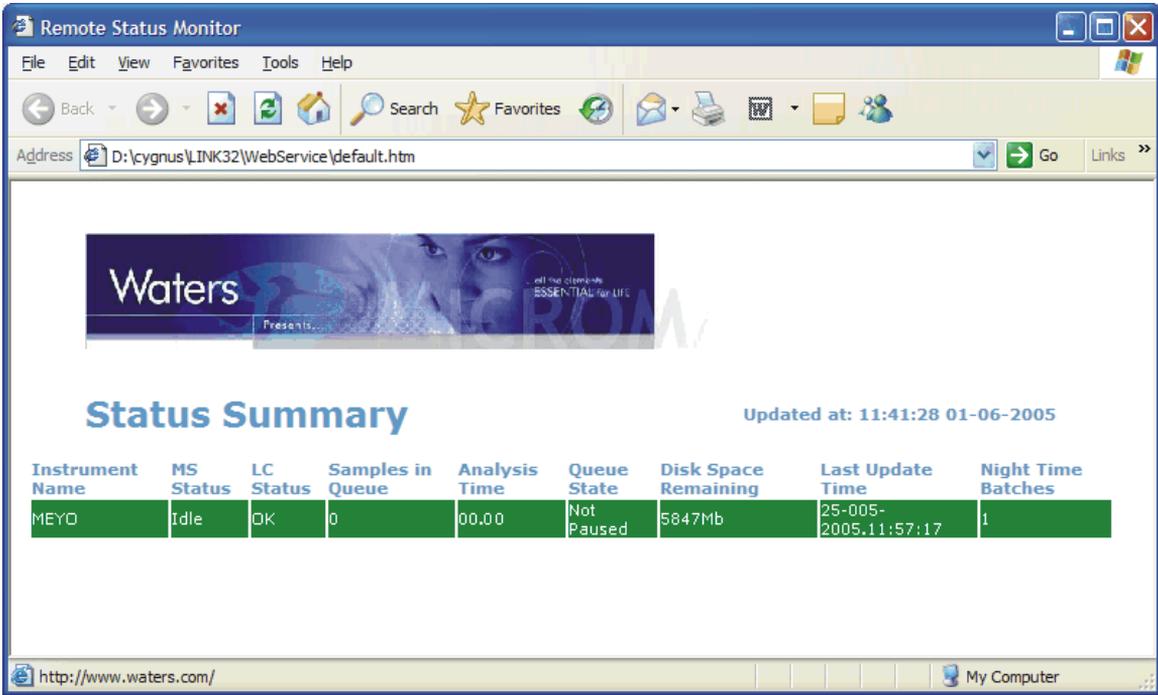
The Status Summary page opens in the browser and contains a list of Acquisition PCs and the number of samples in their queues in a table. The colors are:

Red = the instrument is inactive

Green = the instrument is active

Amber = the instrument is off line.

Remote Status Monitor - Status Summary page:



The screenshot shows a web browser window titled "Remote Status Monitor". The address bar displays "D:\cygnus\LINK32\WebService\default.htm". The page content includes a Waters logo banner with the text "Waters" and "all the elements ESSENTIAL for LIFE". Below the banner is the heading "Status Summary" and a timestamp "Updated at: 11:41:28 01-06-2005". A table displays the status of an instrument named "MEYD".

Instrument Name	MS Status	LC Status	Samples in Queue	Analysis Time	Queue State	Disk Space Remaining	Last Update Time	Night Time Batches
MEYD	Idle	OK	0	00.00	Not Paused	5847Mb	25-005-2005.11:57:17	1

The browser's status bar at the bottom shows the URL "http://www.waters.com/" and a "My Computer" icon.

2. To display more detailed information about an instrument, click anywhere in the instrument row. An instrument summary page opens.

Remote Status Monitor - instrument details:

Summary Page

Updated at: 11:45:28 01-06-2005

MEYO

MS Status
 HV Electronics: Operating
 Mass Spectrometer: Idle

Inlet System
 Inlet system healthy
 Ready to inject next sample

Flow Rates

%A	%B	%C	%D	LC (ml/min)
100.00	000.00	000.00	000.00	0.000

MassLynx Queue Queue Status : Not Paused

No queue

Open Access Batches Estimated Total Time : 00.00

Batch ID	User Name	Num Samples	Est. Runtime (Mins)	Priority	Night-Time
div10	berty	1	0.00	Yes	Yes
div11	berty	1	0.00	Yes	No

- To return to the Status Summary, click Summary Page at the top-right corner of the page.

Installing Diversity browser

Diversity browser is used to view, create, or print reports on a PC that does not have MassLynx installed on it.

To install Diversity browser:

1. Log on to the PC using a user account with permission to install software – usually an administrator account.
2. Insert MassLynx 4.1 CD 2 into the appropriate drive.
3. Use Windows Explorer to navigate to the Diverse directory, then double-click setup.exe; the Diversity Browser installer is displayed.
4. Click Next, confirm that you accept the license agreement, then click Next again to accept the installation directory for Diversity Browser.
5. Click Install to begin the installation process.
6. When prompted, browse to the location of the key disk that has been supplied. If you do not have the appropriate key disk, contact your MassLynx system administrator.

Result: The Diversity browser is installed.

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