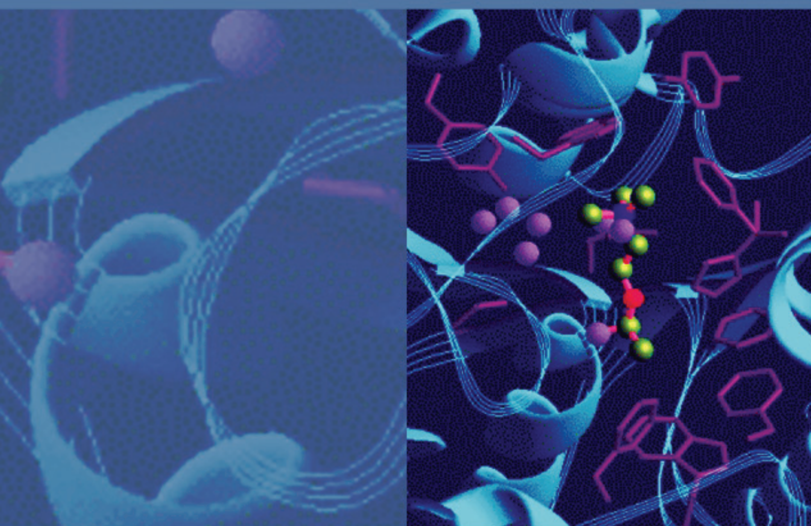

Thermo

EnviroLab Forms 3.0

User Guide

XCALI-97292 Revision A May 2010

DOCUMENTATION SURVEY

Release history: Revision A

Minimum software requirements: Xcalibur 2.1.0; Microsoft Windows XP Professional SP 3

For Research Use Only. Not for use in diagnostic procedures.

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Contents

Preface

The EnviroLab Forms 3.0 application is next in the series of Thermo Scientific GC-MS analytical software.

Contents

❖ To suggest changes to documentation or to Help

Complete a brief survey about this document by clicking the link below. Thank you in advance for your help.

Related Documentation

The EnviroLab Forms documentation includes Help that you can access from the application and also includes the *EnviroLab Forms User Guide* and three quick reference guides as PDF files that you can access from the Start menu.

❖ To view the EnviroLab Forms user guide or quick reference guides

Go to **Start > All Programs > Thermo EnviroLab Forms 3.0 > Manuals** and choose one of the following documents:

– ***EnviroLab Forms User Guide***

– ***EnviroLab Forms Administrator Quick Reference Guide***

– ***EnviroLab Forms Production Quick Reference Guide***

– ***EnviroLab Forms Data Review Quick Reference Guide***

❖ **To open EnviroLab Forms Help**

From the EnviroLab Forms window, choose **Help > EnviroLab Forms Help.**

To find a particular topic, use the Help Contents, Index, or Search panes.

For more information, including upcoming application notes, visit www.thermo.com.

Special Notices

This guide includes the following types of special notices:

IMPORTANT Highlights information necessary to prevent damage to software, loss of data, or invalid test results; or might contain information that is critical for optimal performance of the system.

Note Highlights information of general interest.

Tip Highlights helpful information that can make a task easier.

System Requirements

Your system must meet these minimum requirements.

System	Requirements
PC	• 2.33 GHz processor dual core with 2 GB RAM • CD/R-ROM drive • Video card and monitor capable of 1280 × 1024 resolution (XGA) • 75 GB available on the C: drive • NTFS format
Instruments (supported or required)	Autosamplers: • Triplus™ • AS3000 GC Devices: • Focus GC™ • Trace GC Ultra™ GC-MS mass spectrometers
Software	• Microsoft™ Windows™ XP Professional SP3 • Microsoft Office 2007 SP2 or Excel™ 2007 SP2 • Microsoft .NET Framework 3.5 SP 1 • Thermo Foundation™ 1.0.1 (available on the Xcalibur 2.1.0 CD) • Xcalibur™ 2.1 and Xcalibur 2.1.QF

Contacting Us

There are several ways to contact Thermo Fisher Scientific for the information you need.

❖ To contact Technical Support

Phone	800-532-4752
Fax	561-688-8736
E-mail	us.techsupport.analyze@thermofisher.com
Knowledge base	www.thermokb.com

Find software updates and utilities to download at mssupport.thermo.com.

❖ To contact Customer Service for ordering information

Phone	800-532-4752
Fax	561-688-8731
E-mail	us.customer-support.analyze@thermofisher.com
Web site	www.thermo.com/ms

❖ To copy manuals from the Internet

Go to mssupport.thermo.com and click **Customer Manuals** in the left margin of the window.

❖ To suggest changes to documentation or to Help

- Fill out a reader survey online at http://www.surveymonkey.com/s.aspx?sm=R7gKOvhLXn3NTkpK2BefHQ_3d_3d.
- Send an e-mail message to the Technical Publications Editor at techpubs-lcms@thermofisher.com.

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Introduction

This chapter describes the general features of EnviroLab Forms 3.0 quantitative software.

Contents

About the EnviroLab Forms Application

The EnviroLab Forms application is next in the series of Thermo Scientific GC-MS analytical software. The application focuses on environmental markets, creating the workflows that laboratories use.

In a single software package, the EnviroLab Forms application supports a focused workflow for specific non-bioanalytical laboratory use, instrument control, and method development functionality. The EnviroLab Forms application is the primary application for the ISQ single quadrupole and the TSQ Quantum™ XLS triple quadrupole mass spectrometers.

The EnviroLab Forms application can export SRM data in .xml format so that other applications can import the files into their databases.

The EnviroLab Forms application can import the following file types:

- Sample lists in .csv or .xml format
- Processing (.pmd) and instrument (.meth) method files from the Xcalibur data system
- Compounds from .xml files that use the datastore format
- Batches or methods from the LabForms 2.5 application or later versions

The EnviroLab Forms application checks the accuracy and precision of data against systems that have previously been certified against a standard processing program, such as the Statistical Analysis System (SAS).

Supported File Types

The EnviroLab Forms application supports the following file types:

- Comma-separated values (.csv): A textual representation of value fields that are denoted as separated from a stream of alpha-numeric values that may be associated by a comma.
- Extensible Markup Language (.xml): A generic framework for storing any amount of text or any data whose structure can be represented as a tree. The only indispensable syntactical requirement is that the document has exactly one root element (also called the document element). This means that the text must be enclosed between a root start-tag and a corresponding end-tag.
- Instrument method (.meth): A proprietary file format for the Xcalibur software suite that contains specific instructions that let connected scientific instruments perform data acquisition.
- Processing method (.pmd): A proprietary file format for the Xcalibur software suite with specific instructions about how to process data that was acquired through the instruments attached to the system.
- Raw data (.raw): A file type used for acquired samples on the system.

EnviroLab Forms Directory Structure

The EnviroLab Forms application creates folders for projects/subprojects/batches, and templates in the ..\Thermo\EnviroLab Forms directory. Within each batch folder, the application creates folders for data, methods, and reports.

IMPORTANT You cannot rename or move the folders created by the EnviroLab Forms application.

EnviroLab Forms Feature Summary

The EnviroLab Forms system provides a workflow-oriented approach to high-throughput quantitation. The system uses a batch-centric approach and tools to automate and speed up the processes of method creation, loading samples, automatically generating data, manually reviewing and editing results, and finalizing the data review and reporting process.

The EnviroLab Forms software package includes data acquisition, processing, reviewing, and reporting capabilities designed to assist analysts in environmental and food safety applications. The application has a fully automated acquisition mode and a manual review mode. You can use the data acquisition system to create and submit batches and monitor real-time review of results.

The EnviroLab Forms application uses a comprehensive processing method to provide improved handling of ion ratio calculations, reviewing, and reporting. In addition, the application provides a mass spectral comparison capability and an integrated connection between the processes of data review and reporting.

Key features include the following:

- Role-based authorization for Manager, IT Administrator, Supervisor, Technician, and QAQC (quality assurance) roles
- Configuration mode with user administration, project administration, datastore administration, and application administration
- Method Development mode with instrument method editor, processing parameters, QAQC parameters, and reporting options
- Production mode with batch views, data review, local method views, and report views
- Database-capable method development
- Quantification workflows, supporting capabilities present in the LCquan and LabForms 2.5 applications
- Customized report formats

Features of the common workflow core include the following:

- Acquisition and processing
- Peak detection
- Quantification to include calibration
- QAQC analysis and flag setting
- Reporting
- Data persistence
- Raw data file handling

Reporting Features

The report engine can generate several different types of reports designed to meet the needs of the laboratory, the laboratory's customers, and key regulatory agencies that might review the results. The EnviroLab Forms application can produce both standard reports and custom reports. The following types of reports meet the requirements of various methods and worldwide regulatory agencies and are designed to help track the performance of the GC system and method. The reports are divided into two groups: Standard and Custom.

Standard Report Types

- Batch Report
- Blank Report
- Breakdown Report
- Calibration Report
- Check Standard Report
- Chromatogram Report
- Compound Calibration Report
- Confirmation Report
- Confirmation Report 2
- High Density Internal Standard Report
- High Density Internal Standard Report Long
- High Density Sample Report 1
- High Density Sample Report 1 Long
- High Density Sample Report 2
- High Density Sample Report 2 Long
- High Density Sample Report 3
- High Density Sample Report 3 Long
- Internal Standard Summary Report
- Ion Ratio Failure Report
- LCSLCSD Report
- Manual Integration Report
- Method Detection Limit Report
- Method Report
- Method Validation Report
- MSMSD Report
- Quantitation Report
- Quantitation Report - 2
- Solvent Blank Report
- Surrogate Recovery Report
- TIC Report
- TIC Summary Report
- Tune Report

Example PDFs of standard report formats are located in the following folder:

C:\Thermo\Shared\ExampleReports

Custom Report Types

- AltCalibrationReport
- BatchReport
- BlankReport
- CalibrationDensityReport
- CalibrationReport
- CheckStandardReport
- CompoundCalibrationReport
- ConfirmationReport
- ConfirmationReport2
- DCCReport
- HighDensitySampleReport1Long
- HighDensitySampleReport2Long
- HighDensitySampleReport3Long
- HighDensitySampleReport4
- HighDensitySampleReport5
- QuantitationReport

For additional information about custom and standard reports and a sample of each standard report type, see "Reports" on page 261.

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Getting Started

This chapter describes the basic EnviroLab Forms workflow and the procedures for getting started with the EnviroLab Forms application.

Contents

EnviroLab Forms Workflow

The EnviroLab Forms application is structured with a typical laboratory workflow in mind—the user creates a batch and the system injects samples into the instrument, runs the samples, analyzes the data, and generates a report. You can set up a master method for specific compound groups or assays you expect to run in your lab. When you are ready to run a particular type of sample, select the appropriate method and you are ready to start.

When using the EnviroLab Forms application, follow these basic steps:

1. Create and save a master method in the Method Development mode.

   A master method combines the instrument method and processing method that define how the raw data is acquired and processed, how the QAQC information evaluates the results, and how the results appear in reports.

2. Create and submit a batch in the Production mode.

   A batch lists samples for processing and reporting using a specified method. Each row of a batch represents a unique sample.

3. Monitor the status of the batch in the Real Time Status view.

   The real-time display is visible from the dashboard and all the EnviroLab Forms modes. You can begin another batch while you watch the real-time display of the currently acquiring batch.

4. Evaluate the data in the Production mode.

   The Production mode includes views where you can review batches, batch data, reports, and local methods.

5. View and print reports in the Report View of the Production mode.

   Use the Report View to view or print the reports for the currently selected batch.

Installing the EnviroLab Forms Application

Follow these instructions to install, start, and log on to the EnviroLab Forms application.

❖ **To install the EnviroLab Forms application**

1. Follow the instructions on the included CDs to install the Xcalibur 2.1 data system and your instrument drivers.

2. Install the driver for your GC device and autosampler.

3. Insert the EnviroLab Forms 3.0 CD in the drive, and follow the on-screen instructions.

   If the install windows do not automatically open, navigate to the Xinstall.exe file and launch it.

❖ **To start the EnviroLab Forms application**

1. Configure your instruments.

   You cannot configure your instruments while the EnviroLab Forms application is running.

2. Double-click the EnviroLab Forms 3.0 application icon on your desktop, or go to **Start > All Programs > Thermo EnviroLab Forms 3.0 > Thermo EnviroLab Forms 3.0.**

   By default, user security is not enabled and the application does not require a password. To enable user security, follow the instructions "To enable user security" on page 36.

   IMPORTANT If you are the administrator logging on for the first time with user security enabled, use **Administrator/Password** as the *username/password*.

❖ **To log on to the EnviroLab Forms application (when user security is enabled)**

1. Enter your assigned user name.

   Before you can log on to the EnviroLab Forms application, a system administrator must set up a user account for you. The administrator assigns you a user name and password and gives you permission to access specific modes.

2. Enter your password.

   If your user name and password do not match, the system reports this error:

   Correct the user name or password, or contact your system administrator.

3. Click **Login**.

   The EnviroLab Forms dashboard opens. See "EnviroLab Forms Dashboard" on page 14.

4. To exit the EnviroLab Forms application without logging on, click **Exit EnviroLab Forms**.

> **IMPORTANT** If you are the administrator logging on with user security enabled, use **Administrator/Password** as the *username/password*.

Figure 1. EnviroLab Forms logon screen

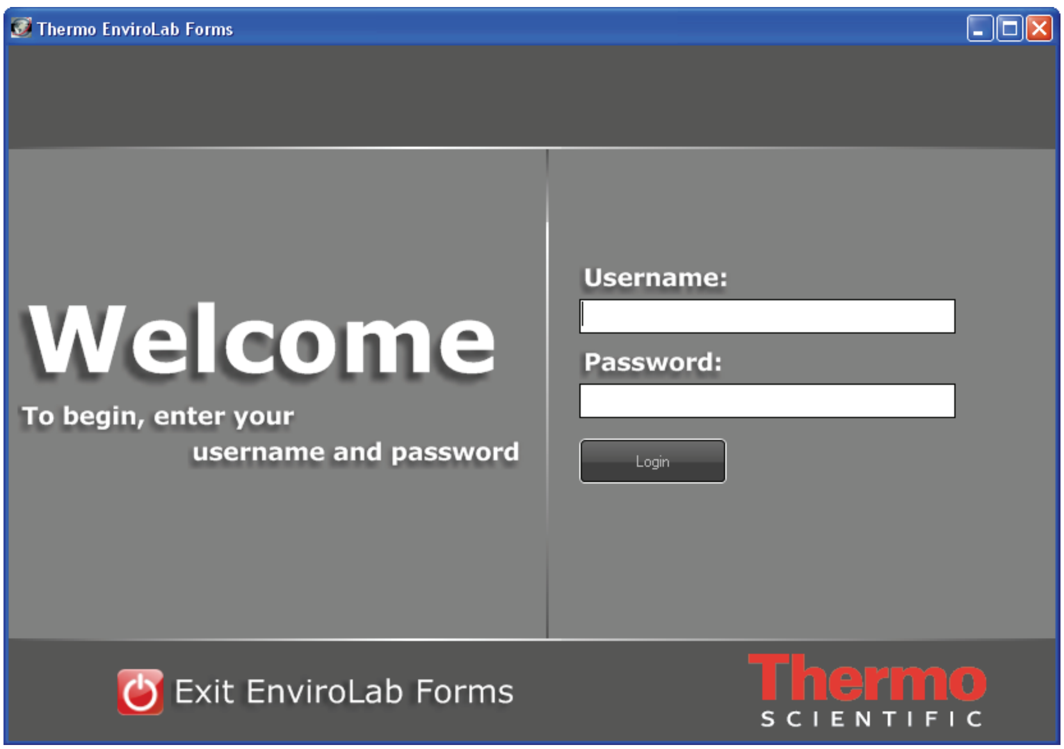


Table 1. Logon screen parameters

Parameter	Description
Username	The user's assigned user name.
Password	The assigned password for the user name.
Login	Verifies the user name and password, and displays the dashboard.
Exit EnviroLab Forms	Quits the EnviroLab Forms application.

Installing the QED and NIST Libraries

When you are using triple quad instruments, follow these instructions to install the NIST and QED libraries.

❖ To install the NIST library

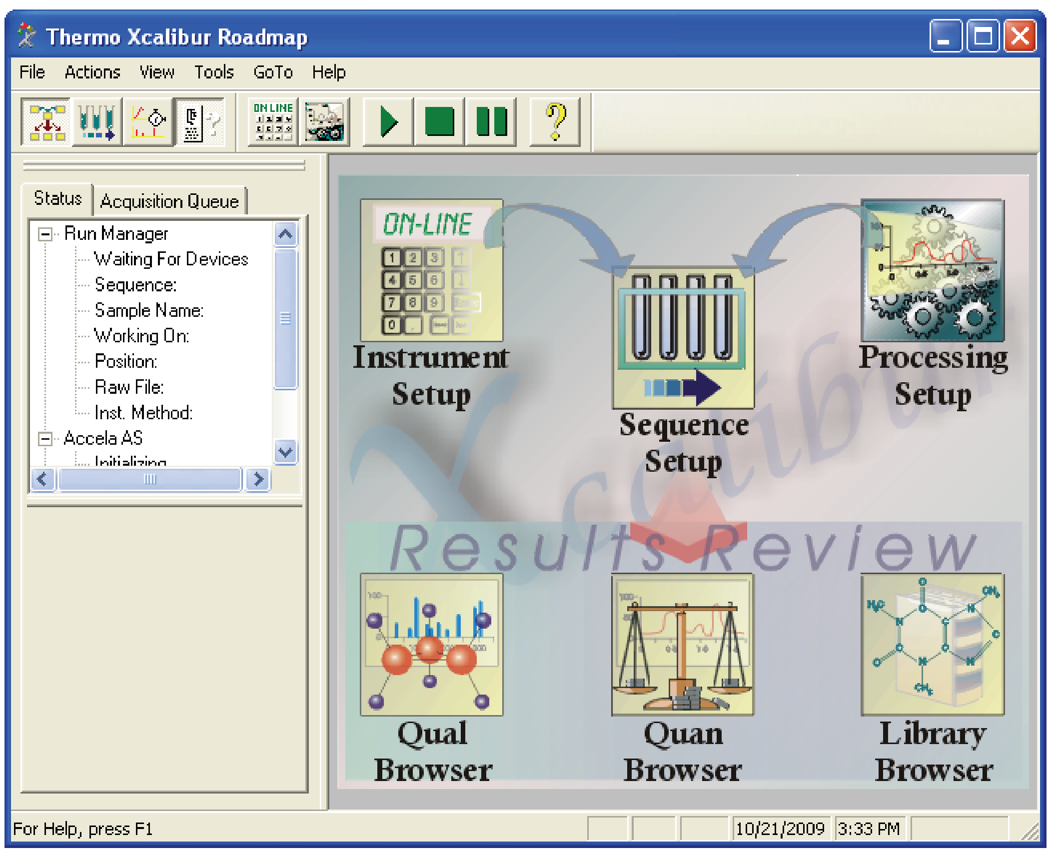
1. Launch the XInstall executable file.
2. Click the **NIST** button.

   The NIST 08 MS Search and AMDIS Setup wizard opens.
3. Follow the instructions in the setup wizard.
4. When the wizard prompts you to select a program folder, select **C:\Thermo**.

❖ To install the QED library

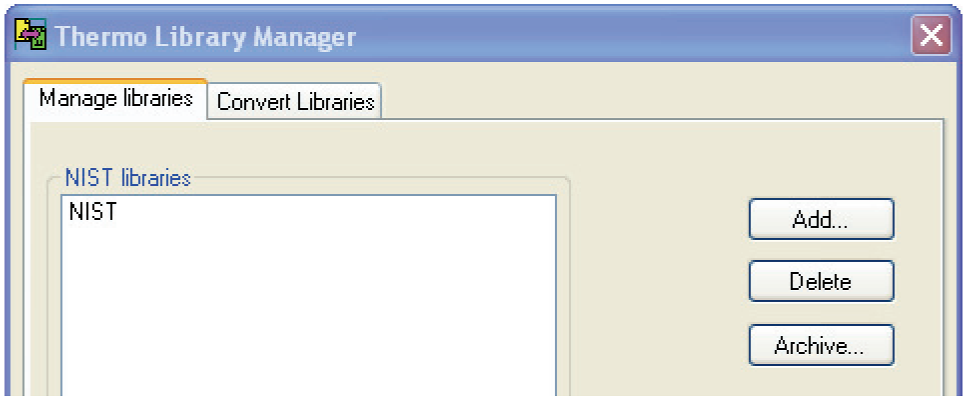
1. On your desktop, double-click the **Xcalibur** icon, .

   The Thermo Xcalibur Roadmap opens.



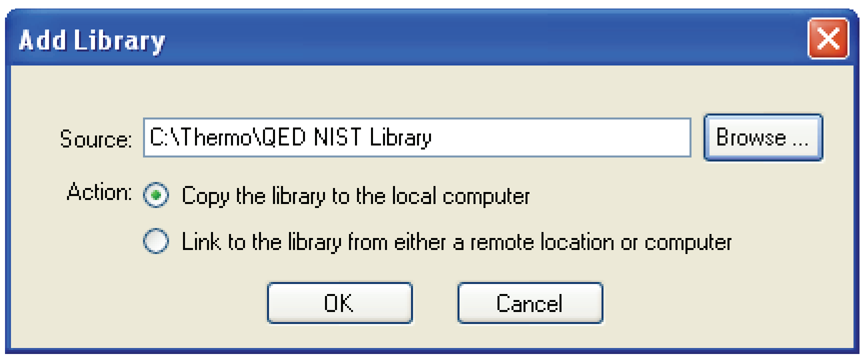
2. Select **Tools > Library Manager**.

   The Thermo Library Manager dialog box opens. The NIST library is displayed in the NIST Libraries list.



3. Click **Add**.

   The Add Library dialog box opens.

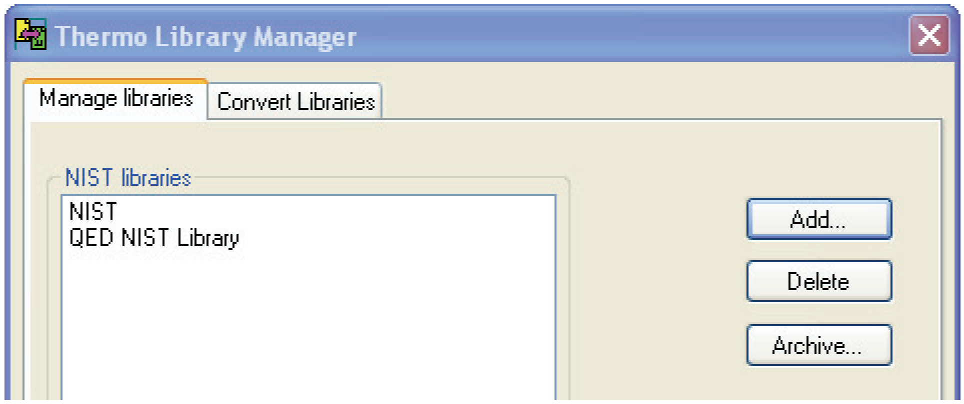


4. Click **Browse**, and locate your QED library in the C:\Thermo folder.
5. Click **OK**.

   The Xcalibur application reports that it has added the library to the NIST software.

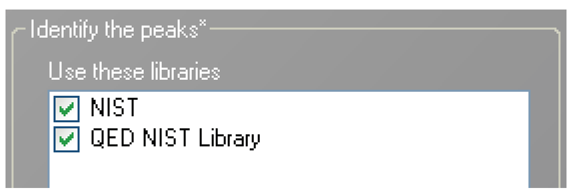
6. Click **Dismiss** to close the message box.

   The application adds the QED library to the NIST Libraries list in the Library Manager dialog box.



7. Click **Exit** in the Thermo Library Manager dialog box.
8. Start the EnviroLab Forms application.
9. Go to the Method Development mode.
10. Click **Method View** in the navigation pane.
11. Choose **File** > **New** > **Method template** from the main menu.

    The QED NIST Library is listed in the Use These Libraries list on the Method Template Editor.



Choosing a Mode

When user security is enabled, the dashboard provides the current user with options applicable to the role assigned to that user. The following table shows the available modes for each user role.

Table 2. User roles and permissions

User role	Method Development	Production	Configuration
Manager	×	×	×
IT Administrator			×
Supervisor	×	×	
Technician		×	
QAQC		×	

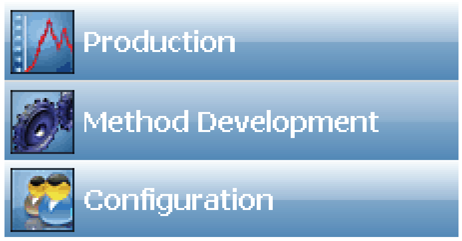
Note When user security is not enabled, all modes are available to all users.

❖ To choose a mode

1. From the dashboard, click the mode in which you want to work.

   Your dashboard shows only the modes that you have permission to use. See "EnviroLab Forms Dashboard" on page 14.

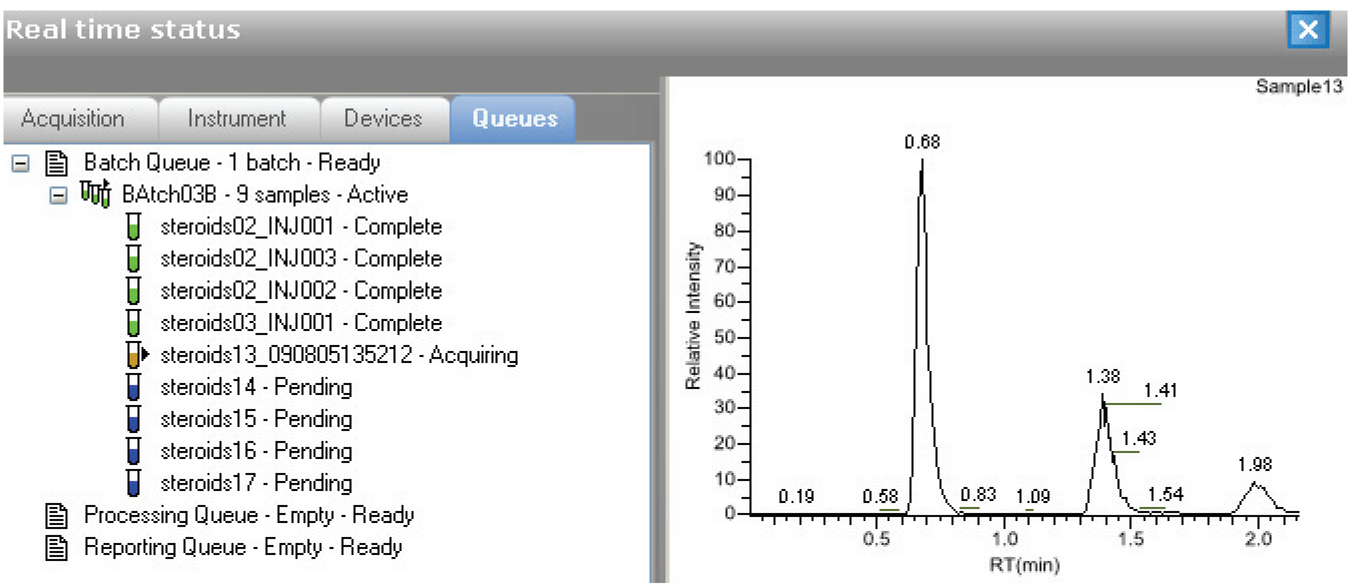
2. To change modes from within any of the EnviroLab Forms application modes, click a mode button in the lower left corner of the window.



❖ To watch the real-time display from the dashboard

Click **Real Time Status**.

The real-time status is displayed at the bottom of the dashboard.



For descriptions of all the features of the real-time display, see "Real-time Display" on page 185.

EnviroLab Forms Dashboard

A dashboard for a Manager, who has permission for all modes, looks like this:

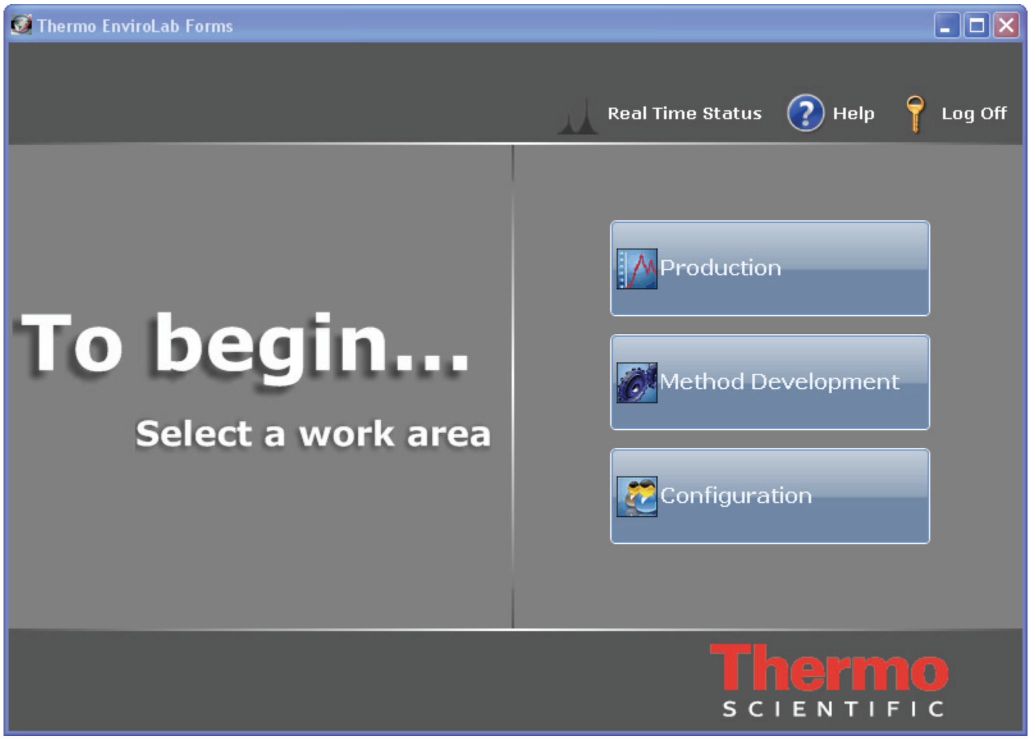


Table 3. EnviroLab Forms dashboard parameters

Parameter	Description
Real Time Status	Opens the real-time display for the current acquisition. The acquisition progress is displayed within the current mode window.
Help	Opens the EnviroLab Forms Help.
Log Off	Logs off the current user and displays the logon screen. This function is available only when user security is enabled. See "Specifying the General Configuration" on page 35.
Production	Opens the Production mode where you can create and review batches, batch data, reports, and local methods. See "Using the Production Mode" on page 169.
Method Development	Opens the Method Development mode where you can create a master method, an instrument method, or a development batch. See "Using the Method Development Mode" on page 47.
Configuration	Opens the Configuration mode where you can set permissions, assign users to roles, configure available reports and import new reports, and maintain the various databases, including the Compound Datastore. See "Using the Configuration Mode" on page 15.

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Using the Configuration Mode

This chapter discusses the configuration tasks assigned to the IT Administrator and Manager roles.

Contents

If your role is that of an IT Administrator or Manager, you are responsible for the following:

- Handling the databases
- Applying roles to users
- Understanding security, users, and groups
- Creating local users and network groups
- Creating projects and subprojects
- Maintaining compounds in the compounds datastore

❖ To access the Configuration mode

Click **Configuration** from the dashboard or the navigation pane.

The Configuration navigation pane opens.

Figure 2. Configuration navigation pane

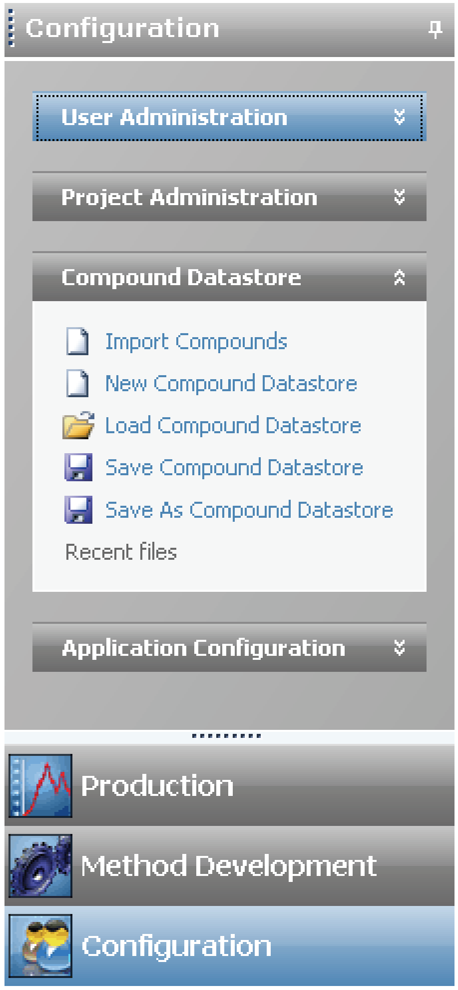


Table 4. Configuration navigation pane functions (Sheet 1 of 2)

Function	Description
User Administration	Opens the User Administration view where you can add, remove, or edit user accounts and permissions. See "User Administration" on page 18. This task pane is available only when you have selected Enable User Security on the General page of the Application Configuration view. See "Application Configuration" on page 35.
Project Administration	Opens the Project Administration view where you can create and manage projects and subprojects. See "Project Administration" on page 26.

Table 4. Configuration navigation pane functions (Sheet 2 of 2)

Function	Description
Compound Datastore	Opens the Compound Datastore view where you can manage the definition of compounds in the current datastore. See "Compound Datastore" on page 28. This task pane is available only when you have selected Enable Compound Datastore on the General page of the Application Configuration view. See "Application Configuration" on page 35.
Application Configuration	Opens the Application Configuration view where you can specify a compound datastore to use for the gas chromatography technology and specify defaults to use for laboratory name, instrument name, and mass precision. See "Application Configuration" on page 35.

User Administration

In the User Administration view of the Configuration mode, in the role of Manager or IT Administrator, you can add, remove, or edit user accounts and permissions.

For detailed descriptions of each user role and the permissions and responsibilities for each role, see "User Roles" on page 23.

Follow these procedures:

- To open the User Administration view
- To add a user
- To edit user information
- To remove a user

❖ To open the User Administration view

1. Click **Configuration** from the dashboard or the navigation pane.

The Configuration navigation pane opens.

> **Note** The User Administration view is available only when you enable user security. Follow the instructions "To enable user security" on page 36.

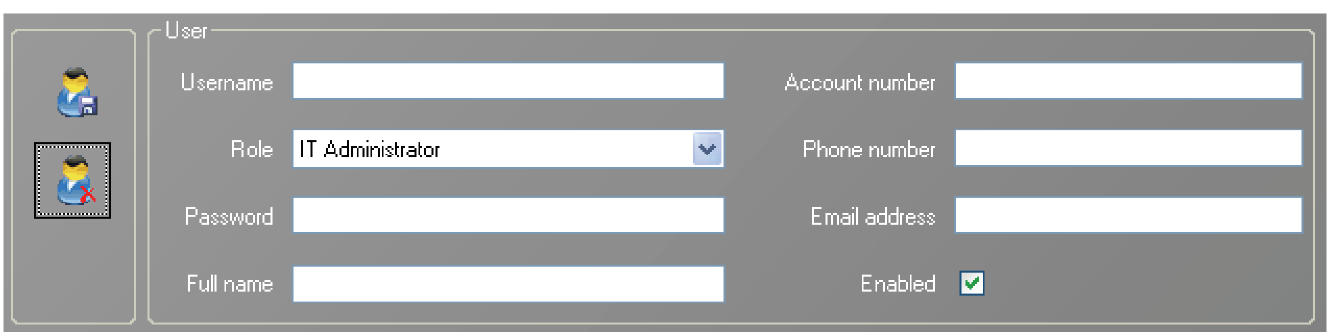
2. Click the **User Administration** task pane.

The User Administration view opens. See "User Administration view" on page 21.

❖ To add a user

1. Click the **Add User** icon, .

The parameters in the User area at the bottom of the view are enabled.



2. Enter a unique name in the Username field.

3. Select a role from the Role list.

   All users must be assigned to one of these defined roles. For detailed information about the permissions allowed for each role, see “User Roles” on page 23.

4. Enter the user’s password.

   There is no confirmation for the encrypted password you enter, so carefully type it and make sure to communicate it to the user.

5. (Optional) Enter the user’s full name, account number, phone number, and E-mail address.

6. To enable this user logon, select the **Enabled** check box.

   You can disable a user logon without deleting the user’s information. Follow the instructions “To edit user information” on page 19.

7. Do one of the following:

   - When all the user information is correct, click the **Save Changes** icon, .

     The EnviroLab Forms application adds the new user to the User Listing table, and the parameters in the User area are unavailable.

     –Or–

   - To discard all information and not create a new user from the parameter values you entered, click the **Cancel Changes** icon, .

     All information is discarded and the parameters in the User area are unavailable.

❖ To edit user information

1. In the User Listing table, select a user.

User Listing

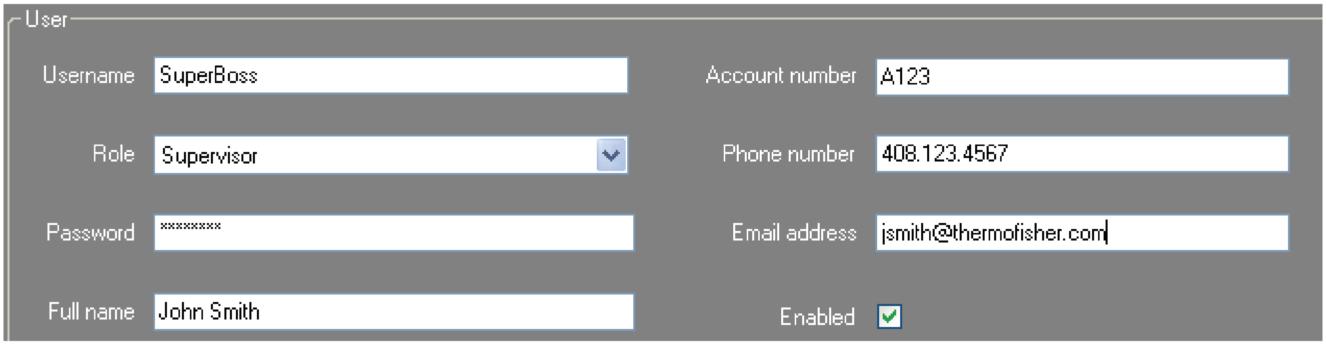
	Username	Role	Account Number	Phone Number	Email Address	Enabled
1	Admin	IT Administrator				✓
2	Manager	Manager				✓
▶ 3	QAQC	QAQC				✓
4	Supervisor	Supervisor				✓
5	Technician	Technician				✓

   Note Clicking anywhere in the row selects the user.

   The user information populates the parameter fields in the User area.

2. Click the **Edit User** icon, .

The parameters in the User area are enabled.



3. Edit any of the parameter values.

   If you are editing your own user name, the Enabled check box is unavailable because you cannot make your own account unavailable.

4. Do one of the following:

   - When all the user information is correct, click the **Save Changes** icon, .

     The EnviroLab Forms application adds the new parameter values to the User Listing, and the parameters in the User area are unavailable.

     – Or–

   - To discard all changes and not save the edits, click the **Cancel Changes** icon, .

     All changes are discarded, and the parameters in the User area are unavailable.

❖ To remove a user

1. In the User Listing table, select a user.

   Note Clicking anywhere in the row selects the user.

   The user information populates the parameter fields in the User area.

2. Click the **Remove User** icon, .

   If you select your current user name, the Remove User icon is unavailable. You cannot remove yourself.

3. When prompted, confirm that you want to remove this user.

   If the user is currently logged on to the EnviroLab Forms application, the user's current session is not affected.

4. Click **OK**.

Note Rather than completely removing the user, you can disable a user logon without removing all the user information from the system. Follow the instructions "To edit user information" on page 19.

Figure 3. User Administration view

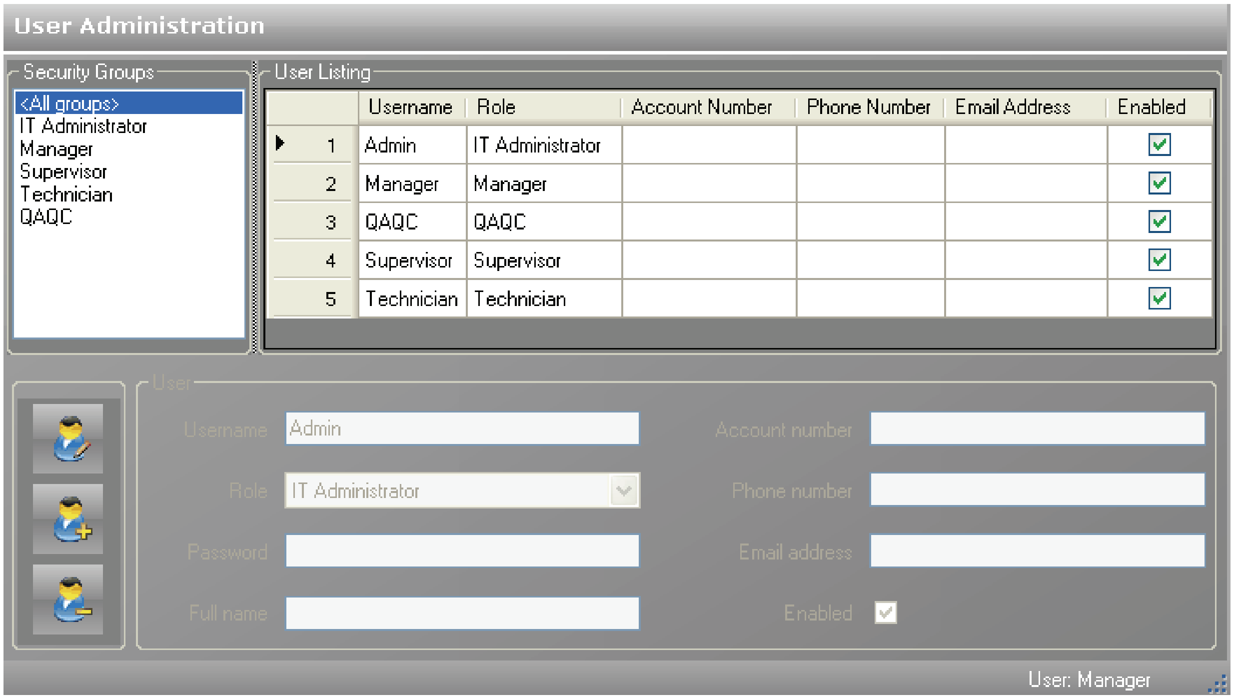


Table 5. User Administration parameters (Sheet 1 of 2)

Parameter	Description
Security Groups	All permission levels defined in the EnviroLab Forms application. For detailed descriptions of user permissions, see “User Roles” on page 23.
User Listing	
Username	User logon names.
Role	The security group that defines user permissions.
Account Number	User account numbers.
Phone Number	User telephone numbers.
Email Address	User e-mail addresses.
Enabled	Available or unavailable status for the user account.
User	
Username	Logon name for this user.
Role	Security group that defines this user’s permissions.
Password	Logon password for this user.
Full name	The user’s actual name.
Account number	Optional account number for this user.

Table 5. User Administration parameters (Sheet 2 of 2)

Parameter		**Description**
Phone number		Optional telephone number for this user.
Email address		E-mail address for this user. Used to notify user of a randomly generated password.
Enabled		Allows or disallows access for this user. When this user is currently logged on, disallowing takes effect after the user logs off.
Icon	**Function**	
	Add user	Enables the fields in the User area where you can enter information for a new user.
	Remove user	Deletes all information for the selected user.
	Edit user	Enables the User area where you can edit any of the parameters for the selected user.
	Save changes	Adds the new parameter values to the User Listing table and disables the parameters in the User area.
	Cancel changes	Discards all new or edited information.

User Roles

This section describes the responsibilities for five different types of users: Manager, IT Administrator, Supervisor, Technician, and QAQC.

User Permissions

A Manager or an IT Administrator assigns you to a role that gives you permission to access specific modes of the EnviroLab Forms application. When you log on, the dashboard displays links to only the modes that you can access.

Table 6. User roles and permissions

User role	Method Development	Production	Configuration
Manager	×	×	×
IT Administrator			×
Supervisor	×	×	
Technician		×	
QAQC		×	

Manager

As a user in the role of Manager, you review graphically applicable data and manipulate data, batches, methods, and instruments.

A manager is responsible for these tasks:

- Creating or editing methods for new levels of detection or adding new compounds to the existing database
- Reviewing data from the mass spectrometer
- Running samples and reviewing data collected by others
- Reporting the data
- Understanding the results and giving final approval of the released data before archiving

IT Administrator

As a user in the role of IT Administrator, you set security, manage users into roles, and manipulate the various databases. You are responsible for adding compounds into the various compound databases.

An IT administrator is responsible for these tasks:

- Handling the databases
- Applying roles to users
- Understanding security, users, and groups
- Creating local users and network groups

Supervisor

As a user in the role of Supervisor, you are responsible for putting samples on the instrument and using previously built sequences and methods for processing and acquiring data. You also develop and edit methods for processing and acquiring data, review the data, and distinguish between the need to rerun samples or pass reports up to the lab manager or QAQC technician for final review. On a daily basis, you establish the priority for a list of samples to run and create the sequence of events.

A supervisor is responsible for these tasks:

- Submitting samples
- Creating and submitting batches
- Reporting the data to management
- Creating or editing methods for new levels of detection or adding new compounds to the existing database
- Reviewing data from the mass spectrometer
- Understanding the results, who ran the batch, and who passed along the results before giving intermediate approval and sending the data to management
- Modifying new compounds or adjusting methods for specific result sets

Technician

As a user in the role of Technician, you are responsible for putting samples on the instrument and using previously built sequences and methods for processing and acquiring data. You also edit existing methods for processing and acquiring data and are responsible for reviewing collected data and distinguishing between the need to rerun samples or pass reports up to the supervisor. On a daily basis, you are responsible for gathering the list of samples to run and creating the sequence of events.

A technician is responsible for these tasks:

- Submitting samples
- Creating and submitting batches
- Creating data to be reviewed by management
- Receiving instructions for new sets of samples for the EnviroLab Forms application to analyze after finishing the current analysis
- Reviewing data from the mass spectrometer
- Understanding the resulting data, making integration changes, and passing those changes up for further approval.

QAQC

As a user in the role of a QAQC technician, you review graphically applicable data and interpret the data, but you do not manipulate the data.

A QAQC user is responsible for these tasks:

- Reviewing data from the mass spectrometer
- Understanding the results and who ran and passed along the results before giving intermediate approval and sending the data to management
- Receiving instructions for new sets of samples for the EnviroLab Forms application to analyze after finishing the current analysis

Note A user in the role of a QAQC technician cannot submit batches for acquisition from the Production mode.

Project Administration

In the role of Manager or IT Administrator, you can create and manage projects and subprojects in the Project Administration view of the Configuration mode.

Follow these procedures:

- To open the Project Administration view
- To create projects or subprojects
- To delete projects or subprojects

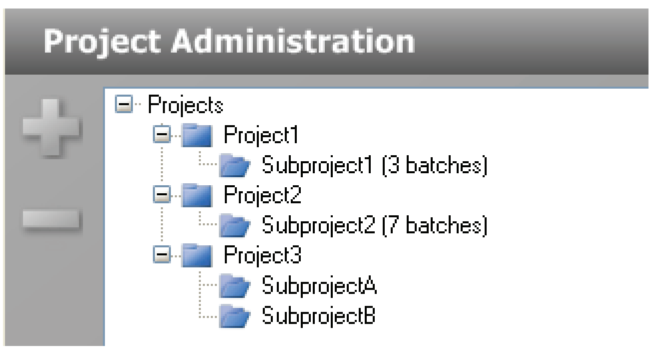
❖ **To open the Project Administration view**

1. Click **Configuration** from the dashboard or the navigation pane.

The Configuration navigation pane opens.

2. In the Configuration navigation pane, click **Project Administration**.

The Project Administration view opens.



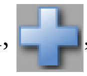
All projects are created under a main Projects folder on the C: drive:

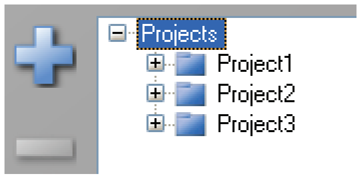
C:\Thermo\EnviroLab Forms\Projects

❖ To create projects or subprojects

1. Select the top-level project.

   You can select the main Projects folder and create a new project under it, or you can select one of your existing projects and create a subproject under it.

   When you select a project folder, the application enables the plus sign icon, , indicating that you can create a folder within the selected folder.

2. Click the plus sign.

   The EnviroLab Forms application creates a new, unnamed project folder under the selected project.

3. While the new project is still highlighted, type a new name.

   Project names can contain spaces and special characters, except for the following special characters: \ / : * ? “ < > |

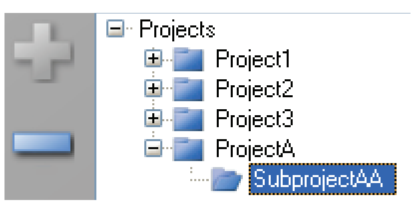
   Note After you add a subproject to a project, you cannot rename the project.

4. To save the new name, press ENTER or click anywhere in the view.

❖ To delete projects or subprojects

1. Select the project or subproject you want to delete.

   You can delete any project that contains no subprojects. You can delete any subproject that contains no batches. When the selected project or subproject is available for deletion, the application enables the minus sign icon,  .

2. Click the minus sign, or right-click and choose **Remove Project** or **Remove Subproject** from the shortcut menu.

3. At the prompt, click **Yes** to remove the selected project or subproject.

Compound Datastore

In the role of Manager or IT Administrator, you can manage compounds definitions in the current datastore in the Compound Datastore view of the Configuration mode.

The current default datastore is the datastore specified for the current technology in the Application Configuration view. See “Application Configuration” on page 35.

Follow these procedures:

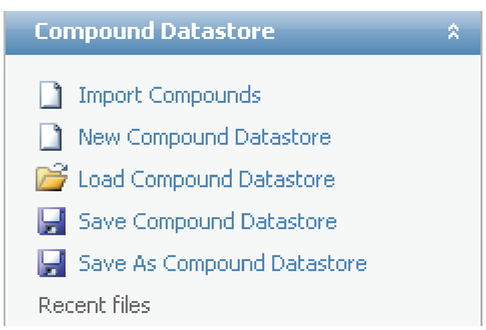
- To open the Compound Datastore editor
- To open a compound datastore
- To create a new compound datastore
- To import compounds
- To add a single compound
- To save a datastore
- To save a datastore to a new name
- To remove a compound or a compound’s transition information
- To filter the compound list

❖ To open the Compound Datastore editor

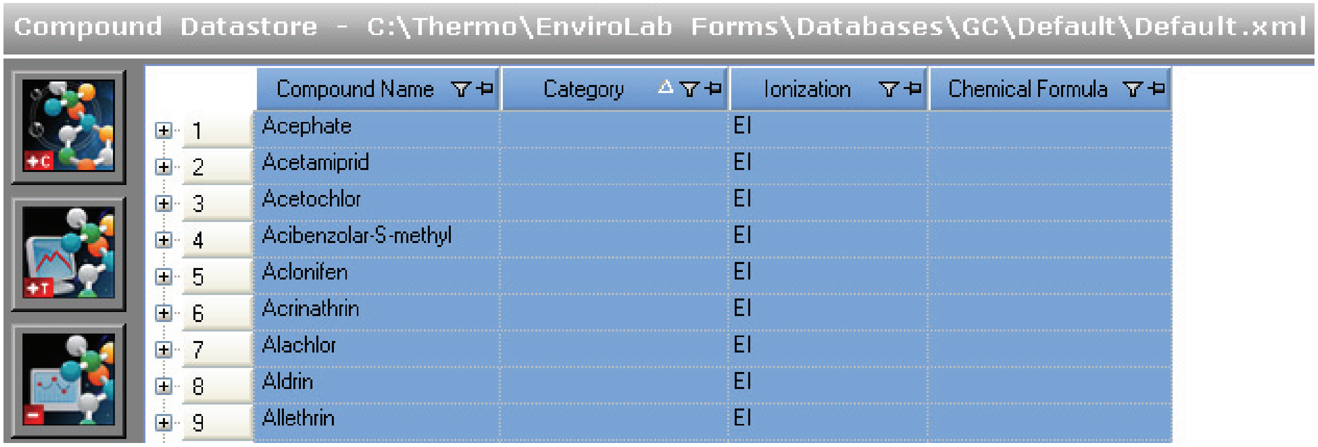
1. Click **Configuration** from the dashboard or the navigation pane.

The Configuration navigation pane opens.

2. Click the **Compound Datastore** task pane.



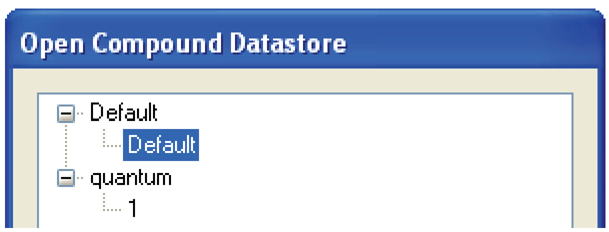
The current datastore opens in the Compound Datastore view.



❖ To open a compound datastore

1. Click **Load Compound Datastore** in the Compound Datastore task pane.

   The Open Compound Datastore dialog box opens.

2. To expand the folder, click the plus sign before the folder name.

3. Double-click the name of the datastore you want to open.

   The selected datastore opens in the Compound Datastore view. See "Compound Datastore view" on page 33.

❖ To create a new compound datastore

Click **New Compound Datastore** in the Compound Datastore task pane.

A new, empty datastore opens in the Compound Datastore view. You can import a file of compounds into the new datastore (following the instructions, To import compounds), or you can manually add compounds one at a time (following the instructions, To add a single compound).

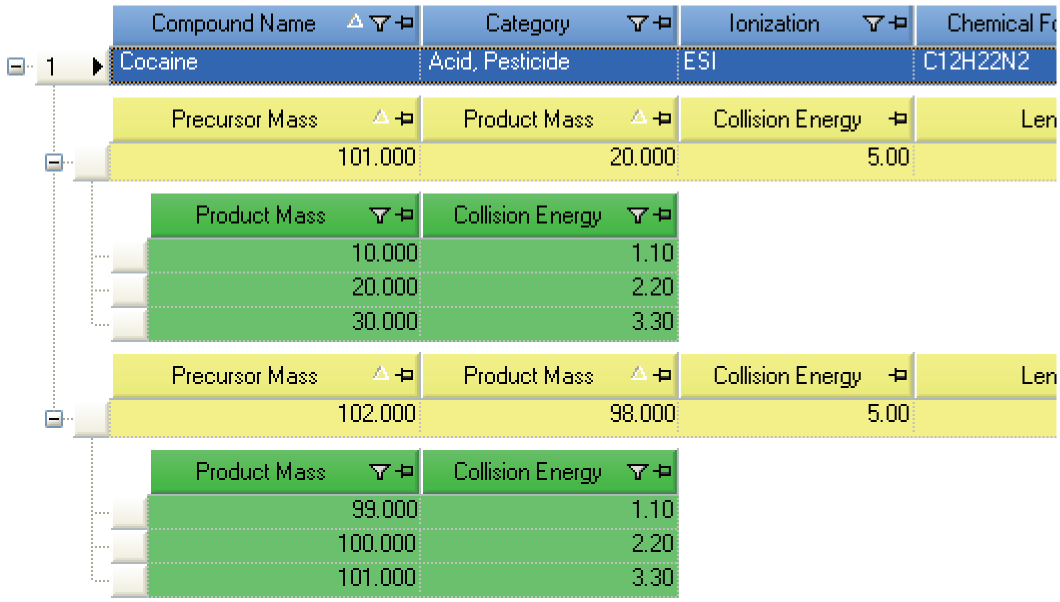
❖ To import compounds

1. Click **Import Compounds** in the Compound Datastore task pane.

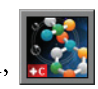
2. Browse to a .csv or .xml compounds file and click **Open**.

   The EnviroLab Forms application imports the compounds from the imported file, adds them to any compounds already in the datastore, and alphabetically sorts them.

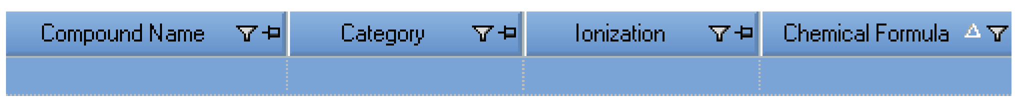
When the application imports a compound that contains multiple quan peaks, it lists all the peaks under a single compound name, as in this example for Cocaine:



❖ To add a single compound

1. To add a single compound to the datastore, click the **Add Compound** icon, , or right-click the compounds list and choose **Add Compound** from the shortcut menu.

   A new empty compound row is added to the bottom of the compounds table.



2. Click the first table cell, and enter the required Compound Name parameter.

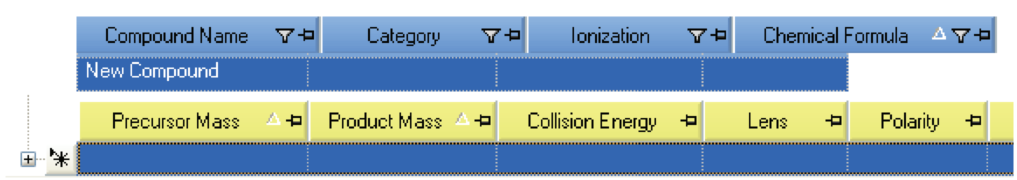
3. (Optional) Enter values for the Category, Ionization, or Chemical Formula columns.

4. To add a transition to the compound, do the following:

   a. Select the compound.

   b. Click the **Add Transition Information** icon, , or right-click and choose **Add Transition Information** from the shortcut menu.

   A new empty transition row is added to the compound. A transition includes quantitative values for the compound. Each compound requires at least one transition.



5. Enter all required parameters.

   For a list of required and optional parameters, see the list of "Compound Datastore parameters" on page 33.

   Tip You cannot add another new compound or save the compound datastore until you enter all required transition parameters or remove the transition from the compound. To remove a transition, right-click the row and choose **Cancel**.

6. To save the new datastore, click **Save Compound Datastore** in the Compound Datastore task pane.

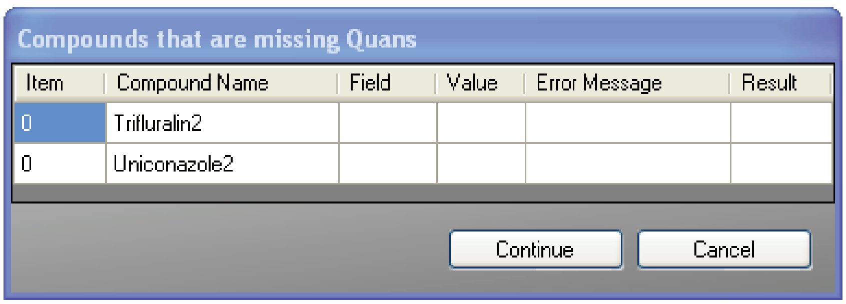
❖ To save a datastore

1. Click **Save Compound Datastore** in the Compound Datastore task pane.

   The database is stored as

   ..\Thermo\EnviroLab Forms\Databases\foldername\filename.xml

   If the datastore contains any compounds that do not have an associated transition, the Compounds That are Missing Quans dialog box opens, listing the compounds.



2. Do one of the following:

   - To remove the listed compounds from the datastore and save the datastore, click **Continue**.

     –Or–

   - To keep the listed compounds and return to the datastore, click **Cancel**.

   Note You cannot save a compound that does not have an associated transition.

❖ To save a datastore to a new name

1. Click **Save As Compound Datastore** in the Compound Datastore task pane.

   The Save Compound Datastore dialog box opens. See "Save Compound Datastore dialog box" on page 32.

2. Enter a file name for the new compound datastore.

3. (Optional) Click **Add Folder** and enter the name for a new folder to be created in the ..\Thermo\EnviroLab Forms\Databases folder.

4. Click **Save**.

   The database is stored as

   ..\Thermo\EnviroLab Forms\Databases\foldername\filename.xml

Figure 4. Save Compound Datastore dialog box

Table 7. Select Compound Datastore parameters

Parameter	Description
Compounds	Lists the datastores you have created for this technology.
Default	The default datastore defined for this technology.
File Name	File name for the new datastore.
Save	Writes the new datastore to the specified folder.
Add Folder	Adds a new folder where you can save the datastore.
Cancel	Closes the dialog box and makes no changes to the datastore.

❖ To remove a compound or a compound's transition information

1. In the Compound Datastore view, select the row you want to delete.

   You can remove either of the following:

   - An entire compound, including all associated transition information
   - A row of transition information

2. Click the **Remove Transition** icon, , or right-click and choose **Remove Transition** from the shortcut menu.

3. If you are sure you want to delete the selected row, at the prompt, click **Yes** .

   The selected row and all items within it are deleted.

> **Tip** If you add a row of compound or transition information and do not complete all the required values, you can right-click and choose **Cancel** to remove the entire row. You can cancel only incomplete compound or transition rows.

❖ To filter the compound list

1. To display a filtered list of compounds, click the funnel icon, , in the column header.

   For each column, filterable criteria is displayed in a list. In all lists, you can choose to filter by All, Blanks, NonBlanks, or by custom filter criteria. Other filter criteria are specific to the individual columns.

2. To create a custom filter based on column values, choose **Custom** from the list.

   For detailed instructions about creating a custom filter, see Appendix C, "Using Filter Criteria."

Figure 5. Compound Datastore view

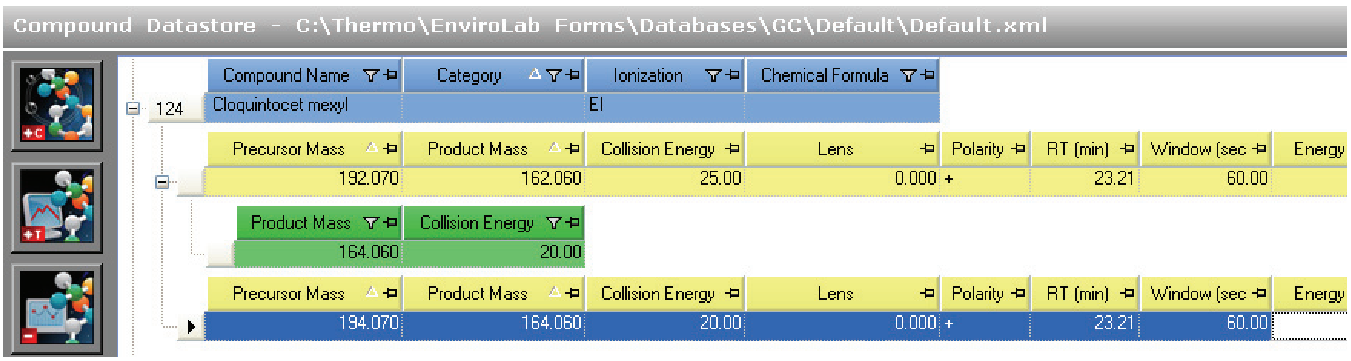


Table 8. Compound Datastore parameters (Sheet 1 of 2)

Parameter	Description
Function icons	
	Adds a compound transition to the datastore.
	Adds a quantitation items row to the selected compound transition, or adds a confirming items row to the selected quantitation item.
	Deletes the selected compound transition.
Compound parameters	
Compound Name	Alphanumeric name assigned to the compound.
Category	(Optional) Alphanumeric identifier.
Ionization	(Optional) Alphanumeric identifier. Valid values: ESI, APCI, EI, CI, APPI
Chemical Formula	(Optional) Alphanumeric chemical identifier.

Table 8. Compound Datastore parameters (Sheet 2 of 2)

Parameter	Description
Precursor Mass	The mass-to-charge ratio of a precursor ion. The location of the center of a target precursor-ion peak in mass-to-charge ratio (*m/z*) units. Default: 0.0 Range: 10.000 to 2999.999
Product Mass	The mass-to-charge ratio of the quan ion. The location of the center of a target quan-ion peak in mass-to-charge ratio (*m/z*) units. Default: 0.0 Range: 10.000 to 2999.999
Collision Energy	The energy used when ions collide with the collision gas. Range: –250.00 to 250.00
Lens	(Optional) Range: –400 to 400
Polarity	+ (positive) or –(negative)
RT (min)	Retention time. The application uses RT and Window values to determine the start and stop time for the acquisition. Range: 0.00 to 999.00 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Window (sec)	Acquisition window. The application uses RT and Window values to determine the start and stop time for the acquisition. Range: 0.00 to 499.50 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Energy Ramp	(Optional) Range: 0.00 to 200.00
Color coding	• Blue indicates a compound. • Yellow indicates a quantitative transition. • Green indicates a confirming transition. • Pink fields are editable when you import new transitions into the datastore from the method editor.

Application Configuration

This section includes instructions for the following groups of tasks:

- Specifying the General Configuration
- Specifying the Reports Configuration

Specifying the General Configuration

In the role of Manager or IT Administrator, you can specify a default compound datastore and specify defaults to use for laboratory name, instrument name, and mass precision in the Application Configuration view of the Configuration mode.

Follow these procedures:

- To open the General page of the Application Configuration view
- To enable user security
- To specify a datastore to use in method development
- To specify a default laboratory name, instrument name, and mass precision
- To specify a default chromatogram intensity display

❖ To open the General page of the Application Configuration view

1. Click **Configuration** from the dashboard or the navigation pane.

   The Configuration navigation pane opens.

2. Click **Application Configuration**.

   The General page of the Application Configuration view opens. See "General page" on page 38.

❖ To enable user security

In the User Security area, select the **Enable User Security** check box.

When checked, all users are required to log on to the EnviroLab Forms application and have access to only those modes assigned to their user role. See "User Roles" on page 23.

When cleared, users are not required to log on to the EnviroLab Forms application. When they start the application, the dashboard is the first screen the users see and all modes are available to them. However, the User Administration view in Configuration mode is hidden and cannot be edited.

> **Note** By default, user security is not enabled.

> **IMPORTANT** If you are the administrator logging on with user security enabled, use **Administrator/Password** as the username/password. Immediately create an account with Manager or IT Administrator permissions for yourself.

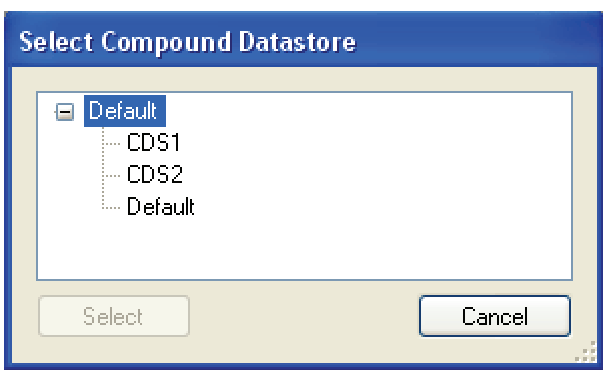
❖ To specify a datastore to use in method development

1. In the Compound Datastore Selection area, select the **Enable Compound Datastore** check box.

   > **Note** By default, the Enable Compound Datastore option is not selected.

2. Click **Select**.

   The Select Compound Datastore dialog box opens.



3. Select a compound datastore from the list.
4. Do one of the following:
   - To use the selected datastore for all methods, click **Select**.

     –Or–

   - To close the Select Compound Datastore dialog box and keep the currently specified datastore, click **Cancel**.
5. In the Application Configuration view, click **Apply**.

6. When you are prompted to restart your application, click **Yes**.

   When the application restarts, the following changes are implemented:

   - The application displays the Acquisition List page on the Compounds page in the Master Method View. See "Editing the Compounds Page" on page 77.
   - The application displays the Compound Datastore task pane on the Configuration mode navigation pane. See "Compound Datastore" on page 28.
   - The application enables the Export SRM Data command in the Method Development mode. See "Exporting SRM Data" on page 156.

❖ To specify a default laboratory name, instrument name, and mass precision

1. In the Defaults area, type the name of your laboratory in the Lab Name box.

   When you create a method, this default laboratory name is used for the Laboratory Name value on the General page of the Master Method View. This laboratory name is also used in the headings of reports.

   Note This default laboratory name is not applied to previously created methods. By default, the laboratory name is ThermoFisher Laboratory.

2. In the Defaults area, type the name of your instrument in the Instrument Name box.

   When you create a batch, this default instrument name is used for the Instrument Name value. This instrument name is also used in the headings of reports.

   Note This default instrument name is not applied to previously created batches. By default, the instrument name is ThermoFisher Instrument.

3. In the Defaults area, in the Display Mass Precision box, set the mass precision decimal places value to an integer from 0 through 5.

   The default mass precision is 2. The EnviroLab Forms application uses this mass precision value in the following locations:

   - Reports:
     – Confirmation report (data spectra, library spectra, quan ion display, and qual ion display)
     – High Density reports (*m/z* values)
     – Ion Ratio Failure Report (quan ion and qual ion)
     – Manual Integration Report (*m/z* value)
     – Quantitation Report (QIon)
   - All peaks on the Detection pages in the Method Development mode
   - The spectrum display in the Data Review view in the Production mode
   - The spectrum display in the Method Forge dialog box

4. In the Application Configuration view, click **Apply**.

❖ To specify a default chromatogram intensity display

In the Defaults area, select **Relative** or **Absolute** from the Chromatogram Intensity Scale list.

This sets the default display type for both quan and qual chromatograms displayed in data review and reports.

Figure 6. General page

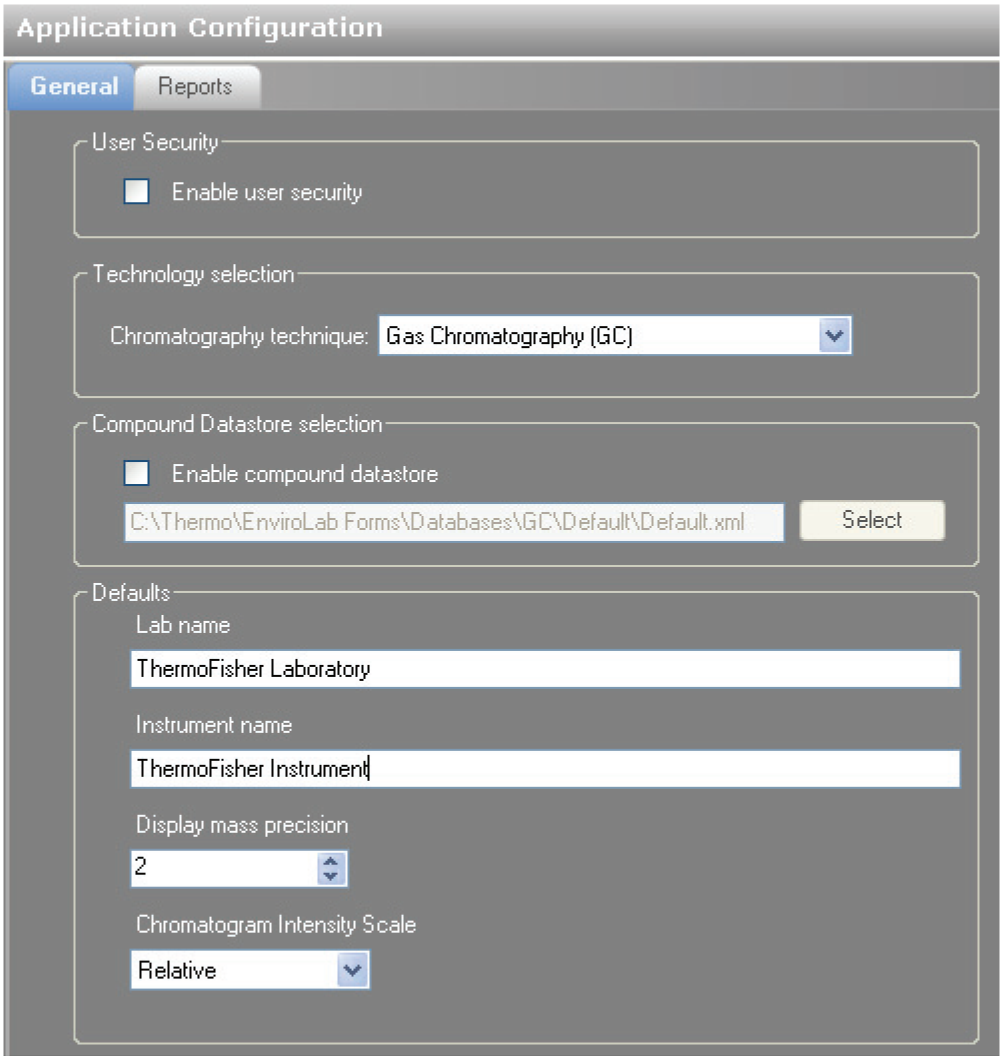


Table 9. General configuration parameters (Sheet 1 of 2)

Parameter	Description
User Security	Enables application level security.
Technology selection	Defaults to Gas Chromatography (GC).

Table 9. General configuration parameters (Sheet 2 of 2)

Parameter	Description
Compound Datastore selection	Enable compound datastore: Enables the Acquisition List page on the Compounds page in the Master Method View and displays the Compound Datastore task pane on the Configuration mode navigation pane. Select: Opens a browser where you can select a saved datastore .xml file.
Defaults	
Lab name	Specifies the default laboratory name used for methods. Default: ThermoFisher Laboratory
Instrument name	Specifies the default instrument name used for batches. Default: ThermoFisher Instrument
Display mass precision	Specifies the number of decimal places used to display mass precision. Valid values: any integer between 0 and 5, inclusive.
Chromatogram Intensity Scale	Specifies the type of chromatogram display in data review and reports.

Specifying the Reports Configuration

In the Application Configuration view of the Configuration mode, as a user in the role of Manager or IT Administrator, you can configure a list of reports that are available to users when they generate reports from the Method Development or Production modes. From the Reports page, you can configure standard reports or custom reports.

This section includes configuration instructions for the following reports:

- Standard Reports
- Custom Reports

❖ **To open the Reports page of the Application Configuration view**

1. Click **Configuration** from the dashboard or the navigation pane.

   The Configuration navigation pane opens.

2. Click **Application Configuration**.

   The General page of the Application Configuration view opens.

3. Click the **Reports** tab.

   The Reports page of the Application Configuration view opens.

Standard Reports

The EnviroLab Forms application supplies standard reports. Example PDFs of standard report formats are located in the following folder:

C:\Thermo\Shared\ExampleReports

Follow these procedures:

- To specify which standard reports are available
- To import new standard report types

❖ To specify which standard reports are available

1. Click the **Standard Reports** tab.

   The Standard Reports page opens. This page is the default when you first open the Reports page. See "Standard Reports page" on page 42.

2. Use the directional arrows to move reports from the Installed Reports pane to the Displayed Reports pane.

   Tip Use the CTRL or SHIFT keys to select multiple reports.

   All reports in the Displayed Reports pane are available to users in the Method Development and Production modes.

3. Do one of the following:

   - To return the report selections to their original state (when you first opened this page), click **Undo Changes**.

     –Or–

   - To apply the current selections, do the following:

     a. Click **Apply**.

        A message reminds you that you must restart the EnviroLab Forms application before your report selections are reflected in the reports available for the Method Development and Production modes.

     b. To restart the EnviroLab Forms application now, click **Yes,** or to remain on the Reports page, click **No**.

❖ To import new standard report types

1. Click **Import**.

2. In the browser, locate a Crystal Reports .dll file and open the file.

   The application writes the imported report to the EnviroLab Forms installation directory.

   The Installed Reports pane displays the new report.

Figure 7. Standard Reports page

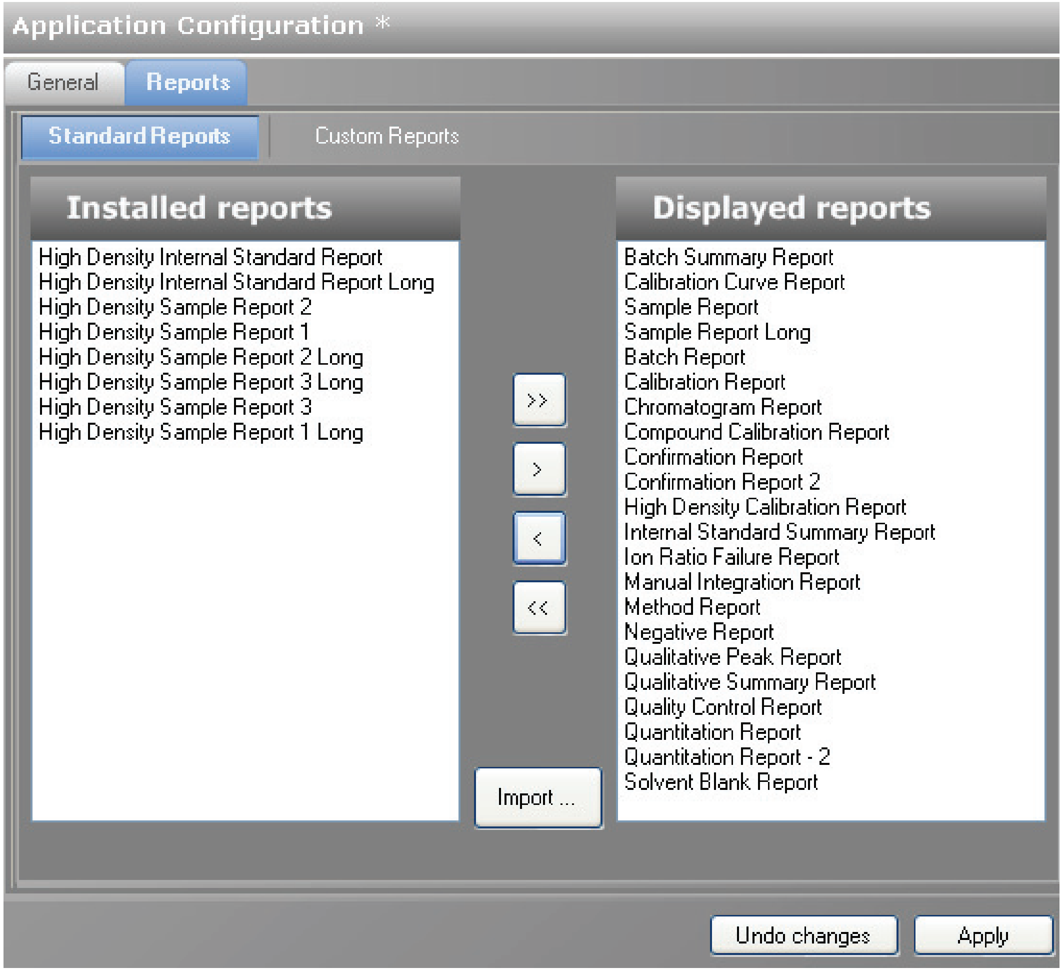


Table 10. Standard Reports parameters (Sheet 1 of 2)

Parameter	Description
Standard Reports	Displays all available standard reports.
Custom Reports	Displays all available custom reports.
Installed reports	All reports listed in the Installed Reports pane are potentially available for this application but are not selected for the Method Development or Production modes.
Displayed reports	All reports listed in the Displayed Reports pane are selected for the Method Development and Production modes. By default, the application displays all reports.
>>	Moves all reports from the Installed Reports list to the Displayed Reports list.
>	Moves the selected reports from the Installed Reports list to the Displayed Reports list.

Table 10. Standard Reports parameters (Sheet 2 of 2)

Parameter	Description
<	Moves the selected reports from the Displayed Reports list to the Installed Reports list.
<<	Moves all reports from the Displayed Reports list to the Installed Reports list.
Import	Opens a browser where you can choose a report file to add to the Installed Reports list.
Undo changes	Returns the report selections to their original state (when you first opened this page).
Apply	Applies the current selections, and reminds you that you must restart the application before the report selections are available for the Method Development and Production modes.

Custom Reports

Use the EnviroLab Forms application to configure and import custom reports.

Follow these procedures:

- To specify which custom reports are available
- To import new custom report types

❖ To specify which custom reports are available

1. Click the **Custom Reports** tab.

   The Custom Reports page opens. See "Custom Reports page" on page 45.

2. Use the directional arrows to move reports from the Installed Reports pane to the Displayed Reports pane.

   Tip Use the CTRL or SHIFT keys to select multiple reports.

   All reports in the Displayed Reports pane are available to users in the Method Development and Production modes.

3. To create a single report for an entire batch (rather than separate reports for each sample), select the **Batch Level Report** check box for the report type.

   Rather than creating separate reports for each sample, the application uses data from only the last sample to create a single report for the entire batch. Batch-level reports are prepended with a **B** to differentiate them.

4. Do one of the following:

   - To return the report selections to their original state, click **Undo Changes**.

     –Or–

   - To apply the current selections, do the following:

     a. Click **Apply**.

        A message reminds you that you must restart the EnviroLab Forms application before your report selections are reflected in the reports available for the Method Development and Production modes.

     b. To restart the EnviroLab Forms application now, click **Yes,** or to remain on the Reports page, click **No**.

❖ To import new custom report types

1. Click **Import**.

2. In the browser, locate a Custom Reports .xltm file and open the file.

   The application writes the imported report to the following folder:

   ..\Thermo\EnviroLab Forms\Templates\Reports

   The Installed Reports pane adds the new report to the list.

Figure 8. Custom Reports page

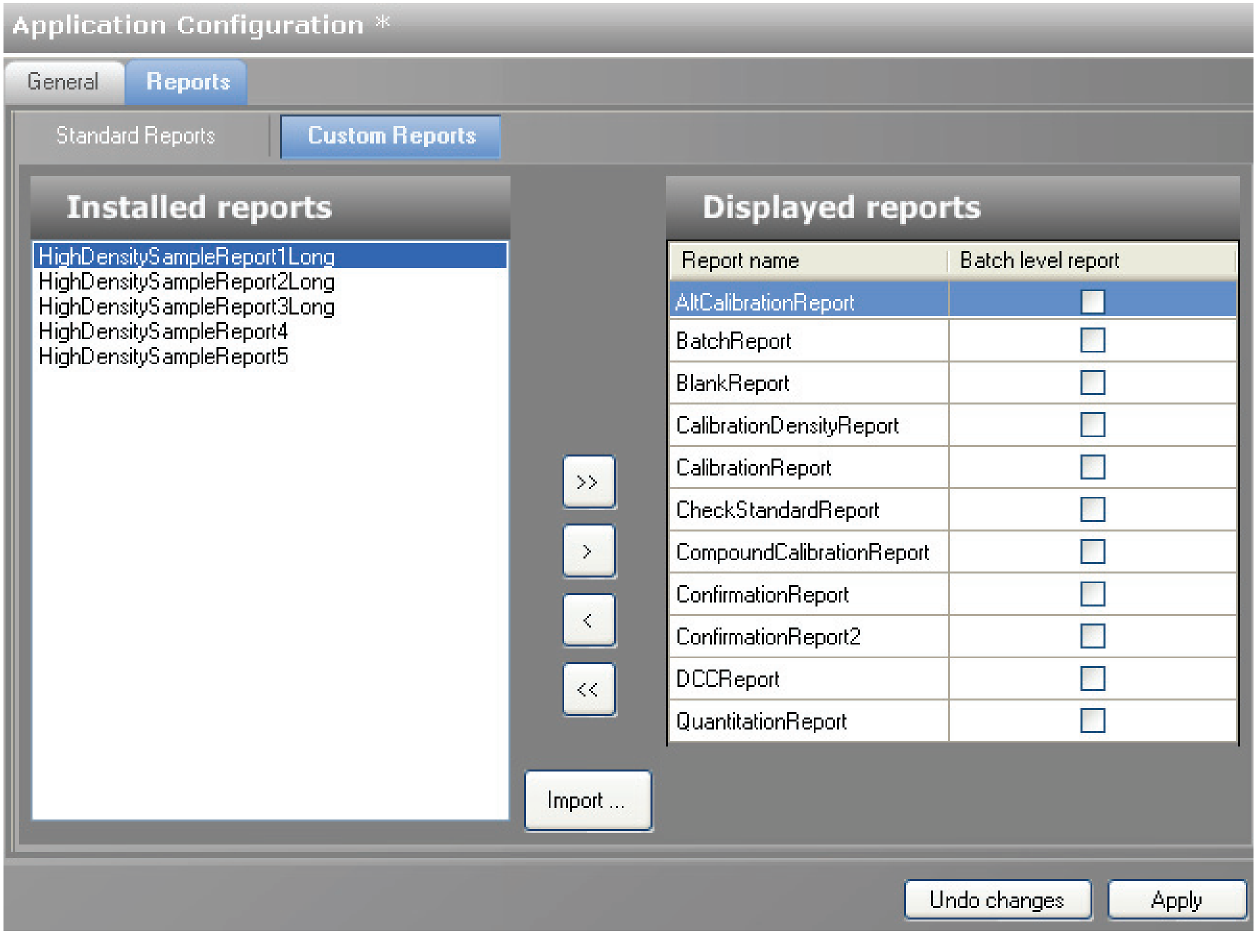


Table 11. Custom Reports parameters (Sheet 1 of 2)

Parameter	Description
Standard Reports	Displays all available standard reports.
Custom Reports	Displays all available custom reports.
Installed reports	All reports listed in the Installed Reports pane are potentially available for this application but are not selected for the Method Development or Production modes.
Displayed reports	All reports listed in the Displayed Reports pane are selected for the Method Development and Production modes. By default, the application displays all reports.
>>	Moves all reports from the Installed Reports list to the Displayed reports list.
>	Moves the selected reports from the Installed Reports list to the Displayed Reports list.

Table 11. Custom Reports parameters (Sheet 2 of 2)

Parameter	Description
<	Moves the selected reports from the Displayed Reports list to the Installed Reports list.
<<	Moves all reports from the Displayed Reports list to the Installed Reports list.
Batch level report	Creates a single report for the entire batch by using data from only the last sample, rather than creating separate reports for each sample. Batch-level reports are prepended with a **B** to differentiate them.
Import	Opens a browser where you can choose a report file to add to the Installed Reports list.
Undo changes	Returns the report selections to their original state (when you first opened this view).
Apply	Applies the current selections, and reminds you that you must restart the application before the report selections are available.

4

Using the Method Development Mode

This chapter includes method development tasks assigned to the Supervisor or Manager roles.

Contents

From the Method Development mode, you can create a master method or an instrument method, and you can create a development batch to test your instrument method with a sample batch.

❖ To access the Method Development mode

Click **Method Development** from the dashboard or the navigation pane.

The Method Development navigation pane opens.

Figure 9. Method Development navigation pane

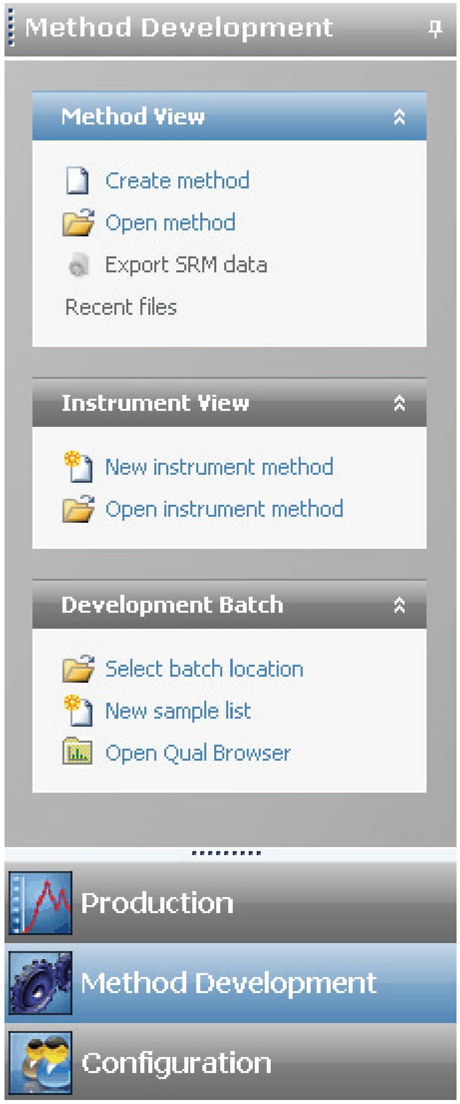


Table 12. Method Development navigation pane functions (Sheet 1 of 2)

Function	Description
Method View	See "Working with Master Methods" on page 50.
Create method	Opens the Create Master Method dialog box where you can choose the process you want to use to begin your master method.
Open method	Opens the Open Master Method dialog box where you can choose a master method to open.

Table 12. Method Development navigation pane functions (Sheet 2 of 2)

Function	Description
Export SRM data	Writes the selected reaction monitoring (SRM) table to the following file: `..\Thermo\EnviroLab Forms\Methods\`*`methodname`*`.xml` You can use the data in this file in the instrument method editor when you open the TSQ 2.1 application. This command is available only when you have selected Enable Compound Datastore on the General page of the Application Configuration view. See "Application Configuration" on page 35.
Recent Files	Displays recently saved master methods.
Instrument View	See "Working with Instrument Methods" on page 157.
New instrument method	Opens the Instrument View where you can specify instrument settings for your configured instruments. If the instrument you want to use is not configured, close the EnviroLab Forms application, configure the instrument, and then reopen the EnviroLab Forms application. You cannot configure an instrument while the EnviroLab Forms application is running.
Open instrument method	Opens a browser where you can choose an instrument method to open.
Development Batch	See "Working with Development Batches" on page 161.
Select batch location	Specifies a location to store temporary development batch raw data files.
New sample list	Removes acquired samples from your development batch so you can begin a new sample list.
Open Qual Browser	Opens the Qual Browser where you can monitor the acquisition of your samples.

Working with Master Methods

The EnviroLab Forms application uses a master method to specify the nature and types of acquisition, processing, and reporting that occur with a batch of samples. When you are testing for compounds in an assay, you can create a method designed specifically for that type of application.

When you create a master method, the EnviroLab Forms application uses the method to determine how the software works with a set of samples to provide a set of meaningful results. The application uses an instrument method to define how raw data is acquired. The rest of the master method defines how the raw data is processed, how the flags information evaluates the results, and how the reporting functionality defines the way your data and results are output into reports.

The EnviroLab Forms application applies your master method to a batch, which is a list of one or more samples to be processed and reported. Together, the master method and batch provide a workflow-oriented approach to the processing of data and the reporting of information for small and large sets of samples.

To speed up the creation of master methods, you can create a method template. Using a method template helps you to develop methods faster because all of your commonly used method settings, such as number of confirming ions, are saved in a template.

This section includes instructions for the following tasks:

- Creating a New Master Method
- Editing a Master Method
- Creating a Method Template
- Exporting SRM Data

Creating a New Master Method

You can use any of four different procedures to begin a master method:

- Creating a Method with Method Forge
- Importing an Xcalibur Method
- Associating a Raw Data File
- Selecting Compounds from the Compound Datastore

Each procedure lets you begin the method in a specific way and then use the common features of the Master Method View to complete and save your master method.

Creating a Method with Method Forge

With Method Forge, you can create a new master method by manually selecting peaks, selecting multiple compounds, renaming peaks, or comparing mass spectra from the library searches. You can also choose to let the EnviroLab Forms application automatically create a master method for you.

When the EnviroLab Forms application automatically creates a master method for you, it performs the following functions:

- Reviews your raw data file and identifies compounds that are present in your sample.
- Uses your mass spectral reference libraries to assign compound names and CAS numbers.
- Uses mass spectral information to select potential quantification and confirming ions and a reference mass spectrum for the compound.

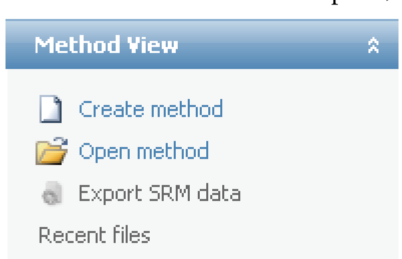
A master method contains a list of compounds and an initial set of information for detecting, processing, and reporting those compounds.

Follow these procedures:

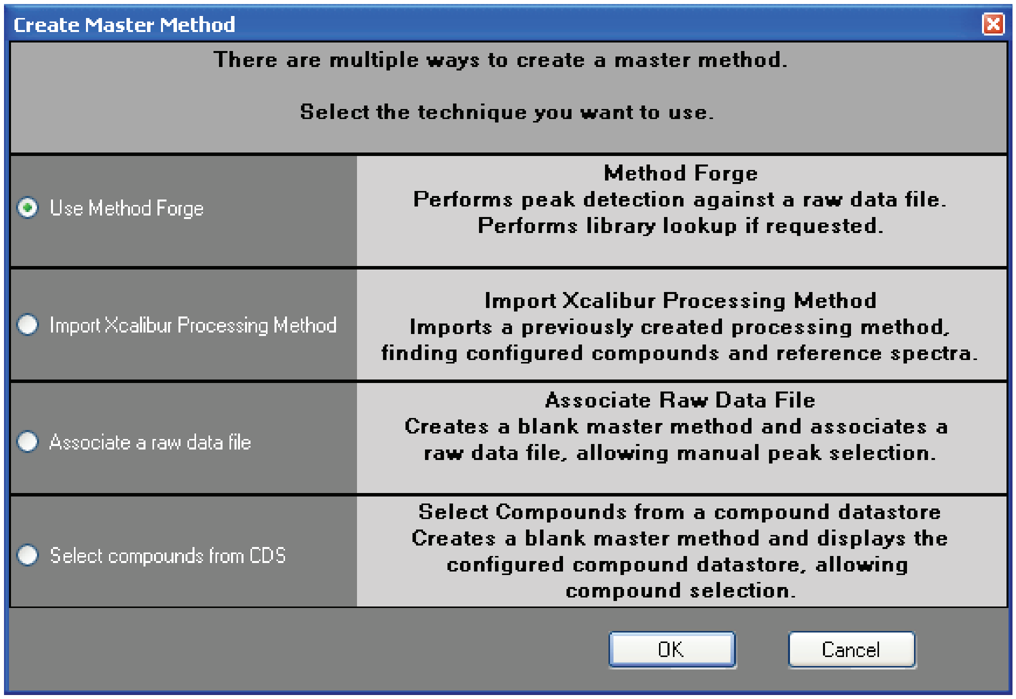
- To automatically select compounds to create a new method
- To manually select compounds to create a method

❖ To automatically select compounds to create a new method

1. From the Method View task pane, click **Create Method**.



The Create Master Method dialog box opens.



2. Select **Use Method Forge**.

3. Click **OK**.

   The Method Forge dialog box opens. See “Method Forge” on page 58.

   Use the Method Forge to create a master method from an existing raw data file or to create a new raw data file to use for the master method.

4. In the Method Forge dialog box, do one of the following:

   - Select the **Use the Default Template** option.

   –Or–

   - Select the **Select a Custom Template** option and highlight your custom template in the Method template table.

     For detailed instructions on creating a custom method template, see “Creating a Method Template” on page 147.

5. Select the **Name the Master Method** check box and type a name for your master method.

   You can enter an existing method name and overwrite it when you create the method. If you do not specify a name, the method is named for the raw file used to create the method.

6. Select the **Automatically Create the Master Method** check box.

7. Do one of the following:

   a. In the Raw File Selection area, choose **Use an Existing Raw Data File**.

   b. Click the browse button and locate a raw data file to use for the method.

   –Or–

   a. In the Raw File Selection area, choose **Acquire a New Raw Data File**.

   b. From the Instrument method list, select a method (.meth) file to use for acquiring the data.

   c. In the Raw Filename box, type the name of the file where the EnviroLab Forms application will write the raw data.

   d. In the Path box, type a path or click the browse button and locate a folder where the application will save the raw data file.

   e. (Optional) Type a comment about the acquired sample or the data file.

8. If you chose to acquire a new raw data file, do one of the following:

   - Choose **Manual Injection**.

   –Or–

   - Do the following:

     a. Choose **Use Autosampler**.

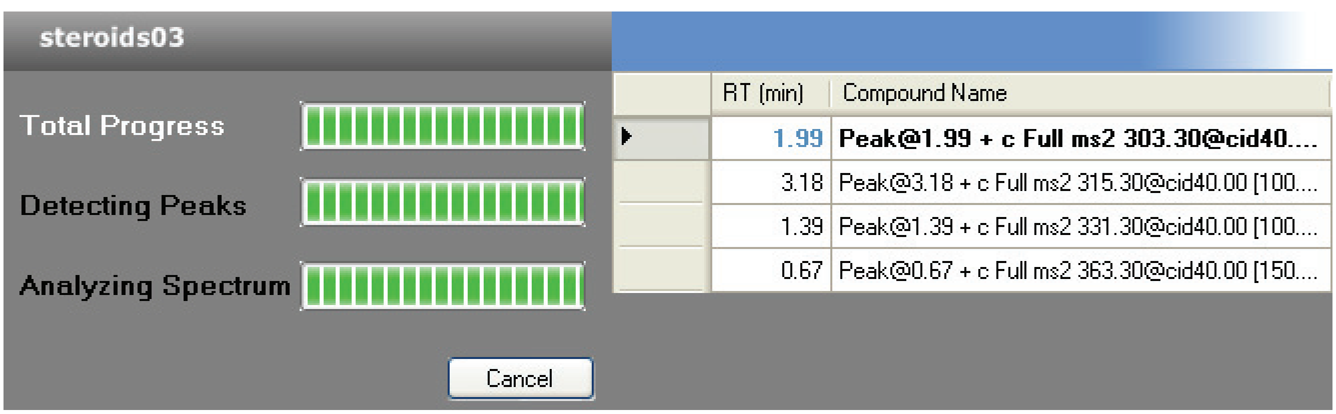
     b. In the Vial Position box, type a vial position.

     c. In the Injection Volume box, type an injection volume.

        The minimum injection volume value allowed is 0.05 µL.

9. To automatically create the master method, click **OK** (or **Overwrite**).

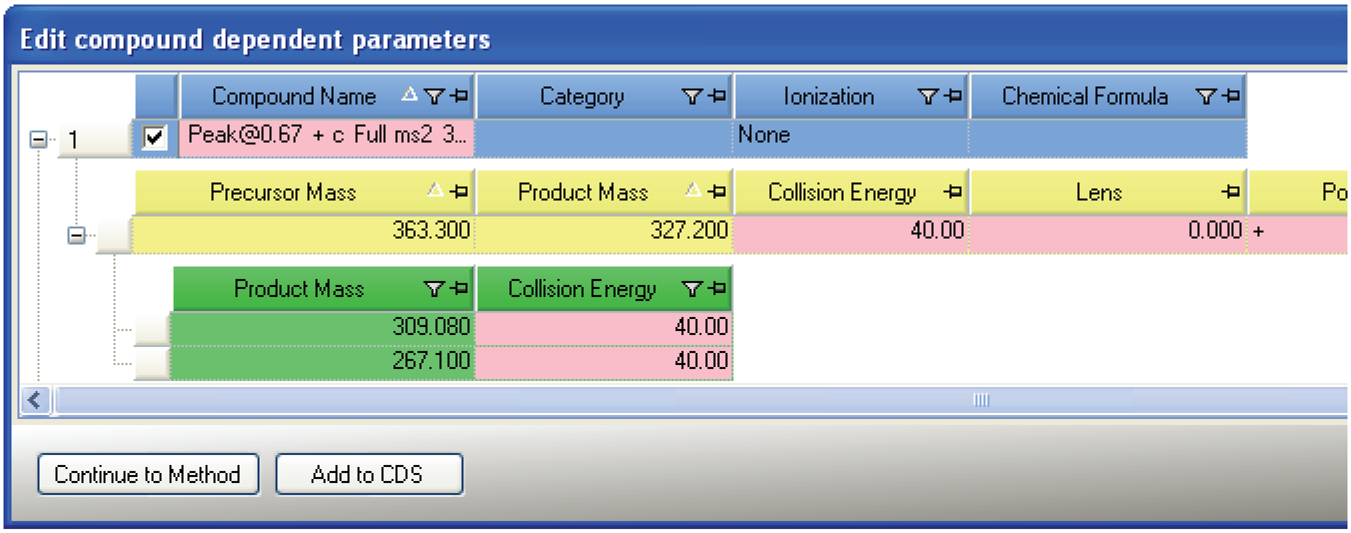
   As the Method Forge creates the method, it displays the following status:



Note When you have a compound datastore enabled, the Method Forge process searches the library and displays the identified compound names instead of peak times.

When the acquisition completes, Method Forge performs peak detection, datastore searching, and characteristic ion and reference spectrum identification. Method Forge then loads this information into a new master method. This process occurs immediately if you selected a previously acquired raw file.

If the compounds in the raw data file you used to create the method are not in the Compound Datastore, the EnviroLab Forms application displays the compounds in the Edit Compound Dependent Parameters dialog box.



10. (Optional) Select the compounds that you want to add to the compound datastore and click **Add to CDS**.

    The selected compounds are added to the current compound datastore.

    Note To add these compounds to the datastore, you must use the Add to CDS command before you continue to the method.

11. To use these compounds in your method and close the dialog box, click **Continue to Method**.

    All compounds found in the raw data file are used in your method. The EnviroLab Forms application displays the General page of the Master Method View.

12. From the Instrument Method list on the General page, select an instrument method.

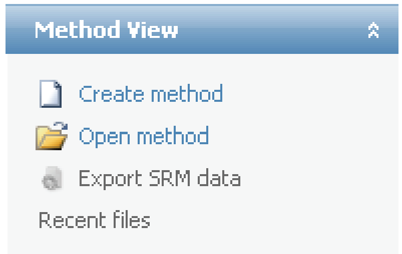
13. From the Tune/Breakdown method list, select a tune/breakdown method (if different from your instrument method).

14. To save the new method, choose **File > Save** from the main menu.

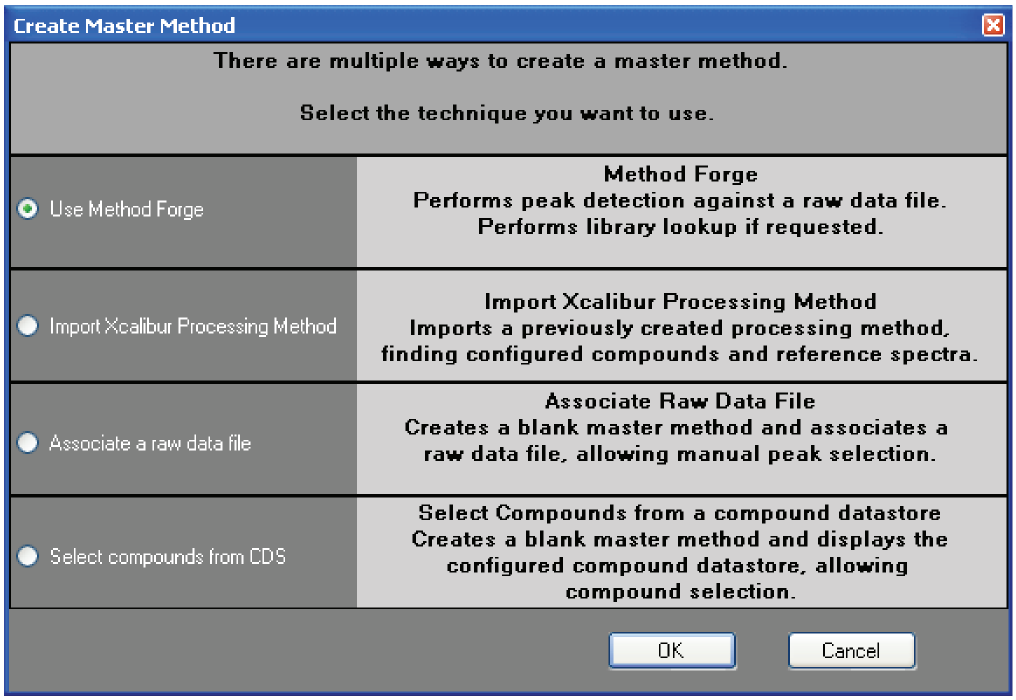
    For a detailed description of how to modify a master method, see "Editing a Master Method" on page 68.

❖ To manually select compounds to create a method

1. From the Method View task pane, click **Create Method**.



The Create Master Method dialog box opens.



2. Select **Use Method Forge**.

3. Click **OK**.

   The Method Forge dialog box opens. See "Method Forge" on page 58.

4. In the Method Forge dialog box, do one of the following:

   - Select the **Use the Default Template** option.

   –Or–

   - Select **Select a Custom Template** and highlight your custom template in the Method Template table.

     For detailed instructions about creating a custom method template, see "Creating a Method Template" on page 147.

5. Select the **Name the Master Method** check box and type a name for your master method.

   You can enter an existing method name and overwrite it when you create the method. If you do not specify a name, the method is named for the raw file used to create the method.

6. Ensure that the **Automatically Create the Master Method** check box is not selected.

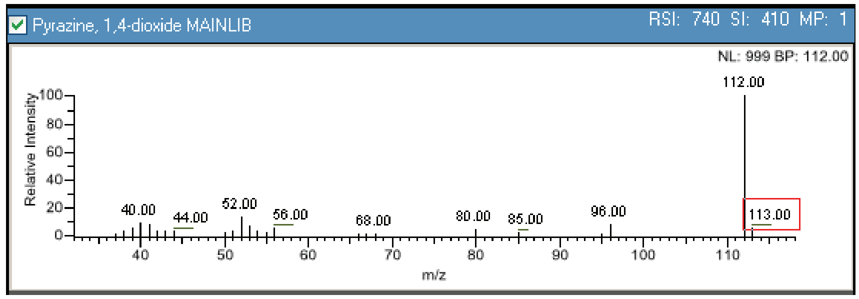
7. To select a raw data file, click the browse button and locate the file.

8. To manually create the master method, click **OK** (or **Overwrite**).

   The Master Method View displays a list of possible matches in the Library Results pane. The EnviroLab Forms application displays the best match in the Compound Name list and displays the peak spectrum for that compound.

9. To use a compound other than the compound chosen by the EnviroLab Forms application, scroll to the spectrum for that compound and select the compound name in the header of the spectrum pane.

Select compound



10. After you manually select your compound, click **Create** to create the master method.

    All compounds found in the raw data file are used in your method. The EnviroLab Forms application displays the General page of the Master Method View.

11. From the Instrument Method list on the General page, select an instrument method.

12. From the Tune/Breakdown method list, select a tune/breakdown method (if different from your instrument method).

13. To save the new method, choose **File > Save** from the main menu.

    For a detailed description of how to modify a master method, see "Editing a Master Method" on page 68.

Figure 10. Method Forge

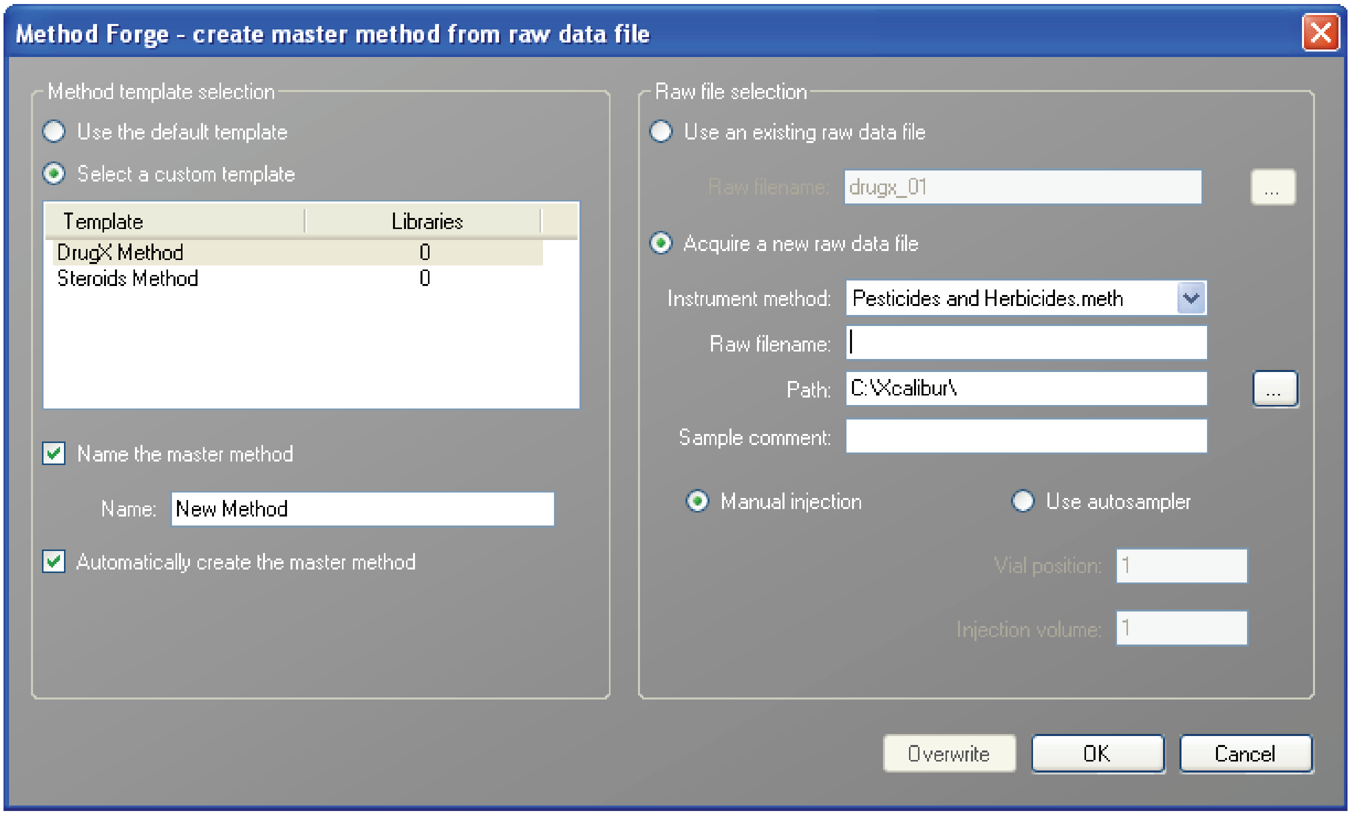


Table 13. Method Forge parameters (Sheet 1 of 2)

Parameter	Description
Method template selection	
Use the default template	Creates a new method with the default template.
Select a custom template	Lists all the available method templates. For detailed instructions about creating a custom method template, see "Creating a Method Template" on page 147.
Name the master method	The name for the new master method.
Automatically create the master method	When the acquisition completes, Method Forge performs peak detection, library searching, and characteristic ion and reference spectrum identification. This information is loaded into a new master method. This process occurs immediately when you specify an existing raw data file.

Table 13. Method Forge parameters (Sheet 2 of 2)

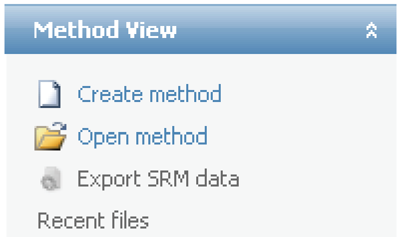
Parameter	Description
Raw file selection	
Use an existing raw data file	Enables the Raw Filename box where you can select a raw data file to use to create the master method.
Acquire a new raw data file	Enables functions to acquire data to create a raw file to use to create the master method.
Instrument method	The saved method (.meth) file to use for acquiring the data.
Raw filename	The file name where the EnviroLab Forms application will write the raw data.
Path	The location where the EnviroLab Forms application will save the raw data file.
Sample comment	(Optional) Comment about the acquired sample or the data file.
Manual injection	Performs a manual acquisition.
Use autosampler	Performs an autosampled acquisition.
Vial position	The tray vial number used for the autosampler acquisition.
Injection amount	The volume (in milliliters) injected by the autosampler acquisition.
Function button	
Overwrite	Overwrites the specified master method name. This function is enabled only when the specified master method name already exists.
OK	Creates a master method using the data and parameters you specified.
Cancel	Closes the Method Forge and does not create a master method.

Importing an Xcalibur Method

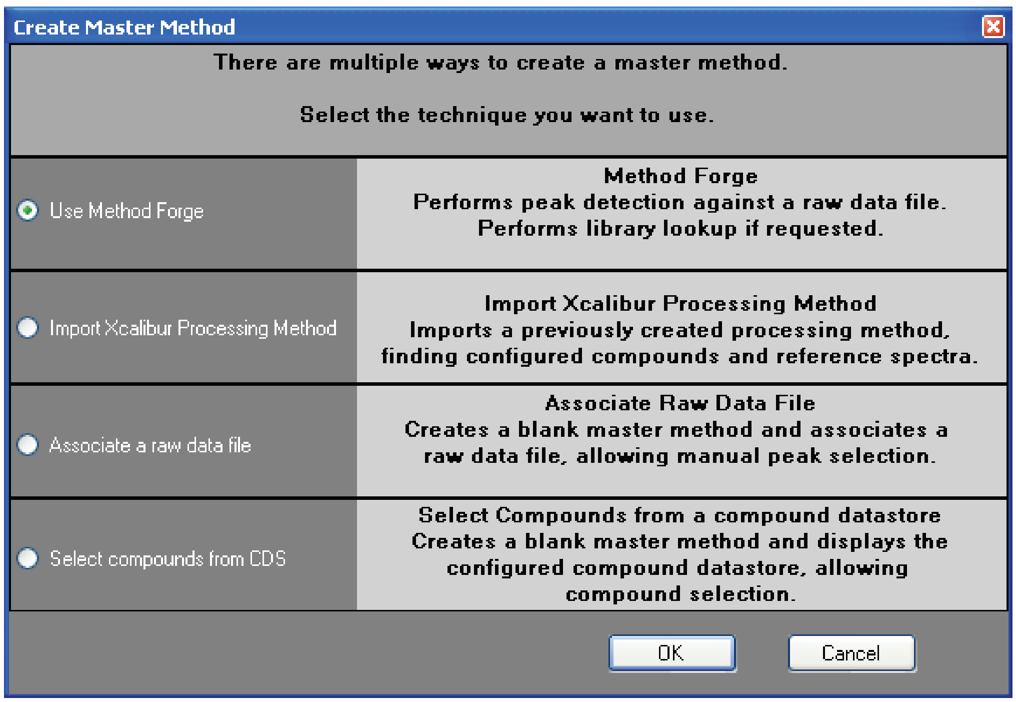
You can create a new master method from an existing Xcalibur processing method.

❖ To import an Xcalibur method

1. From the Method View task pane, click **Create Method**.



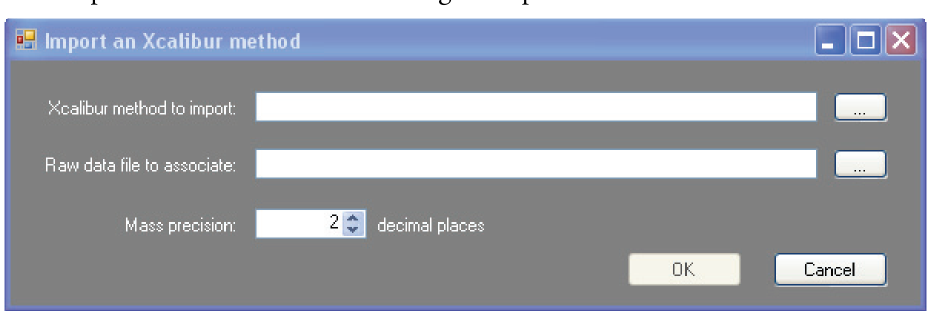
The Create Master Method dialog box opens.



2. Select **Import Xcalibur Processing Method**.

3. Click **OK**.

The Import an Xcalibur Method dialog box opens.



4. To select an Xcalibur processing method file to import, click the browse button for the **Xcalibur Method to Import** box.

5. Browse to the Xcalibur processing method file and open the file.

   The EnviroLab Forms application imports the compound information from the Xcalibur method file.

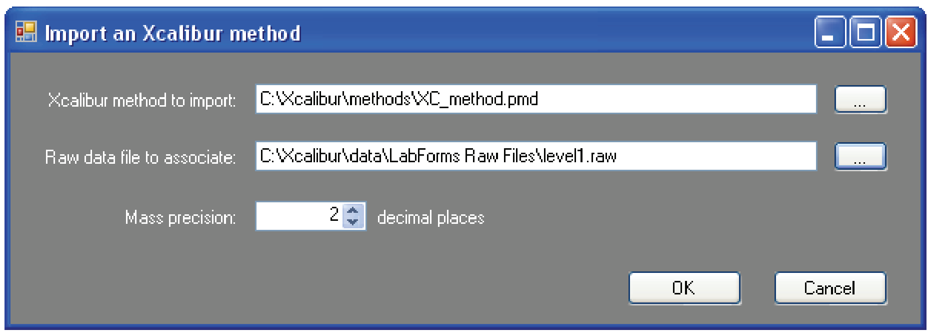
6. To associate a raw data file with this method, click the browse button for the **Rawfile to Associate** box.

7. Browse to the raw data file and open the file.

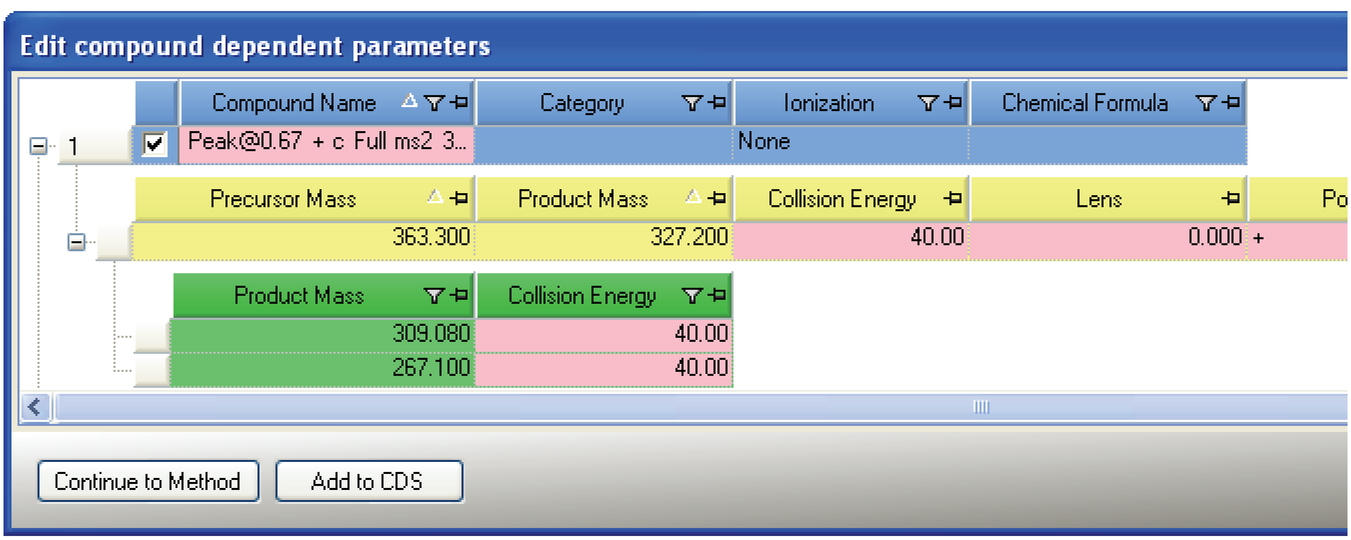
8. (Optional) Change the number of decimal places in the Mass Precision box.

   You can set the mass precision decimal places to any integer between 0 and 5, inclusive.

9. Click **OK**.



If the compounds in the imported Xcalibur method file are not in the Compound Datastore, the EnviroLab Forms application displays the compounds in the Edit Compound Dependent Parameters dialog box.



10. (Optional) Select the compounds you want to add to the Compound Datastore and click **Add to CDS**.

The selected compounds are added to the current compound datastore.

Note To add these compounds to the datastore, you must use the Add to CDS command before you continue to the method.

11. To add these compounds to your method and close the dialog box, click **Continue to Method**.

    All compounds found in the imported Xcalibur method are added to your method. The EnviroLab Forms application displays the General page of the Master Method View.

12. From the Instrument Method list on the General page, select an instrument method.

13. From the Tune/Breakdown method list, select a tune/breakdown method (if different from your instrument method).

14. To save the new method, choose **File > Save** from the main menu.

    For a detailed description of how to modify a master method, see "Editing a Master Method" on page 68.

Associating a Raw Data File

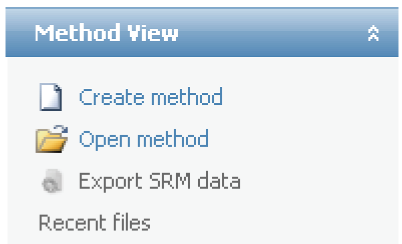
You can use the compounds in a previously acquired raw data file to create a new master method.

Follow these procedures:

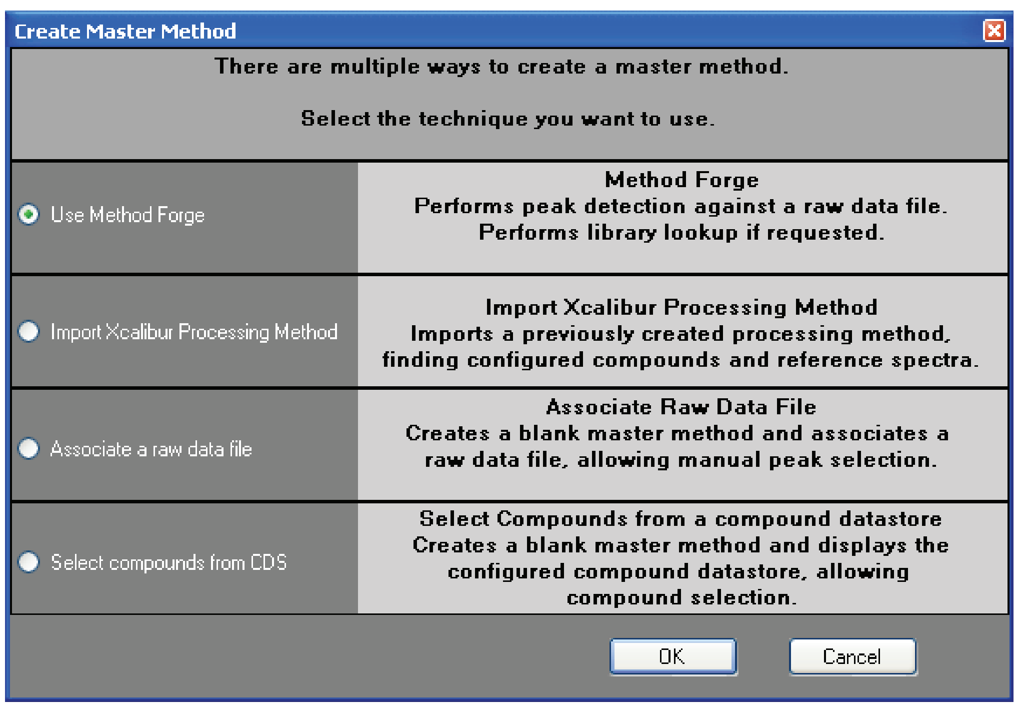
- To associate a raw data file with the method
- To add compounds to the method

❖ To associate a raw data file with the method

1. From the Method View task pane, click **Create Method**.

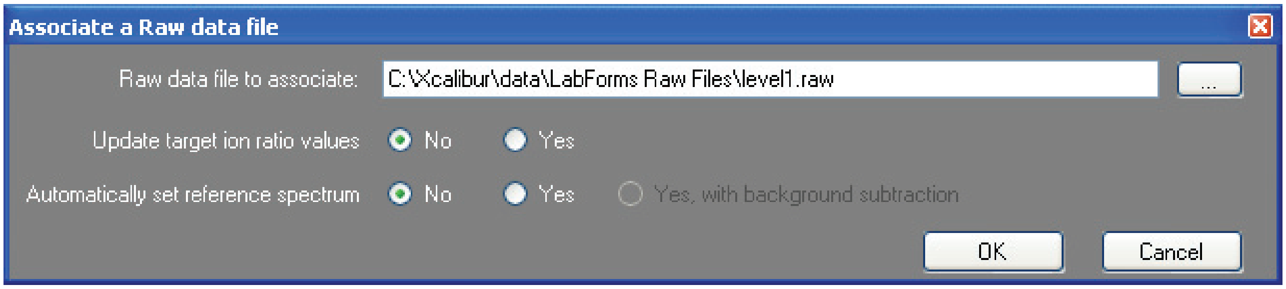


The Create Master Method dialog box opens.



2. Select **Associate a Raw Data File**.

   The Associate a Raw Data File dialog box opens.



3. Click the browse button and locate a raw data file to associate with the method.
4. To update the target ion ratio values when you associate this raw data file, click **Yes**.
5. To set a reference spectrum, do one of the following:
   - Click **Yes**.

   – Or –

   - Click **Yes, with Background Subtraction.**

     This feature is available only when you have set background subtraction values on the General page of the Master Method View. See “Editing the General Page” on page 70.
6. Click **OK**.

   All compounds found in the raw data file are added to your method. The EnviroLab Forms application displays the General page of the Master Method View.
7. From the Instrument Method list on the General page, select an instrument method.
8. From the Tune/Breakdown method list, select a tune/breakdown method (if different from your instrument method).
9. To save the new method, choose **File > Save** from the main menu.

   If the compounds in the associated raw data file are not found in the Compound Datastore, the EnviroLab Forms application will not let you save the method. Follow the instructions “To add compounds to the method” on page 65.

   For a detailed description of how to modify a master method, see “Editing a Master Method” on page 68.

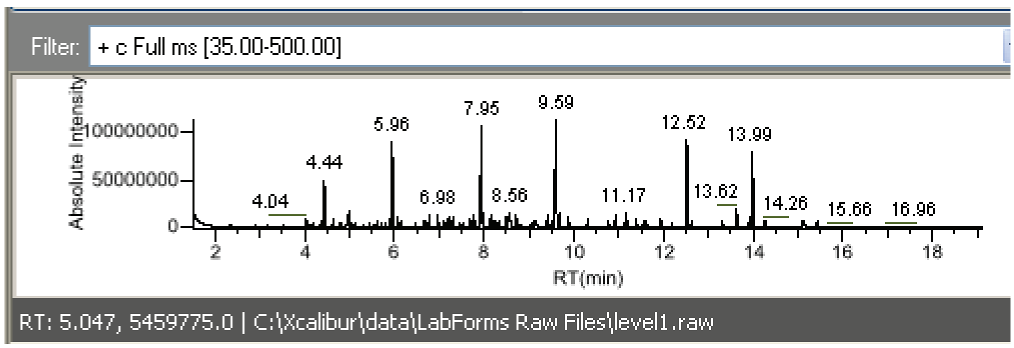
❖ To add compounds to the method

1. Click the **Compounds** tab.

   The **Detection** page is selected by default.

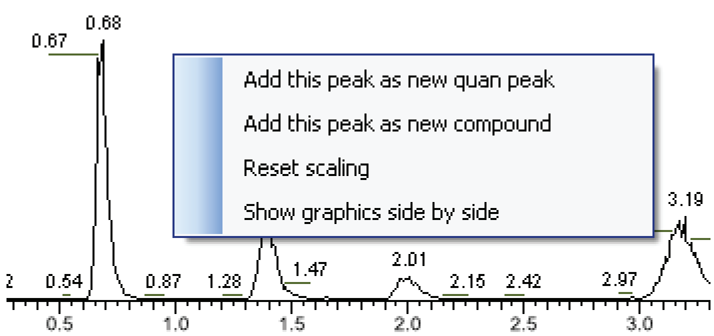
   The Detection page shows an empty Compound list and displays the chromatographic data for the compounds in the raw file.

2. Select a filter from the Filter list.

3. Click the peak in the chromatogram that represents the compound you want to add to the method.

4. Right-click and choose **Add this Peak as New Compound** from the shortcut menu.

   The EnviroLab Forms application adds the new compound and displays the quantitation peak information for the compound.

5. Repeat these steps for each compound you want to add to the method.

   For a detailed description of all parameters on the Detection page, see "Editing the Compounds Page" on page 77.

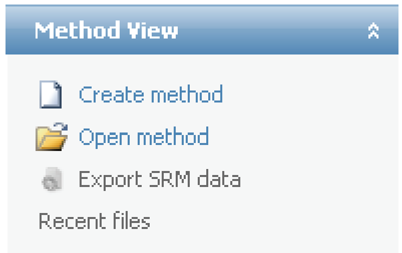
   For a detailed description of how to modify a master method, see "Editing a Master Method" on page 68.

Selecting Compounds from the Compound Datastore

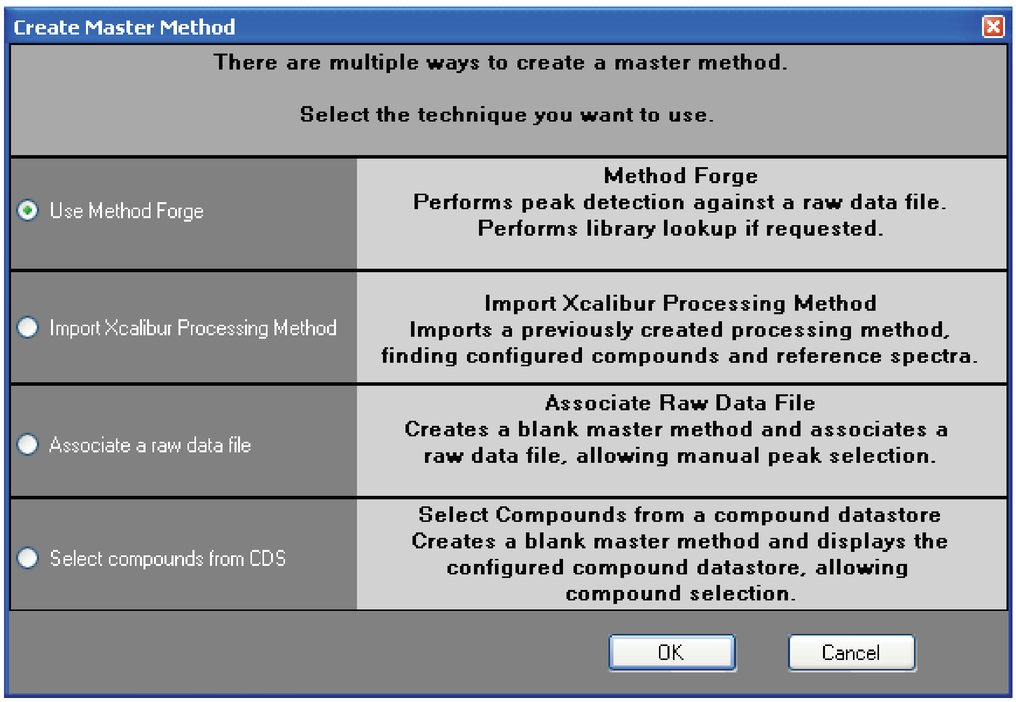
You can select compounds from the compound datastore to create a new master method.

❖ To select compounds from the datastore

1. From the Method View task pane, click **Create Method**.

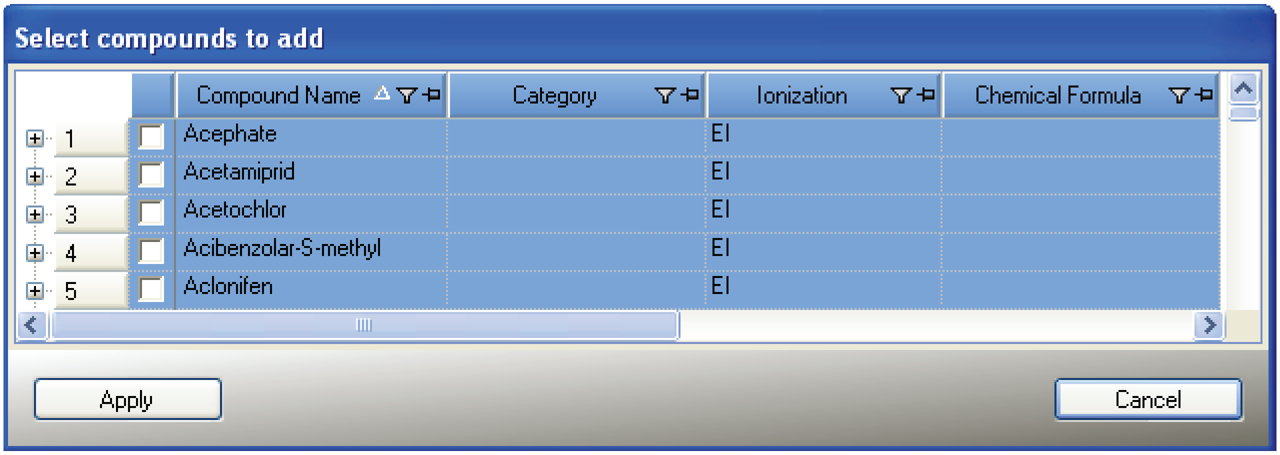


The Create Master Method dialog box opens.



2. Select **Select Compounds from CDS**.

   The Select Compounds to Add dialog box opens, listing all the compounds defined in the compound datastore specified for the gas chromatography technology.



3. Select the check box for each compound you want to add to the method and click **Apply**.

   The EnviroLab Forms application adds the selected compounds to the Master Method View.

4. From the Instrument Method list on the General page, select an instrument method.

5. From the Tune/Breakdown method list, select a tune/breakdown method (if different from your instrument method).

6. To save the new method, choose **File > Save** from the main menu.

   For a detailed description of how to modify a master method, see "Editing a Master Method" on page 68.

Editing a Master Method

You can open a master method to view or edit the compounds, method instructions, and reporting options in the method.

This section includes instructions for the following tasks:

- Opening a Master Method
- Editing the General Page
- Editing the Compounds Page
- Editing the QAQC Page
- Editing the Groups Page
- Editing the Reports Page

Opening a Master Method

The EnviroLab Forms application lets you open a master method that was created and saved in the EnviroLab Forms 3.0 application or one that was created and saved in the EnviroLab Forms 2.5 application.

Follow these procedures:

- To open a saved master method
- To open a saved master method from the Recent Files list

❖ To open a saved master method

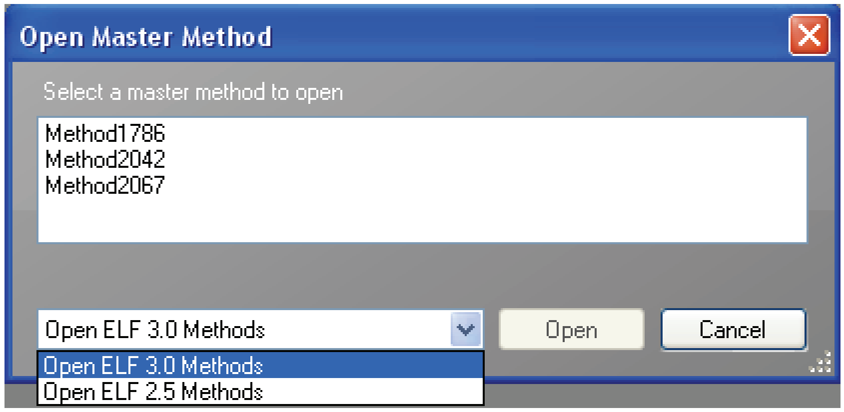
1. Click **Method Development** from the dashboard or the navigation pane.

   The Method Development navigation pane opens.

2. In the Method View task pane, click **Open Method,** or choose **File > Open > Master Method** from the main menu.

   The Open Master Method dialog box opens where you can select a master method.



3. Select either **Open ELF 3.0 Methods** or **Open ELF 2.5 Methods**.

   The EnviroLab Forms application displays all available methods for the specified version of the application. The list of EnviroLab Forms 2.5 methods can include any method created with EnviroLab Forms 2.5 or greater.

4. Select a master method and click **Open**.

   The selected master method opens in the Master Method View.

   When you open a LabForms 2.5 method, the EnviroLab Forms application copies all components of the selected method including its associated instrument method.

   - If the LabForms 2.5 master method does not have an associated instrument method, the Master Method View for the imported method indicates that you need to select an instrument method.

   - If you open a LabForms 2.5 master method that uses an instrument method name already used in your Xcalibur\methods folder, you are prompted to overwrite the instrument method or use the method with the same name already in your methods folder.

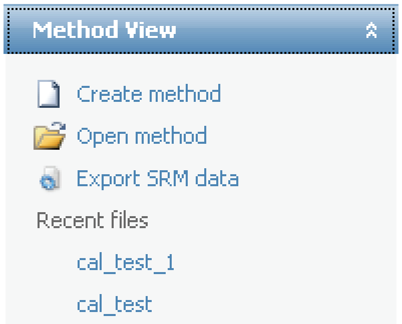
❖ To open a saved master method from the Recent Files list

1. Click **Method Development** from the dashboard or the navigation pane.

   The Method Development navigation pane opens.

   When you save a method, it is added to the Recent Files list. The Recent Files list displays a list of your most recently saved master method files.



2. Click the method name in the Recent Files list. Do not double-click.

   The General page for the selected method opens in the Method View. See "General page" on page 74.

Editing the General Page

The General page defines basic information about the master method.

Follow these procedures:

- To specify general information for a master method
- To edit the instrument or tune/breakdown method parameters
- To set automated background subtraction options
- To specify a chromatogram reference sample

❖ To specify general information for a master method

1. In the Lab Name box, type the name to be displayed on the top of each printed, saved, or exported report.

   The default name is ThermoFisher Laboratory.

2. In the Assay Type box, type the assay type to be targeted by the method.

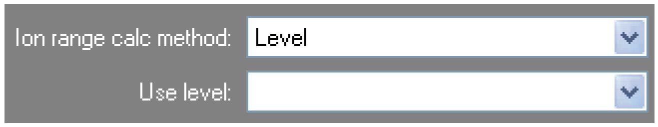
3. From the Injection Volume box, select the injection volume (in µL) to be used for sample injection.

   Use either the up/down arrows to change the volume in increments/decrements of 1 µL, or the keyboard to enter non-integer injection volumes.

   > **IMPORTANT** The EnviroLab Forms application uses the injection volume you specify here in the master method, not the injection volume from the instrument method.

4. From the Ion Range Calc Method box, select a method for calculating the ion ratio range windows.

When you select **Level**, the EnviroLab Forms application displays an additional list box where you can choose a calibration level. To define the calibration levels on the Compounds page, see "Editing the Compounds Page" on page 77.



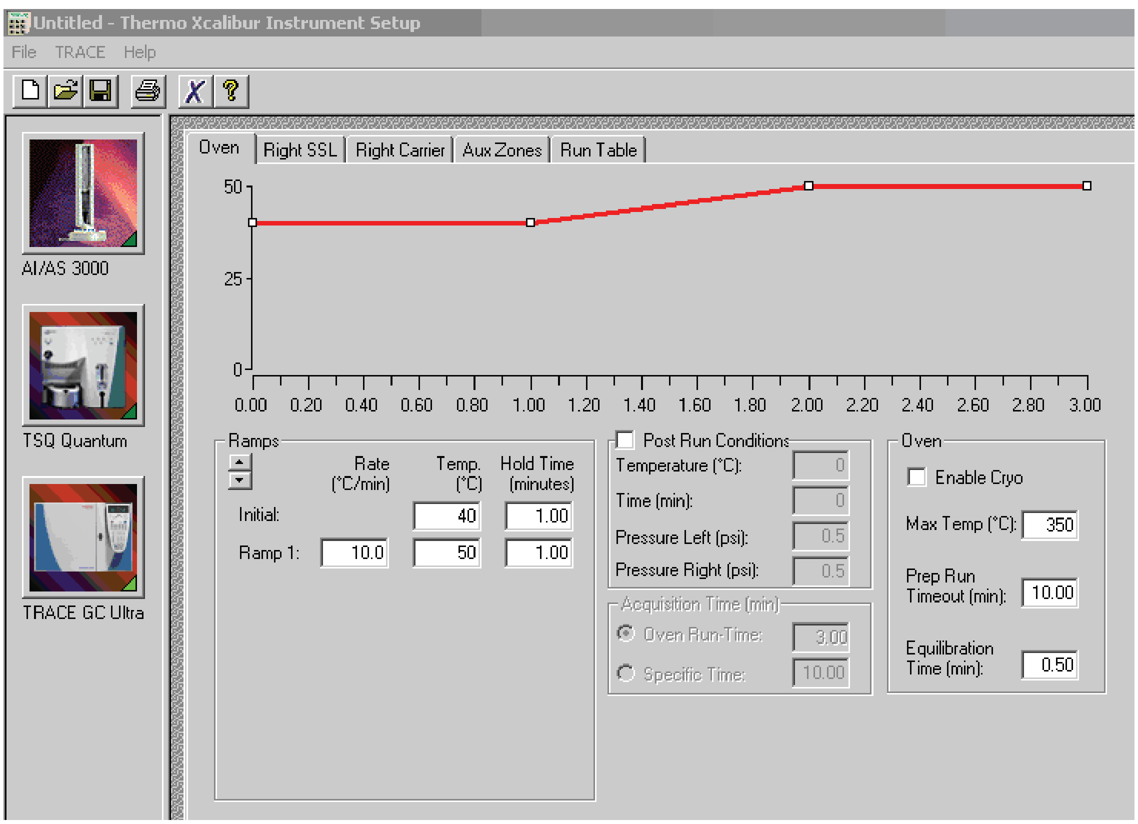
5. From the Qualitative Peak Processing Template box, select a template for performing peak detection on quantitative samples following target compound analysis.

❖ To edit the instrument or tune/breakdown method parameters

1. From the Instrument Method list on the General page, select an instrument method.
2. From the Tune/Breakdown method list, select a tune/breakdown method (if different from your instrument method).
3. To edit the instrument or tune/breakdown methods for this master method, click **Edit** next to the appropriate box.

   The Thermo Xcalibur Instrument Setup dialog box opens.

   This example instrument setup shows multiple configured instruments.



4. Edit the values on the instrument page.

5. From the main menu on the Thermo Xcalibur Instrument Setup dialog box, choose **File > Save** and then choose **File > Exit**.

   The EnviroLab Forms application returns you to the General page.

6. To update any changes that were made to the instrument method, tune method, or breakdown method after you created this master method, click **Update** next to the appropriate box.

❖ To set automated background subtraction options

1. Click **Range Option** and select how you want the subtraction range determined.

   - **Before Peak**: Averages and subtracts a specified number of scans before the apex of the peak.
   - **After Peak**: Subtracts a specified number of scans following the apex of the peak.
   - **Both Sides of Peak**: Subtracts a specified number of scans from each side of the apex of the peak.

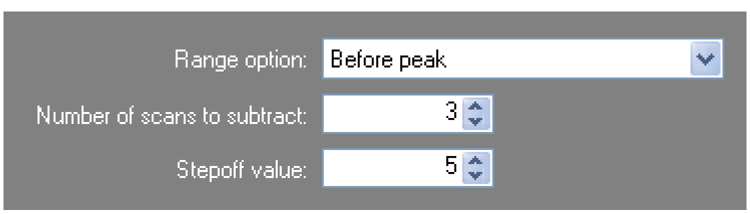
2. Click **Number of Scans to Subtract**, and use the spin box to select a number or type a number in the box.

   After averaging, this is the number of scans that the EnviroLab Forms application subtracts from the background. If you specified to subtract scans from both sides of the peak, the application subtracts this number of scans from EACH side of the peak.

3. Click **Stepoff Value**, and use the spin box to select a number or type a number in the box.

   This offset value lets the EnviroLab Forms application average and subtract scans that are not adjacent to the apex of the peak.

   For example:

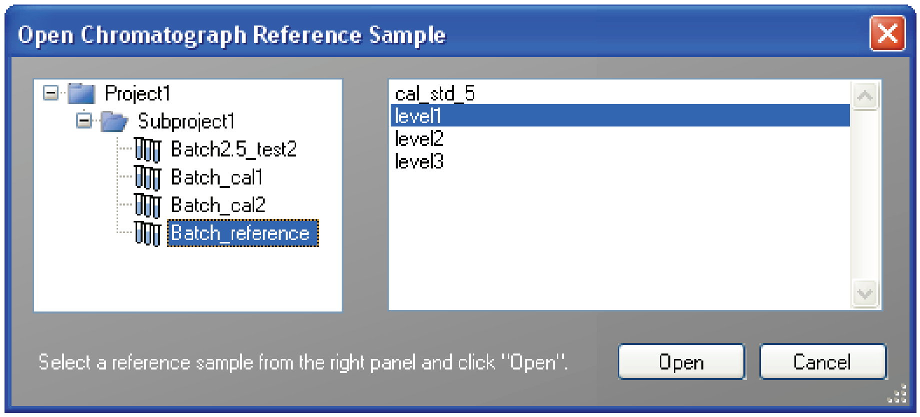


   If you have specified to subtract 3 scans before the peak and the Stepoff value is 5, the EnviroLab Forms application ignores the first 5 scans to the left of the peak and applies the averaging and subtraction to the 6th, 7th, and 8th scans to the left of the peak.

❖ To specify a chromatogram reference sample

1. Click **Set Chromatogram Reference Sample** and select **External** from the list.
2. Click **Select File**.

   The Open Chromatograph Reference Sample dialog box opens.



> **Note** If you are using a EnviroLab Forms 2.5 method, you will not see any reference samples here. You must first create and save a batch using the EnviroLab Forms 2.5 method.

3. Select a project from the list of projects.
4. Select a subproject from the list of subprojects.
5. Select a batch from the list of batches.

   The EnviroLab Forms application displays only batches that were created using the same master method as the current batch.

6. Select a sample from the list of processed samples.

   The EnviroLab Forms application displays all the processed samples in the selected batch. To use a sample as a reference sample, it must have been acquired and processed with the current master method.

7. Click **Open**.

   The selected sample is displayed as the chromatogram reference sample in the Master Method View.

> **Tip** To clear the reference sample from the master method, click **Set Chromatogram Reference Sample** and select **None** from the list.

Figure 11. General page

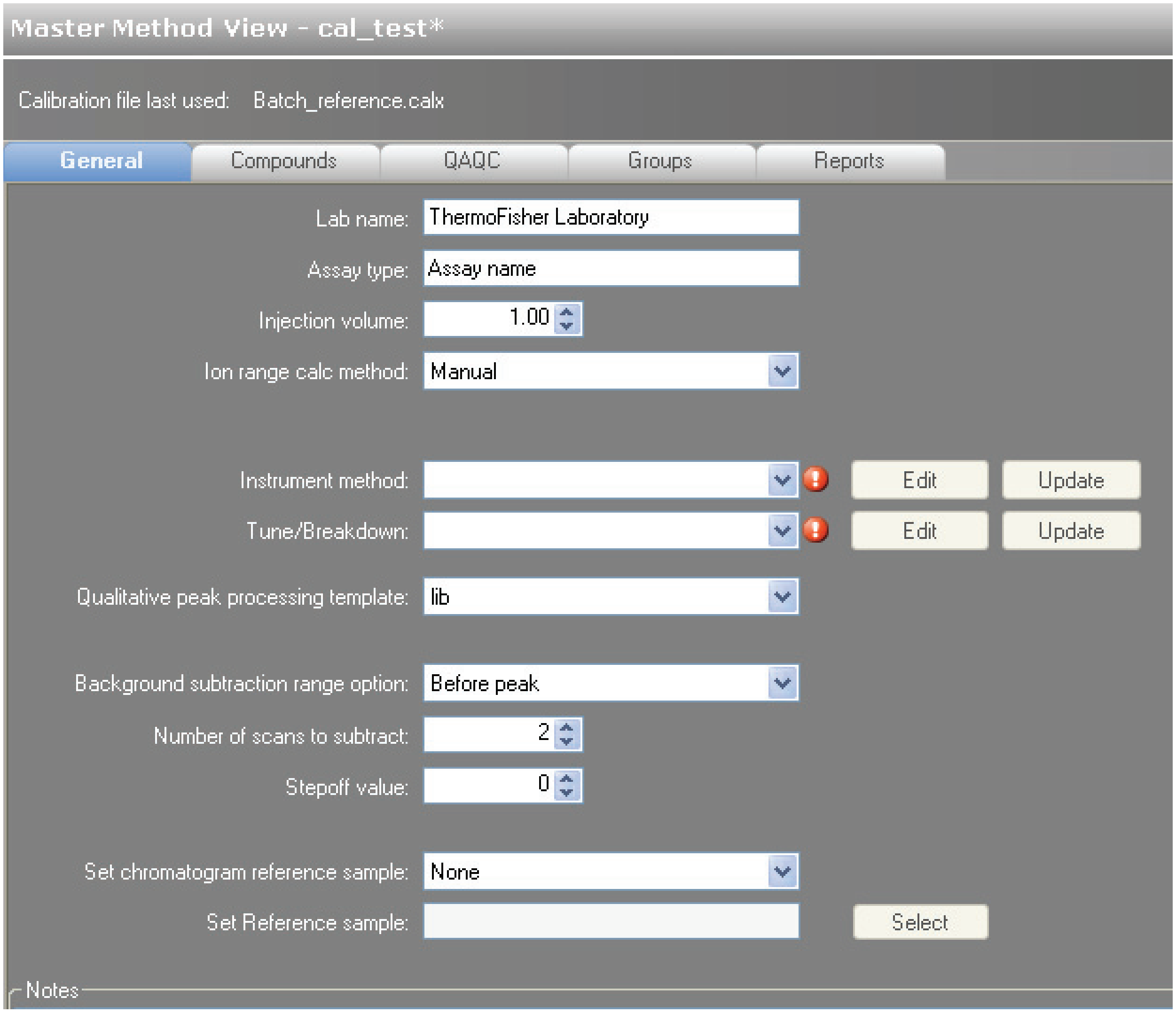


Table 14. General parameters (Sheet 1 of 2)

Parameter	Description
Lab name	The laboratory name to be displayed on the top of each printed, saved, or exported report. Default: ThermoFisher Laboratory To specify this default laboratory name, see "Specifying the General Configuration" on page 35.
Assay type	The name for the analysis type to be targeted by the method. The assay type associates the method with the analysis of a compound or specific class of compounds (for example, an assay type of PAH might be used for the analysis of Polynuclear Aromatic Hydrocarbons). The EnviroLab Forms application uses this assay type in the batch template.
Injection volume	The system use the injection volume (in µL) for sample injection. Certain autosamplers, such as the AI/AS 3000, use the injection volume specified in the associated instrument method. For those autosamplers, the value entered in this field is ignored and the instrument uses a default method injection volume. Other autosamplers, such as the TriPlus, use the EnviroLab Forms application method injection volume for sample analysis and override the instrument method. For a more detailed explanation, refer to the documentation for the autosampler.
Ion range calc method	The EnviroLab Forms application uses the selected ion range calc method to calculate the ion ratio range windows: Manual (default), Average, Level, or Weighted average. When you select **Level**, an additional list box is displayed where you can choose a calibration level amount. To define these calibration levels on the Compounds page, see "Editing the Compounds Page" on page 77.
Instrument method	Instrument method used for processing samples.
Tune/Breakdown	Breakdown or tune method used for processing samples.
Edit	Opens the Thermo Xcalibur Instrument Setup dialog box where you can edit the instrument method, tune method, or breakdown method.
Update	Updates any changes to the instrument method, tune method, or breakdown method after you created this master method.
Qualitative peak processing template	The EnviroLab Forms application uses the qualitative peak processing template to perform peak detection on quantitative samples following compound analysis.

Table 14. General parameters (Sheet 2 of 2)

Parameter	Description
Background subtraction range option	Valid values: None, Before Peak, After Peak, Both Sides of Peak Default: None
Number of scans to subtract	Valid values: Even numbered integers Default: 0
Stepoff value	Offset from the selected peak to the first subtracted peak.
Set chromatogram reference sample	Valid values: None, External Default: None
Set Reference sample	This parameter is enabled only when Set Chromatogram Reference Sample is set to **External**. The **Select** button lets you choose a reference sample from the project folders.
Notes	Notes you add about the method.

Editing the Compounds Page

Use the Compounds page to set all parameters for the identification, detection, and quantification for the target compound list.

From the Compounds page of the Master Method View, you can access the following pages:

- Acquisition List
- Identification
- Detection
- Calibration
- Calibration Levels
- QC Levels

Acquisition List

The Acquisition List page displays all compounds defined for the current method. From this page, you can add or delete compounds from the method. See "Acquisition List page" on page 79.

The Acquisition List page is displayed only when the Enable Compound Datastore option is checked on the General page on the Application Configuration view. See "Application Configuration" on page 35.

Follow these procedures:

- To filter the compound list
- To delete a compound from the list
- To add a compound transition to the list

❖ To filter the compound list

1. To display a filtered list of compounds, click the funnel icon, , in the column header.

   For each column, a list of filterable criteria is displayed in a list box. On all list boxes, you can choose to filter by All, Blanks, NonBlanks, or by custom filter criteria. Other filter criteria are specific to the individual columns.

2. Choose the type of compound you want to display.

   For example, if you choose **All** in the Compound Name column, the EnviroLab Forms application displays all compounds; if you choose **Blanks** in the Compound Name column, the application displays only blank compound types.

3. (Optional) To create a custom filter based on compound values in a specific column, choose **Custom** from the column list box.

   For detailed instructions about creating a custom filter, see Appendix C, "Using Filter Criteria."

❖ To delete a compound from the list

1. Select the compound to remove from the list.
2. Click the **Remove Compound Transition** icon, , or right-click and choose **Remove Compound Transition** from the shortcut menu.

   A confirmation dialog box opens, listing the compound to be removed.

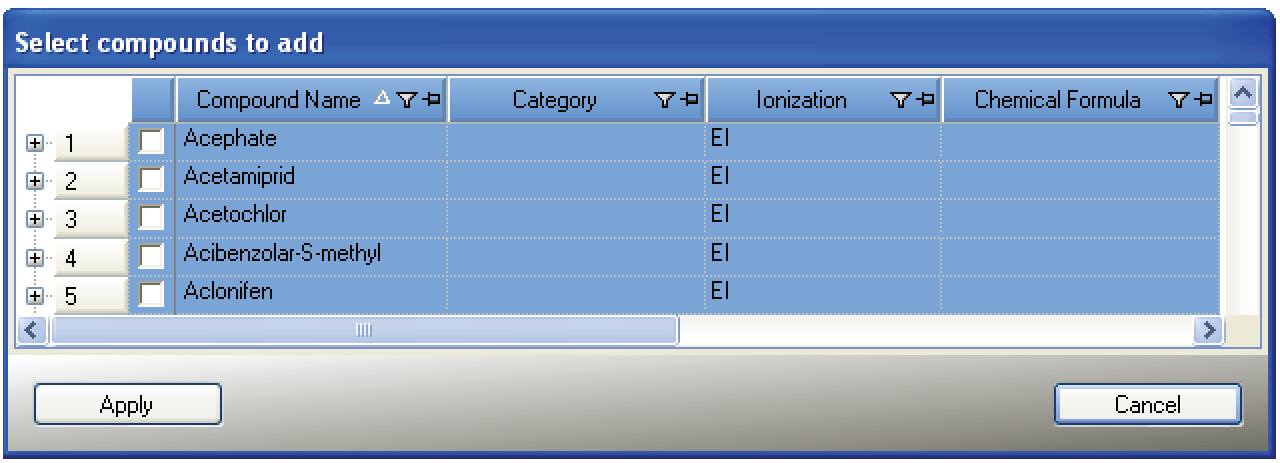
3. To confirm the deletion, click **Yes**.

   The selected compound is removed from the acquisition list.

❖ To add a compound transition to the list

1. Click the **Add Compound Transition** icon, , or right-click and choose **Add Compound Transition** from the shortcut menu.

   The Select Compounds to Add dialog box opens, listing all the compounds defined in the compound datastore specified for the gas chromatography technology.



2. Select the check box for each of the compounds you want to add to the method and click **Apply**.

   The EnviroLab Forms application adds the compounds to the Acquisition List and Compounds pages of the Master Method View.

Figure 12. Acquisition List page

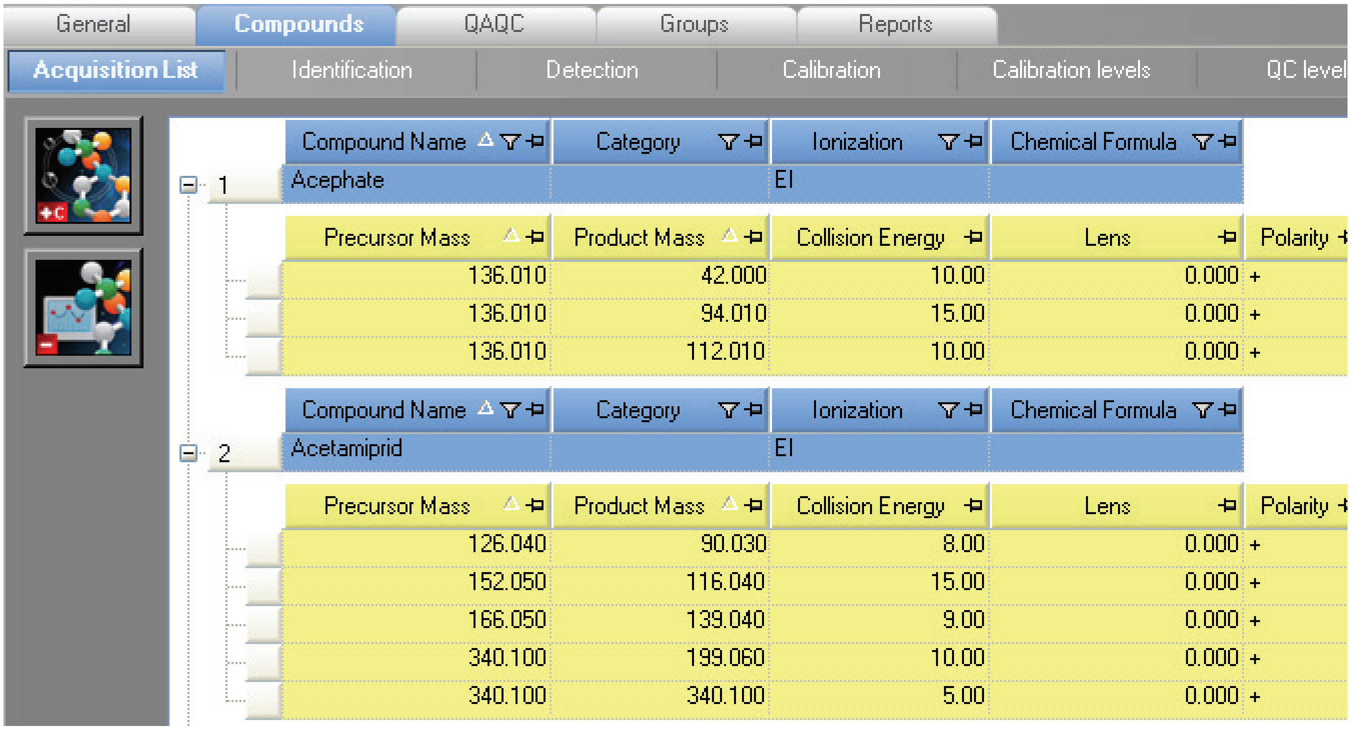


Table 15. Acquisition List parameters (Sheet 1 of 2)

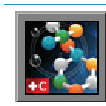
Parameter	**Description**
Function Icon	
	Opens the Select Compounds to Add dialog box that lists all the compounds defined in the compound datastore specified for the gas chromatography technology.
	Deletes the selected compound transition. The icon is unavailable when no row is selected. If you have used the filters to display a subset of compounds, the selected compound might not be visible in the Acquisition List page.
Compound parameter	
Compound Name	Alphanumeric name assigned to the compound.
Category	(Optional) Alphanumeric identifier.
Ionization	(Optional) Alphanumeric identifier. Valid values: ESI, APCI, EI, CI, APPI
Chemical Formula	(Optional) Alphanumeric chemical identifier.

Table 15. Acquisition List parameters (Sheet 2 of 2)

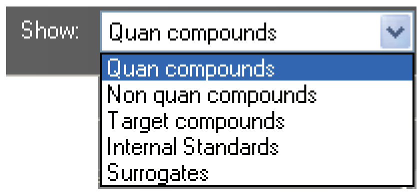
Parameter	Description
Precursor Mass	The mass-to-charge ratio of a precursor ion. The location of the center of a target precursor-ion peak in mass-to-charge ratio (*m/z*) units. Default: 0.0 Range: 10.000 to 2999.999
Product Mass	The mass-to-charge ratio of the quan ion. The location of the center of a target quan-ion peak in mass-to-charge ratio (*m/z*) units. Default: 0.0 Range: 10.000 to 2999.999
Collision Energy	The energy used when ions collide with the collision gas. Range: –250 to 250
Lens	(Optional) Range: –400 to 400
Polarity	**+** (positive) or **–** (negative)
RT (min)	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column. RT and Window values are used to determine the start and stop time for the acquisition. Range: 0.00 to 999.00 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Window (sec)	Acquisition window. RT and Window values are used to determine the start and stop time for the acquisition. Range: 0.00 to 499.50 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Energy Ramp	(Optional) Range: 0.00 to 200.00

Identification

The Identification page lists the compounds that are targeted for analysis, reporting, and other compound-specific values.

❖ To filter the displayed compounds

From the **Show** list box, select the type of compounds you want to display in the compounds list.



Compound Type	Description
Quan compounds	Displays only quan compounds, such as target compounds, internal standards, and surrogates.
Non quan compounds	Displays only non-quan compounds, such as native, breakdown, and tune compounds.
Target compounds	Displays only target compounds.
Internal Standards	Displays only internal standard compounds.
Surrogates	Displays only surrogate compounds.

Figure 13. Identification page

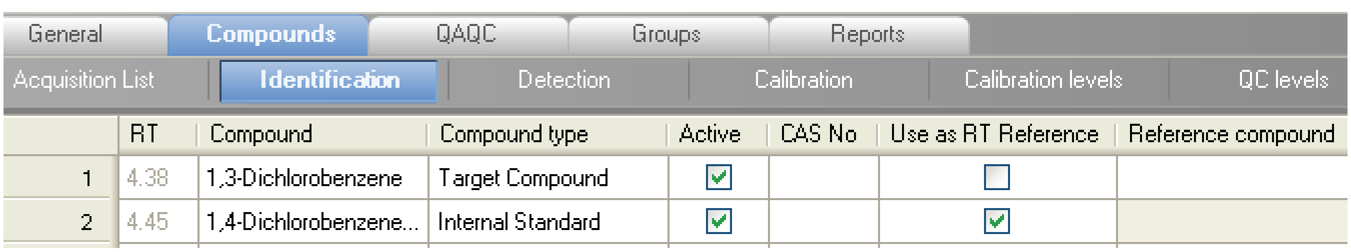


Table 16. Identification parameters

Parameter	Description
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column. RT and Window values are used to determine the start and stop time for the acquisition. Range: 0.00 to 999.00 Start time = RT – (Window/2) Stop time = RT + (Window/2) Start and stop range: 0.00 to 999.00
Compound	A list of compounds that have been identified. To customize the compound names, click the cell and type a new name. To display a filtered list of compounds, use the Show list box.
Compound type	Compound types are Target Compound, Internal Standard, Surrogate, Native, Breakdown, or MSTune. The EnviroLab Forms application uses target compounds, internal standards, and surrogates in quantitative analysis, and it uses native, breakdown, and tune compound types in system evaluation, as defined on the Breakdown page. See "Breakdown page" on page 125.
Active	Identifies each compound to be included in data review and reporting. By default, all added compounds are set to active.
CAS No	The Chemical Abstract Service (CAS) number that the EnviroLab Forms application matched with each compound. To change or add a number, click the CAS No cell and enter a new number.
Use as RT Reference	When performing peak detection with retention time standards, the EnviroLab Forms application first identifies those compounds identified as retention time standards and then uses their observed retention times to adjust any associated target compound.
Reference compound	Reference compound to be used for retention time adjustment for a compound. This list includes all compounds that are selected in the Use as RT Reference column.

Detection

Use the Detection page to customize peak detection and integration for any ions that define peaks and compounds.

On the Detection page, you can configure how characteristic ions for targeted compounds are detected and integrated. You can also edit the list of characteristic ions for a specific compound. Refining these parameters in the master method for each compound and its ions can reduce the degree of manual integration that would otherwise be required.

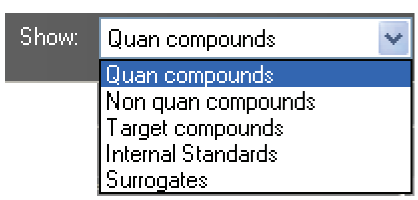
You can change the parameters used to identify a quantification peak, mass range, or confirming ion. The EnviroLab Forms application automatically assumes the first match it finds is the compound name, the base peak of the mass spectrum is the quan peak, and the second and third largest ions are the confirming ions.

Follow these procedures:

- To filter the displayed compounds
- To add compounds to the method
- To change the compound reference spectrum
- To replace a quan mass
- To add a mass to the existing quan mass ranges
- To add a quan peak
- To add a mass as a new compound
- To replace a confirming ion
- To add a mass as a new confirming ion
- To save the new method

❖ To filter the displayed compounds

From the **Show** list box, select the type of compounds you want to display in the compounds list.

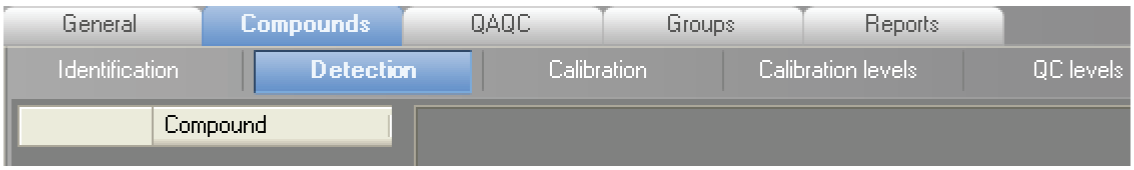


Compound Type	Description
Quan compounds	Displays only quan compounds, such as target compounds, internal standards, and surrogates.
Non quan compounds	Displays only non-quan compounds, such as native, breakdown, and tune compounds.

Compound Type	Description
Target compounds	Displays only target compounds.
Internal Standards	Displays only internal standard compounds.
Surrogates	Displays only surrogate compounds.

❖ To add compounds to the method

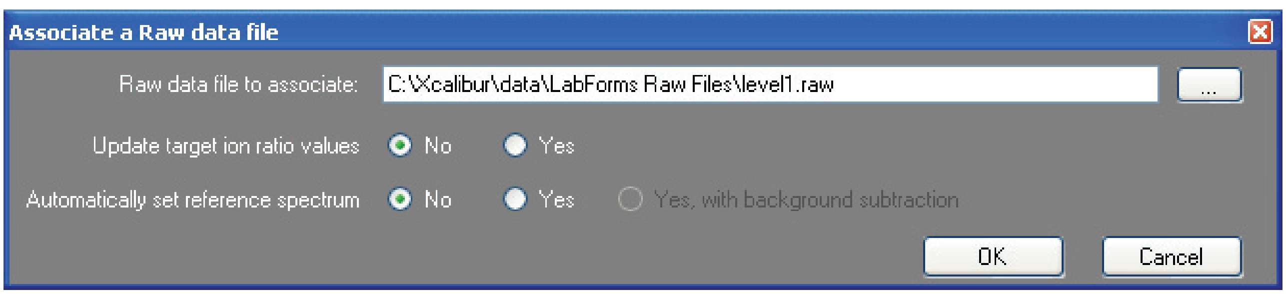
1. Click the **Compounds** tab.
2. Click the **Detection** tab.



The Detection page shows an empty Compound list.

3. From the main menu, choose **Master Method > Associate a Raw Data File**.

The Associate a Rawfile dialog box opens.



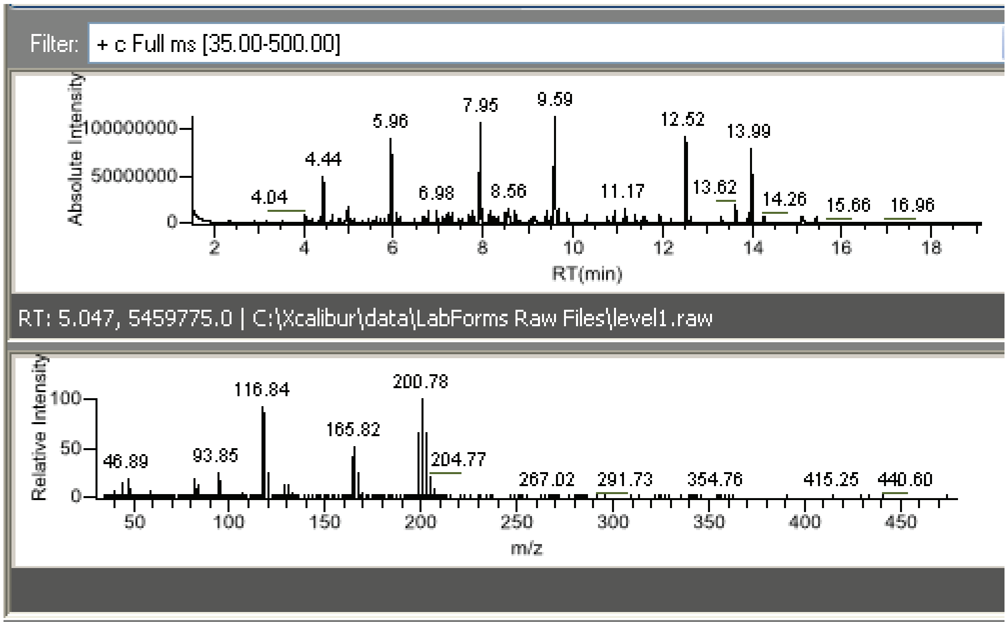
4. Browse to a raw data file to associate with the method and open the file.
5. To update the target ion ratio values when you associate this raw data file, click **Yes**.
6. To set a reference spectrum, do one of the following:
   - Click **Yes**.

   – Or –

   - Click **Yes, with Background Subtraction.**

     This feature is available only when you have set background subtraction values on the General page of the Master Method View. See "Editing the General Page" on page 70.
7. Click **OK**.

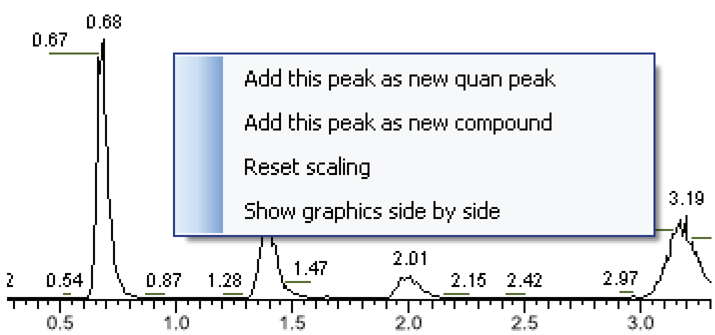
The EnviroLab Forms application displays the chromatographic and spectrum data for the compounds in the selected raw file.



8. Select a filter from the Filter list.

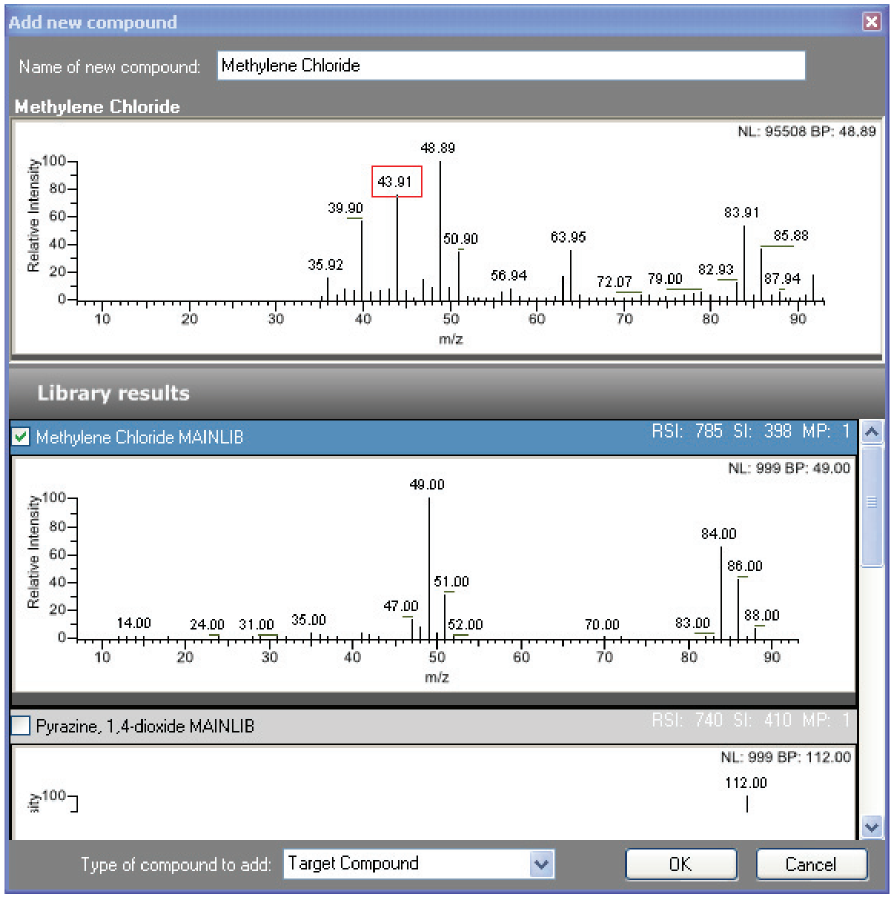
9. Click the peak in the chromatogram that represents the compound you want to add to the method.

10. Right-click and choose **Add This Peak as New Compound** from the shortcut menu.



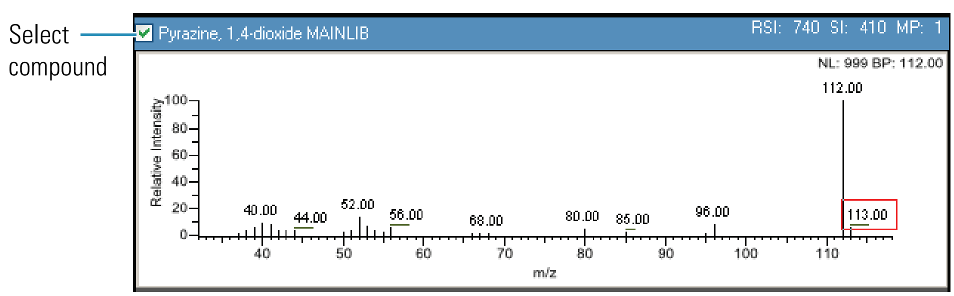
The EnviroLab Forms application performs a library search for the selected compound. The application uses the first match it finds as the compound name, the base peak of the mass spectrum as the quan peak, and the second and third largest ions as the confirming ions.

If the name of the first match is already in the library, the Add New Compound dialog box opens.



11. (Optional) In the Add New Compound dialog box, do the following:

    a. To use a compound other than the compound already in the library, scroll to the spectrum for that compound and select the compound name in the header of the spectrum pane.



    b. In the Type of Compound to Add list, select a compound type.

    c. Click **OK**.

12. Repeat these steps for each compound you want to add to the method.

    For a detailed description of all parameters on the Detection page, see “Editing the Compounds Page” on page 77.

❖ To change the compound reference spectrum

1. In the raw file chromatogram pane, select a peak.

   The EnviroLab Forms application displays the spectrum for the selected peak in the spectrum pane.

2. In the raw file spectrum pane, right-click and choose **Use This Spectrum for Compound Reference Spectrum** from the shortcut menu.

3. Choose either **Update Spectrum Only** or **Update Spectrum and Ion Ratios**.

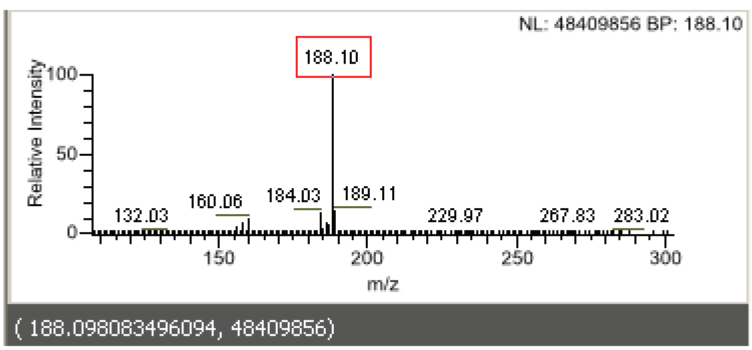
   The EnviroLab Forms application replaces the spectrum in the Spectrum page of the quan peak pane with this spectrum. If you choose to update the spectrum and the ion ratios, the application also replaces the ion ratios for the confirming peaks. You can see the updated ion ratios on the Ratios page for the confirming ions. See "Ratios" on page 109.

❖ To replace a quan mass

1. Click the pane for the quan mass that you want to replace.

2. In the raw file spectrum pane, pause the cursor over a peak.

   The red box indicates the selected peak.



3. Right-click and choose **Set This Mass as Quan Mass** from the shortcut menu.

4. Choose either **Don't Update Ion Ratios** or **Update Ion Ratios Using This Spectrum**.

   You can see the updated ion ratios on the Ratios page for the confirming ions. See "Ratios" on page 109.

❖ To add a mass to the existing quan mass ranges

1. In the raw file spectrum pane, pause the cursor over a peak.

   The red box indicates the selected peak.

2. Right-click and choose **Add This Mass to Existing Quan Mass Ranges** from the shortcut menu.

3. Choose either **Don't Update Ion Ratios** or **Update Ion Ratios Using This Spectrum**.

The EnviroLab Forms application adds the selected mass to the existing quan mass ranges to increase the signal.

If you chose to update the ion ratios, you can see the updated ion ratios on the Ratios page for the confirming ions. See “Ratios” on page 109.

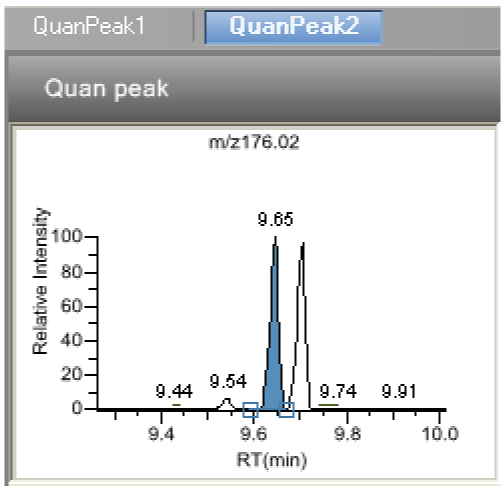
❖ To add a quan peak

1. In the raw file spectrum pane, pause the cursor over a peak.

   The red box indicates the selected peak.

2. Right-click and choose **Add This Mass as New Quan Peak** from the shortcut menu.

   A new quan peak is added to the compound.

   You can use the shortcut menu on the spectrum pane for this new quan peak to perform any of the tasks you could perform on the original quan peak.

❖ To add a mass as a new compound

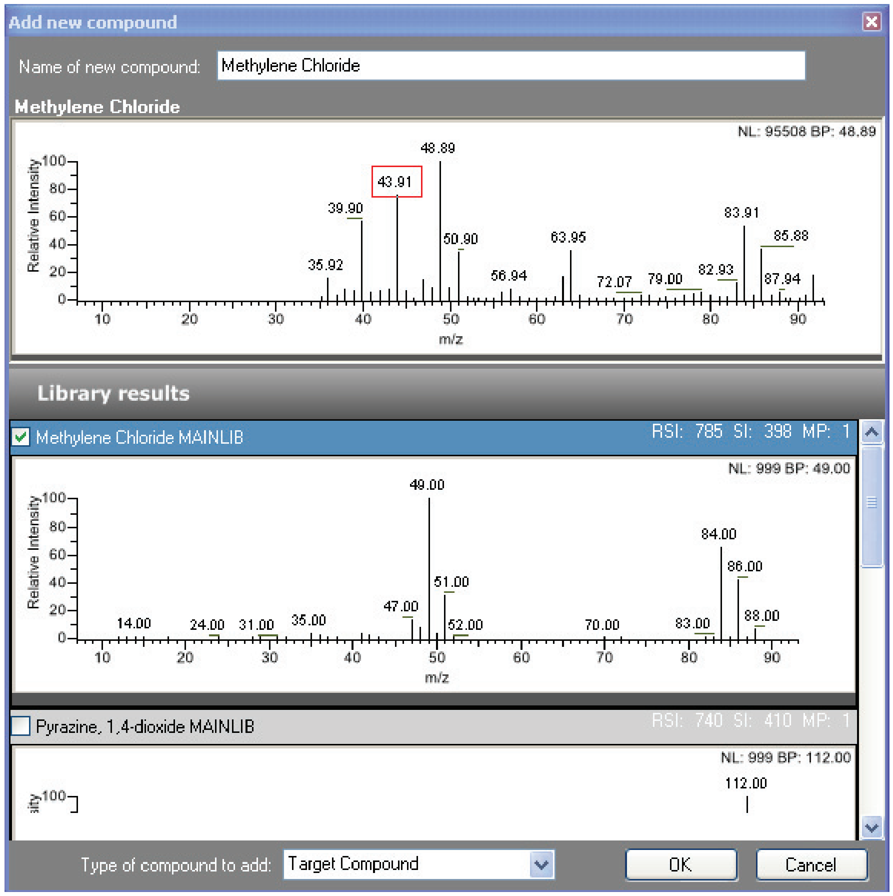
1. In the raw file spectrum pane, pause the cursor over a peak.

   The red box indicates the selected peak.

2. Right-click and choose **Add This Mass as New Compound** from the shortcut menu.

   The EnviroLab Forms application performs a library search for the selected compound. The application uses the first match it finds as the compound name, the base peak of the mass spectrum as the quan peak, and the second and third largest ions as the confirming ions.

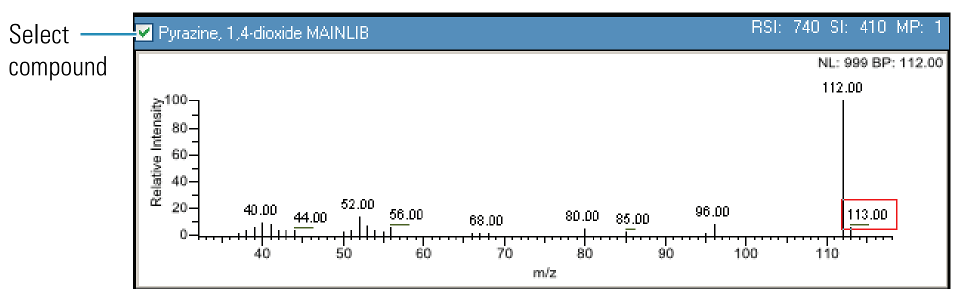
   If the name of the first match is already in the library, the Add New Compound dialog box opens with the matching compound selected.



3. (Optional) In the Add New Compound dialog box, make any of the following changes:

   a. Change the name for the compound in the Name of New Compound box.

   b. To use a compound other than the compound chosen by the EnviroLab Forms application, scroll to the spectrum for that compound and select the compound name in the header of the spectrum pane.



   c. Click the Type of Compound to Add list and select a compound type.

4. Click **OK**.

❖ To replace a confirming ion

1. Click the pane for the confirming ion that you want to replace.
2. In the raw file spectrum pane, pause the cursor over a peak.

   The red box indicates the selected peak.
3. Right-click and choose **Set this Mass as New Confirming Ion** from the shortcut menu.

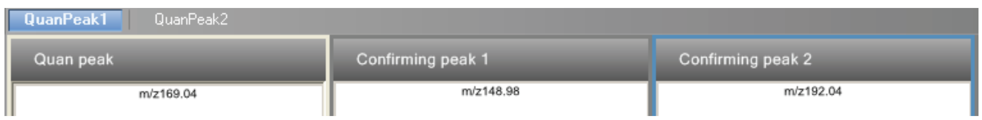
   The EnviroLab Forms application replaces the confirming ion with the selected mass.

❖ To add a mass as a new confirming ion

1. Click the pane for the quan mass to which you want to add a confirming ion.
2. In the raw file spectrum pane, pause the cursor over a peak.

   The red box indicates the selected peak.
3. Right-click and choose **Add this Mass as New Confirming Ion** from the shortcut menu.

   The EnviroLab Forms application adds the confirming ion to the quan peak.

   You can use the shortcut menu on the spectrum pane for this new confirming ion to perform any of the tasks you could perform on the original confirming ions.

❖ To save the new method

1. Choose **File > Save**.

   The Save Master Method dialog box opens.
2. Do one of the following:

   - Type a new name for the master method and click **OK**.

   –Or–

   - Select a method name to overwrite and click **Overwrite**.

   The EnviroLab Forms application saves the new method data in the following folder:

   ..\Thermo\EnviroLab Forms\Methods

Figure 14. Detection page

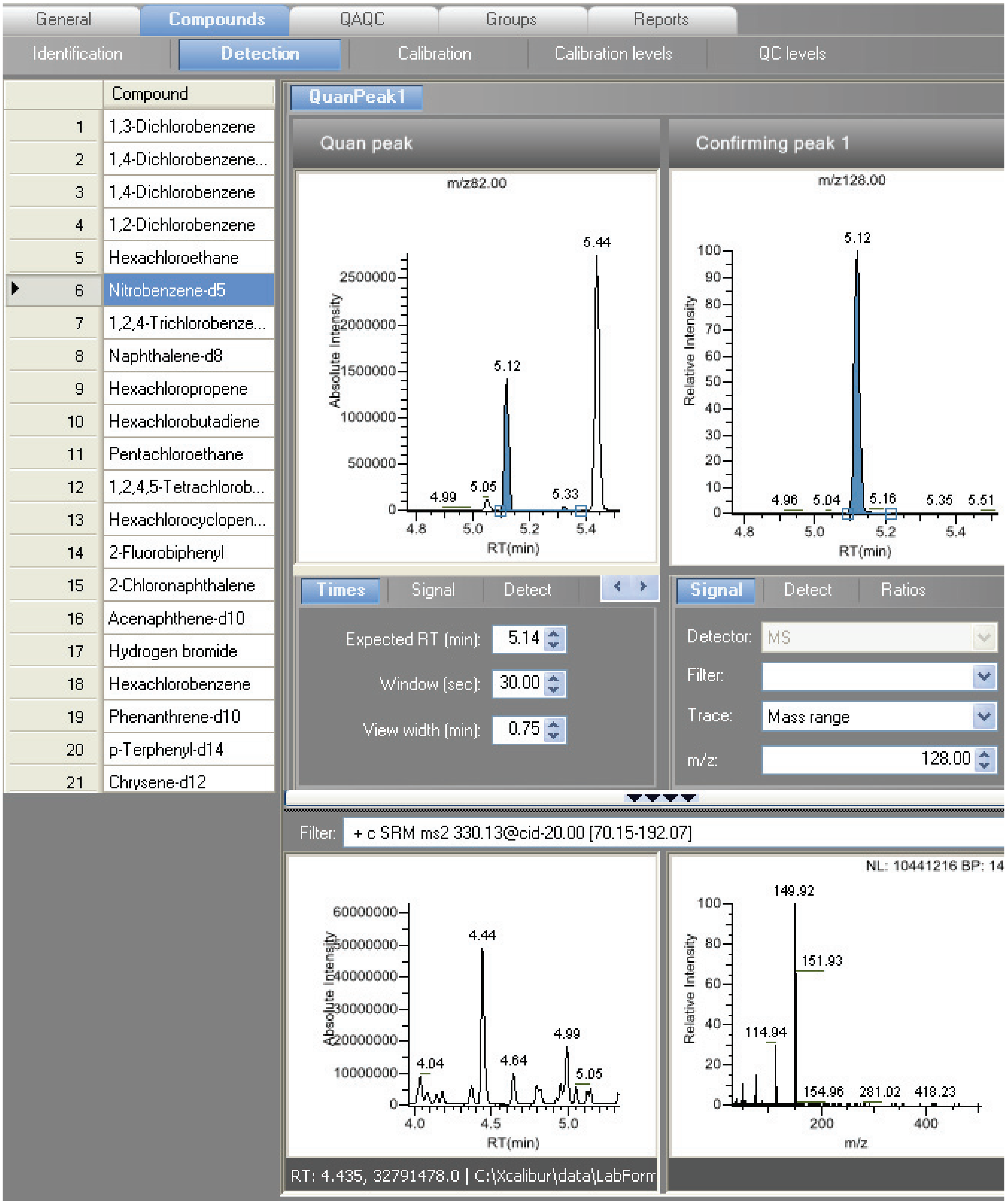


Table 17. Detection page parameters

Parameter	Description
Compound list	Lists all compounds in the master method.
Quan peak	Displays a chromatogram for the quan peak and its confirming ions. The quan peak and confirming ion panes include additional pages for retention time, signal, detection, spectrum, and ratio parameters.
Filter	Displays the filter used for the raw data file.
Reference chromatogram and spectra	Displays a reference chromatogram and spectra for the raw data file.
Additional pages	
Times	Defines the retention time and window for a quan peak. See "Times" on page 93.
Signal	Defines the detector and its parameters used to display each chromatogram trace. See "Signal" on page 94.
Detect	Defines the peak detection algorithm and its options. See "Detect" on page 96.
Spectrum	Defines a reference mass spectrum for a quan peak or compound. See "Spectrum" on page 104.
Ratios	Defines the criteria for evaluating, confirming, or qualifying ions. See "Ratios" on page 109.

Times

Use the Times page to define the retention time and window for a quan peak.

Figure 15. Times page

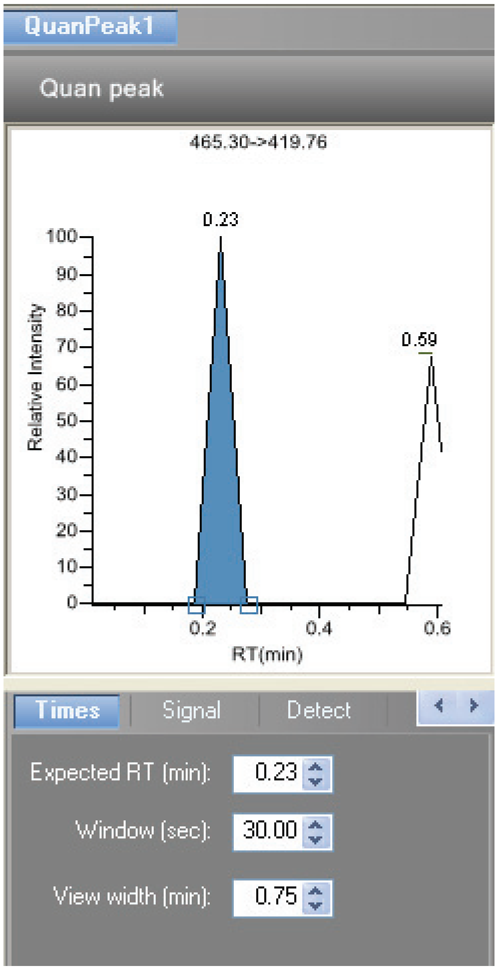


Table 18. Times parameters

Parameter	Description
Expected RT (min)	Expected retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Window (sec)	Width of the window (in seconds) of how far around the expected retention time the system will look for a peak apex.
View width (min)	Viewable size of the ion chromatogram display. Changing the view width does not affect the process of peak detection; the EnviroLab Forms application uses it only for graphical display.

Signal

Use the Signal page to define the detector and its parameters as you display each chromatogram trace.

Figure 16. Signal page

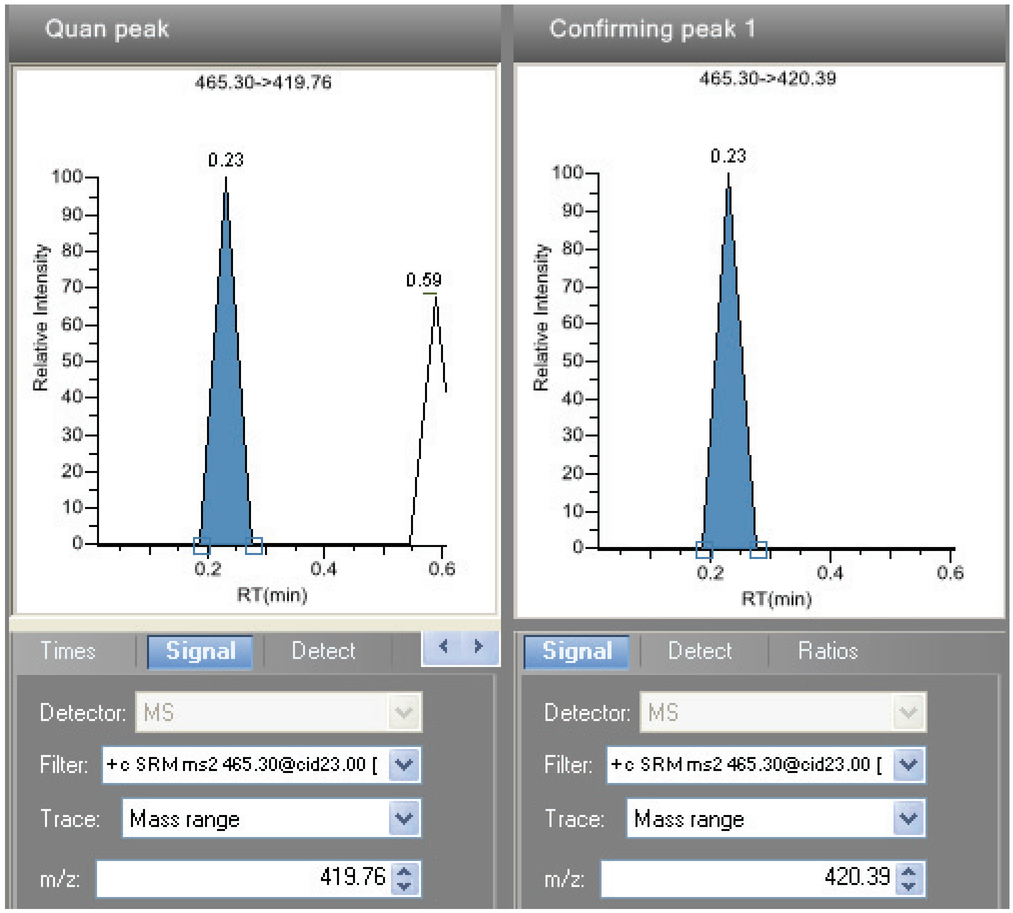


Table 19. Signal parameters (Sheet 1 of 2)

Parameter	Description
Detector	MS: Mass spectrometers. Analog: Supplemental detectors (for example, FID, ECD). AD card: If you have a detector not under data system control, you can capture the analog signal and convert it to digital using an interface box (for example, SS420X) for storage in the raw file.
Filter	Represents a particular data acquisition channel. For example, the filter option *+ c Full ms [35.00-500.00]* represents a positive ion centroid signal acquired in single-stage, full-scan mode from *m/z* 35 to 500.
Trace	Represents a specific range of the data. In conjunction with the filter, the EnviroLab Forms application uses the trace to identify the characteristic ions for a compound. The options are: Mass Range, TIC, or Base Peak.

Table 19. Signal parameters (Sheet 2 of 2)

Parameter	Description
Ranges	A range of ions for detection and integration. Entering a single value in the Start *m/z* cell defines a range of one amu centered on that value. To specify a range that is narrower or wider than this range, specify both a start and end value. Multiple ions are summed by adding rows to the Ranges grid.
m/z	The initial mass to charge ratio.

Detect

Use the Detect page to define the peak detection algorithm and its options and to determine the area under a curve. There are two different modes - Standard (Genesis) and High (ICIS). On this page, you can specify how you want each mode to run.

Figure 17. Detect page for Standard (Genesis)

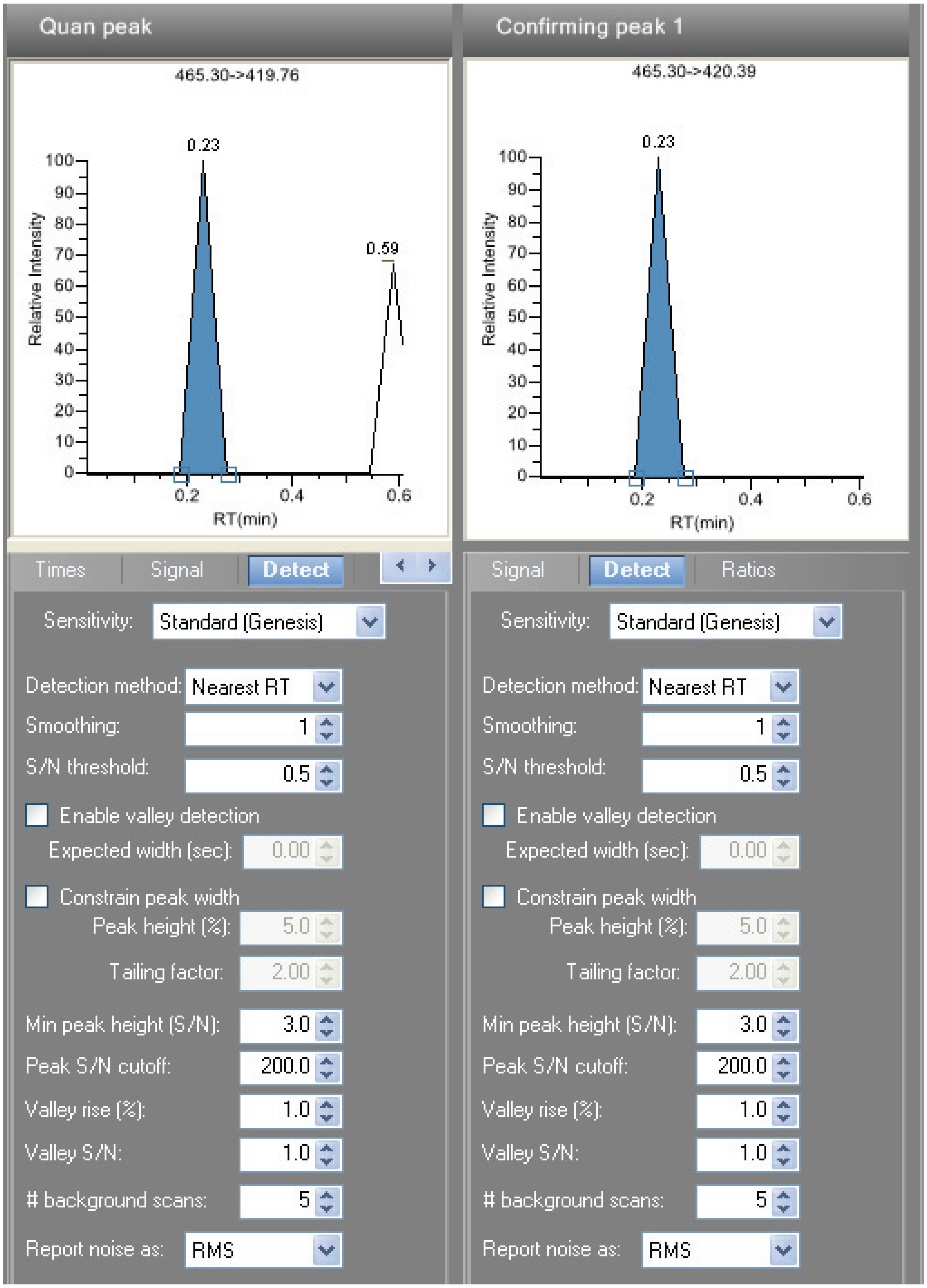


Table 20. Detect parameters for Standard (Genesis) (Sheet 1 of 3)

Parameter	Description
Sensitivity	Specifies the Standard (Genesis) peak detection algorithm.
Detection method	Highest peak: Uses the highest peak in the chromatogram for component identification. Nearest RT: Uses the peak with the nearest retention time in the chromatogram for component identification.
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. The ICIS peak detection algorithm uses this value. Range: Any odd integer from 1 through 15 points Default: 1
S/N threshold	Current signal-to-noise threshold for peak integration. Peaks with signal-to-noise values less than this value are not integrated. Peaks with signal-to-noise values greater than this value are integrated. Range: 0.0 to 999.0
Enable valley detection	Uses the valley detection approximation method to detect unresolved peaks. This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak.
Expected width (sec)	The expected peak width parameter (in seconds). This parameter controls the minimum width that a peak is expected to have if valley detection is enabled. With valley detection enabled, any valley points nearer than the [expected width]/2 to the top of the peak are ignored. If a valley point is found outside the expected peak width, the EnviroLab Forms application terminates the peak at that point. The application always terminates a peak when the signal reaches the baseline, independent of the value set for the expected peak width. Range: 0.0 to 999.0
Constrain peak width	Constrains the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. Selecting the Constrain Peak Width check box enables the Peak Height (%) and Tailing Factor options.

Table 20. Detect parameters for Standard (Genesis) (Sheet 2 of 3)

Parameter	Description
Peak height (%)	A signal must be above the baseline percentage of the total peak height (100%) before integration is turned on or off. This text box is active only when the Constrain Peak Width check box is selected. Range: 0.0 to 100.0%
Tailing factor	A factor that controls how the EnviroLab Forms application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when the Constrain the Peak Width check box is selected. Range: 0.5 through 9.0
Min peak height (S/N)	For the valley detection approximation method to use the Nearest RT Peak Identification criteria, this peak signal-to-noise value must be equaled or exceeded. For component identification purposes, the EnviroLab Forms application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value. Range: 0.0 (all peaks) through 999.0
Peak S/N cutoff	The peak edge is set to values below this signal-to-noise ratio. This test assumes it has found an edge of a peak when the baseline adjusted height of the edge is less than the ratio of the baseline adjusted apex height and the peak S/N cutoff ratio. When the S/N at the apex is 500 and the peak S/N cutoff value is 200, the EnviroLab Forms application defines the right and left edges of the peak when the S/N reaches a value less than 200. Range: 50.0 to 10000.0

Table 20. Detect parameters for Standard (Genesis) (Sheet 3 of 3)

Parameter	Description
Valley rise (%)	The peak trace can rise above the baseline by this percentage after passing through a minimum (before or after the peak). This method drops a vertical line from the apex of the valley between unresolved peaks to the baseline. The intersection of the vertical line and the baseline defines the end of the first peak and the beginning of the second peak. When the trace exceeds rise percentage, the EnviroLab Forms application applies valley detection peak integration criteria. This test is applied to both the left and right edges of the peak. The rise percentage criteria is useful for integrating peaks with long tails. Range: 0.1 to 500.0
Valley S/N	Specifies a value to evaluate the valley bottom. Using this parameter ensures that the surrounding measurements are higher. Range: 1.0 to 100.0 Default: 2.0
# background scans	Number of background scans performed by the EnviroLab Forms application.
Report noise as	Determines if the noise used in calculating S/N values is calculated using an RMS calculation or peak-to-peak resolution threshold. Options are RMS or Peak to Peak.

Figure 18. Detect page for High (ICIS)

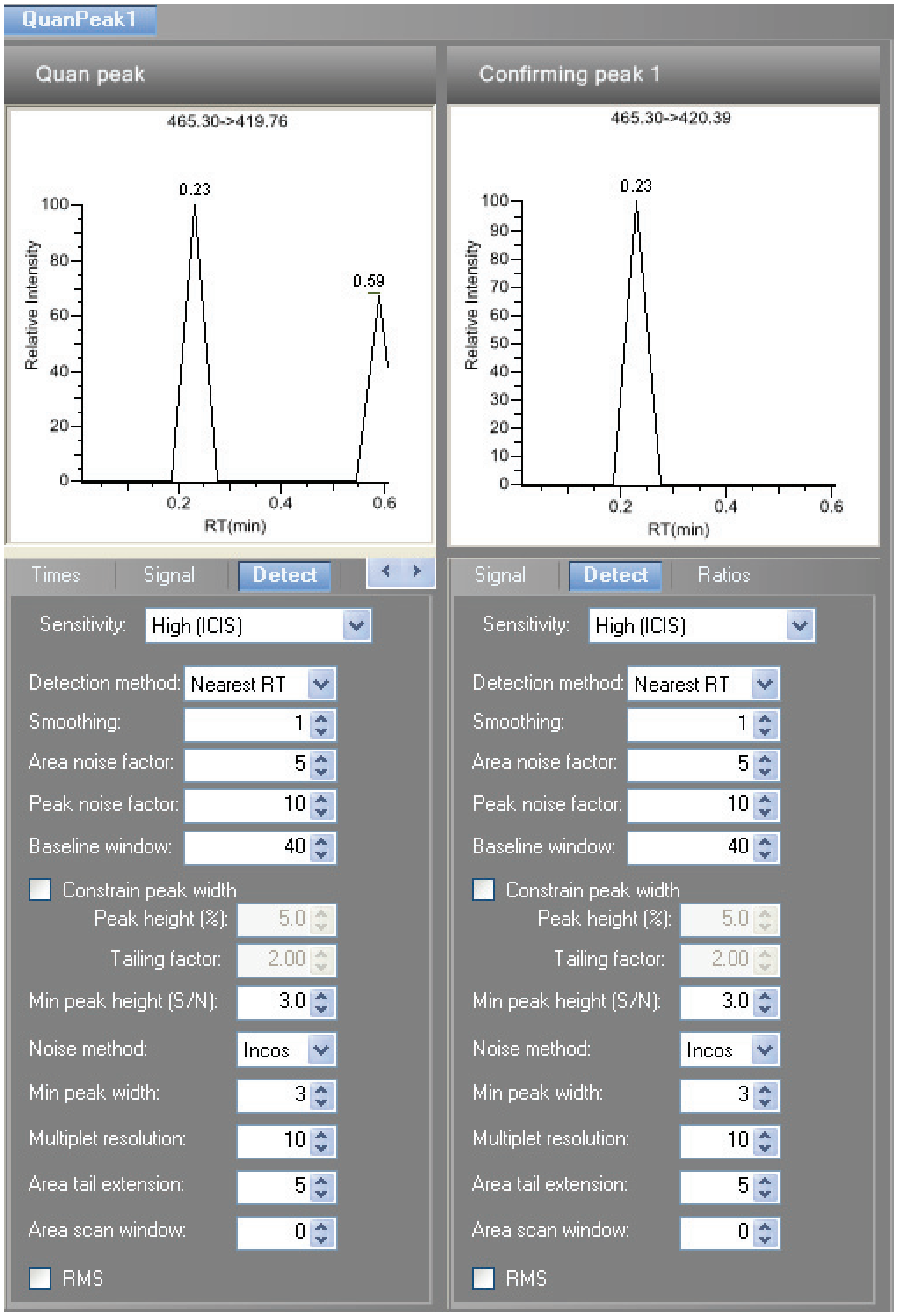


Table 21. Detect parameters for High (ICIS) (Sheet 1 of 3)

Parameter	Description
Sensitivity	Specifies the High (ICIS) peak detection algorithm.
Detection method	Highest peak uses the highest peak in the chromatogram for component identification. Nearest RT uses the peak with the nearest retention time in the chromatogram for component identification.
Smoothing	Determines the degree of data smoothing to be performed on the active component peak prior to peak detection and integration. The ICIS peak detection algorithm uses this value. Range: Any odd integer from 1 through 15 points Default: 1
Area noise factor	The noise level multiplier used to determine the peak edge after the location of the possible peak. The ICIS peak detection algorithm uses this value. Range: 1 through 500 Default: 5
Peak noise factor	The noise level multiplier used to determine the potential peak signal threshold. The ICIS peak detection algorithm uses this value. Range: 1 through 1000 Default: 10
Baseline window	The EnviroLab Forms application looks for a local minima over this number of scans. The ICIS peak detection algorithm uses this value. Range: 1 through 500 Default: 40
Constrain peak width	Constrains the peak width of a component during peak integration of a chromatogram. You can then set values that control when peak integration is turned on and off by specifying a peak height threshold and a tailing factor. Selecting the Constrain Peak Width check box enables the Peak Height (%) and Tailing Factor options.

Table 21. Detect parameters for High (ICIS) (Sheet 2 of 3)

Parameter	Description
Peak height (%)	A signal must be above the baseline percentage of the total peak height (100%) before integration is turned on or off. This text box is active only when the Constrain Peak Width check box is selected. Range: 0.0 to 100.0%
Tailing factor	A factor that controls how the EnviroLab Forms application integrates the tail of a peak. This factor is the maximum ratio of the trailing edge to the leading side of a constrained peak. This text box is active only when the Constrain the Peak Width check box is selected. Range: 0.5 through 9.0
Min peak height (S/N)	For the valley detection approximation method to use the Nearest RT Peak Identification criteria, this peak signal-to-noise value must be equaled or exceeded. For component identification purposes, the EnviroLab Forms application ignores all chromatogram peaks that have signal-to-noise values that are less than the S/N Threshold value. Range: 0.0 (all peaks) through 999.0
Noise method	The options are INCOS or Repetitive. INCOS uses a single pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value. Repetitive uses a multiple pass algorithm to determine the noise level. The ICIS peak detection algorithm uses this value. In general, this algorithm is more accurate in analyzing the noise than the INCOS Noise algorithm, but the analysis takes longer.
Min peak width	The minimum number of scans required in a peak. The ICIS peak detection algorithm uses this value. Range: 0 to 100 scans Default: 3
Multiplet resolution	The minimum separation in scans between the apexes of two potential peaks. This is a criteria to determine if two peaks are resolved. The ICIS peak detection algorithm uses this value. Range: 1 to 500 scans Default: 10

Table 21. Detect parameters for High (ICIS) (Sheet 3 of 3)

Parameter	Description
Area tail extension	The number of scans past the peak endpoint to use in averaging the intensity. The ICIS peak detection algorithm uses this value. Range: 0 to 100 scans Default: 5
Area scan window	The number of allowable scans on each side of the peak apex. A zero value defines all scans (peak-start to peak-end) to be included in the area integration. Range: 0 to 100 scans Default: 0
RMS	Specifies that the EnviroLab Forms application calculate noise as RMS. By default, the application uses Peak To Peak for the noise calculation. RMS is automatically selected if you manually determine the noise region.

Spectrum

Use the Spectrum page to store a reference mass spectrum for a quan peak or compound.

Follow these procedures:

- To apply or remove the background subtraction
- To update confirming ion ratios
- To change the quantitation mass used for a quan peak
- To add ions together to get an accumulated signal
- To add a quan peak to an existing compound
- To add one or more confirming ions to an existing compound
- To zoom in the chromatogram or spectrum displays

❖ To apply or remove the background subtraction

1. Right-click the Spectrum pane and choose **Apply Background Subtraction to Peak and Set as Reference Spectrum** from the shortcut menu.

   The EnviroLab Forms application replaces the normal reference spectrum with a background subtracted reference spectrum.

2. To remove the background subtracted reference spectrum, right-click the Spectrum pane and choose **Remove Background Subtracted Reference Spectrum** from the shortcut menu.

   The EnviroLab Forms application removes the applied background subtracted reference spectrum and returns to the normal reference spectrum. When there is no spectrum annotated at the beginning, the application displays "no data".

❖ To update confirming ion ratios

1. Click a peak in the quan peak chromatogram pane.

   The mass spectrum for the peak is displayed in the Spectrum pane.

2. Right-click the Spectrum pane and choose **Update Confirming Ion Ratios with this Spectrum** from the shortcut menu.

❖ To change the quantitation mass used for a quan peak

1. Click a peak in the chromatogram pane.

   The mass spectrum for the peak is displayed in the spectrum pane.

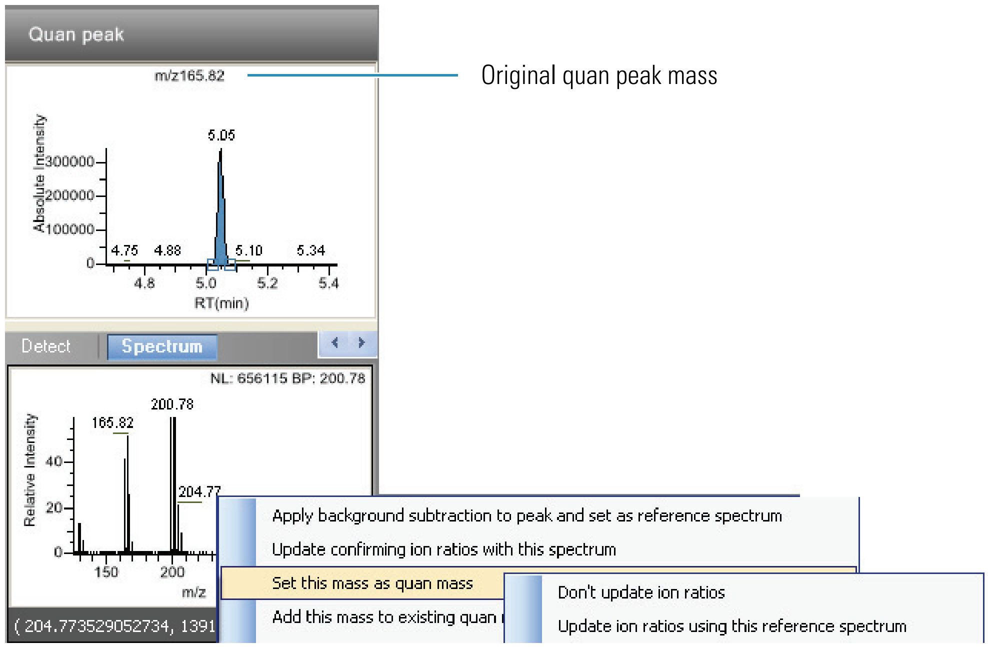
2. In the spectrum pane, pause the cursor over the *m/z* value for an ion.

   A red box around the ion's *m/z* value indicates that the ion is selected.

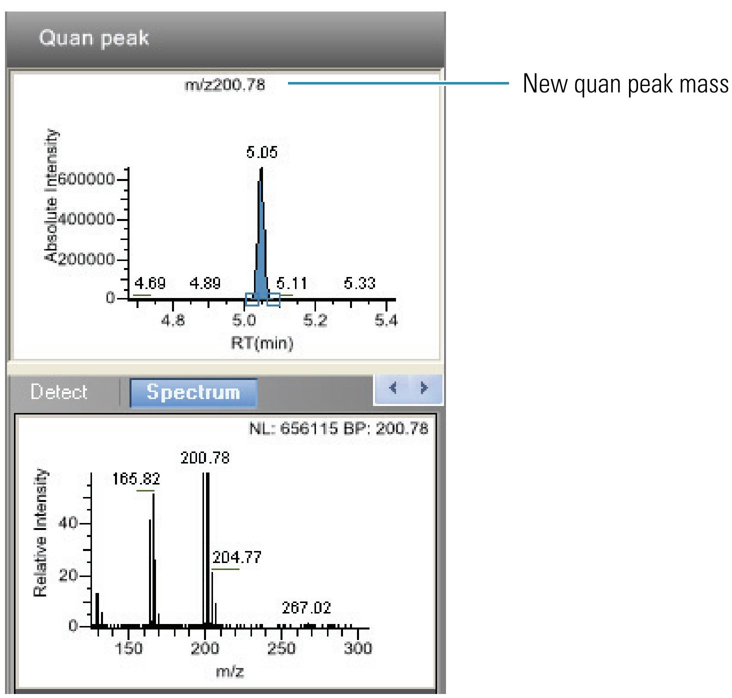
3. Right-click to display the shortcut menu.

4. Pause the cursor over **Set This Mass as Quan Mass** and choose one of the following commands:

   - **Don't Update Ion Ratios**
   - **Update Ion Ratios Using this Reference Spectrum**



The EnviroLab Forms application replaces the original quan mass with the selected mass.



❖ To add ions together to get an accumulated signal

1. Pause the cursor over the *m/z* value for an ion in the Spectrum pane.

   A red box around the ion's *m/z* value indicates that the ion is selected.

2. Right-click and choose **Add This Mass to Existing Quan Mass Range** from the shortcut menu.

   You can now update the ion ratios to adjust the confirming ion comparisons to the new summed quan peak signal.

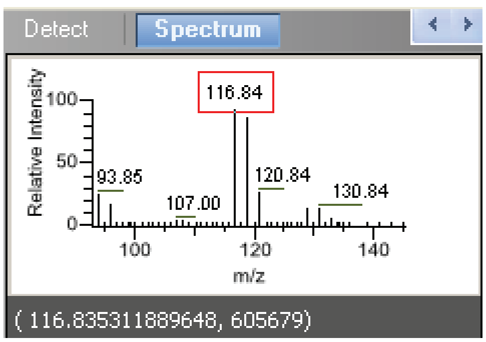
❖ To add a quan peak to an existing compound

1. Click the peak in the Quan Peak chromatogram pane.

   The mass spectrum for the peak is displayed in the Spectrum pane.

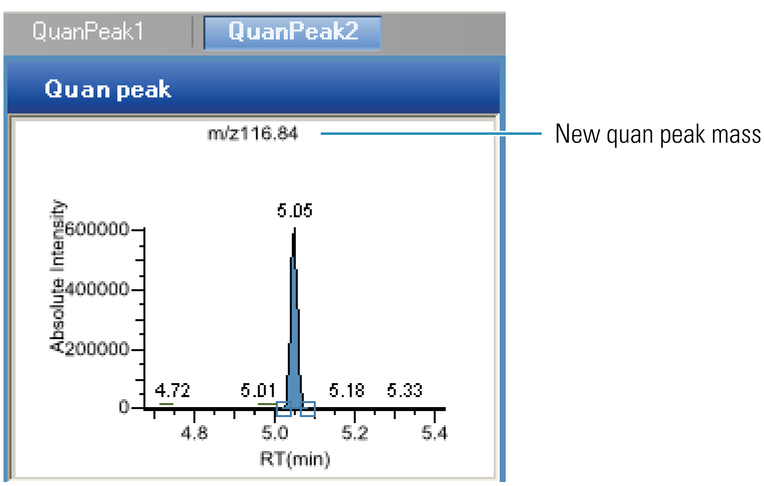
2. In the Spectrum pane, pause the cursor over the *m/z* value for an ion.

   A red box around the ion's *m/z* value indicates that the ion is selected.



3. Right-click and choose **Set This Mass as New Quan Peak** from the shortcut menu.

   The EnviroLab Forms application adds this ion as a new quan peak.



❖ To add one or more confirming ions to an existing compound

1. Click the peak in the chromatogram pane.

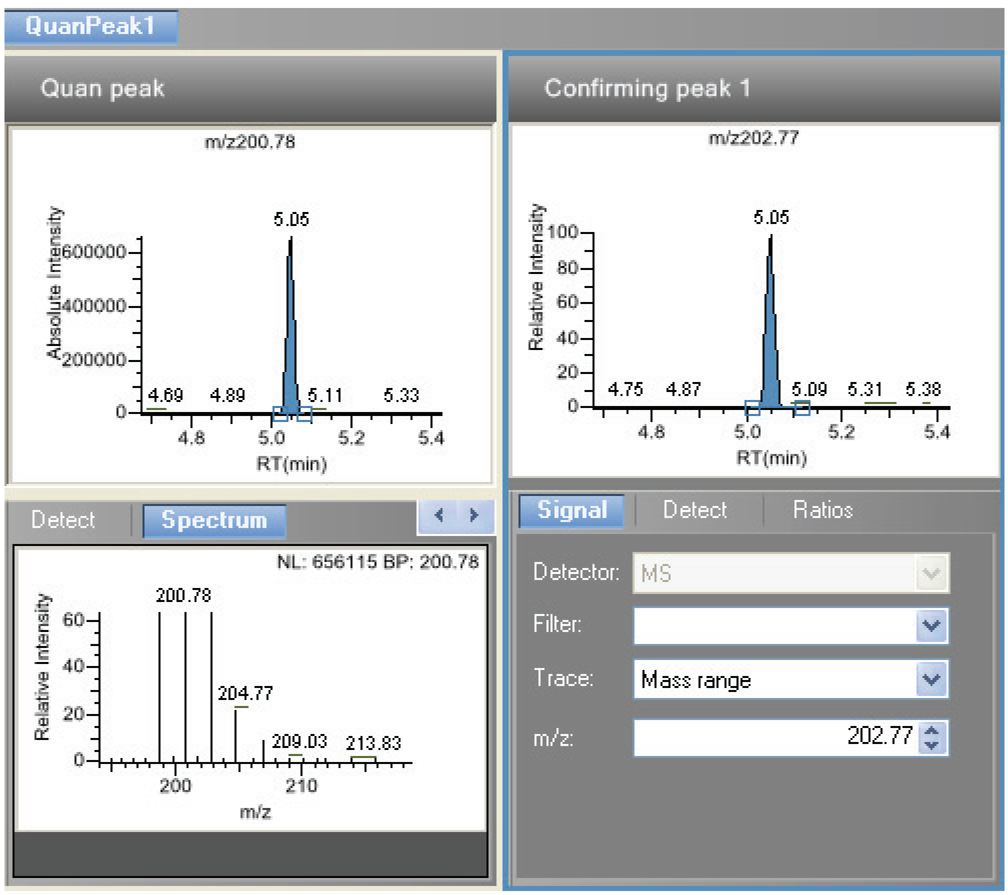
   The mass spectrum for the peak is displayed in the Spectrum pane.

2. In the Spectrum pane, pause the cursor over the *m/z* value for an ion.

   A red box around the ion's *m/z* value indicates that the ion is selected.

3. Right-click and choose to **Add This Mass as New Confirming Ion** from the shortcut menu.

   The EnviroLab Forms application adds the selected mass as a confirming peak for this quan peak.



❖ To zoom in the chromatogram or spectrum displays

1. Drag the cursor to delineate a rectangle.

   The display zooms into the specified rectangle.

2. To return to the original display, right-click and choose **Reset Scaling** from the shortcut menu.

Figure 19. Spectrum page

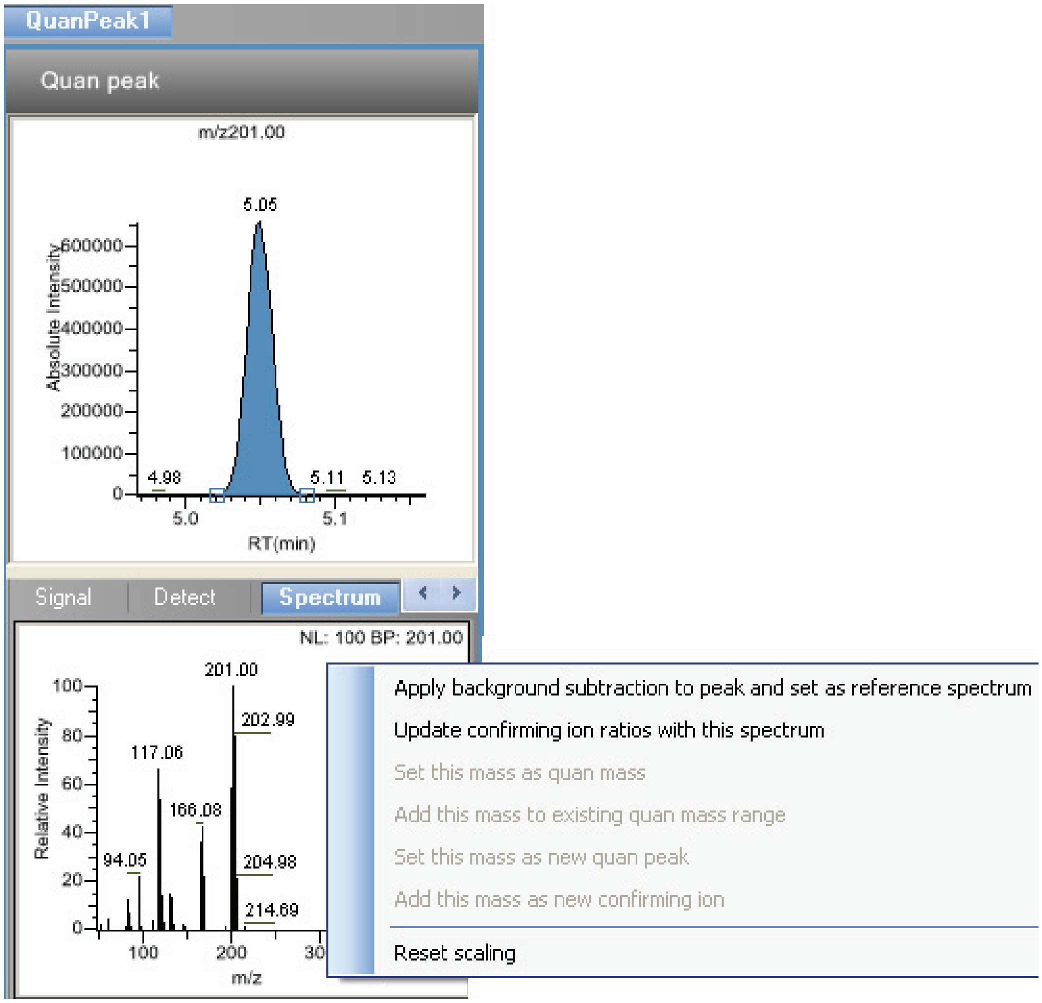


Table 22. Spectrum shortcut menu functions (Sheet 1 of 2)

Functions	Description
Apply background subtraction to peak and set as reference spectrum	Applies the background subtraction values specified on the General page and uses this spectrum as the reference spectrum.
Update confirming ion ratios with this spectrum	Updates the confirming ion ratios using the selected peak.
Set this mass as quan mass	Adds the quan mass of the selected ion to the quantitation mass used for the quan peak. You can choose to update the ion ratios or not update the ion ratios using this reference spectrum.
Add this mass to existing quan mass range	Adds the selected mass to your existing quan mass range. You can choose to update the ion ratios to adjust the confirming ion comparisons to the new summed quan peak signal.

Table 22. Spectrum shortcut menu functions (Sheet 2 of 2)

Functions	Description
Set this mass as new quan peak	Adds a new quan peak to an existing compound.
Add this mass as new confirming ion	Adds one or more confirming ions to an existing compound.
Reset scaling	Returns the chromatogram or spectrum display to its original size.

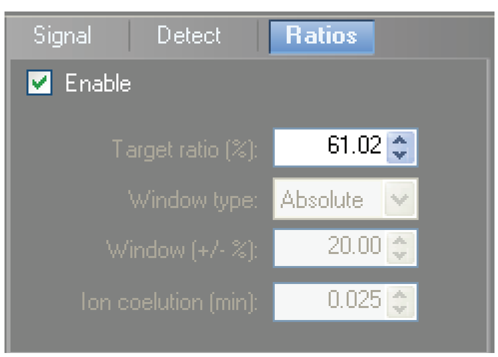
Ratios

Use the Ratios page to define the criteria for evaluating the confirming or qualifying ions. The EnviroLab Forms application detects compounds that have confirming ion values outside their acceptable window and flags them in Production mode and on reports.

❖ To specify ion ratio criteria

1. Enable or disable the use of the particular confirming ion.
2. In the Target Ratio box, select the theoretical ratio of the confirming ion’s response to the quantification ion’s response.
3. In the Window Type box, select **Absolute** or **Relative** as the calculation approach for determining the acceptable ion ratio range.
4. In the Window (+/-%) box, select the acceptable ion ratio range.
5. In the Ion Coelution box, select the maximum difference in retention time between a confirming ion peak and the quantification ion peak.

   In the following example:

   - The target ratio is expected to be 61.02% and the window is Absolute 20%, so the acceptable window for this confirming ion is 41.02% to 81.02%.
   - If, instead, the window type was Relative, the plus or minus value would be 20% of 61.02% (or 12.20%), so the acceptable window for this confirming ion would be 48.82% to 73.22%.

Figure 20. Ratios page

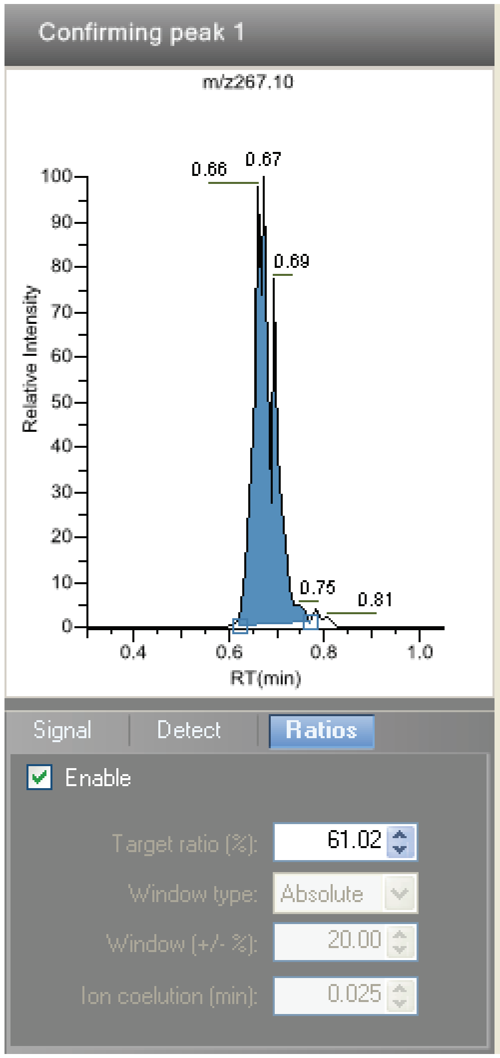


Table 23. Ratios parameters

Parameter	Description
Target ratio (%)	The theoretical ratio of the confirming ion’s response to the quantification ion’s response.
Window type	The absolute or relative calculation approach for determining the acceptable ion ratio range.
Window (+/-%)	The acceptable ion ratio range.
Ion coelution (min)	The maximum difference in retention time between a confirming ion peak and the quantification ion peak.

Calibration

Use the Calibration page to set or edit the mathematical model used for preparing the initial calibration evaluation for one or more calibration standards.

Each target compound can have its own initial calibration settings, independent of the other compounds. You can modify the calibration approach on this page or in Production mode when you view the results of an actual calibration batch.

Figure 21. Calibration page

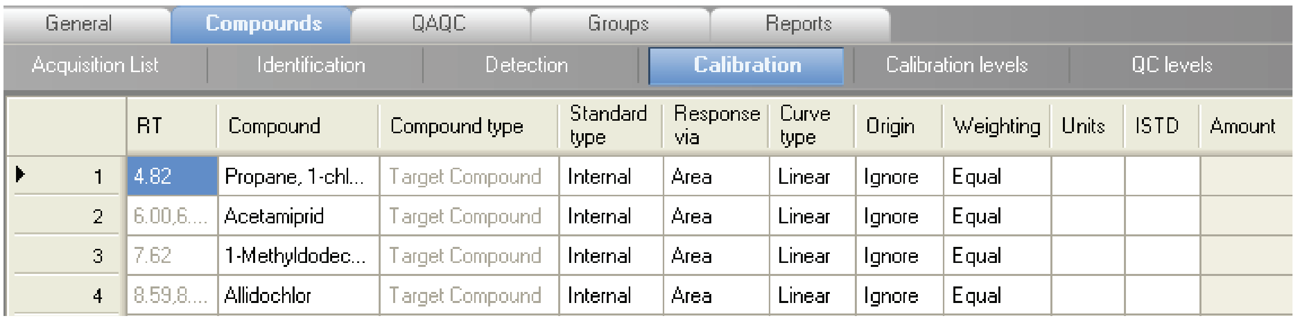


Table 24. Calibration parameters

Parameter	Description
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Compound	The compound name.
Compound type	Displays the compound type as an internal standard, an external standard, or a target compound.
Standard type	Specifies Internal or External standards.
Response via	The use of area or height.
Curve type	Specifies Linear, Quadratic, or AverageRF curve types.
Origin	The origin treatment as Ignore, Include, or Force. The Origin and Weighting columns are active only when you are using Linear or Quadratic curve types.
Weighting	Specifies the weighting as Equal, 1/X, 1/X^2, 1/Y, or 1/Y^2.
Units	The units to be displayed with the calculated values.
ISTD	The internal standard (ISTD) for a target compound or surrogate if the standard type is set to Internal. If you set the standard type to External, this field is inactive.
Amount	The amount of the internal standard for ISTD compounds.

Calibration Levels

On the Calibration levels page for a master method, you can define the standards for calibration. You can edit calibration levels and concentrations for master methods only. The contents of this page are read-only when you are editing a local method.

❖ To specify calibration levels and concentrations

1. Select the compound whose calibration levels and concentrations you want to define.

	RT	Compound
1	6.00...	Acetamiprid
2	7.62	1-Methyldodecylamine

2. In the Manage Calibration Levels area, type a value for the first calibration level.

   The EnviroLab Forms application adds a new, empty calibration level row beneath the edited row.

Manage Calibration levels

	Level
1	cal1
2	

3. Continue adding calibration levels.

Manage Calibration levels

	Level
1	cal1
2	cal2
3	cal3
4	cal4
5	

   When you finish adding calibration levels, you can specify the concentrations for each level for each compound.

4. To enter the concentrations to the table, do the following:

   a. Select the first calibration level table cell.

   b. Click the cell again to make it editable.

   c. Type a concentration value.

Acquisition List | Identification | Detection | Calibration | Calibration levels

	RT	Compound	cal1	cal2	cal3	cal4
1	6.00...	Acetamiprid	10			
2	7.62	1-Methyldodecylamine				

5. Repeat Step 4 for all calibration levels associated with the first compound.

6. To specify the same concentration values for all compounds, select the value you want to copy, right-click, and choose **Copy Down** from the shortcut menu.

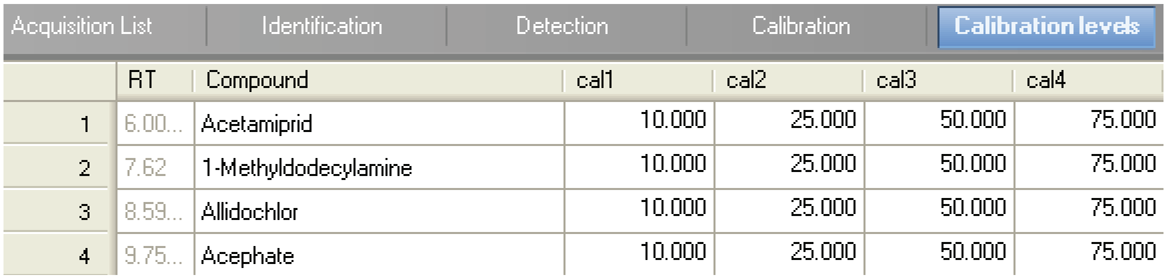


Figure 22. Calibration Levels page

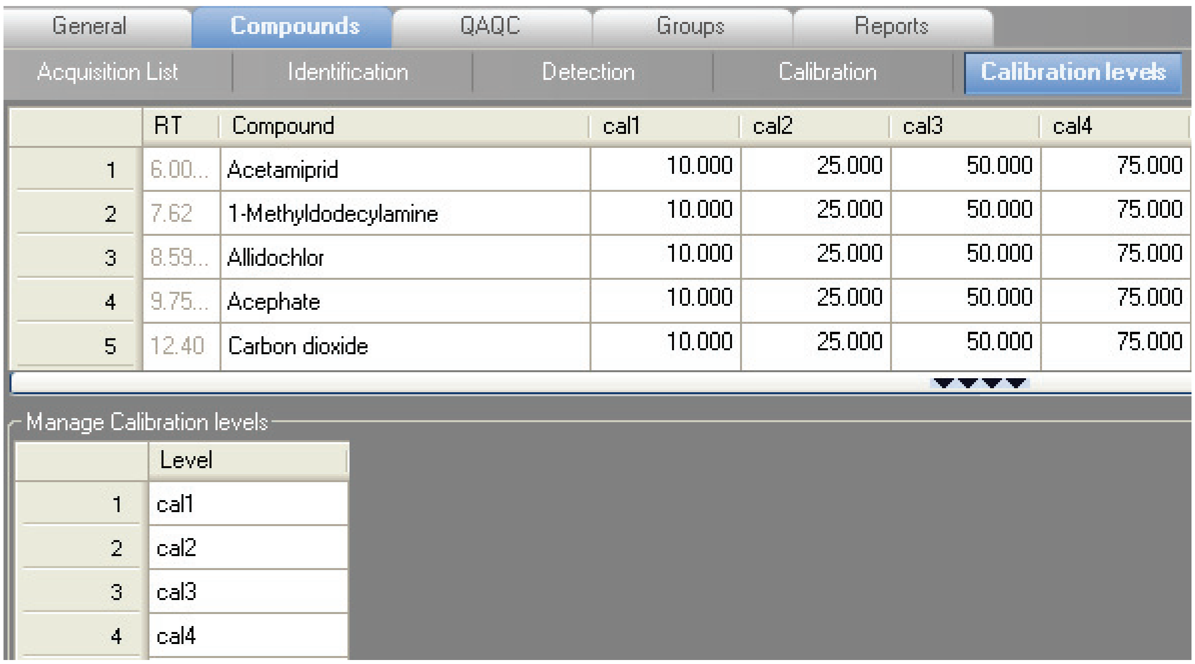


Table 25. Calibration levels parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Compound	The compound name.
cal1-cal*n*	User-defined calibration levels for the compound.
Manage Calibration levels	Defines values for each of the calibration level values for the selected compound.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy Down command, see Appendix B, “Using Copy Down and Fill Down.”

Table 25. Calibration levels parameters (Sheet 2 of 2)

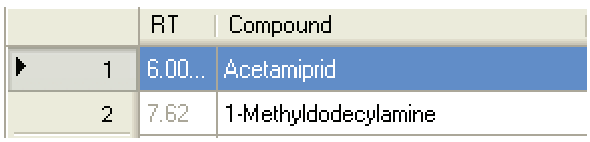
Parameter	Description
Display retention time column	Displays or hides the RT column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

QC Levels

Use the QC levels page for a master method to define the standards for QC levels. You can edit QC levels for master methods only. The contents of this page are read-only when you are editing a local method.

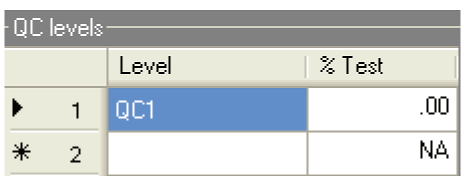
❖ To specify QC levels and concentrations

1. Select the compound whose QC levels, percentage test values, and concentrations you want to define.



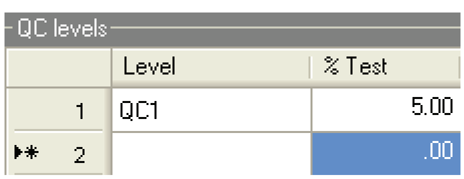
2. In the QC Levels area, type a name for the first QC level.

   The EnviroLab Forms application adds a new, empty QC level row beneath the edited row.



3. Type a value for the % Test.

   The % Test is the acceptable difference (as a percentage) between the known amount and the calculated (measured) amount of each QC level.



4. Continue adding QC levels and values for percentage test.

QC levels

	Level	% Test
1	QC1	5.00
2	QC2	5.00
3	QC3	5.00
▸* 4		.00

When you finish adding QC levels, you can specify the concentrations for each level for each compound.

5. To enter the concentration values to the table, do the following:

   a. Select the first QC level table cell.

   b. Click the cell again to make it editable.

   c. Type a concentration value.

6. Repeat Step 5 for all QC levels associated with the first compound.

Acquisition List | Identification | Detection | Calibration | Calibration levels | QC levels

	RT	Compound	QC1	QC2	QC3
1	6.00,6.00,6.00,...	Acetamiprid	10.000	15.000	25.000
2	7.62	1-Methyldodecylamine			

7. To specify the same concentration values for all compounds, select the value you want to copy, right-click, and choose **Copy Down** from the shortcut menu.

Acquisition List | Identification | Detection | Calibration | Calibration levels | QC levels

	RT	Compound	QC1	QC2	QC3
1	6.00,6.00,6.00,...	Acetamiprid	10.000	15.000	25.000
2	7.62	1-Methyldodecylamine	10.000	15.000	25.000
3	8.59,8.59	Allidochlor	10.000	15.000	25.000
4	9.75,9.75,9.75	Acephate	10.000	15.000	25.000

Figure 23. QC Levels page

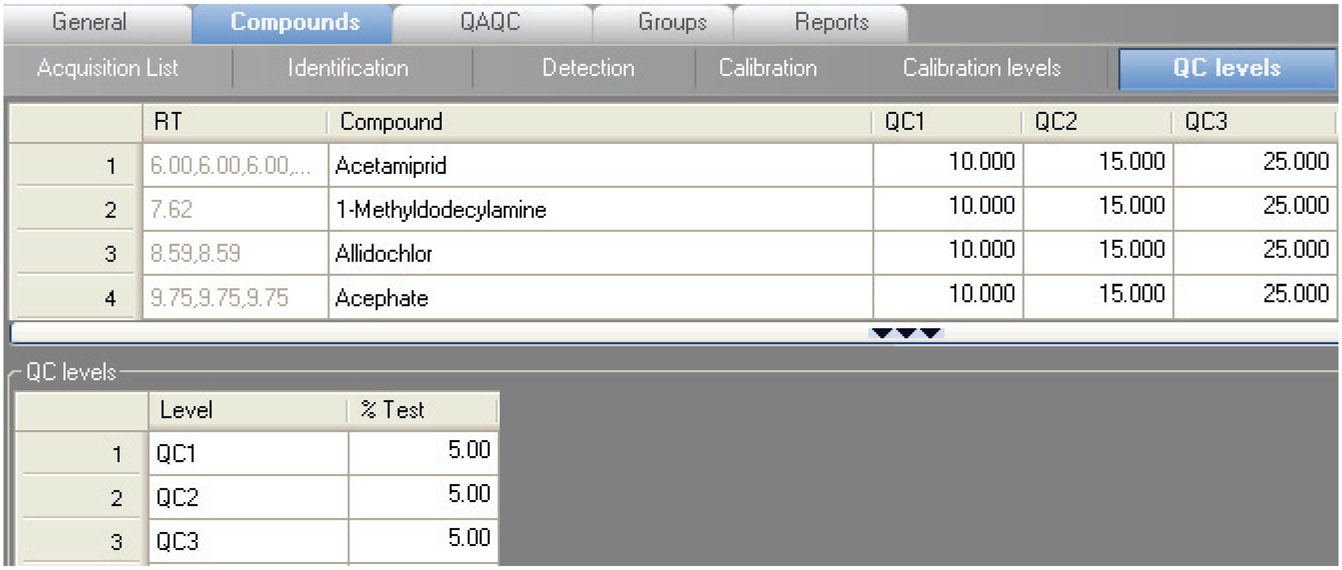


Table 26. QC levels parameters

Parameter	**Description**
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Compound	The compound name.
QC1-QC*n*	User-defined quality control levels for the compound.
QC levels	
Level	User-defined quality control level names.
% Test	A value for the acceptable difference (as a percentage) between the known amount and calculated (measured) amount of each QC level.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy Down command, see Appendix B, “Using Copy Down and Fill Down.”
Display retention time column	Displays or hides the RT column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Editing the QAQC Page

Use the QAQC page to set limits and ranges so the EnviroLab Forms application can review the data and results as an aid to final approval.

From the QAQC page of the Master Method View, you can access these additional pages:

- Limits
- Calibration
- Chk Std
- Lab Control
- Meth Val
- Breakdown
- Blank
- ISTD
- Solvent Blank
- Surrogate
- Matrix Spike
- Tune

Limits

Use the Limits page to define levels of review for quantified results. Quantified results appear on printed and electronic reports. You can also define when a quantified value is reported instead of reporting less than a particular limit.

Figure 24. Limits page

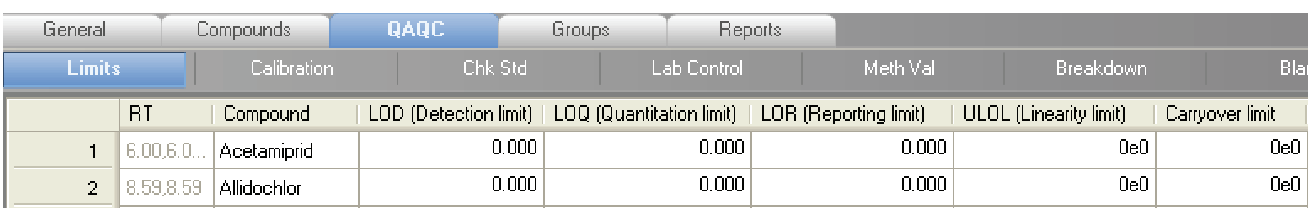


Table 27. Limits parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Compound	The compound name.

Table 27. Limits parameters (Sheet 2 of 2)

Parameter	Description
LOD (Detection limit)	Limit of detection. The lowest amount that can be detected. Usually derived from a method detection limit (mdl) study.
LOQ (Quantitation limit)	Limit of quantitation. The lowest amount that can be confidently and accurately quantitated. This is usually the lowest calibrator amount.
LOR (Reporting limit)	Limit of reporting. Also called cutoff in some industries. This is the highest amount that can be reported, as determined by each laboratory's standard operating practices.
ULOL (Linearity limit)	Upper limit of linearity. This is usually the highest calibrator amount.
Carryover limit	The highest amount of a substance that does not leave a residual amount in the instrument. If a substance has a carryover limit of 5, amounts higher than 5 usually dirty the instrument and leave residue behind, tainting the following sample. A carryover limit of less than 5 does not leave any residual amounts of the substance.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy Down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Calibration

Use the Calibration page to define acceptable criteria for initial calibration. The EnviroLab Forms application makes the evaluation by comparing the initial calibration results for each compound found in the sample to the values defined on this page.

On the Calibration report, the application flags the calculated values for internal standard compounds that exceed these limits.

Figure 25. Calibration page

Table 28. Calibration parameters

Parameter	Description
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Compound	The compound name.
R^2 threshold	The minimum correlation coefficient (r^2) for an acceptable calibration (when in linear or quadratic mode).
Max RSD (%)	The maximum relative standard deviation (RSD) for an acceptable calibration (when in average RF mode).
Min RF	The minimum average response factor (RF) for an acceptable calibration (when in average RF mode).
Max Amt Diff (%)	The maximum deviation between the calculated and theoretical concentrations of the calibration curve data points (when in linear or quadratic mode).
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy Down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Chk Std

Use the Chk Std page to review the calibration on an ongoing basis. The EnviroLab Forms application makes the evaluation by comparing the check standard results for each compound in the sample to the initial calibration using values defined on this page.

On the Check Standard report, the EnviroLab Forms application flags the calculated values for internal standard compounds that exceed these limits.

For linear and quadratic modes, the maximum difference for the calculated concentration in the Chk Std sample versus the theoretical value is set on the QC levels page of the Compounds page.

Figure 26. Chk Std page

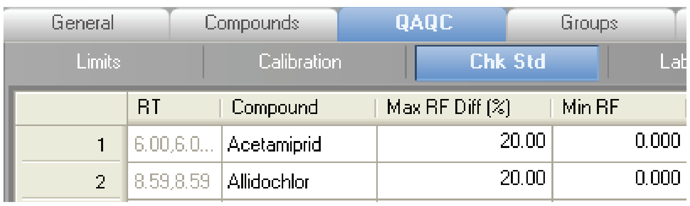


Table 29. Chk Std parameters

Parameter	Description
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Compound	The compound name.
Max RF Diff (%)	The maximum deviation between the response factor (RF) of the Chk Std sample and the average response factor from the calibration (when in average RF mode).
Min RF	The minimum response factor for the Chk Std sample (when in average RF mode).
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy Down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Lab Control

Use the Lab Control page to view and edit QC values for lab control sample (LCS) and lab control sample duplicate (LCSD) analyses. The EnviroLab Forms application makes the evaluation by comparing the calculated concentration for each compound in the sample to the theoretical concentration and range defined on this page.

You can prepare samples (typically known as clean matrices) as LCS or LCSD. These represent samples to which you have added known concentrations of target analytes. To define an LCS and its duplicate in a batch, select the appropriate sample type and a common sample ID.

On the Lab Control report, the EnviroLab Forms application flags the calculated values for spiked compounds that exceed these limits.

Figure 27. Lab Control page

Table 30. Lab Control parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Compound	The compound name.
Theo Conc	Values for each lab control compound that represent the expected theoretical concentration of that compound in the sample.
Min recovery (%)	A range of the allowable minimum recovery percentage and the maximum recovery percentage that the EnviroLab Forms application can determine by comparing the observed calculated concentration in the analysis to the expected concentration. Each LCS or LCSD compound can have its own values for these fields, independent of other LCS or LCSD compounds.
Max recovery (%)	
Max RPD	Specifies a maximum value for relative percent difference (RPD) between two spiked samples.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy Down command, see Appendix B, "Using Copy Down and Fill Down."

Table 30. Lab Control parameters (Sheet 2 of 2)

Parameter	Description
Display retention time column	Displays or hides the RT column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Meth Val

Use the Meth Val page to view or edit QC values for method validation reporting. The EnviroLab Forms application makes the evaluation by comparing the calculated concentration for each compound in the sample to the theoretical concentration and range defined on this page.

You can use these parameters to evaluate the performance of your method. For this evaluation, prepare, analyze, and evaluate a number of samples (typically 4 to 10) to document method accuracy and precision as a comprehensive whole. To define a method validation sample in the batch, select the appropriate sample type.

On the Method Validation report, the EnviroLab Forms application flags the calculated values for method validation compounds that exceed these limits.

Figure 28. Meth Val page

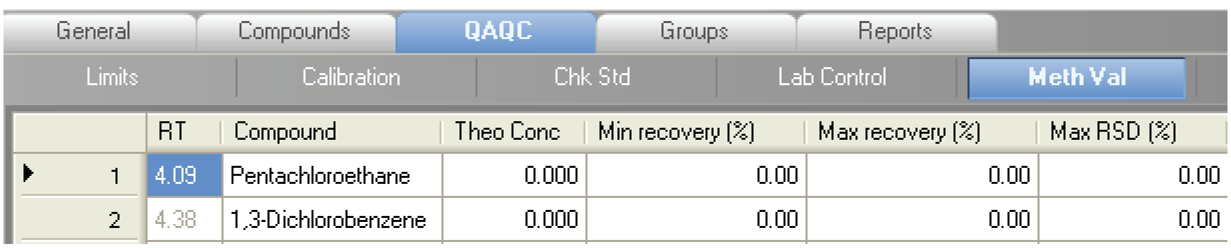


Table 31. Meth Val parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Compound	The compound name.
Theo Conc	Values for each compound that represent the expected theoretical concentration of that compound in the sample.
Min recovery (%)	A range of the allowable minimum recovery percentage and the maximum recovery percentage that the EnviroLab Forms application can determine by comparing the observed calculated concentration in the analysis to the expected concentration. Each method validation compound can have its own values for these fields, independent of other method validation compounds.
Max recovery (%)	
Max RSD (%)	The maximum relative standard deviation of the set of observed concentrations for a component across the set of method validation samples.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy Down command, see Appendix B, "Using Copy Down and Fill Down."

Table 31. Meth Val parameters (Sheet 2 of 2)

Parameter	Description
Display retention time column	Displays or hides the RT column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Breakdown

Use the Breakdown page to view and edit values used for the evaluation of breakdown and degradation reporting. The EnviroLab Forms application makes the evaluation by calculating the ratio of breakdown compounds to the native compounds.

❖ To display the list of compounds in a group

Click anywhere in the group row.

❖ To select a group for breakdown calculation

Select the **Active** check box in the group row.

You can select any group in the method for breakdown calculation, but the EnviroLab Forms application calculates and reports only those that contain breakdown and native compounds.

Figure 29. Breakdown page

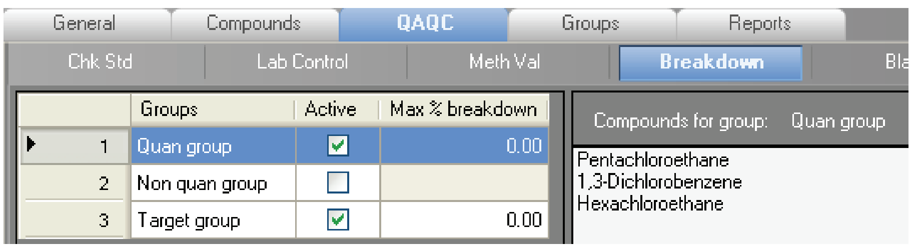


Table 32. Breakdown parameters

Parameter	Description
Groups	Lists all groups created on the Groups page. See "Editing the Groups Page" on page 136.
Active	Specifies which groups are used for analysis.
Max % breakdown	The maximum allowable percentage of breakdown to native compounds. This value is calculated by summing the responses of the breakdown compounds and dividing them by the sum of the native compounds. On the Breakdown Report, the EnviroLab Forms application flags the calculated values for breakdown and native compounds that exceed these limits.
Compounds for group	Lists all compounds in the selected group.

Blank

Use the Blank page to define acceptable levels of target compounds in blank samples. The EnviroLab Forms application makes the evaluation by comparing the calculated concentration for each compound in the sample to the maximum concentration defined on this page. You can enter the maximum concentration as a percentage of a flag value or as a specified value.

On the Blank report, the application flags the calculated values for target compounds that exceed these limits.

❖ To specify the maximum concentration as a percentage

1. From the Method column list box, choose one of the following methods:
   - % of LOD
   - % of LOQ
   - % of LOR
2. In the Percentage column, type a percentage value.

❖ To specify the maximum concentration as an absolute value

1. From the Method column list box, select **Concentration**.
2. In the Max Conc column, type an absolute value.

❖ To specify no maximum concentration

From the Method column list box, select **None**.

Figure 30. Blank page

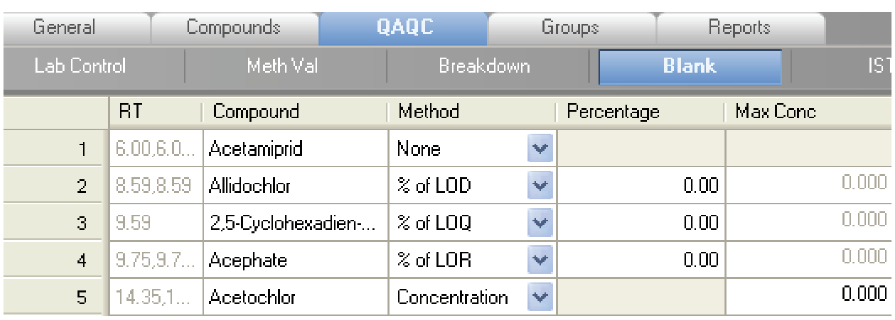


Table 33. Blank parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Compound	The compound name.

Table 33. Blank parameters (Sheet 2 of 2)

Parameter	Description
Method	The evaluation process used for comparing the calculated concentration. You can specify no maximum, a specific concentration, or a percentage of the LOR, LOD, or LOQ.
Percentage	The percentage of the LOR, LOD, or LOQ if you are using the percentage approach.
Max Conc	The maximum concentration if you are using an absolute value.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy Down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

ISTD

Use the ISTD page to review the response and retention time of internal standards (if available). The EnviroLab Forms application makes the evaluation by comparing the area and retention time results for each internal standard compound in the sample to a specified range.

If all of your target compounds are set to external calibration mode or you have not identified any compounds as internal standards, this page does not show any values.

Figure 31. ISTD page

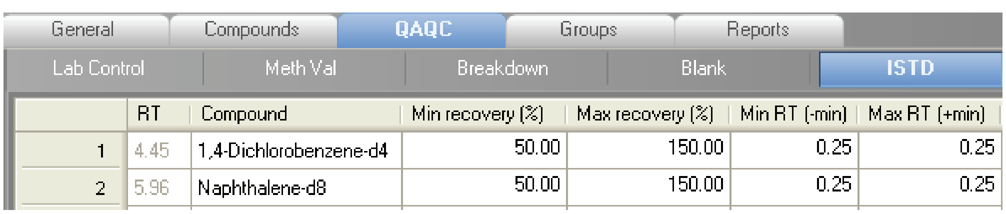


Table 34. ISTD parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Compound	The compound name.

Table 34. ISTD parameters (Sheet 2 of 2)

Parameter	Description
Min recovery (%) Max recovery (%)	The minimum and maximum percent recoveries for the internal standards to define an acceptable range. For check standards, the EnviroLab Forms application compares the response of each internal standard in each sample to a range around the average of the responses of that compound in all of the calibration standards. For all other samples, the application calculates the comparison range around the check standard responses if a check standard is available in the batch. If no check standard is available, the application tests against the initial calibration.
Min RT (–min) Max RT (+min)	The minimum and maximum drift (in minutes) for the internal standards to define an acceptable range. For check standards, the EnviroLab Forms application compares the retention time of each internal standard in each sample to a range around the average of the retention times of that compound in all of the calibration standards. For all other samples, the application calculates the comparison range around the check standard retention times if a check standard is available in the batch. If no check standard is available, the application tests against the initial calibration.
CV Test (%)	Coefficient of Variation test.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy Down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Solvent Blank

Use the Solvent Blank page to view or edit QC values for solvent reporting. The evaluation is made by comparing the calculated response for each compound in the sample to the maximum response defined on this page.

On the Solvent Blank report, the EnviroLab Forms application flags the calculated values for target compounds that exceed these limits.

Figure 32. Solvent Blank page

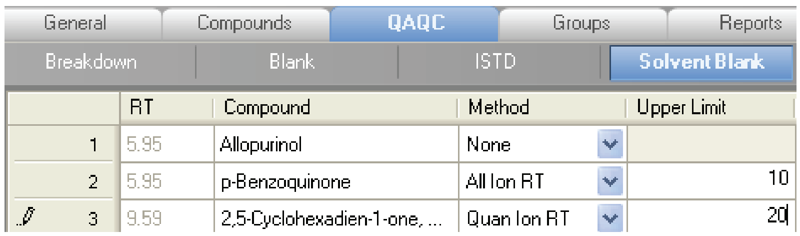


Table 35. Solvent Blank parameters

Parameter	Description
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Compound	The compound name.
Method	The evaluation process to use as a response for the quan ion only (Quan Ion RT) or a summed response for the quan ion and any confirming ions (All Ion RT). To deactivate the solvent blank test for a specific compound, select **None**.
Upper Limit	Specifies an upper limit for each compound in the sample if an evaluation process is selected. These values are not concentrations; they are raw response values.
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy Down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Surrogate

Use the Surrogates page to view or edit QC values for surrogate reporting. The EnviroLab Forms application makes the evaluation by comparing the calculated concentration for each surrogate compound in the sample to the range defined on this page.

On the Surrogate report, the application flags the calculated values for surrogate compounds that exceed these limits.

Figure 33. Surrogate page

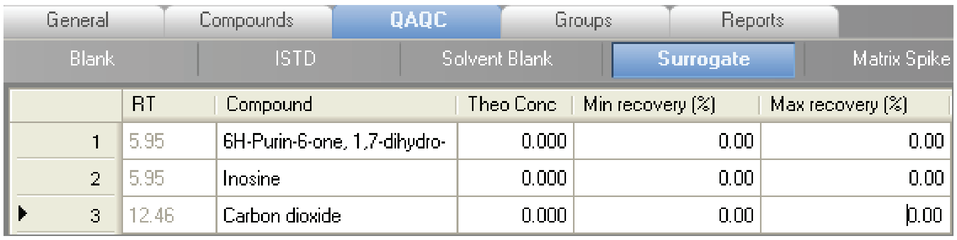


Table 36. Surrogate parameters

Parameter	Description
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Compound	The compound name.
Theo Conc	Values for each surrogate compound that represent the expected theoretical concentration of that compound in the sample. You can apply or not apply the dilution factor for a sample to the calculated surrogate concentrations using the Correct Surrogates option on the Reports page. See "Specifying Report Flag Options" on page 142.
Min recovery (%)	A range of the allowable minimum recovery percentage and the maximum recovery percentage that can be determined by comparing the observed calculated concentration in the analysis to the expected concentration. Each surrogate can have its own values for these fields, independent of other surrogates.
Max recovery (%)	
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy Down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Matrix Spike

Use the Matrix Spike page to view or edit QC values for matrix spike and matrix spike duplicate analyses. The EnviroLab Forms application makes the evaluation by comparing the calculated concentration for each compound in the sample (after subtracting the original sample value) to the theoretical concentration and range defined on this page.

To evaluate matrix spike (MS) or matrix spike duplicate (MSD) compounds, prepare samples as MS or MSD. These represent samples to which you have added known concentrations of target analytes. To define a sample, its MS, and its MSD in the batch, select the appropriate Sample Type and a Sample ID.

> **Note** Sample IDs must be unique. Duplicating Sample IDs can cause incorrect samples to be included in reports.

On the MS/MSD report, the EnviroLab Forms application flags the calculated values for spiked compounds that exceed these limits.

Figure 34. Matrix Spike page

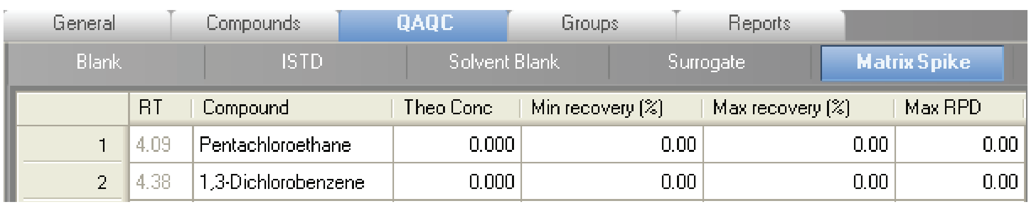


Table 37. Matrix Spike parameters (Sheet 1 of 2)

Parameter	Description
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Compound	The compound name.
Theo Conc	Values for each surrogate compound that represent the expected theoretical concentration of that compound in the sample. You can apply or not apply the dilution factor for a sample to the calculated surrogate concentrations using the Method Options.
Min recovery (%) Max recovery (%)	A range of the allowable minimum recovery percentage and the maximum recovery percentage that can be determined by comparing the observed calculated concentration in the analysis to the expected concentration. Each surrogate can have its own values for these fields, independent of other surrogates.
Max RPD	Specify a maximum value for relative percent difference (RPD) between two spiked samples.

Table 37. Matrix Spike parameters (Sheet 2 of 2)

Parameter	Description
Shortcut menu	
Copy down	Copies the selected column value to all rows in that column. For detailed instructions about using the Copy Down command, see Appendix B, "Using Copy Down and Fill Down."
Display retention time column	Displays or hides the RT column in the compound list.
Delete compound from method	Removes the selected compound from the current master method.

Tune

Use the Tune page to specify mass spectral comparison criteria according to EPA tune methods. Your master method must include one (and only one) compound specified as an MSTune compound type. The QAQC evaluation compares the mass list of the compound to the values in the tune method.

An MSTune sample contains Decafluorotriphenylphosphine (DFTPP) or bromofluorobenzene (BFB) and is handled differently from other samples in the master method. The EnviroLab Forms application handles it as a qualitative examination of the mass spectrum of a specific compound rather than evaluating it on a quantitative basis.

Follow these procedures:

- To select an EPA tune method
- To manually submit a mass spectrum for tune evaluation

❖ To select an EPA tune method

1. Click Method and choose a method from the list.

    - For some methods, the Use Only Selected Method option is available.
    - For some methods, the Perform Background Subtraction option is available.

    The EnviroLab Forms application displays the mass spectral reference for the method.

Eval Mass	Base Peak?	Low Op	Lower Limit %	High Op	High Limit	Relative To
51		>=	10	<=	80	198
68				<	2	69
69		>	0			Base peak
70				<	2	69
127		>=	10	<=	80	198
197				<	2	198
198	Yes			=	100	Base peak
199		>=	5	<=	9	198

2. (Optional) Select the **Use Only Selected Method** check box.

   The EnviroLab Forms application uses only the specified EPA tune method for tune criteria testing.

   If this option is not selected and the tune spectrum fails against the specified tune criteria, the EnviroLab Forms application performs the comparison against other EPA tune method criteria. The Tune report displays the pass/fail status of the tune spectra against all methods used for comparison.

3. (Optional) Select the **Perform Background Subtraction** check box.

   - The 8000 and CLP series methods require background subtraction.

   - The 500 and 600 series do not require background subtraction but you can choose to use it.

   The Tune report displays the retention time and scan range of the spectrum.

4. (Optional) Click **Max Stepoff** and use the spin box to select a number or type a number in the box.

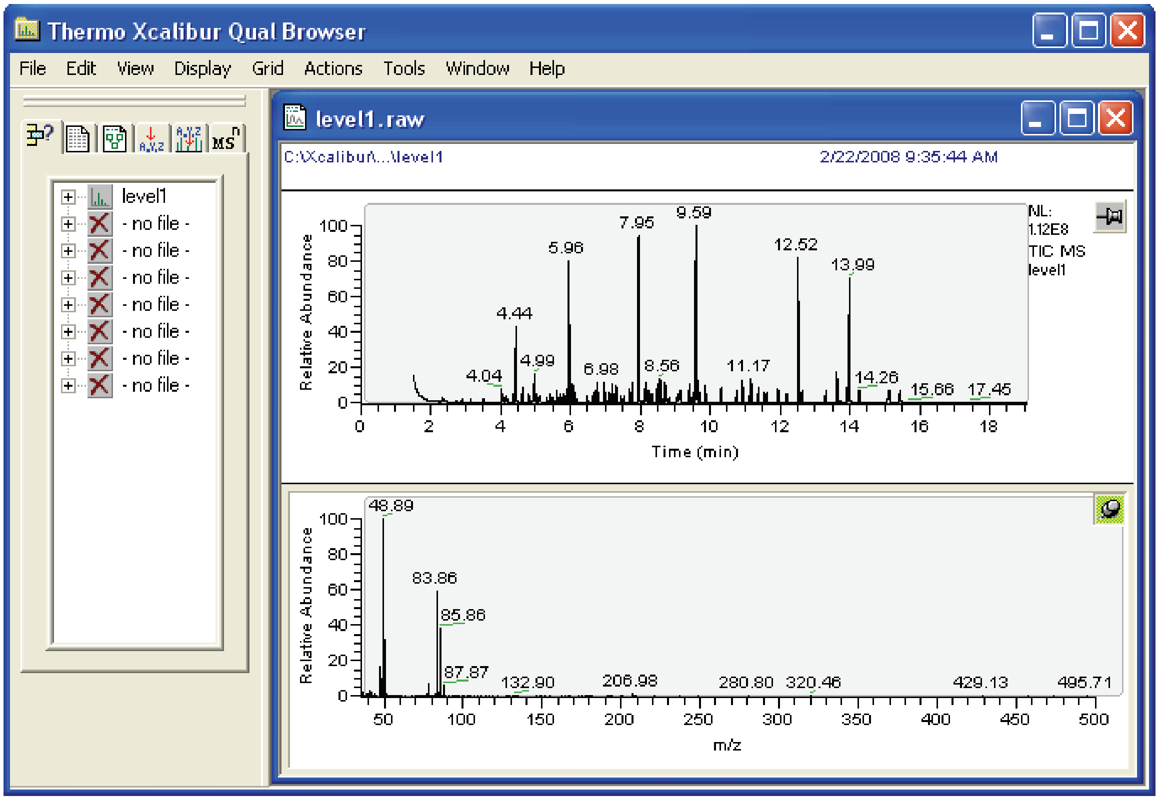
   The Max Stepoff field defines the maximum number of scans as the range before/after the Tune compound peak that is to be used for background subtraction. For example, a maximum stepoff of 1 means that the background spectrum is taken one scan before the left edge of the tune peak or one scan after the right edge of the tune peak. If using the left edge background spectrum fails the tune test, the system automatically tries the right edge of the spectrum. A maximum stepoff of 2 tries up to four tests using four different background spectrum: two scans before the left edge, one scan before the left edge, one scan after the right edge, and two scans after the right edge. EPA guidelines assign a maximum stepoff value of 20.

   Note This Max Stepoff value is not related to the Stepoff Value parameter on the General page of the master method. The Stepoff Value on the General page applies only to the reference spectrum set for the master method and does not affect the Tune method.

❖ To manually submit a mass spectrum for tune evaluation

1. Click **Select File and Mass Spectrum**.
2. In the browser, select a raw data file and click **Open**.

   The Thermo Xcalibur Qual Browser opens.



3. In the Qual browser, do the following:
   a. Select the tune compound peak you want to use.
   b. Select the background subtraction parameters to use and generate the mass spectrum.

      For detailed instructions, refer to the Qual Browser documentation.

   c. When the process is complete, choose **View > Spectrum List**.
   d. Right-click the spectrum list and choose **Export > Clipboard**.
   e. In the LabForms Tune page, click **Create Tune Report as PDF**.

Figure 35. Tune page

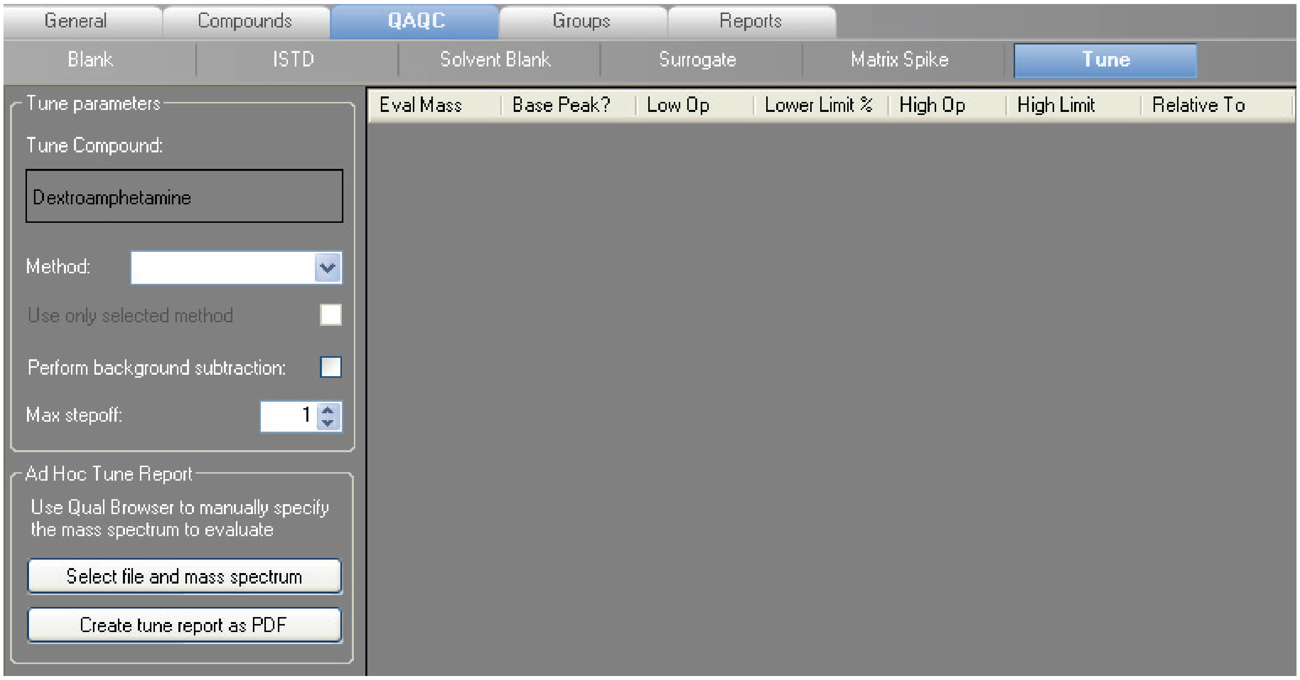


Table 38. Tune parameters

Parameter	Description
Tune parameter	
Tune Compound	Compound specified as a tune compound in the Identification page. See "Identification" on page 81.
Method	Environmental Protection Agency (EPA) methods used for tuning.
Use only selected method	Specifies that the EnviroLab Forms application use only the specified EPA tune method for tune criteria testing.
Perform background subtraction	Specifies that the EnviroLab Forms application average and subtract the mass spectra as specified in the background subtraction settings on the General page for the master method. See "To set automated background subtraction options" on page 72.
Max stepoff	Specifies the maximum number of scans as the range before and after the Tune compound peak to be used for background subtraction.
Ad Hoc Tune Report	
Select file and mass spectrum	Opens a browser where you can select a raw data file to use for the tune report.
Create tune report as PDF	Creates an ad hoc tune report using the mass spectrum data saved on the clipboard.

Editing the Groups Page

Use the Groups page of the Master Method View to organize compounds into functional or logical groups. You can use these groups for creating a subset of target compounds for quantitative processing or a list of non-quantitative compounds for breakdown processing. See "Groups page" on page 137.

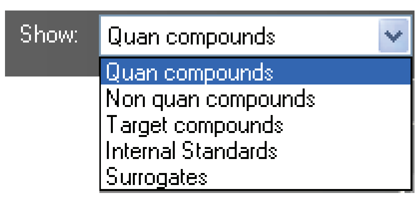
For quantitative processing, the EnviroLab Forms application processes all compounds in the method and stores the complete result set, but only those in the selected group are visible in Production mode. Limiting the displayed compounds to those in the selected group can be useful when working with a master method containing a large list of compounds, only some of which are required for analysis in certain samples. In that case, the application requires only a single method and can reduce the results. To display only those compounds to be used in quantitative processing, select **Quan Compounds** from the Show list box.

For non-quantitative processing, you can select the Breakdown and Native compounds that the EnviroLab Forms application uses for breakdown reporting. To view only those compounds to be used in non-quantitative processing, select **Non Quan Compounds** from the Show list box.

You can create as many quantitative and non-quantitative groups as you want and the same compound can be included in multiple groups.

❖ To create a group

1. From the Show list box, select the type of compounds you want to view.



2. At the bottom of the Groups area, click **Add Group**.

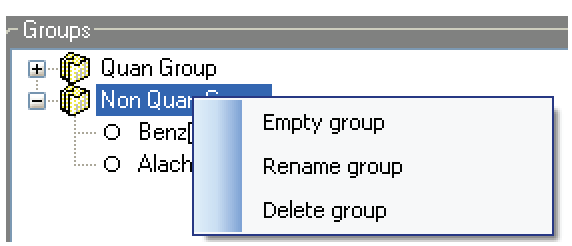
   The Add a New Group dialog box opens.

3. Type a name for the new group and click **OK**.

   The new group appears in the Groups area.

4. Drag a compound from the Compounds area onto a group name (as if you were moving files into a folder).

5. To remove all the compounds from a group, rename the group, or delete it, right-click the group name and choose from the shortcut menu.



6. To remove a single compound, click the compound name in the group, right-click, and choose **Remove from Group** from the shortcut menu.

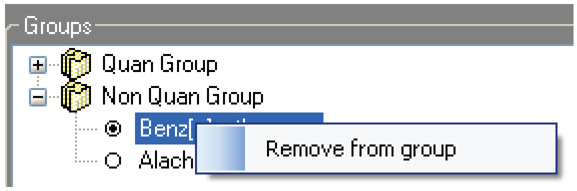


Figure 36. Groups page

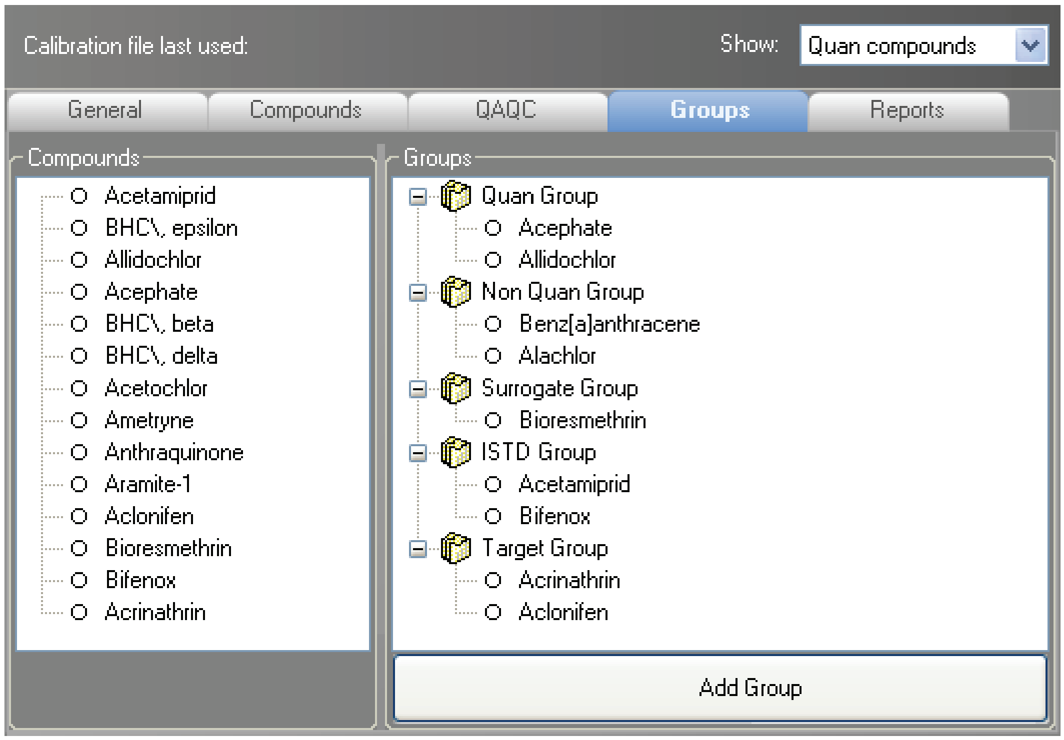


Table 39. Groups parameters

Parameter	Description
Compounds	Lists all available compounds.
Groups	Lists all available groups.
Add Group	Opens the Add a New Group dialog box where you can create a new group.
Shortcut menu	
Empty group	Removes all compounds from the selected group.
Rename group	Changes the name of the selected group.
Delete group	Removes the selected group and all the compounds in it.
Remove from group	Removes the selected compound from its group.

Editing the Reports Page

Use the Standard Reports and Custom Reports pages to specify how you want to save or print your reports.

For the Quantitation Report type, you can modify quan report, user interface, quan flag, and surrogate correction options in the Report Options pane.

This section includes instructions for the following tasks:

- Specifying Report Formats
- Specifying Report Flag Options

Specifying Report Formats

For each standard report you generate, you can create a hardcopy printout, a PDF file, or an XML file. In addition to the report type, you can specify a report title for each of your reports. The default report title is the report name.

For each custom report you generate, you can create a hardcopy printout or an XLS (.xlsm) file. You cannot specify a report title for a custom report.

Follow these procedures:

- To specify standard report types and output formats
- To specify custom report types and output formats

❖ To specify standard report types and output formats

1. Click the **Standard Reports** tab.

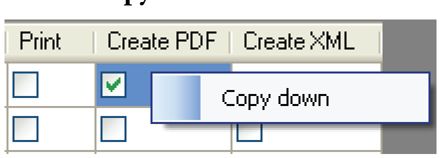
   The Standard Reports page displays the Report Name, Report Title, and the options to create a hardcopy, a PDF file, or an XML file. See "Standard Reports page" on page 140.

2. To edit the Report Title, double-click the name and type your new name.

   The EnviroLab Forms application uses this name for all reports that use this master method. You cannot edit the Report Title from other report views.

3. To specify the type of report output to create for each report type, select the check box in the appropriate column.

4. To duplicate the output type for all reports, click the cell to select it, then right-click and choose **Copy Down** from the shortcut menu.



All check boxes in the column below the selected cell duplicate the selected or cleared state of the selected cell.

By default, all report types are cleared.

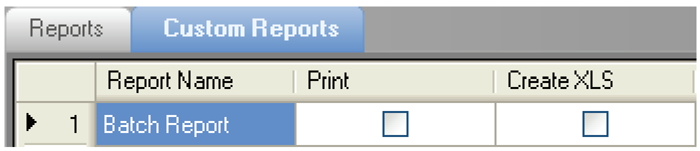
❖ To specify custom report types and output formats

1. Click the **Custom Reports** tab.

   The Custom Reports page lists all the reports that are saved in the following folder:

   `..\Thermo\EnviroLab Forms\Templates\Reports`

   The Custom Reports page displays the Report Name and the options to create a hardcopy printout or XLS file. See “Custom Reports page” on page 141.

2. To specify the type of report output to create for each report type, select the check box in the appropriate column.

3. To duplicate the output type for all reports, right-click the cell and choose **Copy Down** from the shortcut menu.

   All check boxes in the column below the selected cell duplicate the selected or cleared state in the selected cell.

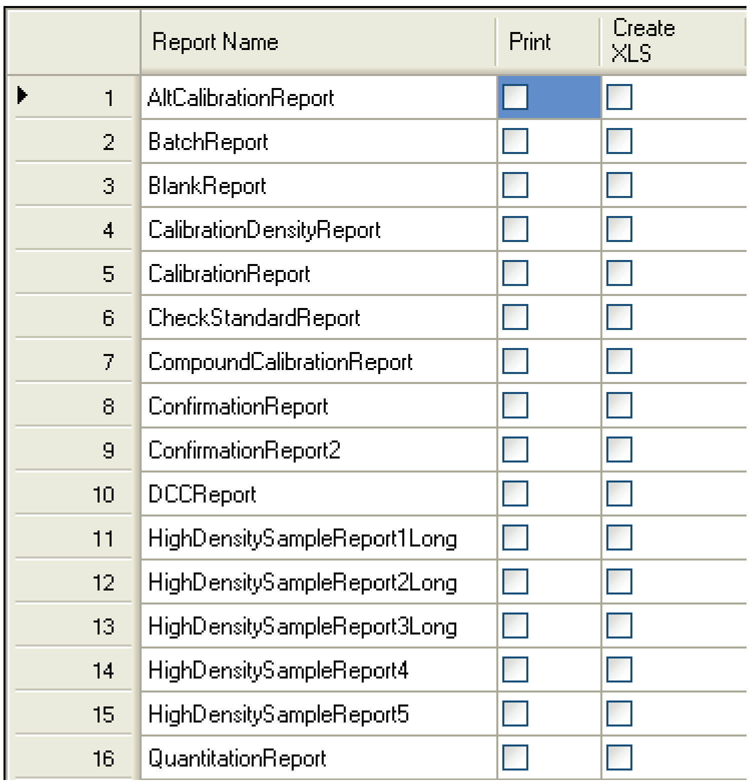
Figure 37. Standard Reports page

	Report Name	Report Title	Print	Create PDF	Create XML
1	Batch Report	Batch Report			
2	Blank Report	Blank Report			
3	Breakdown Report	Breakdown Report			
4	Calibration Report	Calibration Report			
5	Check Standard Report	Check Standard Report			
6	Chromatogram Report	Chromatogram Report			
7	Compound Calibration Report	Compound Calibration Report			
8	Confirmation Report	Confirmation Report			
9	Confirmation Report 2	Confirmation Report 2			
10	High Density Calibration Report	High Density Calibration Report			
11	High Density Internal Standard Report	High Density Internal Standard Report			
12	High Density Internal Standard Report Long	High Density Internal Standard Report Long			
13	High Density Sample Report 1	High Density Sample Report 1			
14	High Density Sample Report 1 Long	High Density Sample Report 1 Long			
15	High Density Sample Report 2	High Density Sample Report 2			
16	High Density Sample Report 2 Long	High Density Sample Report 2 Long			
17	High Density Sample Report 3	High Density Sample Report 3			
18	High Density Sample Report 3 Long	High Density Sample Report 3 Long			
19	Internal Standard Summary Report	Internal Standard Summary Report			
20	Ion Ratio Failure Report	Ion Ratio Failure Report			
21	LCSLCSD Report	LCSLCSD Report			
22	Manual Integration Report	Manual Integration Report			
23	Method Detection Limit Report	Method Detection Limit Report			
24	Method Report	Method Report			
25	Method Validation Report	Method Validation Report			
26	MSMSD Report	MSMSD Report			
27	Quantitation Report	Quantitation Report			
28	Quantitation Report - 2	Quantitation Report - 2			
29	Solvent Blank Report	Solvent Blank Report			
30	Surrogate Recovery Report	Surrogate Recovery Report			
31	TIC Report	TIC Report			
32	TIC Summary Report	TIC Summary Report			
33	Tune Report	Tune Report			

Table 40. Standard Reports parameters

Parameter	Description
Example	Displays a sample of the report type.
Report Name	The name of a report.
Report Title	The user-defined title to be used on a report.
Print	Reports to be sent to the printer.
Create PDF	Reports to be saved as PDF files.
Create XML	Reports to be exported in XML format.

Figure 38. Custom Reports page



	Report Name	Print	Create XLS
1	AltCalibrationReport	☐	☐
2	BatchReport	☐	☐
3	BlankReport	☐	☐
4	CalibrationDensityReport	☐	☐
5	CalibrationReport	☐	☐
6	CheckStandardReport	☐	☐
7	CompoundCalibrationReport	☐	☐
8	ConfirmationReport	☐	☐
9	ConfirmationReport2	☐	☐
10	DCCReport	☐	☐
11	HighDensitySampleReport1Long	☐	☐
12	HighDensitySampleReport2Long	☐	☐
13	HighDensitySampleReport3Long	☐	☐
14	HighDensitySampleReport4	☐	☐
15	HighDensitySampleReport5	☐	☐
16	QuantitationReport	☐	☐

Table 41. Custom Reports parameters

Parameter	Description
Report Name	The name of a report.
Print	Reports to be sent to the printer.
Create XLS	Reports to be exported in Excel spreadsheet (.xlsm) format.

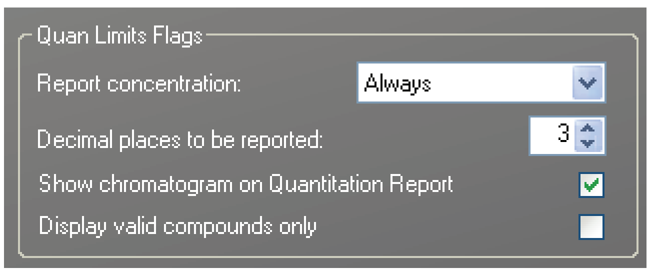
Specifying Report Flag Options

Use the report options to choose parameters for flagging values and displaying information in standard report types.

Follow these procedures:

- To specify quantitation limits
- To specify user interface options
- To specify quantitation flag options
- To correct surrogates
- To track the use of the tune file

❖ To specify quantitation limits



1. To report the calculated concentration at all times or only when the quantified value exceeds LOD, LOQ, or LOR, choose the appropriate value from the Report Concentration list box.

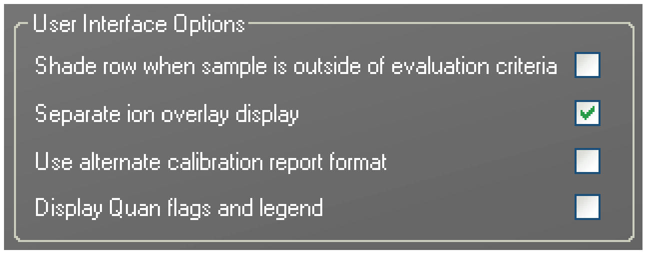
   These concentration limits are defined in "Limits" on page 117.

2. To select the number of decimal places to report for calculated concentrations, set the value in the Decimal Places to be Reported box.

3. To include a chromatogram of the sample in the report, select the **Show Chromatogram on Quantitation Report** check box.

4. To display only valid compounds, select the **Display Valid Compounds Only** check box.

❖ To specify user interface options



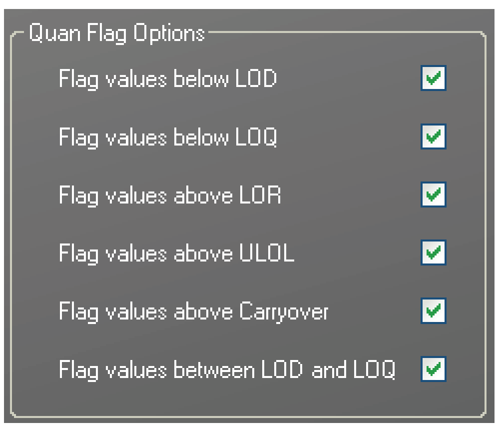
1. To shade a compound row on any of the reports if a value fails one of the criteria used for evaluation, select the **Shade Row when Sample is Outside of Evaluation Criteria** check box.

2. To separate the ion overlay pane from the confirming ion plots, select the **Separate Ion Overlay Display** check box.

3. To use an alternate format for the Calibration Report designed to print more concisely and limit the report to a maximum of 7 calibration standards, select the **Use Alternate Calibration Report Format** check box.

4. To display flags and a legend on high density reports, select the **Display Quan Flags and Legend** check box.

❖ To specify quantitation flag options

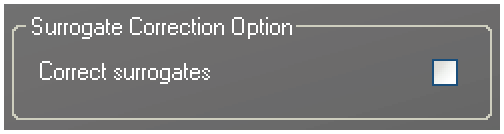


Select the values you want to display in the report.

Values are above or below the limits defined on the Quan page.

These flags appear on a variety of reports and are defined in the Report options parameters table.

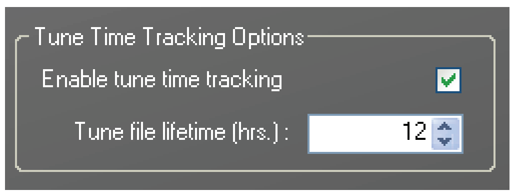
❖ To correct surrogates



Select the **Correct Surrogates** check box.

The EnviroLab Forms application applies the conversion factor (specified in the sample row in the batch) to the sample's calculated concentrations for surrogates as the conversion factor is applied to target compounds.

❖ To track the use of the tune file



1. Select the **Enable Tune Time Tracking** check box.

   This option tracks the number of hours between the last instrument tune and each sample acquisition.

2. Click the **Tune File Lifetime** spin box and set the number of hours you want to allow between the last instrument tune and a sample acquisition.

   Any sample acquired outside this maximum allowable time is flagged on the Batch report.

Figure 39. Report Options

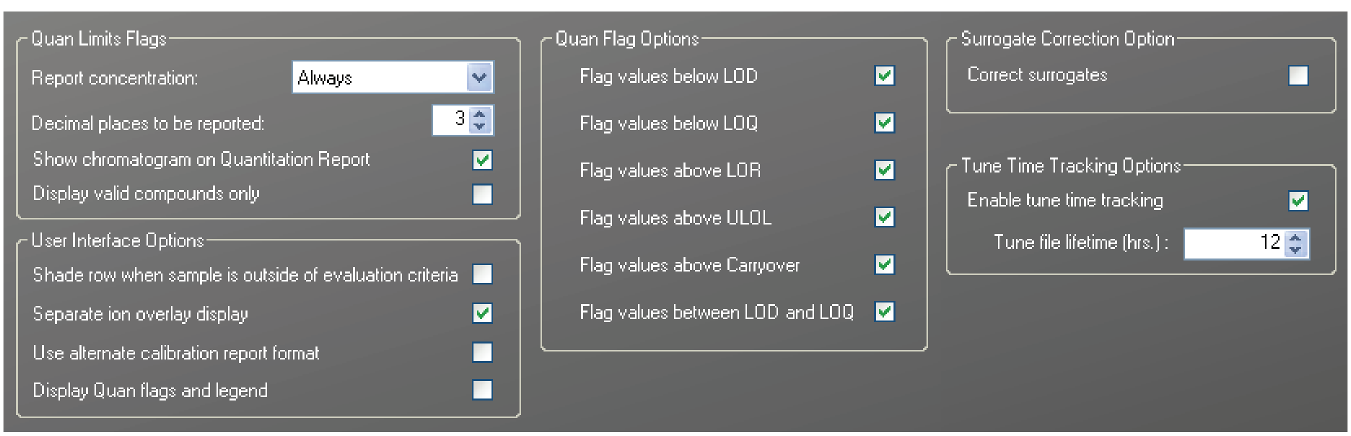


Table 42. Report options parameters (Sheet 1 of 2)

Parameter	Description
Quan Limits Flags	
Report concentration	Reports the concentration at all times or only when the quantified value exceeds either the limit of detection (LOD), the limit of quantitation (LOQ), or the limit of reporting (LOR). Report concentration: Always, >LOD, >LOQ, or >LOR.
Decimal places to be reported	Number of decimal places to be included in the report. Maximum value is 6.
Show chromatogram on Quantitation Report	Displays a chromatogram (TIC trace) of the sample on the quantitation report.
Display valid compounds only	Prints only the positive compounds in a sample. If a compound is valid within a sample and is above the specified Quan Flag Options limits, the EnviroLab Forms application reports the compound.
User Interface Options	
Shade row when sample is outside of evaluation criteria	Shades a compound row on any of the reports if a value fails one of the criteria used for evaluation.
Separate ion overlay display	Separates the ion overlay pane from the confirming ion plots in data review.
Use alternate calibration report format	Uses an alternate format for the Calibration Report that is designed to print more concisely (this report is limited to a maximum of 7 calibration standards).
Display Quan flags and legend	Displays manual flags, confirming manual flags, quan flags, and a legend on high density reports.
Quan Flag Options	Values that are above or below limits defined on the Limits page. These flags appear on a variety of reports.
Flag values below LOD	Flags values below the limit of detection (LOD).
Flag values below LOQ	Flags values below the limit of quantitation (LOQ).
Flag values above LOR	Flags values above the limit of reporting (LOR).
Flag values above ULOL	Flags values above the upper limit of linearity (ULOL).
Flag values above Carryover	Flags values above the carryover limit.
Flag values between LOD and LOQ	Flags values between the limit of detection and the limit of quantitation known as the J flag.

Table 42. Report options parameters (Sheet 2 of 2)

Parameter	Description
Surrogate Correction Option	
Correct surrogates	Applies the conversion factor (specified in the sample row in the batch) to the sample's calculated concentrations for surrogates as the conversion factor is applied to target compounds. For example, if you added surrogates to the sample as part of sample preparation and you require a dilution for analysis, the EnviroLab Forms application dilutes the surrogates and target compounds and applies a dilution correction to correct for this dilution. However, if you added surrogates after a dilution has occurred, then you can leave the option cleared, so that while the target compounds are corrected for the dilution, the surrogates are reported 'as is.'
Tune Time Tracking Options	
Enable tune time tracking	Tracks the number of hours between the last instrument tune and each sample acquisition.
Tune file lifetime	Specifies the maximum number of hours between the last instrument tune and a sample acquisition. Any sample acquired outside this maximum allowable time is flagged on the Batch report.

Creating a Method Template

In the EnviroLab Forms application, you can create a processing method using a method template that contains the basic settings as defined by a user in the role of Manager or Supervisor.

Follow these procedures:

- To create a method template
- To specify peak criteria
- To choose a library
- To specify confirming ions
- To calibrate the compounds
- To enter a note for the method
- To save the method template

❖ To create a method template

1. Click **Method Development** from the dashboard or the navigation pane.

   The Method Development navigation pane opens.

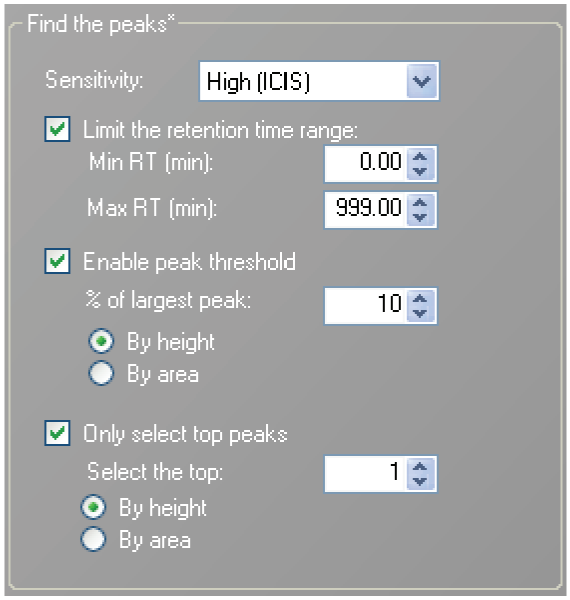
2. Click **Method View** in the navigation pane.

3. From the main menu, choose **File** > **New** > **Method Template**.

   The Method Template Editor opens. See "Method Template Editor" on page 152.

❖ To specify peak criteria



1. In the Find the Peaks area, choose a sensitivity level.

   In selecting the degree of sensitivity, you define how extensively the peak detector algorithm searches for low-level peaks.

   - The High (ICIS) peak detection algorithm is designed for MS data and has superior peak detection efficiency at low MS signal levels.
   - The Standard (Genesis) peak detection algorithm is provided for backward compatibility with Xcalibur 1.0 studies.

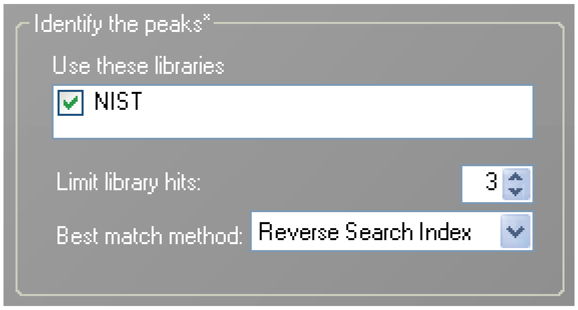
2. To look for peaks only in a certain range of the entire chromatogram, select the **Limit the Retention Time Range** check box and specify a retention time (RT) range.

3. To indicate whether to select peaks by relative height or area and the percentage of the highest peak that will result in compound selection, select the **Enable Peak Threshold** check box.

   To consider a peak for a processing method, the EnviroLab Forms application uses the Enable Peak Threshold filter to determine which peaks meet the specified percentage of the largest peak.

4. To display a specific number of the largest peaks by height or area, select the **Only Select Top Peaks** check box and choose the number of peaks to display.

❖ To choose a library



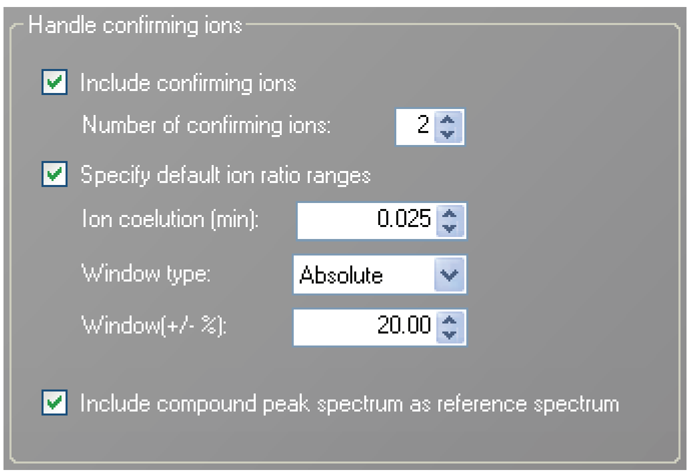
1. In the Use these Libraries box, select the libraries you want to search.

   All libraries loaded on your instrument are displayed in the Use these Libraries box.

2. To limit the number of hits returned when the system searches a spectrum against the selected libraries, set a value in the Limit Library Hits box.

3. To specify how to sort the library searches, choose a value from the Best Match Method list box.

❖ To specify confirming ions



1. To set the number of confirming ions, select the **Include Confirming Ions** check box and set a value in the Number of Confirming Ions box.

   This value is the number of other ions in the spectrum whose ratio is compared to the quantitation ion. Using this ratio, you can then determine if it is the target compound or something else. This value defaults to **2** because you typically perform a 3-ion experiment with one quan mass and two confirming ions.

   The system selects the most intense ion to use as the quantitation mass and uses this mass for the mathematical operations.

2. To define the criteria for evaluating confirming or qualifying ions, select the **Specify Default Ion Ratio Ranges** check box and set the following values:

   a. To specify the maximum difference in retention time between a confirming ion peak and the quantification ion peak, set a value in the Ion Coelution (min) box.

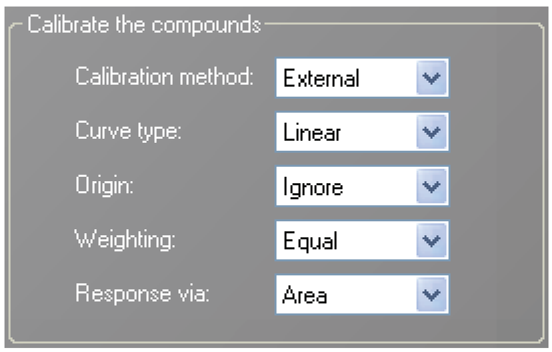
   b. To specify an absolute or relative calculation approach for determining the acceptable ion ratio range, select **Absolute** or **Relative** from the Window type list.

   c. To specify the acceptable ion ratio range, set a value in the Window (+/– %) box.

3. To include the peak spectrum in the processing method, select the **Include Compound Peak Spectrum as Reference Spectrum** check box.

   Use this setting to perform a spectra comparison in Production mode.

❖ To calibrate the compounds



1. From the Calibration method list, select **Internal** or **External**.

2. From the Curve type list, select one of the following:

   - Linear: All other settings are available with this exception: When **Include** is selected in the Origin list, all weighting values are unavailable except for **Equal**.

   - Quadratic: All other settings are available with this exception: When **Include** is selected in the Origin list, all weighting values are unavailable except for **Equal**.

   - Average RF: No selections in the Weighting or Origin lists are available. The Weighting list is set to **Equal**, and the Origin list is set to **Ignore**.

3. From the Origin list, select one of the following:

   - Ignore: Specifies that the origin is not included as a valid point in the calibration curve when the curve is generated. When you select **Ignore**, the calibration curve might or might not pass through the origin.

   - Force: Specifies that the calibration curve passes through the origin of the data point plot when the calibration curve is generated.

   - Include: Specifies that the origin is included as a single data point in the calculation of the calibration curve. When you select **Include**, the calibration curve might or might not pass through the origin.

4. From the Weighting list, select one of the following:

   - Equal: Specifies that the origin is included as a single data point in the calculation of the calibration curve. When you select **Equal**, the calibration curve might or might not pass through the origin.

   - 1/X: Specifies a weighting of 1/X for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their quantity.

   - 1/X^2: Specifies a weighting of 1/X^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their quantity.

   - 1/Y: Specifies a weighting of 1/Y for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their response (or response ratio).

   - 1/Y^2: Specifies a weighting of 1/Y^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their response (or response ratio).

5. From the Response via list, choose **Area** or **Height**.

   - Area: Specifies that the EnviroLab Forms application use this area value in response calculations.

   - Height: Specifies that the EnviroLab Forms application use this height value in response calculations.

❖ To enter a note for the method

Type in the Notes box, or paste text from another application using CTRL-V.

You can add a note to your method template so that there is a record of what makes this template unique.

❖ To save the method template

1. Choose **File > Save** from the Method Template Editor menu.

   The Save Method Template dialog box opens.

2. Do one of the following:

   - Type a new name for the master method and click **OK**.

   –Or–

   - Select a method name to overwrite and click **Overwrite**.

   The EnviroLab Forms application saves the new method template in the following folder:

   ..\Thermo\EnviroLab Forms\Templates\Methods

Figure 40. Method Template Editor

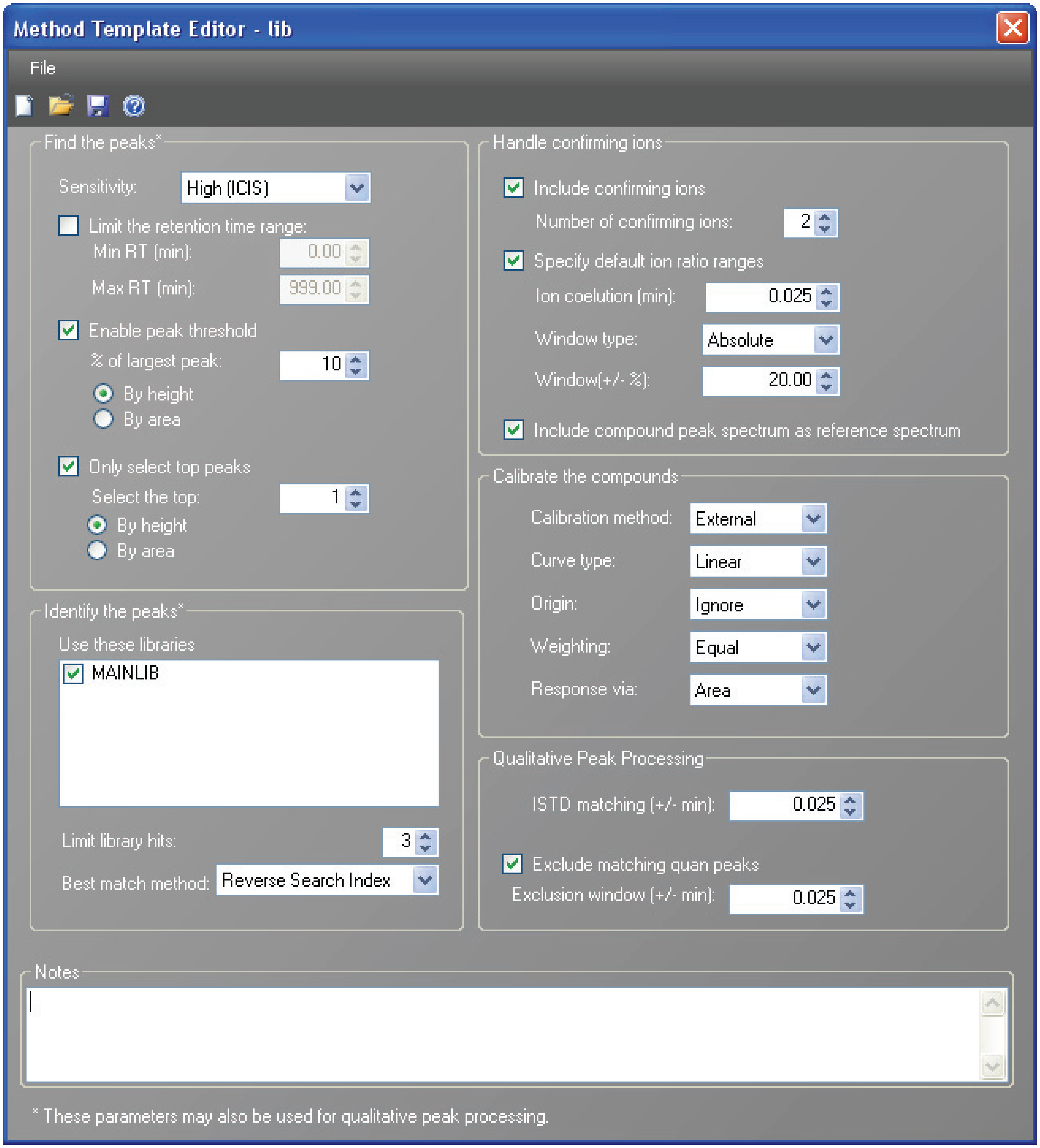


Table 43. Method Template Editor parameters (Sheet 1 of 3)

Parameter	Description
Find the peaks	
Sensitivity	Defines how extensively the peak detector algorithm searches for low-level peaks.
Limit the retention time range	Min RT specifies the beginning of the range. Max RT specifies the end of the range.
Enable peak threshold	Specifies whether to select peaks by relative height or area and the percentage of the highest peak that will result in compound selection.
Only select top peaks	Displays a specific number of the largest peaks by height or area.
Identify the peaks	
Use these libraries	Lists the libraries you can search.
Limit library hits	Specifies the number of hits returned when the system searches a spectrum against the selected libraries.
Best match method	Specifies how to sort the library searches. Valid values: Search Index, Reverse Search Index, Match Probability
Handle confirming ions	
Include confirming ions/ Number of confirming ions	Specifies the number of confirming ions, which are other ions in the spectrum whose ratio is compared to the quantitation ion to identify the compound. This value defaults to 2 because you typically perform a 3-ion experiment with one quan mass and two confirming ions.
Specify default ion ratio ranges	Enables the ion ratio range features. Ion coelution specifies the maximum difference in retention time between a confirming ion peak and the quantification ion peak. Window type specifies an Absolute or Relative calculation approach for determining the acceptable ion ratio range. Window (+/-%) specifies the acceptable ion ratio range.
Include compound peak spectrum as reference spectrum	Includes the peak spectrum in the processing method. Use this setting to perform a spectra comparison in Production.
Calibrate the compounds	
Calibration method	Specifies an internal or external calibration method.
Curve type	Specifies a linear, quadratic, or average RF curve type.

Table 43. Method Template Editor parameters (Sheet 2 of 3)

Parameter	Description
Origin	Specifies that the origin is ignored, forced, or included in the generated calibration curve. • Ignore: Specifies that the origin is not included as a valid point in the calibration curve when the curve is generated. When you select **Ignore**, the calibration curve might or might not pass through the origin. • Force: Specifies that the calibration curve passes through the origin of the data point plot when the calibration curve is generated. • Include: Specifies that the origin is included as a single data point in the calculation of the calibration curve. When you select **Include**, the calibration curve might or might not pass through the origin.
Weighting	Specifies the weighting for the calibration data points. • Equal: Specifies that the origin is included as a single data point in the calculation of the calibration curve. When you select **Equal**, the calibration curve might or might not pass through the origin. • 1/X: Specifies a weighting of 1/X for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their quantity. • 1/X^2: Specifies a weighting of 1/X^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their quantity. • 1/Y: Specifies a weighting of 1/Y for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of their response (or response ratio). • 1/Y^2: Specifies a weighting of 1/Y^2 for all calibration data points during the least-squares regression calculation of the calibration curve. Calibrants are weighted by the inverse of the square of their response (or response ratio).
Response via	Specifies if the EnviroLab Forms application uses area or height in response calculations. • Area: Specifies that the application use this peak area value in response calculations. • Height: Specifies that the application use this peak height value in response calculations.

Table 43. Method Template Editor parameters (Sheet 3 of 3)

Parameter	Description
Qualitative Peak Processing	
ISTD matching (+/- min)	Excludes all the target compounds found in the method and does not list these compounds in the TIC Report or in the Qual Mode view in the Data Review.
Exclude matching quan peaks	Compares the retention time of the internal standard in the method to the found retention time of the internal standard in the library search and excludes peaks outside the range.

Exporting SRM Data

In the EnviroLab Forms application, you can export your selected reaction monitoring (SRM) data to an XML file.

❖ To export SRM data to an XML file

1. Open the master method from which you want to export SRM data.
2. From the Method View task pane, click **Export SRM Data**.

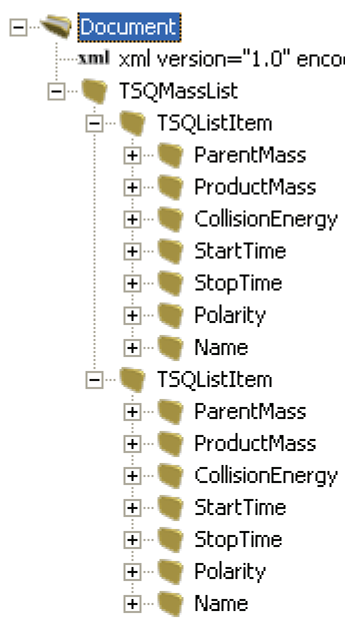
   The EnviroLab Forms application writes the data in the SRM table to the following file:

   `..\Thermo\EnviroLab Forms\Methods\`*`methodname`*`.xml`

   The data in this file matches the TSQ .xml data and can be used in the instrument method editor when you use the TSQ application.

   Note This command is available only when you check the Enable Compound Datastore option on the General page on the Application Configuration view. See "Application Configuration" on page 35.

SRM TSQ Quantum™ example



Working with Instrument Methods

An instrument method is a set of experiment parameters that define the operating settings for an autosampler, gas chromatograph (GC), mass spectrometer, and so on. Instrument methods are saved as file type .meth.

IMPORTANT Do not open the Thermo Foundation Instrument Configuration tool while the EnviroLab Forms application is running.

Follow these procedures:

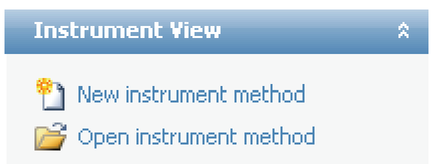
- To open the Instrument View
- To create a new instrument method
- To open an instrument method

❖ To open the Instrument View

1. Click **Method Development** from the dashboard or the navigation pane.

   The Method Development navigation pane opens.

2. Click the **Instrument View** task pane.

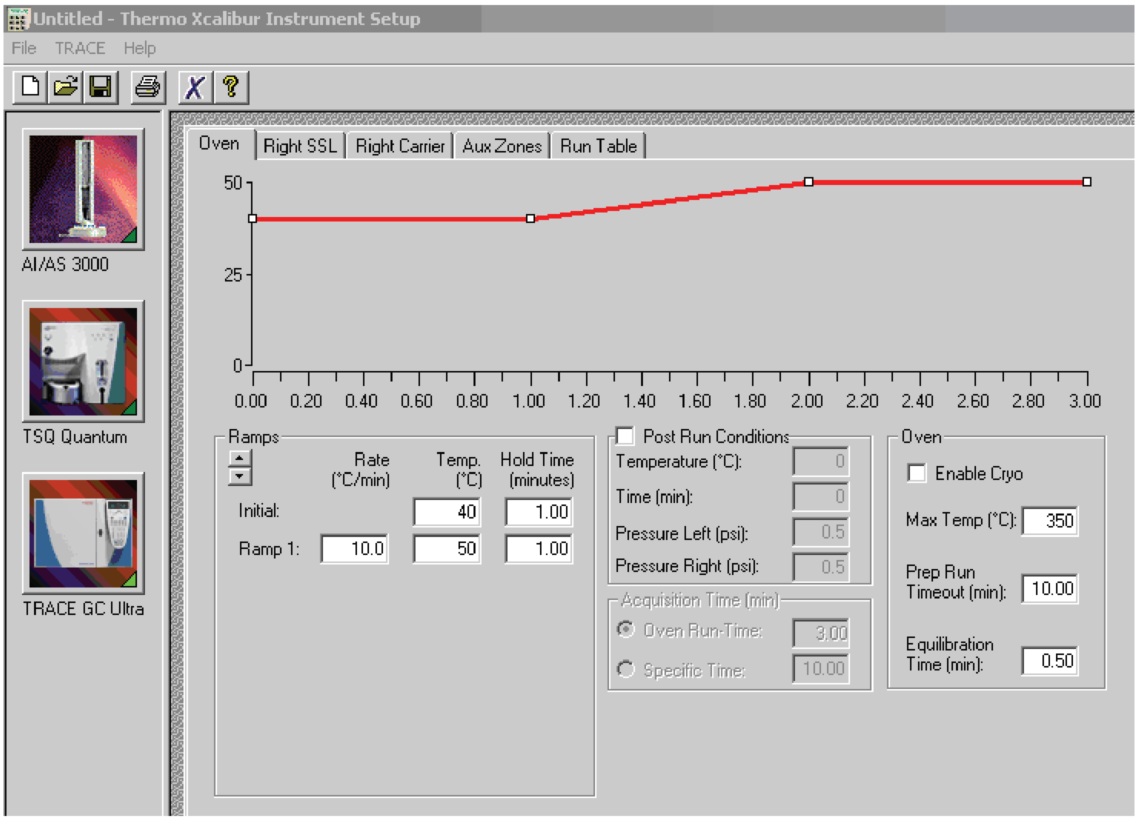


❖ To create a new instrument method

1. Click **New Instrument Method** in the Instrument View task pane.

   The Thermo Xcalibur Instrument Setup opens.

   This example instrument setup shows multiple configured instruments.

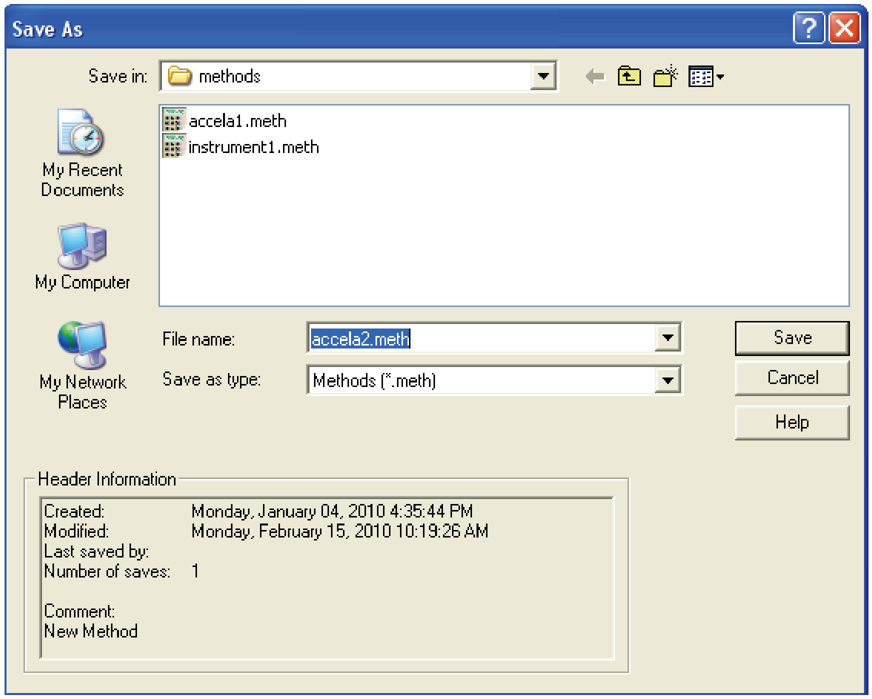


2. Click the icon for the instrument you want to use for the method.

3. Edit the values on the instrument page.

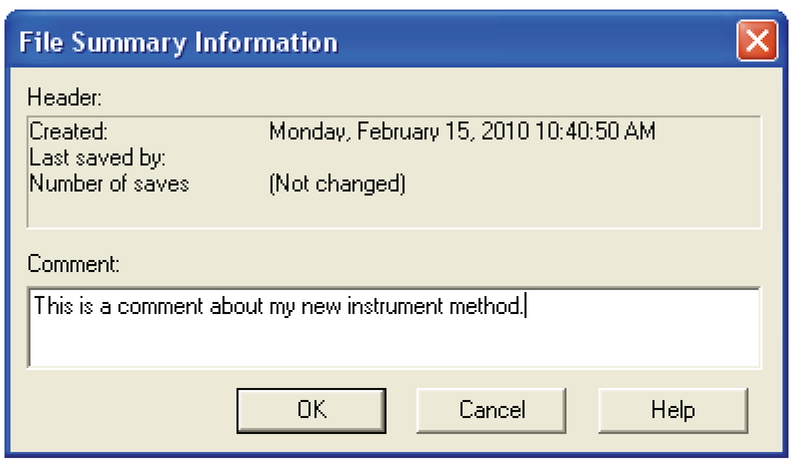
4. From the main menu on Thermo Xcalibur Instrument Setup, choose **File > Save As**.

   The Save As dialog box opens.



5. Select an instrument method name to overwrite or type a new name for the instrument method, and click **Save**.

   The File Summary Information dialog box opens.



6. (Optional) Type a comment about the new instrument method.
7. Click **OK**.

   The EnviroLab Forms application saves the new instrument method in the following folder:

   ..\Xcalibur\methods

❖ To open an instrument method

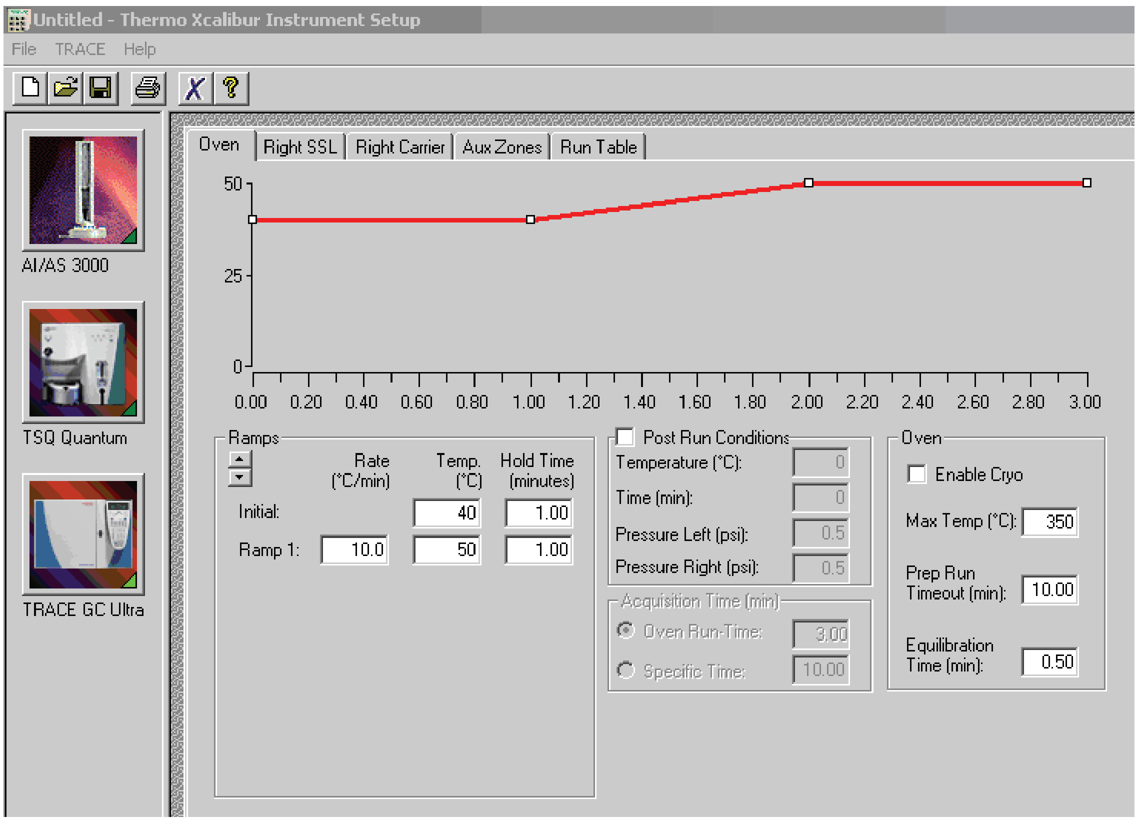
1. Click **Open Instrument Method** on the Instrument View task pane.

   An instrument method browser opens.

2. In the browser, select an instrument method from the list and open the file.

   The selected method opens in the Thermo Xcalibur Instrument Setup. You can edit this method and save the changes, or you can save this method to another name.

   This example instrument setup shows multiple configured instruments.



Note To open Help for any of your configured instruments, click **Help** on the instrument page.

Working with Development Batches

In the Development Batch view, you can test your instrument method in real time by creating and acquiring test samples. Development batches let you test different instrument methods and optimize parameters, such as MS source parameters and autosampler variables, to find the best conditions for a master method. Development batches are not designed for high throughput in everyday analysis.

This section includes instructions for the following tasks:

- Creating a Development Batch
- Editing Samples in a Development Batch
- Acquiring Samples in a Development Batch

Creating a Development Batch

You create a development batch to test your instrument method and use it to acquire samples only once. You cannot save a development batch.

Follow these procedures:

- To open the Development Batch view
- To specify a location for development batch data
- To add samples to the development batch
- To insert samples into the development batch
- To copy a sample

❖ To open the Development Batch view

1. Click **Method Development** from the dashboard or the navigation pane.

The Method Development navigation pane opens.

2. In the Method Development navigation pane, click **Development Batch**.

The Development Batch view opens a new, empty batch.

❖ To specify a location for development batch data

1. To specify a location for the files, click **Select Batch Location** in the Development Batch task pane.

   By default, the EnviroLab Forms application writes the temporary files, raw data files, and .sld method file to the following folder:

   ../Thermo/EnviroLab Forms/Temp

2. In the browser, do one of the following:

   - Locate the folder you want to use for the development batch files and click **OK**.

   –Or–

   - Do the following:

     a. Locate and select the folder where you want to create a new folder for the batch files.

     b. Click **Make New Folder**.

        The EnviroLab Forms application creates a new folder in the selected folder.

     c. Right-click the New Folder filename and choose **Rename** from the shortcut menu.

     d. Type the name for the folder.

     e. Click **OK**.

   The EnviroLab Forms application creates all development batch files in the specified folder.

❖ To add samples to the development batch

Do one of the following:

- Right-click and choose **Add Sample** from the shortcut menu.

–Or–

- Use the spin box to select the number of rows and click the **Add Sample** icon to add multiple sample rows.

New, empty samples appear at the end of the sample list.

❖ To insert samples into the development batch

1. Select the sample above which you want to insert empty samples.
2. Do one of the following:
   - Right-click and choose **Insert Sample** from the shortcut menu.

   –Or–

   - Use the spin box to select the number of rows and click the **Insert Sample** icon to insert multiple sample rows.

   The EnviroLab Forms application inserts new, empty samples above the selected sample.

   > **Note** You cannot insert samples into an empty batch. You must have at least one sample to select before you can use this icon.

❖ To copy a sample

1. Select the sample you want to copy.
2. Right-click and choose **Insert Copy Sample** from the shortcut menu.

   The EnviroLab Forms application adds a copy of the sample above the selected sample.

Figure 41. Completed Development Batch

Development Batch

	Filename	Sample ID	Sample name	Comment	Vial position	Injection volume	Instrument Method
1	File1	1			1	10.0	Pesticides and Herbicides
2	File2	2			2	10.0	Pesticides and Herbicides
3	File3	3			3	10.0	Pesticides and Herbicides
4	File4	4			4	10.0	Pesticides and Herbicides
5	File5	5			5	10.0	Pesticides and Herbicides

Editing Samples in a Development Batch

A development batch requires fewer parameters than a real batch, but the mechanism for managing the information is the same.

For detailed instructions about using the Copy Down or Fill Down commands to enter column values, see Appendix B, "Using Copy Down and Fill Down."

Follow these procedures:

- To enter column values
- To resize or reorganize the columns
- To remove selected samples from the list
- To remove all samples from the list

❖ To enter column values

1. Double-click the Filename column and type a file name for the raw data file.
2. (Optional) Enter values for the Sample Name, Sample ID, or Comment columns.
3. Enter a vial position for each sample.
4. Enter an injection volume for each sample.

   The minimum injection volume value allowed is 0.05 μL.
5. To enter an instrument method for each sample, click the down arrow in the Instrument Method column and select a method from the list.

   This list contains all the available instrument methods.

❖ To resize or reorganize the columns

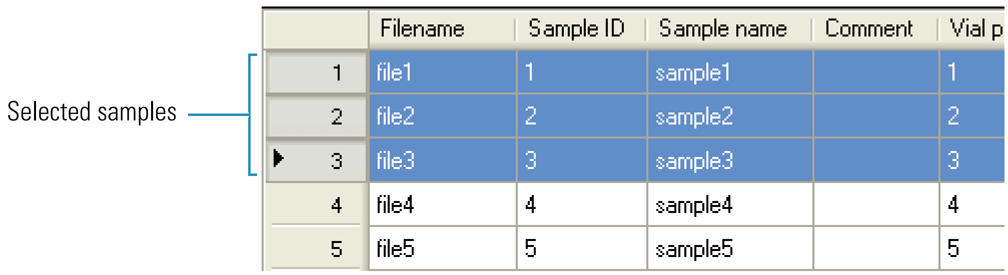
1. To resize a column, drag the header separator on the right side of the column.
2. To move a column, drag the column header.

   You cannot move the Filename column.

❖ To remove selected samples from the list

1. Select the samples you want to remove.

   Ensure that the first column indicates that the samples are selected.



	Filename	Sample ID	Sample name	Comment	Vial p
1	file1	1	sample1		1
2	file2	2	sample2		2
3	file3	3	sample3		3
4	file4	4	sample4		4
5	file5	5	sample5		5

2. Right-click and choose **Remove Selected Samples** from the shortcut menu.

❖ To remove all samples from the list

1. Click **New Sample List** in the Development Batch task pane.

2. One of the following happens:

   - If the samples in the current batch have all been acquired, the list is cleared.
   - If the samples in the current list have not been acquired, a message confirms that you want to clear them and start a new list.

3. To create a new empty list, click **Yes**.

Note You cannot save a development batch when you create a new one; you can only create, acquire, and discard each batch after you use it. The EnviroLab Forms application saves only the generated raw files in the specified batch location.

Acquiring Samples in a Development Batch

In a development batch, you can submit the entire batch for acquisition or submit only selected samples.

Follow these procedures:

- To acquire selected samples
- To acquire the batch
- To open the Qual Browser

❖ To acquire selected samples

1. Select the samples you want to acquire.
2. Right-click and choose **Submit Selected Samples** from the shortcut menu, or click the **Submit Selected Samples** icon, .

   The EnviroLab Forms application creates a raw data file for each selected sample. It writes the raw files and all temporary working files to the following folder:

   `../Thermo/EnviroLab Forms/Temp`

   When the acquisition is complete, the application deletes all the temporary working files. Only the raw files and a MethodDevelopment.sld file remain in the folder.

   If a sample is acquired more than once, the subsequent raw data files are time-stamped with the acquisition time.

❖ To acquire the batch

Right-click and choose **Submit Batch** from the shortcut menu, or click the **Submit Batch** icon, .

The EnviroLab Forms application creates a raw data file for each sample in the batch and a .sld method file. The EnviroLab Forms application writes the raw data files, the .sld method file, and all temporary working files to the specified folder.

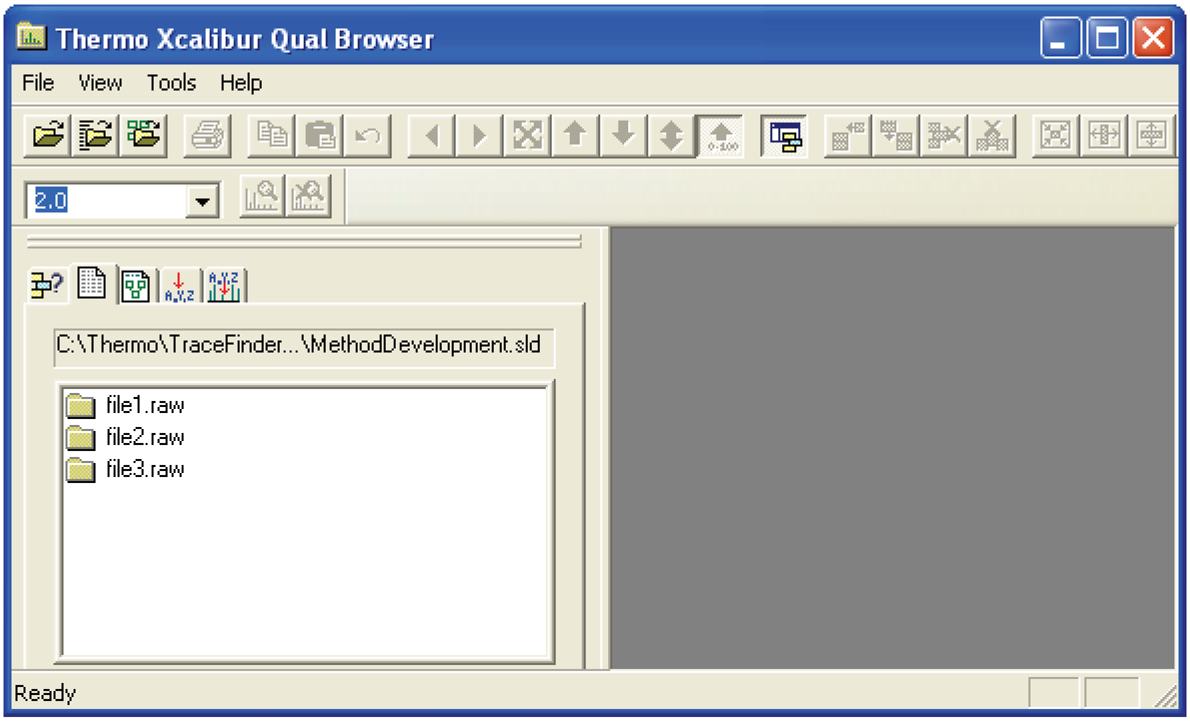
When the acquisition is complete, the application deletes all the temporary working files. Only the raw files and a MethodDevelopment.sld file remain in the folder.

If a sample is acquired more than once, the subsequent raw data files are time-stamped with the acquisition time.

❖ To open the Qual Browser

In the Development Batch task pane, click **Open Qual Browser**.

The Thermo Xcalibur Qual Browser opens.



For detailed instructions about using the Qual Browser, refer to the Qual Browser Help.

Using the Production Mode

This chapter includes instructions for using the features of the Production mode.

Contents

From the Production mode, you can create and review batches, review batch data and reports, and edit local methods.

❖ To access the Production mode

Click **Production** from the dashboard or the navigation pane.

The Production navigation pane opens.

Figure 42. Production navigation pane

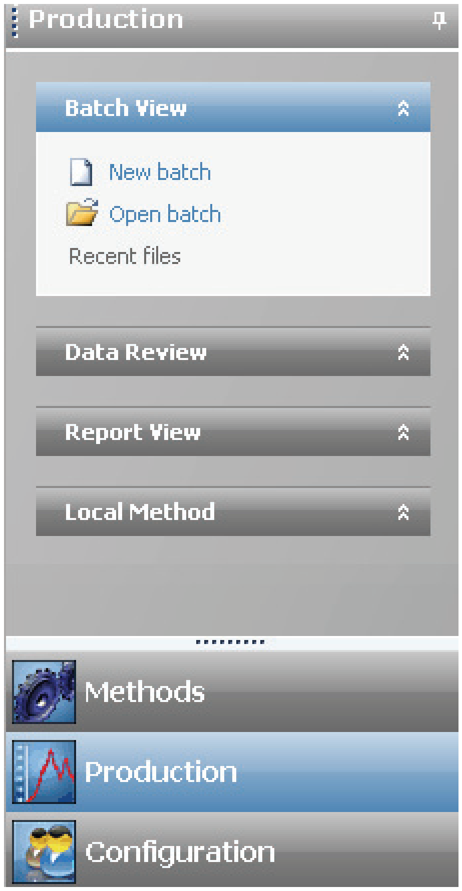


Table 44. Production navigation pane functions

Functions	Description
Batch View	See "Working in Batch View" on page 171.
New batch	Opens a new, unnamed batch with one Unknown sample. See "Creating a New Batch" on page 171.
Open batch	Opens the Open Batch dialog box where you can select a saved batch to edit. "Editing a Batch" on page 176.
Recent Files	Displays recently saved batches.
Data Review	See "Working in Data Review" on page 207.
Report View	See "Working in Report View" on page 239.
Local Method	See "Working in the Local Method View" on page 258.

Working in Batch View

From the Batch view, you can manually create and edit a new batch or open and edit a previously saved batch. You can also use a batch wizard to define a sequence of various sample types to be assembled into a batch of samples. When you submit a batch, you can acquire, process, or create reports for the submitted samples.

This section contains information about the following tasks:

- Creating a New Batch
- Editing a Batch
- Submitting a Batch
- Using a Batch Template
- Creating a Batch Using the Batch Wizard
- Specifying Sample Types

Creating a New Batch

From Batch view, you can create a new batch.

Follow these procedures:

- To create a batch
- To add samples to the list
- To insert samples into the list
- To import samples into the list
- To copy a sample
- To re-inject a sample
- To edit column values
- To rearrange the columns
- To remove samples from the list

❖ To create a batch

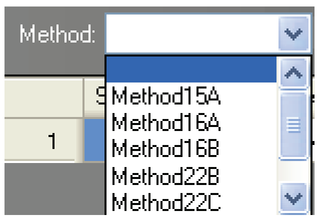
1. Click **Production** from the dashboard or the navigation pane.

The Production navigation pane opens.

2. In the Batch View task pane, choose **New Batch** or choose **File** > **New** > **Batch**.

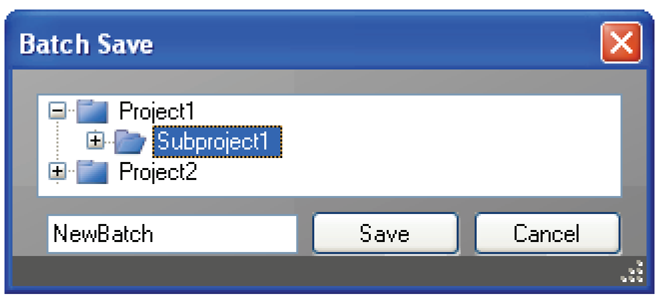
A new, unnamed batch opens with one Unknown sample. You must choose a master method before you can save your new batch.

3. Choose a master method from the Method list.



4. Choose **File** > **Save** > **Batch**.

The Batch Save dialog box opens.



5. Select a project and a subproject and enter a name for your new batch.

> **Tip** To enable the Save button, you must select a subproject and enter a unique batch name. If the Save button is not enabled, either you have entered a name that is already used or you have not selected a subproject.

6. Click **Save**.

❖ To add samples to the list

Right-click the sample list pane and choose **Add Sample** from the shortcut menu, or use the **Add Sample** icon to add multiple sample rows.

Add Sample icon

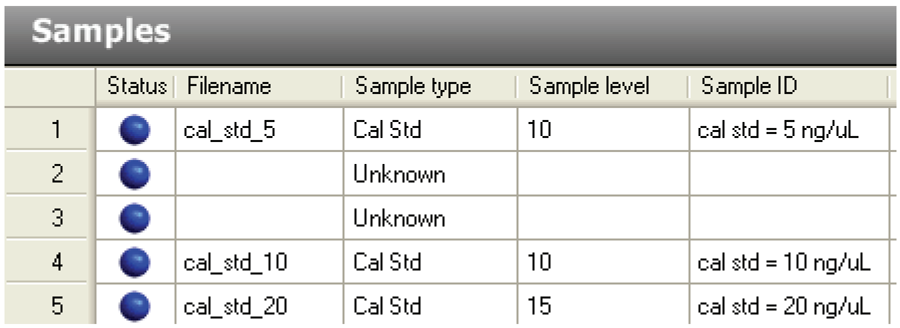
The EnviroLab Forms application adds the specified number of new, empty samples to the end of the sample list.

❖ To insert samples into the list

1. Select the sample above which you want to insert empty samples.
2. Right-click the sample list pane and choose **Insert Sample** from the shortcut menu, or use the Insert Sample icon to insert multiple sample rows.

   The new, Unknown samples are inserted above the selected sample.

   Samples

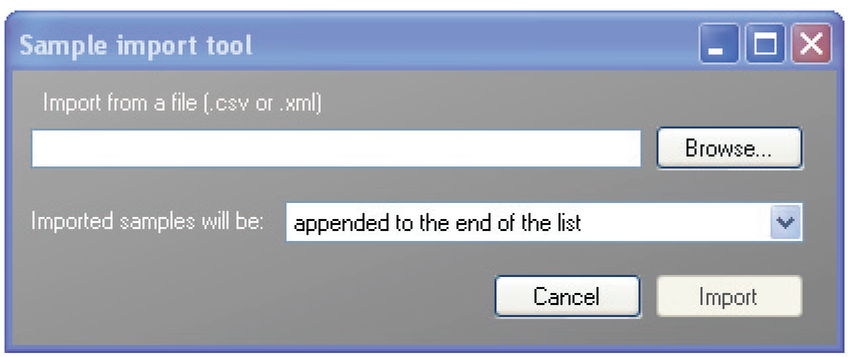
	Status	Filename	Sample type	Sample level	Sample ID
1		cal_std_5	Cal Std	10	cal std = 5 ng/uL
2			Unknown		
3			Unknown		
4		cal_std_10	Cal Std	10	cal std = 10 ng/uL
5		cal_std_20	Cal Std	15	cal std = 20 ng/uL

❖ To import samples into the list

1. Click **Import**.

   The Sample Import Tool dialog box opens.

   From this dialog box, you can import samples from a .csv file or .xml file.

2. Click **Browse** and select a .csv or .xml file that contains the samples you want to import.
3. From the Imported Samples Will be list, select **Appended to the End of the List** or **Inserted at the Selected Row**.
4. Click **Import**.

   The Sample Import Tool dialog box closes and the EnviroLab Forms application adds the specified samples to the Samples list.

❖ To copy a sample

1. Select the sample you want to copy.
2. Right-click and choose **Insert Copy Sample** from the shortcut menu.

   The EnviroLab Forms application inserts the copy above the selected sample.

❖ To re-inject a sample

1. From the Samples list, select the sample you want to re-inject.
2. Right-click and choose **Reinject this Sample** from the shortcut menu.

   The EnviroLab Forms application creates a copy of the selected sample and appends INJ001 to the file name. Additional re-injections of the same sample are numbered INJ002, INJ003, and so forth.

   The EnviroLab Forms application copies all parameter values from the original sample.

❖ To edit column values

1. For each sample, double-click the Filename column (or right-click and choose **Browse in Raw File** from the shortcut menu) and locate the raw data file to use for the sample.

   You can also browse in multiple raw data files to create multiple samples.
2. For each added sample, click the Sample Type column and select a sample type from the list.

Available ELF sample types			
Matrix Blank	Solvent	MS	MDL
Cal Std	Breakdown	MSD	Unknown
Chk Std	Tune	Tune/Breakdown	Unknown/TIC
LCS	LCSD	Meth Val	

3. For each Cal Std or Chk Std sample, click in the Sample Level cell and select a level from the list.

   The sample levels were defined in the master method. If there is nothing to select in the Sample Level list, do the following:

   a. Return to the Method Development mode.
   b. Open the method.
   c. Click the **Compounds** tab.
   d. Click the **Calibration Levels** tab.
   e. Add the levels.
   f. Save the method.
   g. Return to the Production mode, and begin this batch again.

   You must close your original batch without saving and start a new batch. For detailed instructions, see Chapter 4, "Using the Method Development Mode."

4. Enter or edit the values for the remaining columns.

   When you use the scroll bar at the bottom of the Samples list, the Status and Filename columns remains fixed and only the other columns scroll right and left.

   For instructions on automatically copying or filling values in these columns, see Appendix B, "Using Copy Down and Fill Down."

❖ To rearrange the columns

Do one of the following:

- To resize a column, drag the header separator on the right side of the column.
- To move a column, drag the column header.

When you close the EnviroLab Forms application, it saves the new column order and width.

> **Note** The Status and Filename columns can be swapped with each other, but they cannot be moved to any other location in the table.

❖ To remove samples from the list

1. Select the samples you want to remove.

   Ensure that the first column indicates that the samples are selected.

2. Right-click and choose **Remove Selected Samples** from the shortcut menu, or click the **Remove Samples** icon, .

Editing a Batch

In Batch view, you can open a saved batch and edit the list of samples. You can add, edit, or remove samples. If the batch has already been acquired, you can select specific samples for re-injection.

Follow these procedures:

- To open a saved batch
- To edit column values
- To re-inject a sample from a previously acquired batch
- To submit all samples in the batch
- To submit selected samples

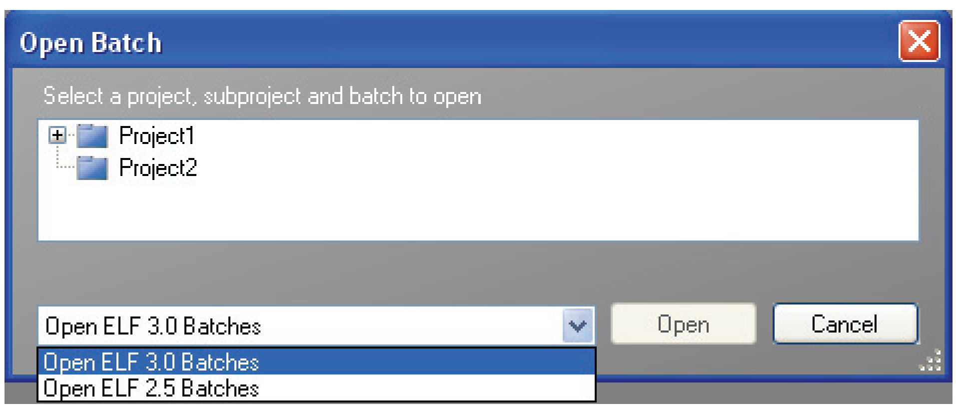
❖ To open a saved batch

1. Click **Production** from the dashboard or the navigation pane.

The Production navigation pane opens.

2. In the Batch View task pane, click **Open Batch** or choose **File > Open > Batch**.

The Open Batch dialog box opens where you can select a saved batch.



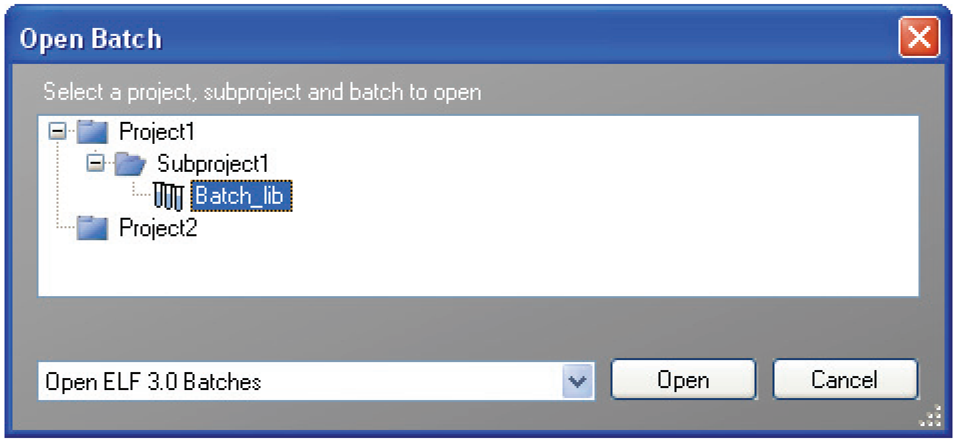
3. Select either **Open ELF 3.0 Batches** or **Open ELF 2.5 Batches**.
   - To open a ELF 3.0 batch, go to Step 4.
   - To open a ELF 2.5 batch, go to Step 5.
4. To open a ELF 3.0 batch, do the following:

   a. Select a project from the list of projects.

   b. Select a subproject from the list of subprojects.

c. Select a batch from the list of batches.

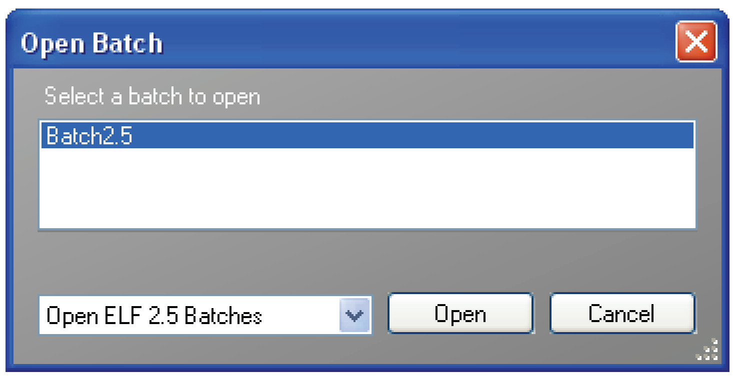
d. Click **Open**.



5. To open an ELF 2.5 batch, do the following:

a. Select a batch from the list of batches.

b. Click **Open**.



c. Edit the batch as you would any other batch.

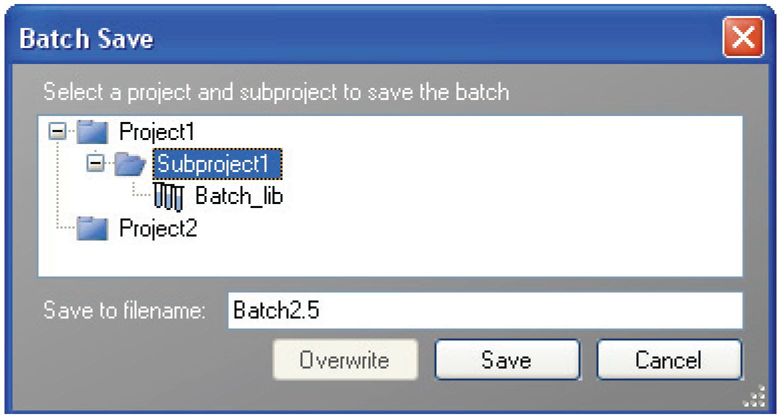
You cannot submit the batch for processing until you save it.

d. To save the batch, choose **File > Save > Batch** or click the **Save** icon, .

A text message informs you that the master method and instrument method for the batch will also be imported.

e. Click **OK** to dismiss the text message and continue saving the batch, or click **Cancel** to terminate the Save process.

The Batch Save dialog box opens.



f. Select a project and subproject where you will save the batch.

g. Type a name for the batch.

h. Do one of the following:

- Type a new name for the batch and click **OK**.

  –Or–

- Select a batch name to overwrite and click **Overwrite**.

❖ To open a batch from the Recent Files list

1. Click **Production** from the dashboard or the navigation pane.

   The Production navigation pane opens.

   When you save a batch, it is added to the Recent Files list. The Recent Files list displays a list of your most recently saved batches.

2. Click the batch name in the Recent Files list. Do not double-click.

   The selected batch opens in the Batch View.

❖ To edit column values

1. Type a file name in the Filename column for each sample, or right-click and choose **Browse in Raw File** from the shortcut menu.

You can also browse in multiple raw data files to create multiple samples.

2. Select a sample type from the Sample Type list box for each sample.

Available ELF sample types			
Matrix Blank	Solvent	MS	Unknown
Cal Std	Breakdown	MSD	LCS
Unknown/TIC	Tune	Tune/Breakdown	MDL
Chk Std	LCSD	Meth Val	

For a detailed description of sample types, see "Specifying Sample Types" on page 205.

3. For each Cal Std or Chk Std sample, select a level from the Sample Level list.

   The sample levels are defined in the master method. If there are no levels to select from the Sample Level list, ask a user with Supervisor or Manager permissions to edit the method and specify the levels.

   For detailed instructions about defining sample levels, see Chapter 4, "Using the Method Development Mode."

4. Type a vial position in the Vial Position column for the new sample.

5. Type a volume in the Injection Volume column for the new sample.

   The minimum injection volume value allowed is 0.05 µL.

❖ To re-inject a sample from a previously acquired batch

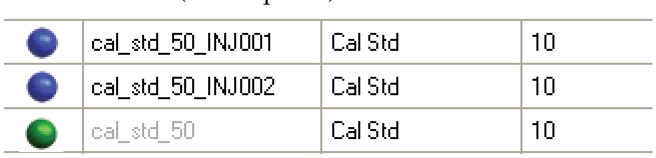
1. From the Samples list, select the sample you want to re-inject.

2. Right-click and choose **Reinject this Sample** from the shortcut menu.

   The EnviroLab Forms application creates a copy of the selected sample and appends INJ001 to the file name. Additional re-injections of the same sample are numbered INJ002, INJ003, and so forth.

   The EnviroLab Forms application copies all parameter values from the original sample.

   Previously acquired samples are indicated with a green status indicator (acquired and processed) and are grayed out. Samples created for re-injection are indicated with a blue status indicator (not acquired).



	cal_std_50_INJ001	Cal Std	10
	cal_std_50_INJ002	Cal Std	10
	cal_std_50	Cal Std	10

3. To save this batch with the new samples for re-injection, choose **File > Save > Batch** from the main menu.

Figure 43. Batch View page

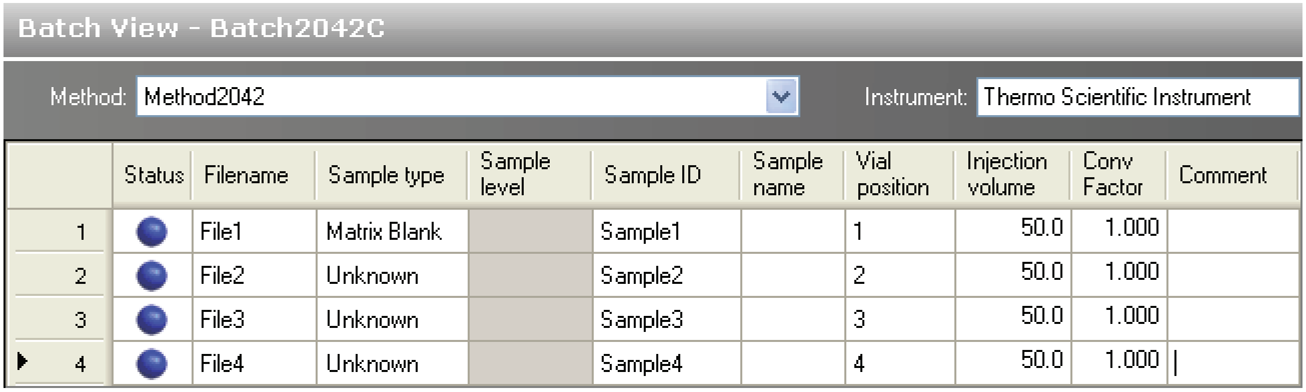


Table 45. Batch View parameters (Sheet 1 of 2)

Parameter	**Description**
Method	Method to use for acquiring or processing the batch.
Instrument	Instrument specified in the method used for the batch.
Column values	
Status	• Orange for samples that are currently acquiring • Blue for samples that have not been acquired • Yellow for samples that have been acquired and not processed • Green for samples that have been acquired and processed
Filename	Name of the raw data file that contains the sample data.
Sample type	Defines how the EnviroLab Forms application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, MDL, Solvent, Cal Std, MSD, Breakdown, Unknown, Unknown/TIC, Chk Std, MS, LCS, LCSD, Meth Val, Tune, or Tune/Breakdown
Sample level	The level defined for a calibration sample or quality control sample.
Sample ID	A user-defined alphanumeric string that identifies a sample.
Sample name	A user-defined name that identifies a sample.
Vial Position	The tray vial number used for the autosampler acquisition.

Table 45. Batch View parameters (Sheet 2 of 2)

Parameter	Description
Injection volume	The injection volume in microliters of sample to be injected. Minimum value: 0.05 When you are using an autosampler, you can set the default injection volume in the autosampler dialog box in the Instrument View. The minimum and maximum injection volumes that you can use depend on the autosampler you configure. The usable range depends on the injection mode and might be smaller than the range displayed.
Conv Factor	Adjustment made to the injected concentration.
Comment	A user-defined comment for the sample.
Shortcut menu commands	
Add sample	Adds a single empty row to the sample grid.
Insert sample	Inserts a single empty row to the sample grid above the selected row.
Insert copy sample	Copies the currently selected row and inserts a copy above the row.
Reinject this sample	Creates a copy of the selected sample and appends INJ001 to the file name. Additional re-injections of the same sample are numbered INJ002, INJ003, and so forth.
Remove selected samples	Removes selected samples from the sample grid.
Import samples	Opens the Sample Import Tool. Follow the instructions "To import samples into the list" on page 173.
Submit selected samples	Submits all selected samples to be acquired or processed.
Submit batch	Submits all samples in the batch to be acquired or processed.
Browse in raw file	Opens a dialog box where you can select a raw data file to use for the selected sample row. You can also browse in multiple raw data files to create multiple samples.

Submitting a Batch

In Batch view, you can submit an entire batch or only selected samples in the batch. When you submit a batch, you can choose to acquire, process, or create reports for the submitted samples.

❖ To submit all samples in the batch

1. Do one of the following:
   - Right-click and choose **Submit Batch** from the shortcut menu.

     –Or–
   - Click the **Submit Batch** icon, .
2. From the Submit Options dialog box, select if you want to process data and create reports in addition to acquiring the samples.
   - You can choose to process samples that have already been acquired.
   - You can choose to acquire and process unacquired samples (including re-injections).
   - You can choose to create reports for all submitted samples.
3. Click **OK**.

❖ To submit selected samples

1. Select the samples you want to submit.
2. Do one of the following:
   - Right-click and choose **Submit Selected Samples** from the shortcut menu.

     –Or–
   - Click the **Submit Selected Samples** icon, .
3. From the Submit Options dialog box, select if you want to process data and create reports in addition to acquiring the samples.
   - You can choose to process samples that have already been acquired.
   - You can choose to acquire and process unacquired samples (including re-injections).
   - You can choose to create reports for all submitted samples.
4. Click **OK**.

Observing the Real-time Display

You can access the real-time display from the dashboard and from any mode in the EnviroLab Forms application.

❖ To access the real-time display from the dashboard

Click **Real Time Status**.

The real-time status displays at the bottom of the dashboard.

❖ To access the real-time display from any of the modes

Click **Real time status**.

The real-time status displays at the bottom of the current view.

The real-time status display has four additional pages of information:

- Acquisition Page
- Instrument Page
- Devices Page
- Queues Page

Figure 44. Acquisition page

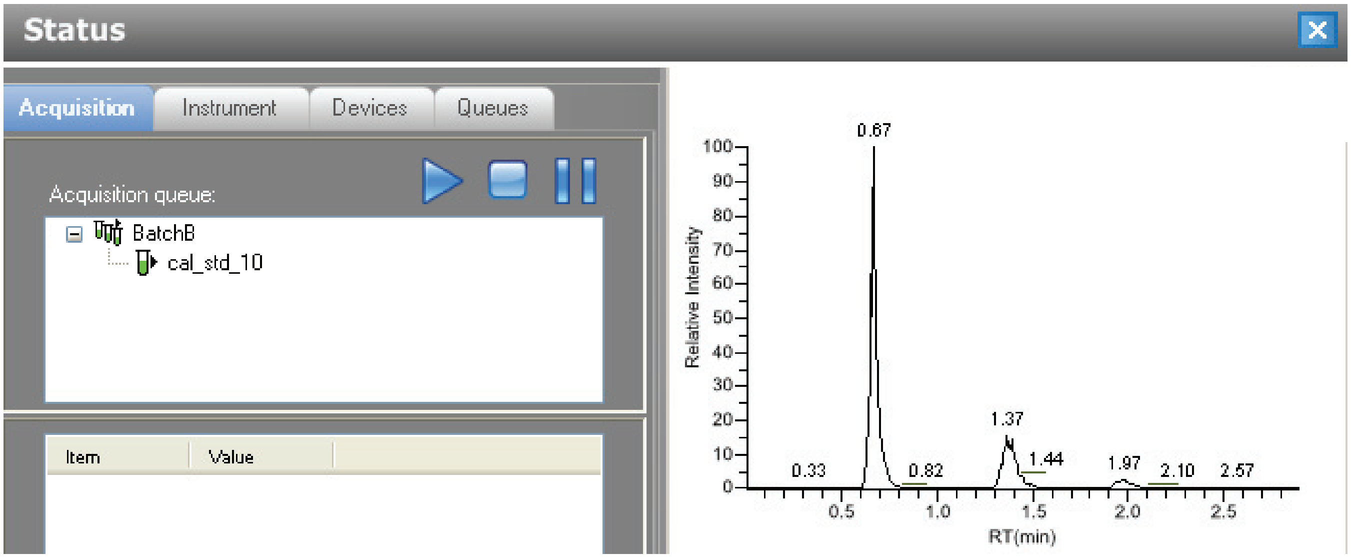


Table 46. Acquisition Queue functions

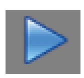
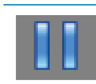
Function	Description
	Start button starts an acquisition.
	Stop button stops the acquisition for the current sample and begins the next sample in the batch.
	Pause button pauses the batch queue. Use the Start button to restart a paused acquisition.

Figure 45. Instrument page

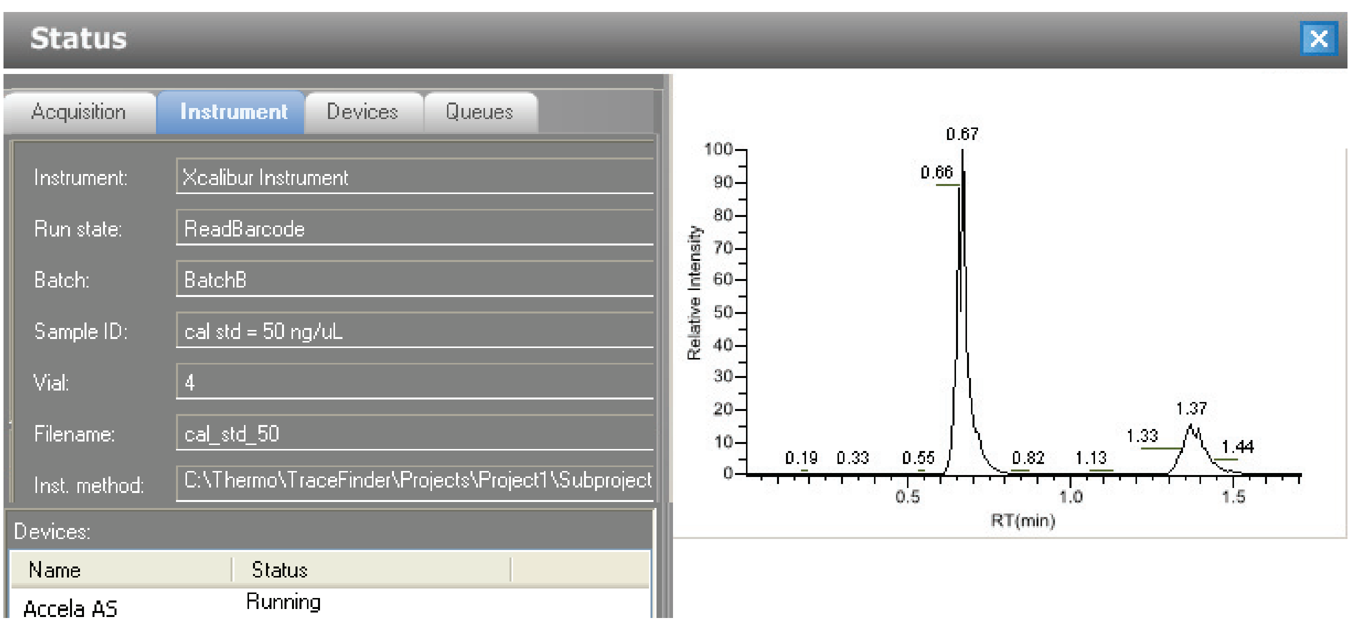


Figure 46. Devices page

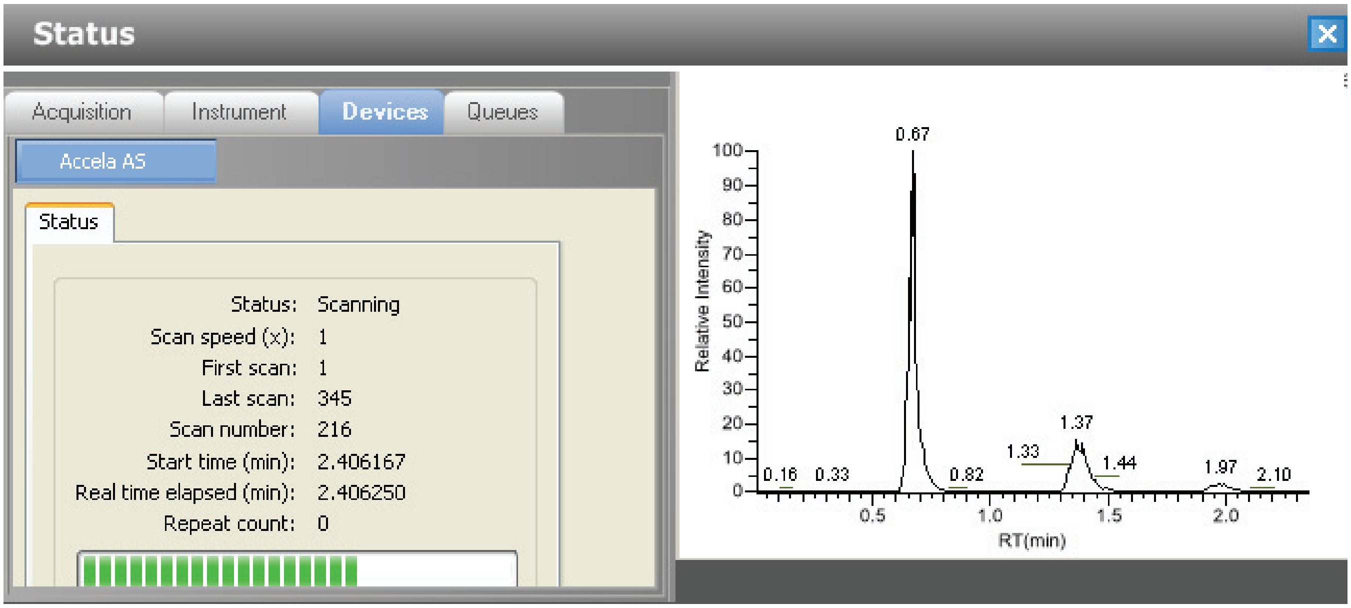
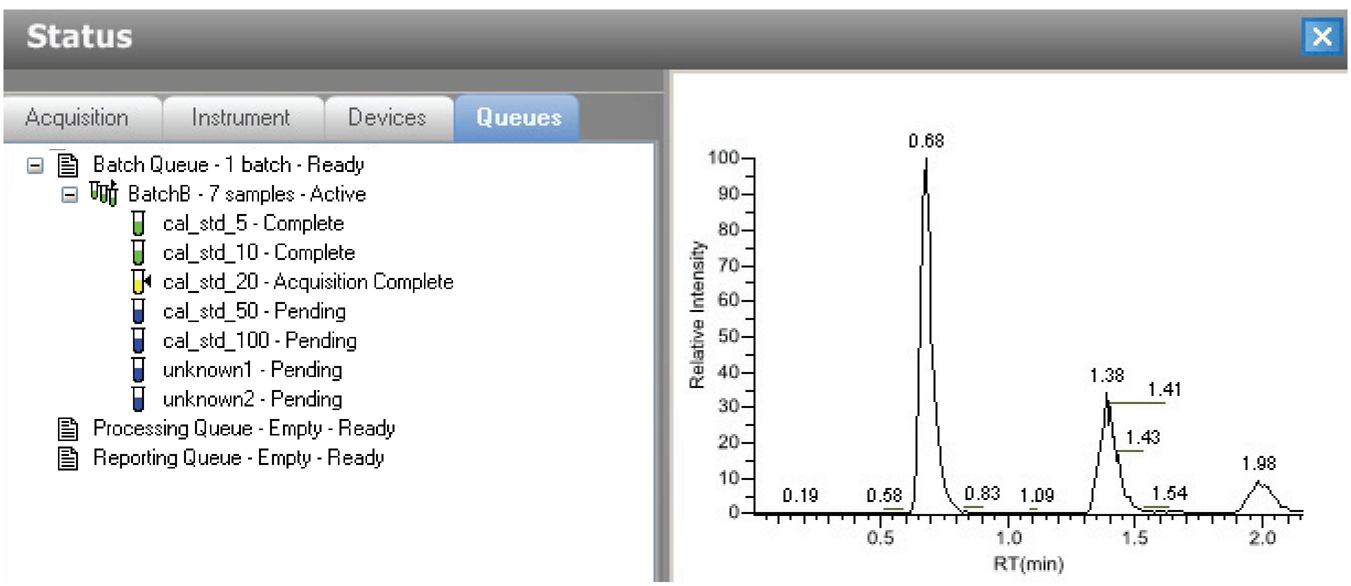


Figure 47. Queues page



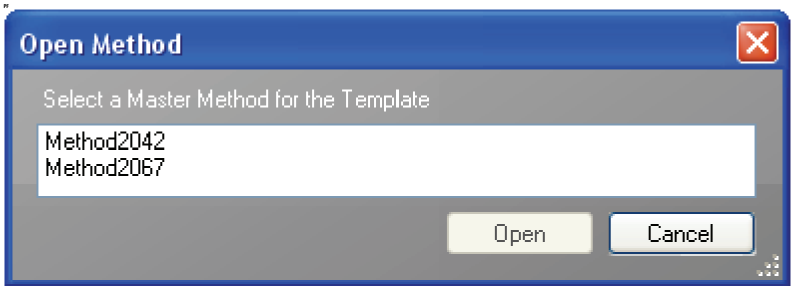
Using a Batch Template

Batches are created as a routine operation and, because the nature and types of batches are often similar (in some cases specified by laboratory operating procedure), you can define a batch template that supplies the basic structure of a batch.

❖ To create a new batch template

1. Choose **New > Batch Template** from the application menu.

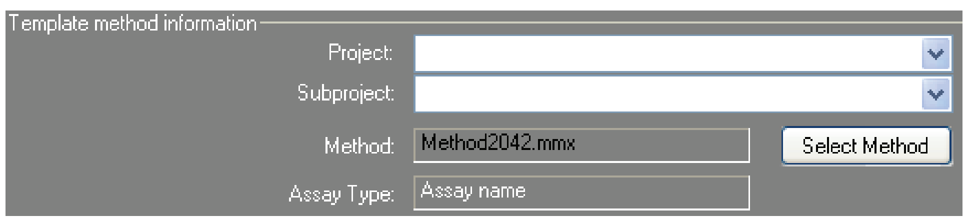
   The Open Method dialog box opens where you can select a master method to use for your template.



2. Select a master method and open the file.

   The Batch Template Editor opens. See "Batch Template Editor" on page 190.

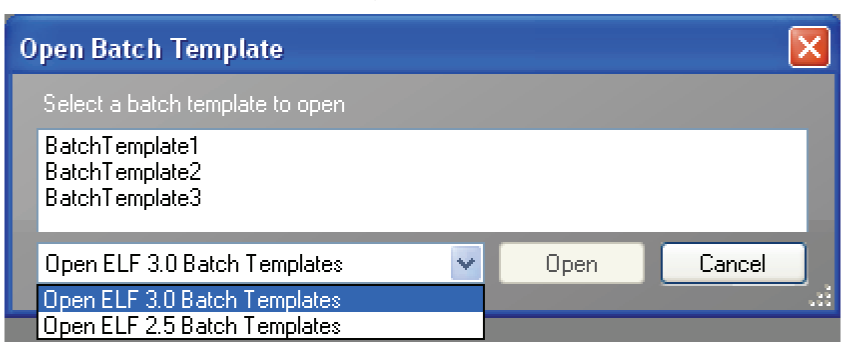
   The editor uses the selected master method for the template.



❖ To open a batch template

1. Choose **File > Open > Batch Template** from the main menu.

   The Open Batch Template dialog box opens.



2. Select the set of batch templates you want to use.

   The EnviroLab Forms 3.0 application lets you use LabForms 2.5 batch templates.

3. Select a batch template and open the file.

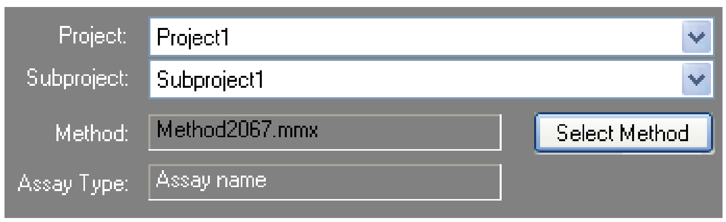
   The Batch Template Editor opens. See "Batch Template Editor" on page 190.

❖ To specify template information

1. From the Project list, select a project name.
2. From the Subproject list, select a subproject name.

> **Tip** If there are no projects or subprojects to choose, go to the Project Administration view of the Configuration mode and create a new subproject. See "Project Administration" on page 26.

3. To change the current method, click **Select Method** and select a new method.



❖ To add a sample to the list

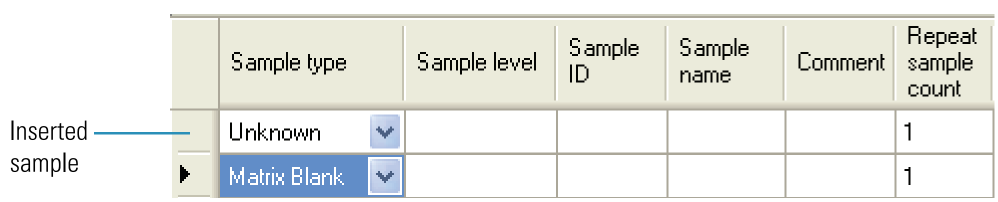
Right-click the sample list pane and choose **Add Sample** from the shortcut menu, or click the **Add Sample** icon, .

The EnviroLab Forms application adds a new, Unknown sample to the end of the Samples list.

❖ To insert a sample into the list

1. Select the sample above which you want to insert a new, Unknown sample.
2. Right-click the Samples list pane and choose **Insert Sample** from the shortcut menu.

   The new, Unknown sample is inserted above the selected sample.



❖ To copy a sample

1. Select the sample you want to copy.
2. Right-click and choose **Insert Copy Sample** from the shortcut menu.

   The EnviroLab Forms application inserts the copy above the selected sample.

❖ To remove samples from the list

1. Select the sample you want to remove.

   Use the Shift or Ctrl keys to select multiple samples.

2. Right-click and choose **Remove Selected Samples** from the shortcut menu, or click the **Remove Sample** icon, .

   The EnviroLab Forms application removes the selected samples from the Samples list.

❖ To edit sample values

1. For each sample, click the Sample Type column and select a sample type from the list.

Available ELF sample types			
Matrix Blank	Solvent	MS	Unknown
Cal Std	Breakdown	MSD	LCS
Unknown/TIC	Tune	Tune/Breakdown	MDL
Chk Std	LCSD	Meth Val	

2. For each Cal Std or Chk Std sample, click in the Sample Level cell and select a level from the list.

   The sample levels were defined in the master method. If there is nothing to select in the Sample Level list, do the following:

   a. Return to the Method Development mode.

   b. Open the method.

   c. Click the **Compounds** tab.

   d. Click the **Calibration Levels** tab.

   e. Add the levels.

   f. Save the method.

   g. Return to the Production mode, and begin this batch again.

   You must close your original batch without saving and start a new batch. For detailed instructions, see Chapter 4, “Using the Method Development Mode.”

3. (Optional) Type a sample ID, sample name, or comment.

❖ To add multiple samples of the same type

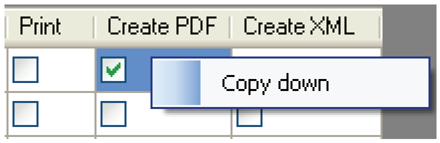
In the Repeat Sample Count column, type the number of samples you want to create for this sample type.

When you use this template to create a batch, the batch will contain this number of individual samples of the specified type.

❖ To specify report options

1. To specify the type of report output to create for each report type, select the check box in the appropriate column.

2. To duplicate the output type for all reports, click the cell to select it, then right-click and choose **Copy Down** from the shortcut menu.



All check boxes in the column below the selected cell duplicate the selected or cleared state of the selected cell.

By default, all report output types are cleared.

❖ To specify active compounds

1. In the sample table, click anywhere in the sample row to select the sample for which you want to specify active compounds.

   Compound selections are specific to a sample. You can select different compounds for each of the samples even if they are the same sample type.

2. In the Compound Active Status area, select the Active check box for each compound you want to identify in the selected sample.

   If you have created compound groups, you can make the entire group active or inactive. Right-click and choose the group from the list.

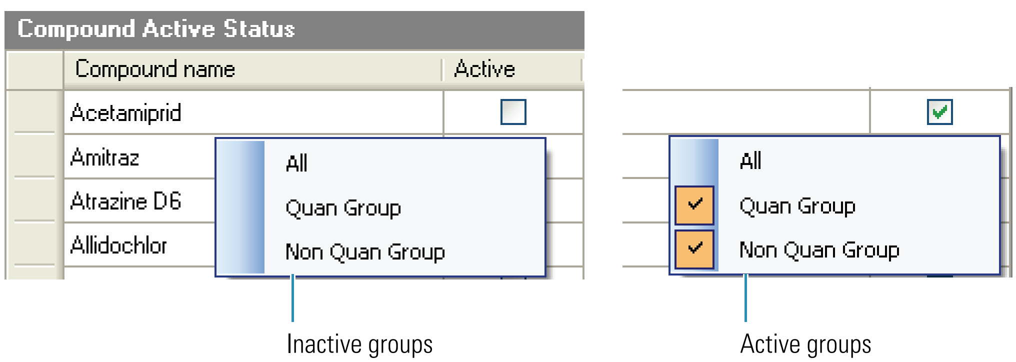


Figure 48. Batch Template Editor

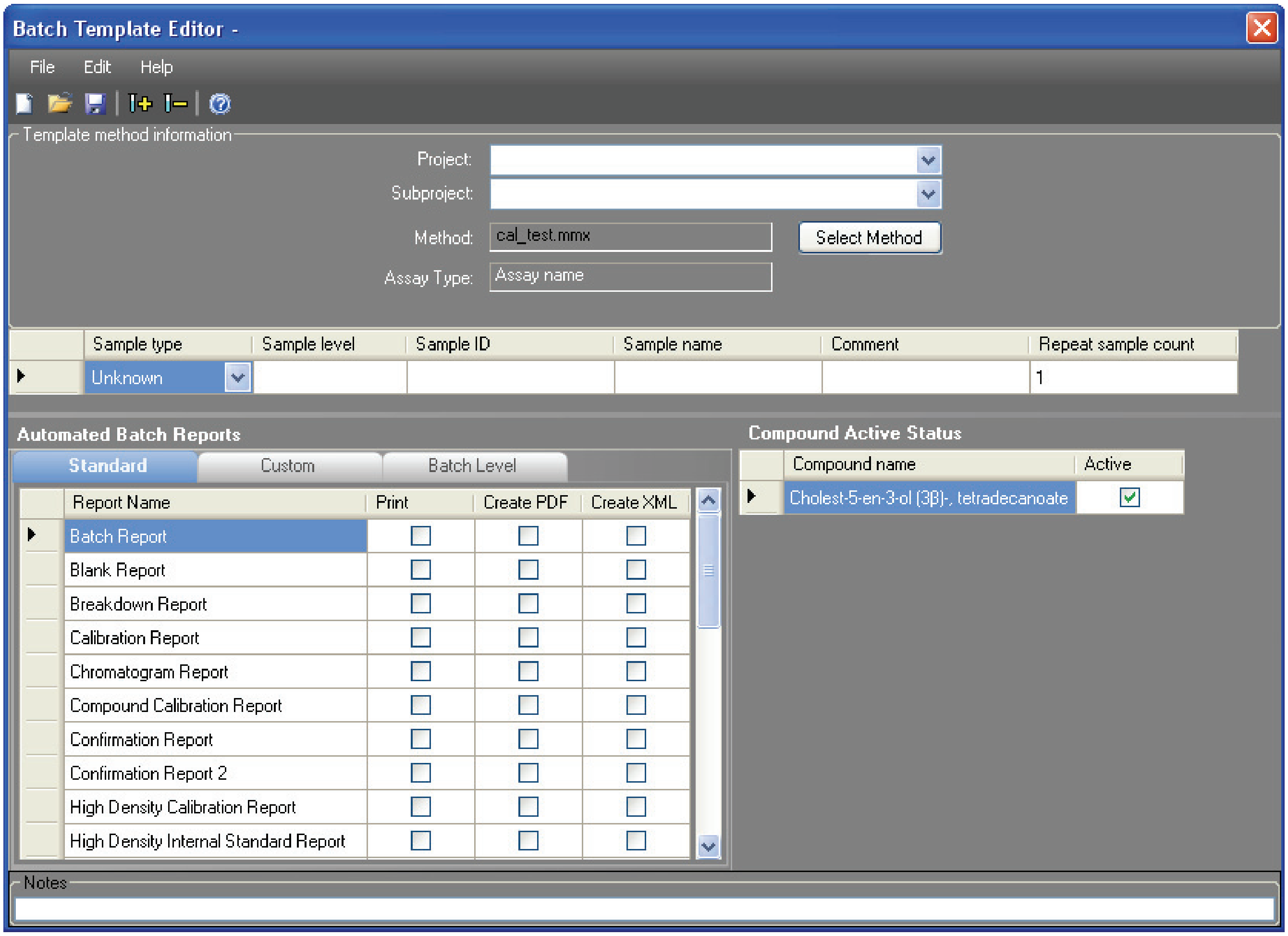


Table 47. Batch Template Editor parameters (Sheet 1 of 2)

Parameter	Description
Template Method Information	
Project	The top-level project for the batch.
Subproject	The lower-level project for the batch.
Method	The master method to use for the batch. The Select Method button opens the Open Method dialog box where you can select a master method for the batch template.

Table 47. Batch Template Editor parameters (Sheet 2 of 2)

Parameter	Description
Assay Type	The name for the analysis type to be targeted by the method. The assay type associates the method with the analysis of a compound or specific class of compounds (for example, an assay type of PAH might be used for the analysis of Polynuclear Aromatic Hydrocarbons). The EnviroLab Forms application uses this assay type in the batch template. You can also select an appropriate combination of method and batch template.
Column values	
Sample type	Defines how the EnviroLab Forms application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, MDL, Solvent, Cal Std, MSD, Breakdown, Unknown, Unknown/TIC, Chk Std, MS, LCS, LCSD, Meth Val, Tune, or Tune/Breakdown
Sample level	The level defined for a calibration sample or quality control sample.
Sample ID	A user-defined alphanumeric string that identifies a sample.
Sample name	A user-defined name that identifies a sample.
Comment	A user-defined comment for the sample.
Repeat sample count	Number of samples to create for this sample type.
Standard	
Report Name	The name of a report.
Print	Reports to be sent to the printer.
Create PDF	Reports to be saved as PDF files.
Create XML	Reports to be exported in XML format.
Custom	
Report Name	The name of a report.
Print	Reports to be sent to the printer.
Create XLS	Reports to be exported in XLS format.
Batch Level	
Report Name	The name of a report.
Print	Reports to be sent to the printer.
Create XLS	Reports to be exported in XLS format.
Compound Active Status	
Compound name	List of all compounds for the method.
Active	Identifies compounds to identify in the selected sample.

Creating a Batch Using the Batch Wizard

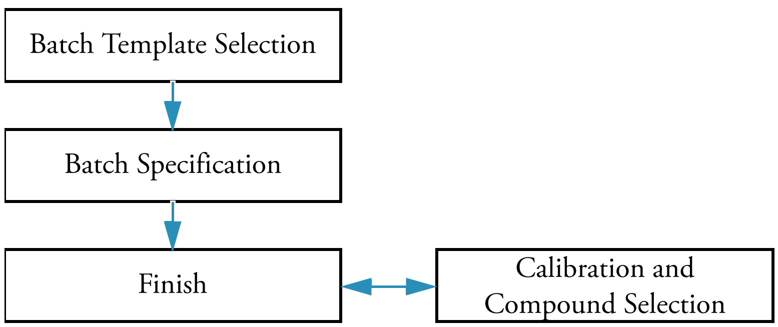
Using the Batch Wizard, you can define a sequence composed of various sample types to be assembled into a batch of samples. The batch wizard requires a batch template and a master method to compile a standardized sample batch.

Before you can create a batch with the Batch Wizard, you must have a master method and a batch template. See “Creating a New Master Method” on page 51 and “Using a Batch Template” on page 186.

Use the following procedures in the Batch Wizard to create and submit a batch:

- Selecting a Batch Template
- Specifying a Batch
- Submitting the Batch
- (Optional) Selecting Calibration Files and Compounds

The Batch Wizard includes the following pages:



❖ To open the Batch Wizard

Choose **File > New > Batch Using Wizard** from the main menu.

The Batch Template Selection page of the Batch Wizard opens. See “Batch Template Selection page” on page 194.

Selecting a Batch Template

From the Batch Template Selection page, you can create a list of samples to acquire or process.

❖ To create a sample list

1. From the Project list, select a project.
2. From the Subproject list, select a subproject.

   The Available Templates area lists all the templates in the specified subproject.

3. Select a starting vial position.

   The default is vial position 1, but you can choose to start your acquisition at any vial position.

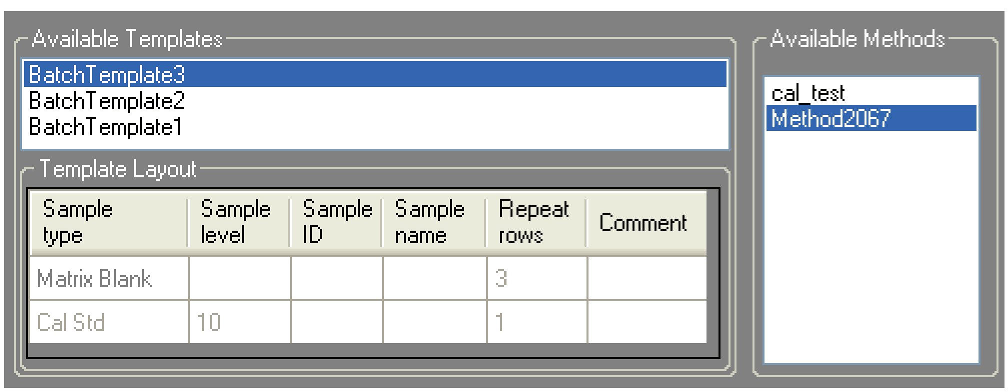
4. (Optional) To simplify the sample list, select the **Quick Mode** check box.

   Quick Mode limits the columns of information in the Batch Specification page to the following:

   - Sample Type
   - Sample ID
   - Injection Volume
   - Conversion factor

5. From the Available Templates list, select a template that defines the layout you want to use.

   The Template Layout area displays sample information in the selected batch template and a list of methods that use the same assay type as your template.

6. Select an available method.

   By default, the method used to create the batch template is selected, but you can choose any method in the Available Methods list.

7. To go to the next wizard page, click **Next**.

   From the Batch Specification page of the wizard, you can customize the batch.

Figure 49. Batch Template Selection page

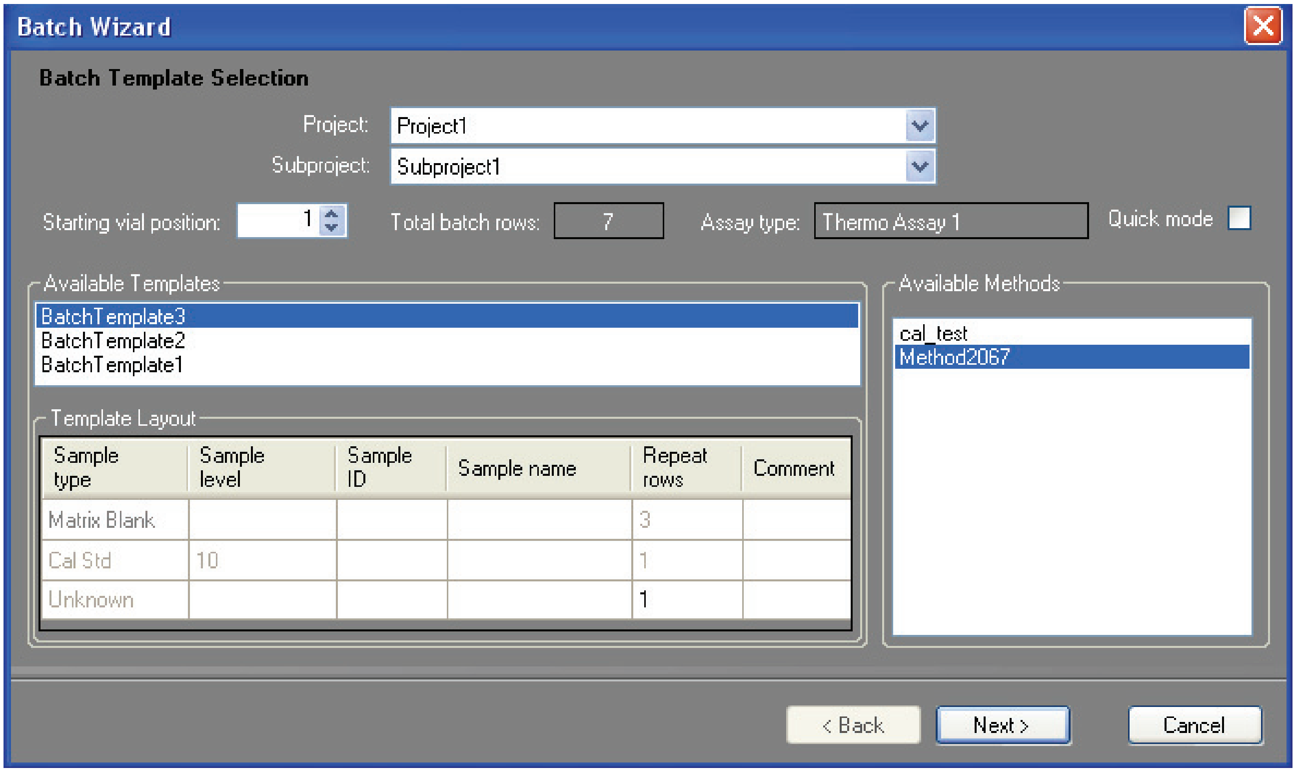


Table 48. Batch Template Selection parameters (Sheet 1 of 2)

Parameter	Description
Starting vial number	The vial position at which you want to begin acquiring samples. Default: 1
Total batch rows	The number of sample rows in the batch template.
Assay type	The assay type specified in the master method used to create the batch template.
Quick mode	Limits the columns of information in the Batch Specification page to the following: • Sample Type • Sample ID • Injection Volume • Conversion Factor
Available Templates	All batch templates saved in the ..\Thermo\EnviroLab Forms\Templates\Batches folder.
Template Layout	Displays sample information in the selected batch template.
Available Methods	Lists all master methods created with the same assay type as the selected batch template.

Table 48. Batch Template Selection parameters (Sheet 2 of 2)

Parameter	Description
Next	Returns you to the Batch Specification page where you can enter a sample ID, a sample name, or comment. You can also add or remove samples from the sample list or edit the column values for the samples. See "Specifying a Batch" on page 195.
Cancel	Immediately exits the Batch Wizard and does not save the batch. There is no confirming message.

Specifying a Batch

From the Batch Specification page, you must enter either a sample ID, sample name, or comment. You can also add or remove samples from the sample list or edit the column values for the samples. The batch template might contain many samples that you do not want to use for your batch. If you do not enter a sample ID, sample name, or comment for these samples, the EnviroLab Forms application discards them when you save the batch.

❖ To enter a sample ID, sample name, or comment

1. In the Sample ID column, type an identifier.

   The identifier can be any text string.

2. In the Sample Name column, type a name.

   The name can be any text string.

3. In the Comment column, type a comment.

   The comment can be any text string.

Note The EnviroLab Forms application requires at least one of these fields to acquire a sample. When the batch begins acquisition, it discards any sample that does not have a value in at least one of these fields.

Follow these procedures:

- To simplify the sample list
- To add samples to the batch
- To remove samples from the batch
- To insert samples into the batch
- To copy a sample
- To move a sample up or down in the sample list
- To browse in a raw data file

❖ To simplify the sample list

Select the **Quick Mode** check box.

In Quick Mode, the Batch Specification page displays only the following columns:

- Sample Type
- Sample ID
- Injection Volume
- Conversion Factor

> **Note** The shortcut menu and its functions are not available when Quick Mode is selected.

❖ To add samples to the batch

1. Right-click and choose **Add Sample** from the shortcut menu, or click the add sample icon, .

   The EnviroLab Forms application adds a new, Unknown sample to the end of the sample list.

2. In the Filename column for each sample, type a file name.

   > **Note** Alternately, you can right-click and choose **Browse in Raw File** from the shortcut menu. Follow the instructions "To browse in a raw data file" on page 198.

3. Select a sample type from the Sample Type list box for each sample.

Available ELF sample types			
Matrix Blank	Solvent	MS	Unknown
Cal Std	Breakdown	MSD	LCS
Unknown/TIC	Tune	Tune/Breakdown	MDL
Chk Std	LCSD	Meth Val	

   For a detailed description of sample types, see "Specifying Sample Types" on page 205.

4. For each Cal Std or Chk Std sample, select a level from the Sample Level list.

   The sample levels are defined in the master method. If there are no levels to select from the Sample Level list, a user with Supervisor or Manager permissions must edit the method and specify the levels.

   For detailed instructions about defining sample levels, see Chapter 4, "Using the Method Development Mode."

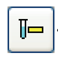
5. In the Vial Position column for the new sample, type a vial position.
6. In the Injection Volume column for the new sample, type a volume.

   The minimum allowed injection volume value is 0.05 µL.

7. (Optional) Type or edit the values for the remaining columns.

> **Note** This function is not available when Quick Mode is selected.

❖ To remove samples from the batch

1. Select the samples you want to remove.
2. Right-click and choose **Remove Selected Samples** from the shortcut menu, or click the remove samples icon, .

   The EnviroLab Forms application removes the selected samples from the sample list.

> **Note** This function is not available when Quick Mode is selected.

❖ To insert samples into the batch

1. Select the sample above which you want to insert a new sample.
2. Right-click and choose **Insert Sample** from the shortcut menu.

   The EnviroLab Forms application inserts a new, Unknown sample above the selected sample.

> **Note** This function is not available when Quick Mode is selected.

❖ To copy a sample

1. Select the sample you want to copy.
2. Right-click and choose **Insert Copy Sample** from the shortcut menu.

   The EnviroLab Forms application inserts the copy above the selected sample.

> **Note** This function is not available when Quick Mode is selected.

❖ To move a sample up or down in the sample list

1. Select the sample you want to move.
2. Right-click and choose **Move Sample Up** or **Move Sample Down** from the shortcut menu.

   The EnviroLab Forms application moves the selected sample up or down one row in the sample list.

> **Note** This function is not available when Quick Mode is selected.

❖ To browse in a raw data file

1. Double-click the Filename column, or right-click and choose **Browse in Raw File** from the shortcut menu.

   A dialog box opens where you can select a raw data file to use for the sample. You can also browse in multiple raw data files to create multiple samples.

2. Locate the raw data file to use for the sample and click **Open**.

Note This function is not available when Quick Mode is selected.

Figure 50. Batch Specification page

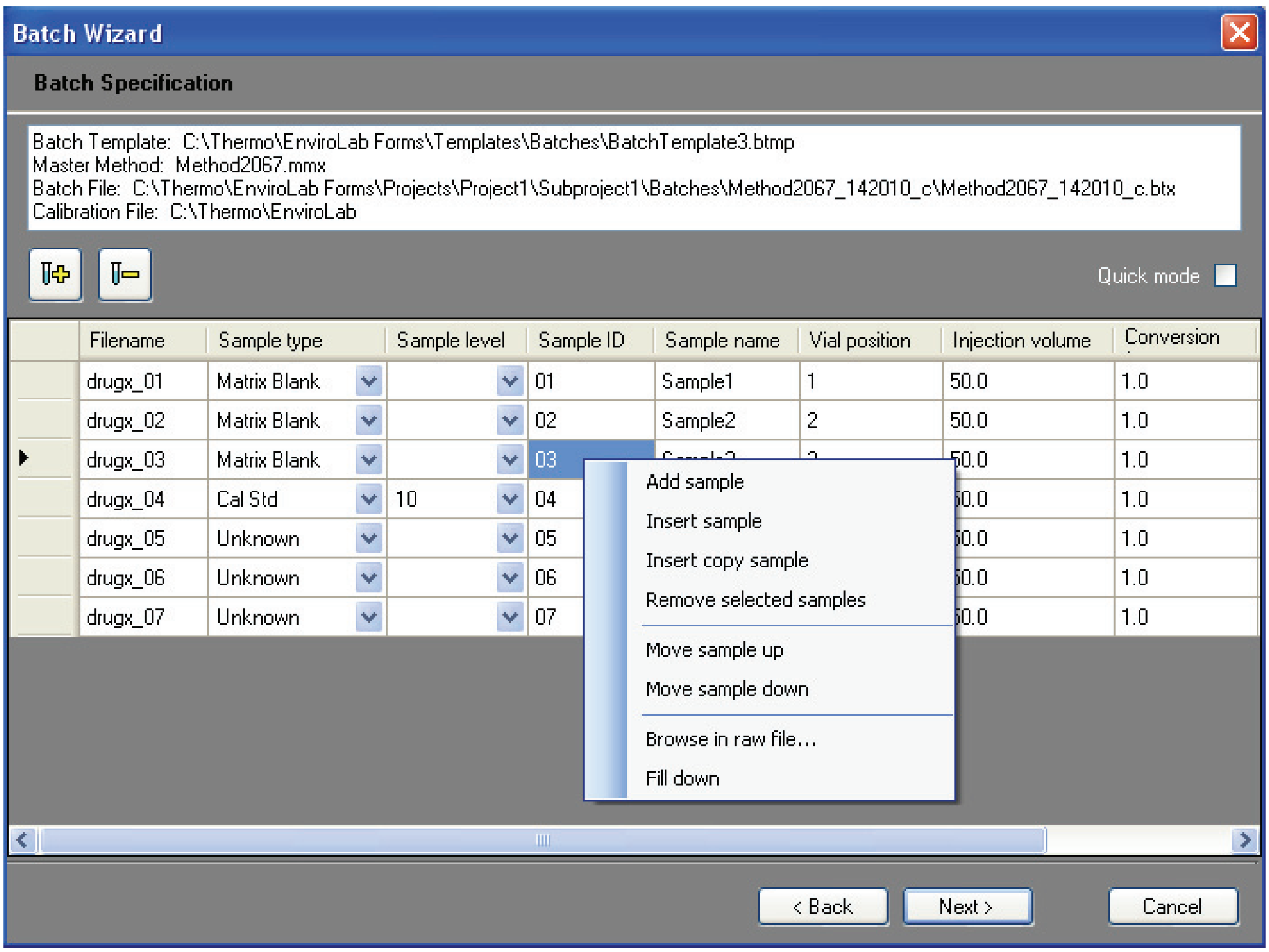


Table 49. Batch Specification parameters (Sheet 1 of 2)

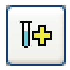
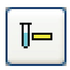
Parameter	Description
Batch Template Master Method Batch File Calibration File	Displays the path names of the batch template, master method, batch file, and calibration file used to create this batch.
	Adds a new, Unknown sample to the end of the sample list. This function is not available when Quick Mode is selected.
	Removes the selected sample. This function is not available when Quick Mode is selected.
Quick mode	Limits the columns of information in the Batch Specification page to the following: • Sample Type • Sample ID • Injection Volume • Conversion Factor In Quick Mode, the shortcut menu and add/remove sample icons are unavailable.
Back	Returns you to the Batch Template Selection page where you can choose a different batch template, master method, or starting vial position.
Next	Takes you to the Finish page where you can submit the batch for acquisition or processing. See “Submitting the Batch” on page 200.
Cancel	Immediately exits the Batch Wizard and does not save the batch. There is no confirming message.
Shortcut Menu	
Add sample	Adds a single empty row to the sample list.
Insert sample	Inserts a new, Unknown sample above the selected row.
Insert copy sample	Copies the currently selected row and inserts a copy above the row.
Remove selected samples	Removes selected samples from the sample list.
Move sample up	Moves the selected sample up one row in the sample list.
Move sample down	Moves the selected sample down one row in the sample list.

Table 49. Batch Specification parameters (Sheet 2 of 2)

Parameter	Description
Browse in raw file	Opens a dialog box where you can select a raw data file to use for the sample row. You can also browse in multiple raw data files to create multiple samples.
Fill down	Enters sequential values in the column starting with the value in the selected row and ending with the last row in the column. For detailed instructions about using the Fill Down command, see Appendix B, "Using Copy Down and Fill Down."

Submitting the Batch

From the Finish page, you can change the name of the batch, access the Calibration and Compound Selection page to edit the calibration file or edit the list of compounds to identify, or save the batch and open it in Batch View.

Follow these procedures:

- To change the name of the batch
- To save the batch
- To edit the calibration file
- To identify specific compounds or groups of compounds

❖ To change the name of the batch

Edit the name in the Batch Name box.

If you enter a name for a batch that already exists, when you click **Finish,** the Batch Save dialog box asks you to enter another name. You cannot overwrite an existing batch name.

❖ To save the batch

Click **Finish**.

The EnviroLab Forms application saves the batch and displays it in Batch View. From Batch View, you can submit the batch for acquisition, processing, or report generation. See "Submitting a Batch" on page 182.

❖ To edit the calibration file

1. Select the **Modify Calibrations or Active Compounds by Group** check box.

   The EnviroLab Forms application replaces the Finish button with a Next button.

2. Click **Next**.

   The Calibration and Compound Selection page opens. See "Selecting Calibration Files and Compounds" on page 202.

❖ To identify specific compounds or groups of compounds

1. Select the **Modify Calibrations or Active Compounds by Group** check box.

   The EnviroLab Forms application replaces the Finish button with a Next button.

2. Click **Next**.

   The Calibration and Compound Selection page opens. See "Selecting Calibration Files and Compounds" on page 202.

Figure 51. Finish page

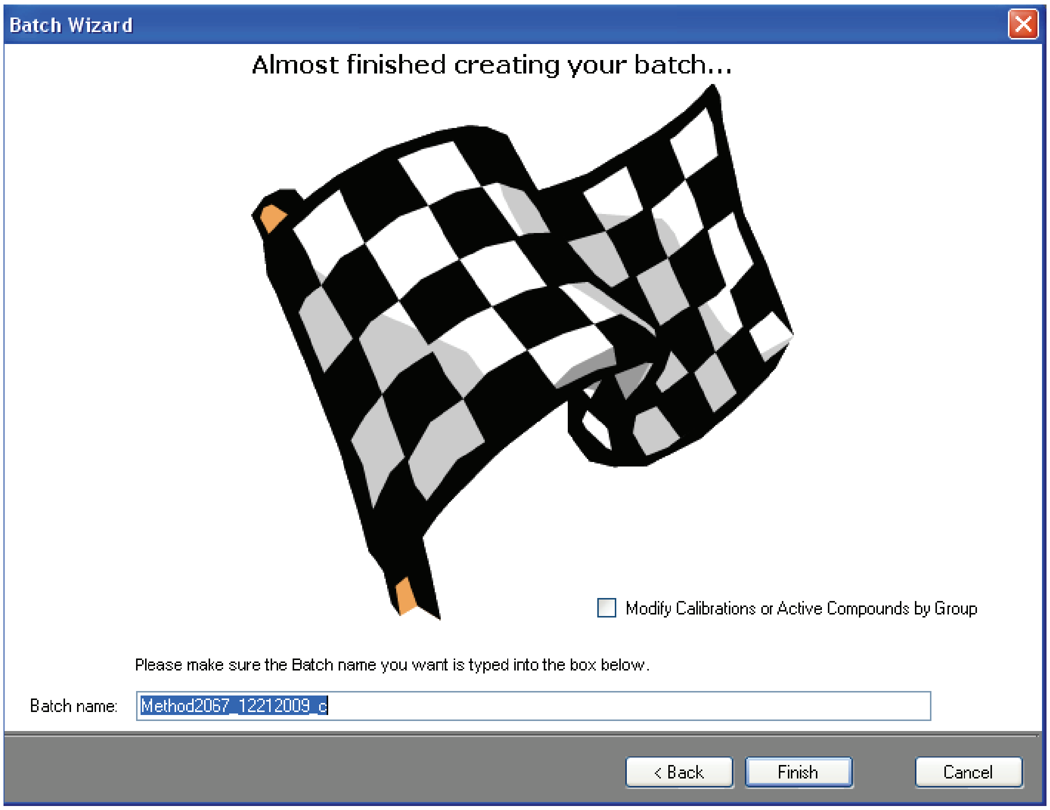


Table 50. Finish parameters (Sheet 1 of 2)

Parameter	Description
Modify Calibrations or Active Compounds by Group	Enables the Next button that lets you access the Calibration and Compound Selection page. If you have already used the Calibration and Compound Selection page, this option is not available.
Batch name	Name of the current batch in the form: *MasterMethodName_MMDDYYYY_*

Table 50. Finish parameters (Sheet 2 of 2)

Parameter	Description
Back	Returns you to the Batch Specification page where you can enter a sample ID, sample name, or comment. You can also add or remove samples from the sample list or edit the column values for the samples. See "Specifying a Batch" on page 195.
Finish	Saves the batch and displays it in Batch View. From Batch View, you can submit the batch for acquisition, processing, or report generation. See "Submitting a Batch" on page 182.
Next	Opens the Calibration and Compound Selection page where you can edit the calibration file or edit the list of compounds you want to identify. Available only when Modify Calibrations or Active Compounds by Group is checked.
Cancel	Immediately exits the Batch Wizard and does not save the batch. There is no confirming message.

Selecting Calibration Files and Compounds

From the Calibration and Compound Selection page, you can edit the calibration file or edit the list of compounds you want to identify.

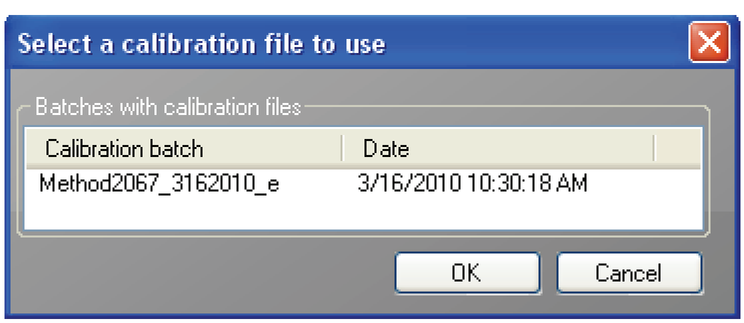
Follow these procedures:

- To add calibration data to the calibration file
- To identify specific compounds or groups of compounds

❖ To add calibration data to the calibration file

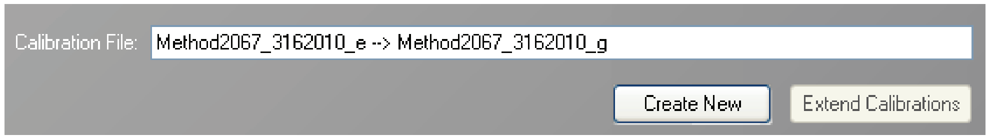
1. To add calibration data from another batch to the current calibration file, click **Extend Calibrations**.

   The Select a Calibration File to Use dialog box opens. The dialog box lists only calibration batches that use the same master method as the current batch.



2. Select a calibration file to append to the current calibration file and click **OK**.

   The EnviroLab Forms application appends the selected calibration file to the current file.



3. To save calibration data from both files into a single file for this batch, click **Create New**.

4. When you are finished with the Calibration and Compound Selection page, click **Next**.

   The Finish page opens. See "Submitting the Batch" on page 200.

❖ To identify specific compounds or groups of compounds

1. In the Compound Groups area, select the groups that include the compounds you want to identify in the samples.

2. In the Included Compounds area, select the **Active** check box for each compound that you want to identify in the samples.

3. When you are finished with the Calibration and Compound Selection page, click **Next**.

   The Finish page opens. See "Submitting the Batch" on page 200.

Figure 52. Calibration and Compound Selection Page

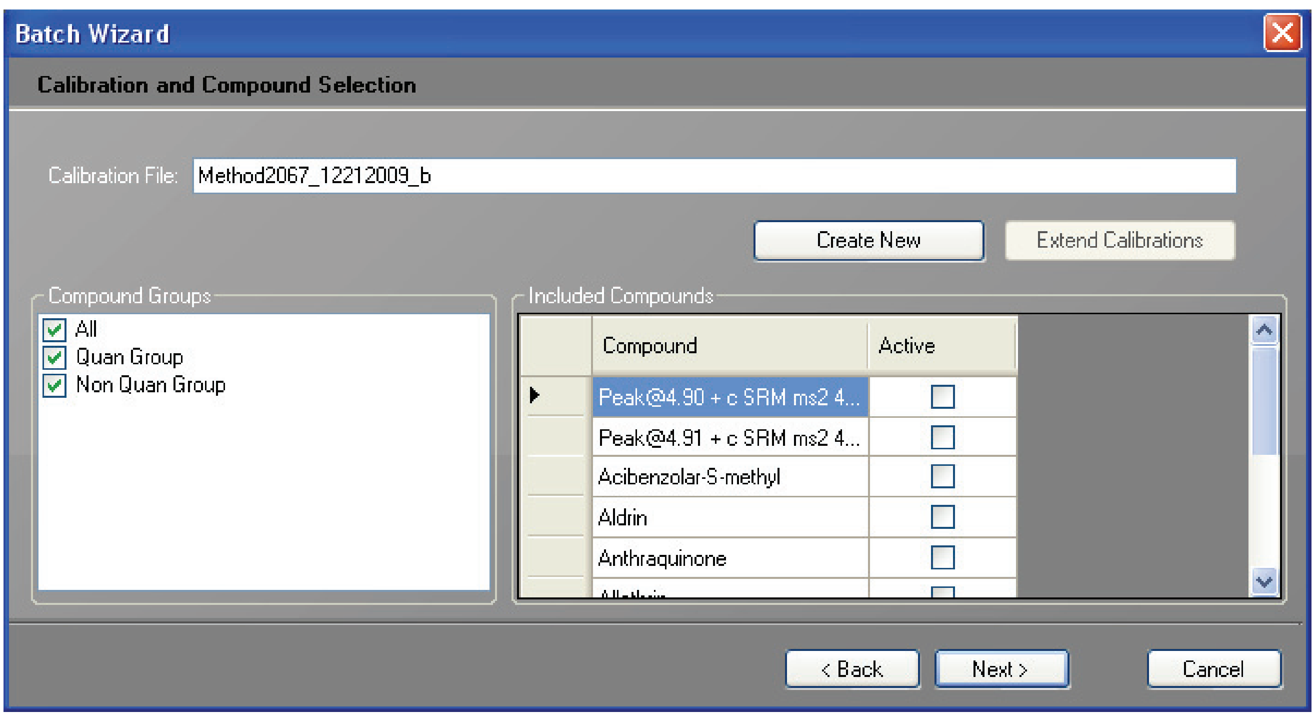


Table 51. Calibration and Compound Selection parameters

Parameter	Description
Calibration File	Name of the current batch in the form: *MasterMethodName_MMDDYYYY_*
Create New	Saves calibration data from all calibration files to the current calibration file. Available only after you use Extend Calibrations to append calibration data from another calibration file.
Extend Calibrations	Adds calibration data from the current batch to the selected calibration file.
Compound Groups	Displays all available groups defined in the Groups page of the Master Method View. See "Editing the Groups Page" on page 136.
Included Compounds	Displays all available compounds that you can identify in the samples. Compounds marked as Active are identified in the batch samples.
Back	Returns you to the Batch Specification page where you can enter a sample ID, sample name, or comment. You can also add or remove samples from the sample list or edit the column values for the samples. See "Specifying a Batch" on page 195.
Next	Opens the Finish page where you can change the name of the batch or save the batch to the Batch View. See "Submitting the Batch" on page 200.
Cancel	Immediately exits the Batch Wizard and does not save the batch. There is no confirming message.

Specifying Sample Types

The EnviroLab Forms application uses the following sample types in all sample definitions and reports.

To view example standard reports specific to each sample type, see Appendix A, "Reports."

Table 52. Sample type definitions (Sheet 1 of 2)

Sample type	Definition
Matrix Blank	Contains no target compounds but might contain an ISTD when you use the internal standard quantitative analysis technique. By analyzing a blank sample, you can confirm that there are no residual compounds in the solvent system that can cause erroneous results.
Cal Std	(Calibration standard) Contains known amounts of all target compounds. The purpose of a calibration standard is to measure the response of the instrument to the target compounds so that the processing software can generate a calibration curve for each compound.
Chk Std	(Check standard) Contains a known amount of one or more specific target compounds. The EnviroLab Forms application places check standard samples in the sequence so that it can test quantitative analysis results for quality assurance purposes. After the application analyzes the check standard sample, it compares the measured quantity with the expected value and an acceptability range. The quantitative analysis of a check standard sample is classified as passed if the difference between the observed and expected quantities is within the user-defined tolerance. A check standard sample is classified as failed if the difference between the observed and expected quantities is outside the user-defined tolerance.
LCS	Lab control sample.
LCSD	Lab control sample duplicate.
MDL	Method detection limits sample.
Meth Val	Method validation sample.
MS	Matrix spike sample.
MSD	Matrix spike duplicate sample.
Tune	Verifies the tune of the system according to EPA guidelines.
Tune/Breakdown	Verifies the tune of the system according to EPA guidelines, allowing for the degradation of compounds.
Breakdown	Checks the degradation of compounds.

Table 52. Sample type definitions (Sheet 2 of 2)

Sample type	Definition
Solvent	Contains only solvent.
Unknown	Used for quantitative analysis of samples.
Unknown/TIC	Used for quantitative and qualitative analysis of samples.

Working in Data Review

From the Data Review view, you can view the data generated by the master method. Use the Data Review view to verify the data for a sample-specific compound before you generate reports. You can use the functions in the Data Review view to investigate and edit the quantification values in a batch.

❖ To open the Data Review view

1. Click **Production** from the dashboard or the navigation pane.

The Production navigation pane opens.

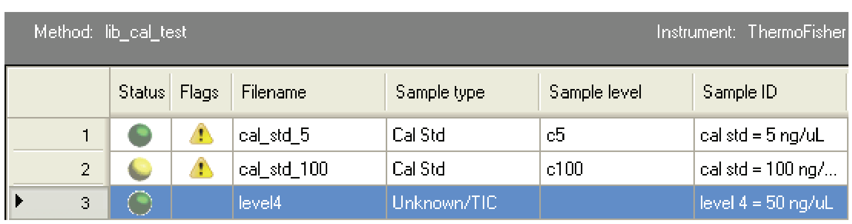
2. From the Production navigation pane, click **Data Review** (to open the Data Review view).

The Data Review view for the currently selected batch opens.

Data Review Panes

The Data Review view uses a Samples list and one of two modes: Quan Mode or Qual Mode. The Qual Mode is available only for Unknown/TIC sample types. When you view the data for one of these sample types, you can toggle between Qual Mode and Quan Mode.

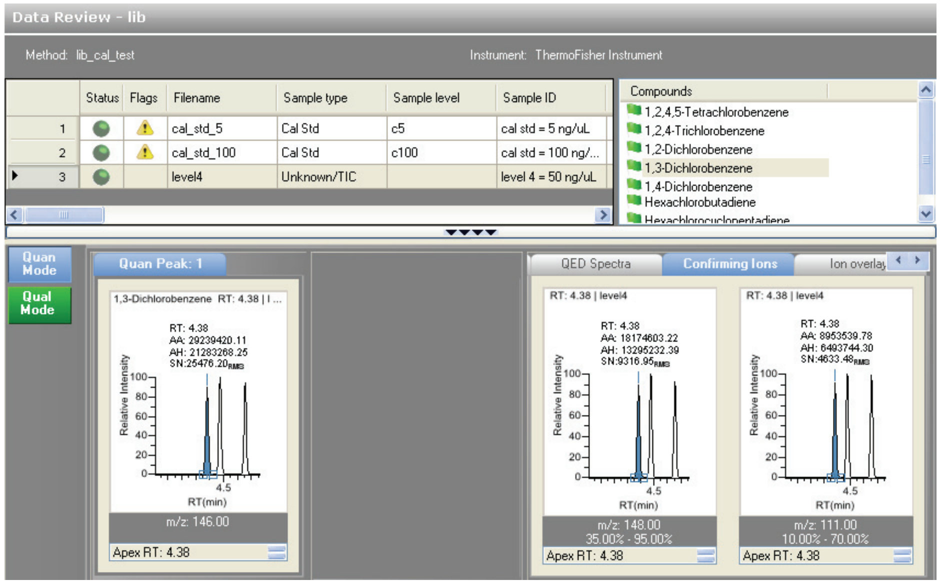
- Use the Samples list to select a particular sample. Status indicators for each sample indicate if the sample is unacquired, acquired, acquiring, or processed. See “Samples List” on page 209.



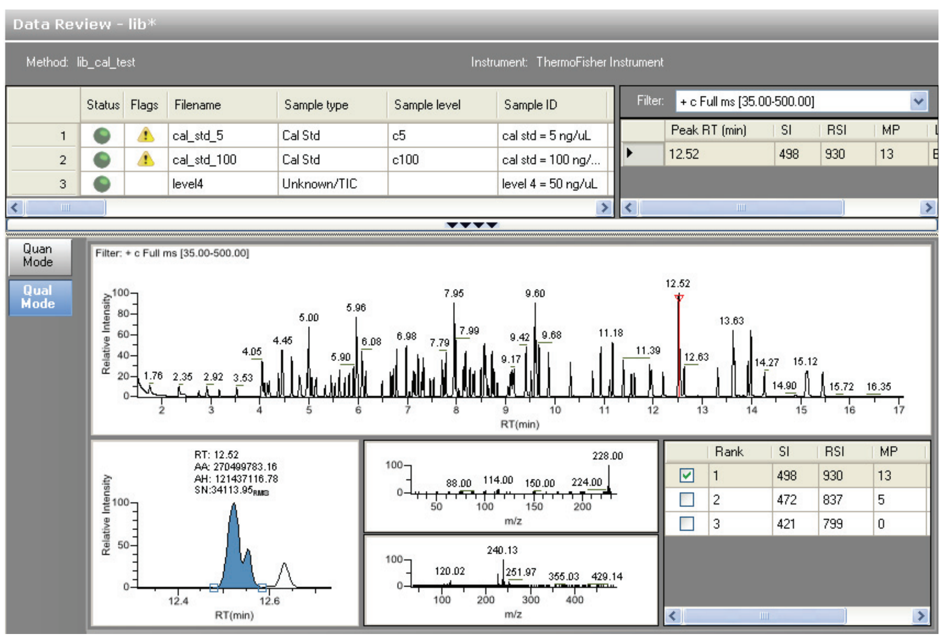
Method: lib_cal_test   Instrument: ThermoFisher

	Status	Flags	Filename	Sample type	Sample level	Sample ID
1			cal_std_5	Cal Std	c5	cal std = 5 ng/uL
2			cal_std_100	Cal Std	c100	cal std = 100 ng/...
3			level4	Unknown/TIC		level 4 = 50 ng/uL

- Use the Quan Mode and the associated Compounds pane to view quantitative information to complement the textual information for the selected sample. See "Quan Mode" on page 214.



- Use the Qual Mode and the associated Peaks pane to view qualitative information that complements the textual information for the selected Unknown/TIC sample. See "Qual Mode" on page 229.



Samples List

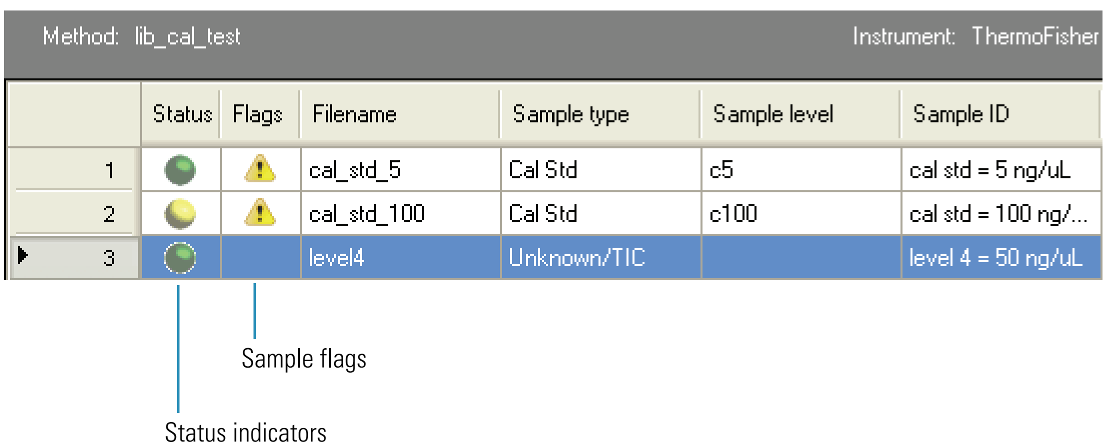
The Samples list is the same in both Quan Mode and Qual Mode and displays all the quantitative data for the samples of a batch.

- In Quan Mode, the Samples list works with the Compounds pane to select a unique sample and compound combination, which then has its textual and graphical values displayed in the Quan Mode pane. The list of compounds that are available for a specific method is displayed in the Compounds pane.

  From the Samples list, you can make a compound active or inactive. Switching a compound to inactive status does not remove its data and calculated values from the result set. Instead, the EnviroLab Forms application masks off the appearance of that compound for that particular sample and grays the compounds in the Compounds list. For a calibration standard, the application no longer uses the data file's calibration point for the calibration and removes it from the graphical view of the calibration curve displayed in the Qualification pane. It is no longer part of the result set.

- In Qual Mode, the Samples list works with the Peaks pane to select a unique sample and peak combination, which then has its textual and graphical values displayed in the Qual Mode pane.

The Flags column in the Samples list displays a caution flag if the sample is not in compliance with the method criteria.



To open a dialog box with a list of problems found in the sample, click the caution flag. The dialog box does not list compounds that are not found in Unknown sample types.

Status Indicators

Status indicators show the current status of each sample during the acquisition and processing:

- Orange for samples that are currently acquiring
- Blue for samples that have not been acquired
- Yellow for samples that have been acquired and not processed
- Green for samples that have been acquired and processed

Sample Flags

Sample flags are displayed when compounds within the samples have an error.

- Sample caution flags remain static when you switch between compounds for chromatogram review until a change is completed, for example, when a compound is manually integrated and no longer falls outside the accepted criteria.
- Sample caution flags list a summary of all compound indicator messages within the sample when you pause the cursor over the flag. The Tooltip does not list compounds that are not found in Unknown sample types.

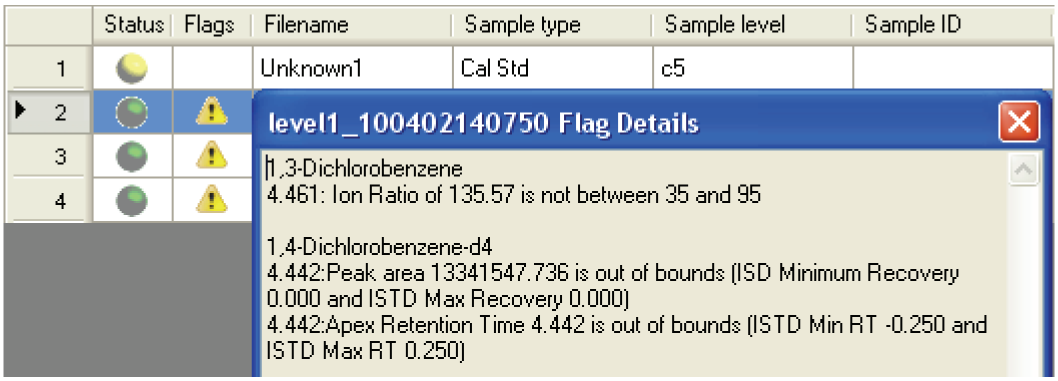


Figure 53. Samples List pane

Method: Batch1680B_Steroid Method Instrument: Thermo Scientific Instrument

	Status	Flags	Filename	Sample type	Sample level	Sample ID	Sample name	Comment	Vial position	Injection volume
1			steroids02...	Unknown		Sample02			1	20.0
2			steroids03	Unknown		Sample03			2	20.0
3			steroids04	Unknown		Sample04			3	20.0
4			steroids05	Unknown		Sample05			4	20.0

Integration mode	Height	*Area	Actual RT	Expected RT	Calc Amt	Theo Amt	Resp ratio	IS Amt	IS Resp
Method	312402	2958671	3.16	3.19	N/A		4.372	0.600	676792
Method	152082	1590374	3.17	3.19	N/A		2.361	0.600	673528
Method	71110	766235	3.15	3.19	N/A		0.992	0.600	772347
Method	583384	6056721	3.11	3.19	N/A		9.472	0.600	639426

Active	Excluded	% Diff	% RSD	% CV
☑	☐	N/A	N/A	N/A
☑	☐	N/A	N/A	N/A
☑	☐	N/A	N/A	N/A
☑	☐	N/A	N/A	N/A

Cells in the Samples list that should not have a value, such as theoretical concentration for an Unknown sample, are shaded and empty. Cells that should have a value, but none exists, report N/A (not available). Results for compounds that are not detected display N/F (not found).

Table 53. Samples List parameters (Sheet 1 of 3)

Parameter	Description
Status	• Orange for samples that are currently acquiring • Blue for samples that have not been acquired • Yellow for samples that have been acquired and not processed • Green for samples that have been acquired and processed
Flags	Displayed only when a compound within the sample has an error. Sample flags are always red.
Filename	Name of the raw data file that contains the sample data.

Table 53. Samples List parameters (Sheet 2 of 3)

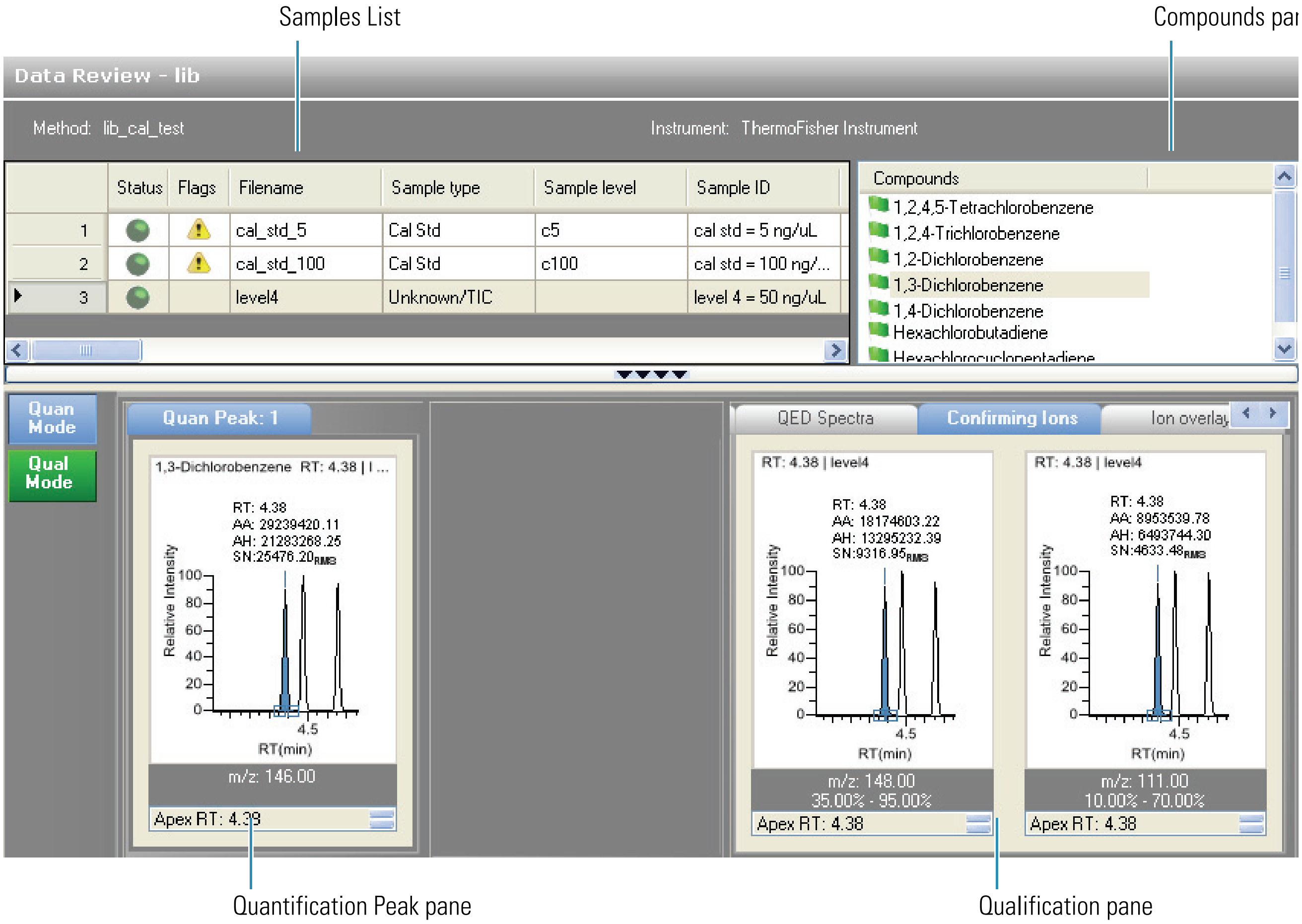
Parameter	Description
Sample type	Defines how the EnviroLab Forms application processes the sample data. Each sample is classified as one of the following sample types: Matrix Blank, MDL, Solvent, Cal Std, MSD, Breakdown, Unknown, Unknown/TIC, Chk Std, MS, LCS, LCSD, Meth Val, Tune, or Tune/Breakdown
Sample level	The level defined for a calibration sample or quality control sample.
Sample ID	A user-defined alphanumeric string that identifies a sample.
Sample name	A user-defined name that identifies a sample.
Comment	A user-defined comment for the sample.
Vial Position	The tray vial number used for the autosampler acquisition.
Injection volume	The injection volume in microliters of sample to be injected. Minimum value: 0.05 When you are using an autosampler, you can set the default injection volume in the autosampler dialog box in the Instrument View. The minimum and maximum injection volumes that you can use depend on the autosampler you configure. The usable range depends on the injection mode and might be smaller than the range displayed.
Integration mode	Indicates whether the peaks have been manually integrated or integrated from the original method.
Height	The distance from the peak maximum to the peak base, measured perpendicular to the ordinate. When the Resp Ratio is specified as Height, this column is indicated with an asterisk (*Height).
Area	The area obtained by integrating peak intensities from the start to the end of the peak. When the Resp Ratio is specified as Area, this column is indicated with an asterisk (*Area).
Actual RT	Actual retention time for the compound. Retention time is the time after injection at which a compound elutes and the total time that the compound is retained on the GC column.
Expected RT	Expected retention time for the compound.
Calc Amt	The amount present in the sample, as determined using the calibration curve and the response ratio.
Theo Amt	Theoretical amount of the compound expected in the sample.

Table 53. Samples List parameters (Sheet 3 of 3)

Parameter	Description
Resp ratio	The ratio of the Response value to the IS Response value. If the Response is specified as Area in the processing method, the units of both Response and IS Response are counts-sec. If the Response is specified as Height in the processing method, the units of both Response and IS Response are counts.
IS Amt	Amount of internal standard.
IS Resp	Response of the internal standard.
Active	Displays or hides a compound for a particular sample. When a calibration standard is marked inactive, the EnviroLab Forms application no longer uses the data file's calibration point for the calibration and removes it from the graphical view of the calibration curve displayed in the Qualification pane. It is no longer part of the result set.
Excluded	Turns a compound on or off in the Calibration curve of the Qualification pane.
%Diff	The calculated amount minus the expected amount, divided by the expected amount, and then multiplied by 100.
%RSD	Standard deviation of the multiple samples of one level, multiplied by 100, and then divided by the average of the multiple samples of that level. This calculation is based on the calculated amounts.
%CV	Coefficient of Variation. Standard deviation of the multiple samples of one level, multiplied by 100, and then divided by the average of the multiple samples of that level. This calculation is based on either the area or height of the peaks.

Quan Mode

The Quan Mode displays quan peak and confirming ion information for selected compounds that are found in the processed samples.



In addition to the Samples List, the Quan Mode view uses the following panes:

- Compounds Pane
- Quantification Peak Pane
- Qualification Pane

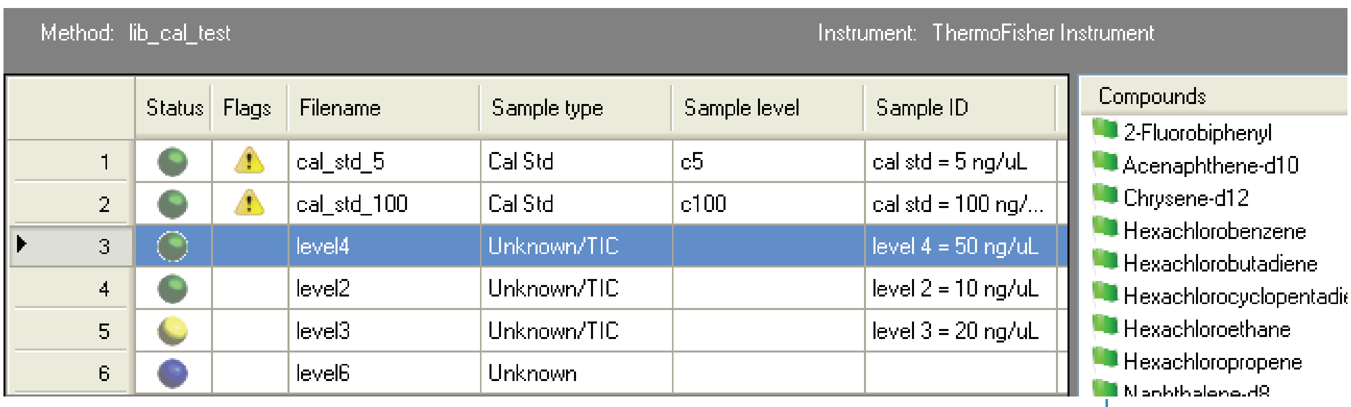
Compounds Pane

In Quan Mode, the Samples list works with the Compounds pane to select a unique sample and compound combination, which then has its textual and graphical values displayed in the Quan Mode pane. The list of compounds that are available for a specific method is displayed in the Compounds pane.

The Compounds pane works with the Samples list to display textual and graphical values for a unique file and compound combination.

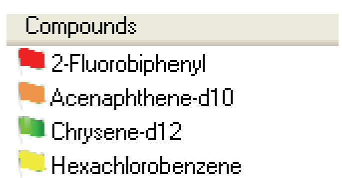
Use the Compounds pane to select a particular compound within that sample's result set. When you select a file and compound, the values displayed in the data grid reflect the quantification data for that unique combination.

From the Samples list, you can make a compound active or inactive. Switching a compound to inactive status does not remove its data and calculated values from the result set; instead, the EnviroLab Forms application masks off the appearance of that compound for that particular sample and grays the compounds in the Compounds list. For a calibration standard, the application no longer uses the data file's calibration point for the calibration and removes it from the graphical view of the calibration curve displayed in the Qualification pane. It is no longer part of the result set.



Compound flags

Compound Flags



When are flags displayed?

The EnviroLab Forms application displays compound flags for any of the following conditions:

- When a compound has violated (or is activated by) any of the values set in the method. See "Editing the QAQC Page" on page 117.
- For compounds that are not found in Cal Std, Chk Std, and Surrogate sample types.
- For compounds that are outside the specified ion ratio range.
- For compounds that are not found.

These criteria do not apply to Matrix Blank sample types when the compound is an internal standard.

What do the flag colors mean?

The EnviroLab Forms application defines the colors of the compound flags as follows:

- Red flags for compounds that have ion ratio failures, method validation failures, or have values above the ULOL or carryover limits.
- Orange flags for compounds that are below the LOQ, below the LOD, or between the LOD and LOQ values specified in the method.
- Green flags for compounds that are over the LOR amount specified in the method.
- Yellow flags for compounds that are below the LOR amount specified in the method.
- No flag for compounds that have no errors or where there were no report options selected.

Follow these procedures:

- To display peaks for a specific compound
- To change the sort order
- To display the compound nonconformance
- To make a compound active or inactive
- To exclude a calibration point

❖ To display peaks for a specific compound

1. From the Samples list, select the sample.

   The Compounds pane lists all compounds specified in the method.

2. From the Compounds pane, select the compound in the sample.

   The Quan peak pane displays the peaks for the selected compound and its internal standard.

❖ To change the sort order

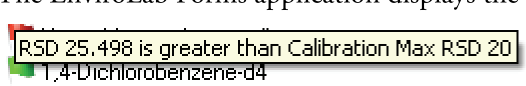
Right-click the Compounds pane and choose one of the following from the shortcut menu:

– Sort by Flag and Alphabetical (the default)
– Sort by Flag and Retention Time
– Sort by Alphabetical
– Sort by Retention Time

❖ To display the compound nonconformance

Pause the cursor over the compound or compound flag.

The EnviroLab Forms application displays the error condition.



❖ To make a compound active or inactive

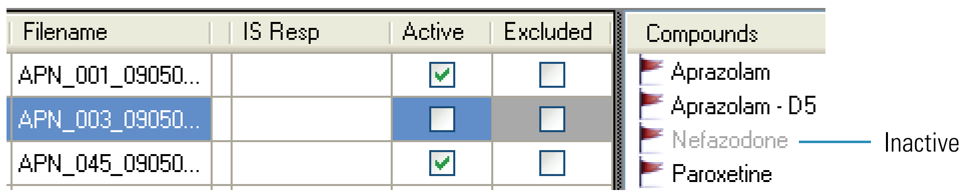
1. Select the sample from the Samples list.

   All compounds in that sample are displayed in the Compounds pane. The status of a compound in a sample is determined by the Component Active Status pane in the Batch View for the batch. Inactive compounds are grayed out.

2. From the Compounds pane, select the compound you want to make inactive.

3. From the Samples list, select or clear the **Active** check box.

   Use the horizontal scroll bar at the bottom of the table to scroll to the Active column.



❖ To exclude a calibration point

From the Samples list, select the **Excluded** check box for the sample.

When a value is no longer used for calibration, it remains part of the calibration dataset and is displayed in the graphical view of the calibration curve.

Quantification Peak Pane

The Quantification Peak pane displays the compound selected in the Samples list and Compounds panes. You can store two peak value sets (method and manual integration settings) with each compound in each file. These settings can result in a different set of stored values. The method values were originally calculated based on the processing method parameters. The manual values are a result of what has been viewed or altered.

When the sample contains an internal standard, the chromatogram shows both the analyte and the internal standard in side-by-side panes.

Follow these procedures:

- To zoom in on a peak
- To manually integrate a quantification or qualification ion
- To manually add a peak
- To remove a manually created peak
- To switch between method and manual integration modes
- To change the displayed information for detected peaks
- To modify the peak detection settings

❖ To zoom in on a peak

1. In the chromatogram plot, drag the cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view to help you examine the peak limits for enhanced review and confirmation.

2. To restore the default view, right-click the chromatogram plot and choose **Reset Scaling** from the shortcut menu.

❖ To manually integrate a quantification or qualification ion

1. Place the cursor over one of the two peak delimiter tags in the Quantification Peak pane.

   When the tag can be selected, the cursor changes to a crosshair style cursor. You can zoom in on the baseline to make it easier to select the tag.

2. Drag the tag to another location, and release the cursor to place the peak delimiter tag at its new location and automatically update the peak values (area, height, and so forth) into the result set.

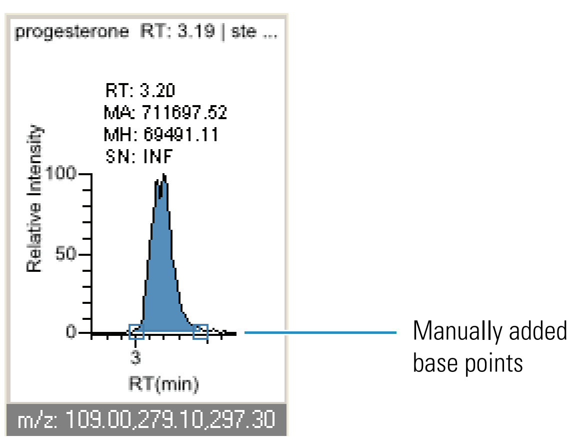
   Both the Quantification Peak pane and the Integration Mode column in the Quantification data pane reflect the change between method and manual modes. The generated reports for these data identify the manual modifications.

❖ To manually add a peak

1. Right-click anywhere in the Quantification Peak pane, and choose **Add Peak** from the shortcut menu.

2. Click to indicate the left and right base points for the peak.

   The EnviroLab Forms application places the peak delimiter tags at these locations and automatically updates the peak values (area, height, and so forth) in the result set.



❖ To remove a manually created peak

Right-click the chromatogram plot, and choose **Remove Peak** from the shortcut menu.

The EnviroLab Forms application removes the manually added peak.

❖ To switch between method and manual integration modes

Right-click the chromatogram view and choose **Method Integration Settings** or **Manual Integration Settings** from the shortcut menu.

Initially, the method and manual integration settings that are stored for a compound and file are identical and when you select one mode it does not affect the saved result set. However, when manual data are available, the chromatogram plots and the result set update as you switch between method and manual modes.

As you switch between modes, the changes are reflected in each pane. The generated reports for this data identify the manual modifications.

❖ To change the displayed information for detected peaks

1. Right-click the quantification chromatogram plot and pause the cursor over **Peak Labels**.
2. Choose to display labels for the peak retention time, peak height, peak area, or signal to noise.

   The label types in the list are selected for displayed labels and cleared for labels that are not displayed.
3. To remove a label, select the label type again and clear it.

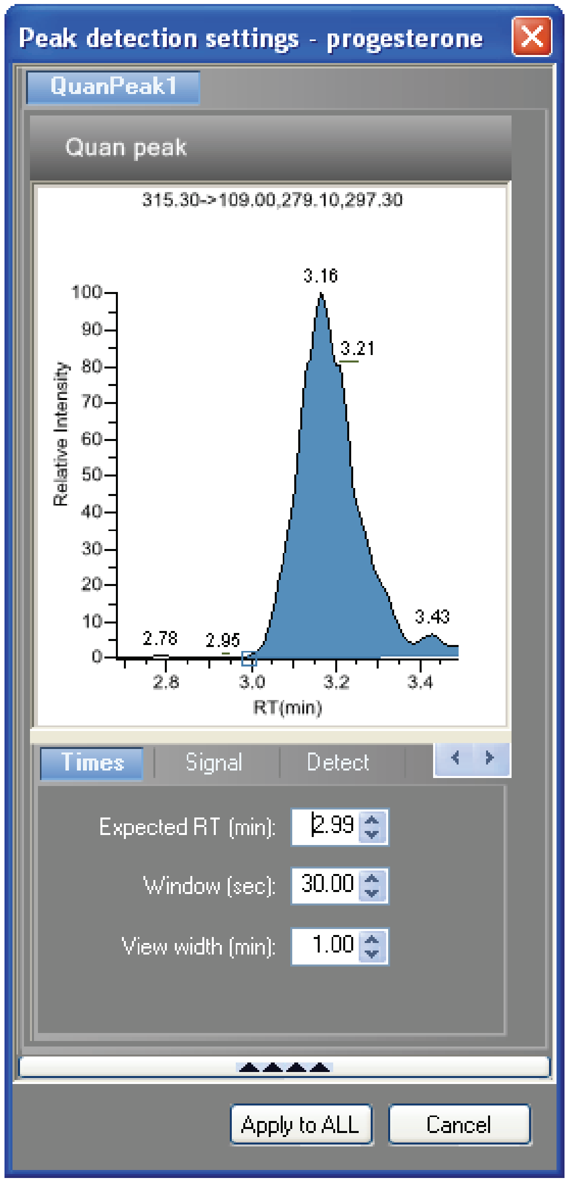
   Label settings are globally applied to quan peaks, confirming peaks, and internal standard peaks.

> **Note** The labels do not always update on all peak displays. To update all labels, select a different compound, and then reselect the compound whose labels you changed.

❖ To modify the peak detection settings

1. Right-click the chromatogram view and choose **Peak Detection Settings** from the shortcut menu.

   The Peak Detection Setting dialog box opens. This dialog box contains the detection settings defined in the method.



2. Edit any of the detection settings.

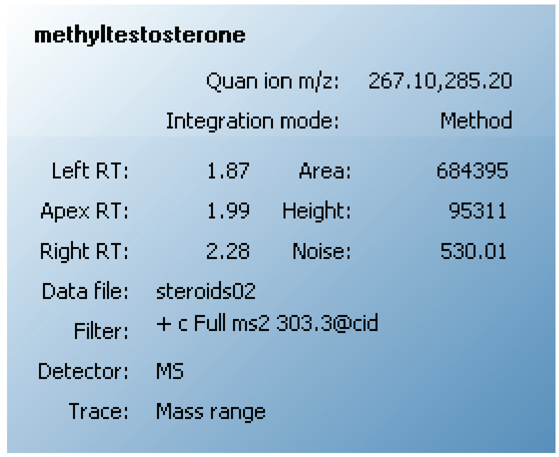
   For a detailed description of all detection settings, see "Detection" on page 83.

3. To save your changes to this compound in all samples in this batch, click **Apply to All**.

Table 54. Quantification Peak shortcut menu (Sheet 1 of 2)

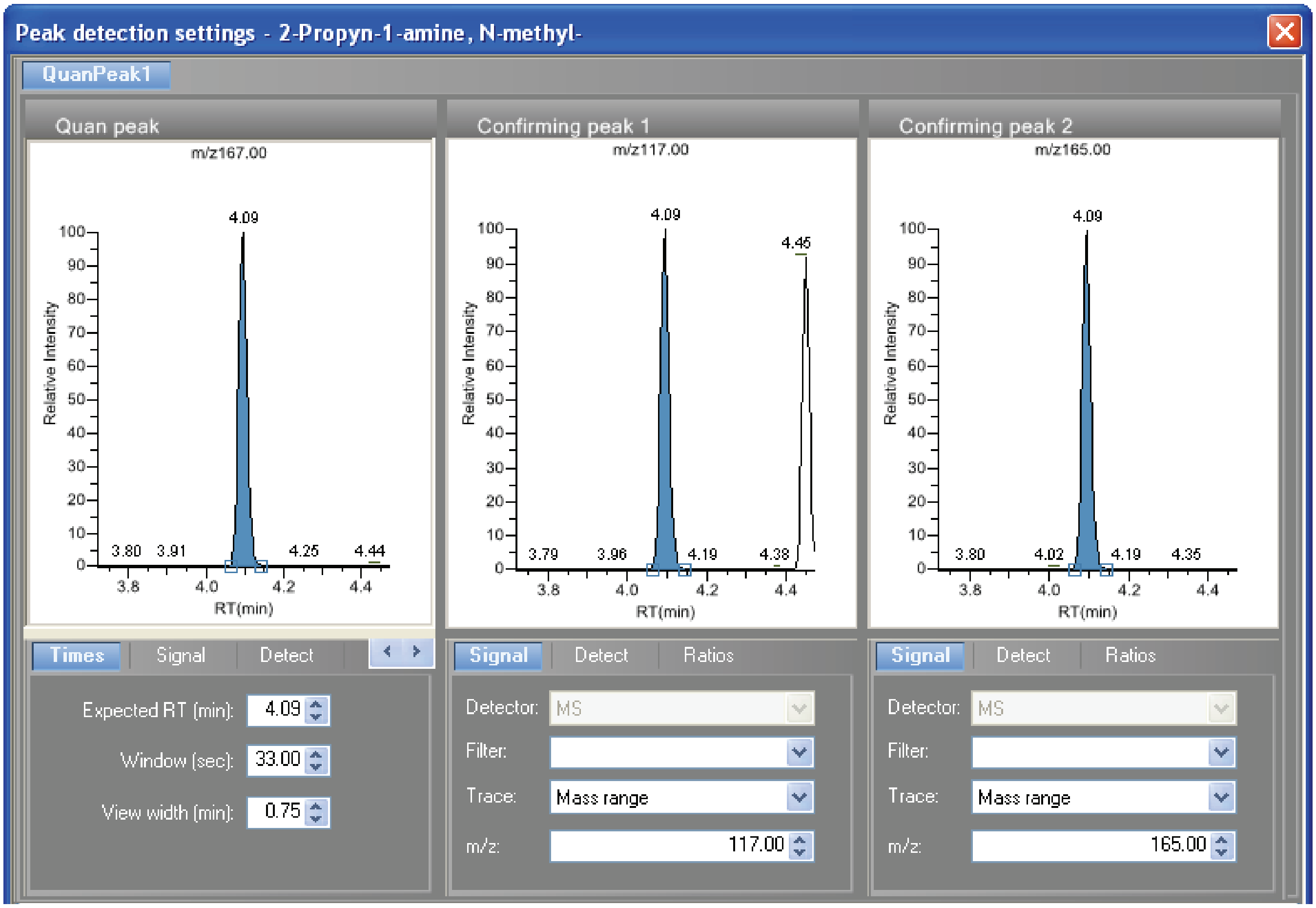
Command	Description
Method integration settings	Displays method integration settings.
Manual integration settings	Displays manual integration settings.
Add peak - Remove peak - Cancel add peak	Adds a peak, removes a peak, or cancels an add peak operation in progress.

Table 54. Quantification Peak shortcut menu (Sheet 2 of 2)

<table>
<tr><th>Command</th><th>Description</th></tr>
<tr><td>Confirming ion list</td><td>Selects the confirming ions to be viewed.</td></tr>
<tr><td>Peak labels</td><td>Displays or hides the peak labels (Label Area, Label Retention Time, Label Height, or Label Signal to Noise).</td></tr>
<tr><td>Show peak info</td><td>Displays peak information for the selected compound. For example:

</td></tr>
<tr><td>Reset scaling</td><td>Resets the original scaling after a zoom operation.</td></tr>
<tr><td>Peak detection settings</td><td>Opens the Peak Detection Settings dialog box for the selected compound. See “Peak Detection Settings” on page 222.</td></tr>
</table>

Peak Detection Settings

Use the Peak Detection Settings dialog box to adjust detection settings that were specified in the method.



For a detailed description of all peak detection settings, see "Detection" on page 83.

Qualification Pane

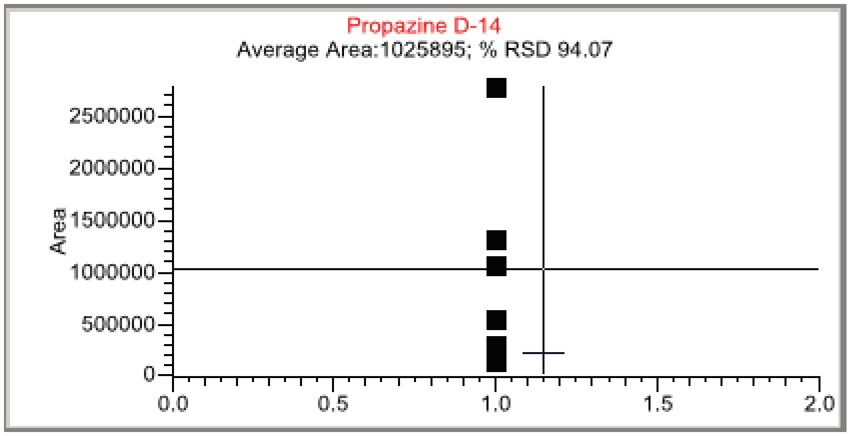
The Qualification pane displays the compound selected in the Quantification data pane and Compounds pane.

The Qualification pane consists of five pages:

- Calibration Curve
- Spectra
- Confirming Ions
- Ion Overlay

Calibration Curve

The Calibration curve page displays a graphical view of the calibration curve for the selected compound and key statistical values for evaluating the quality of the calibration.



❖ To manually exclude a calibration point

From the Samples list, select the **Excluded** check box for the sample.

❖ To zoom in on an area

1. In the Calibration curve plot, drag the cursor to delineate a rectangle around an area.

   The delineated area expands to fill the view.

2. To restore the method default view, right-click the calibration curve plot and choose **Reset Scaling** from the shortcut menu.

   Changes to the calibration settings are immediately applied to the entire results set, but they are saved only when you save the batch.

Table 55. Calibration Curve shortcut menu (Sheet 1 of 2)

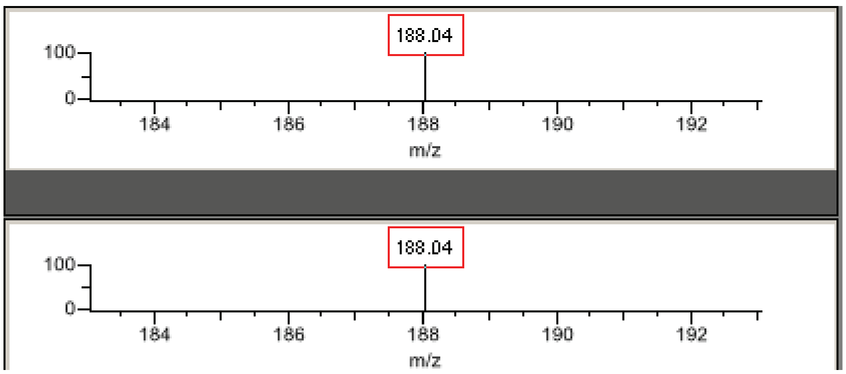
Command	Description
Standard type	Sets the standard type to External or Internal.
Calibration curve type	Sets the calibration curve type to Linear, Quadratic, or Average RF. • Linear: Allows all settings with this exception: When Origin is set to Include, all Weighting values are grayed out and Weighting is set to Equal. • Quadratic: Allows all settings with this exception: When Origin is set to Include, all Weighting values are grayed out and Weighting is set to Equal. • Average RF: Allows no Weighting or Origin selections. All Weighting and Origin values are grayed out. Weighting is set to Equal, and Origin is set to Ignore.

Table 55. Calibration Curve shortcut menu (Sheet 2 of 2)

Command	Description
Response via	Sets the response via to Area or Height.
Weighting	Sets the weighting to equal, 1/X, 1/X^2, 1/Y, or 1/Y^2.
Origin	Sets the origin to Ignore, Force, or Include.
Units	Sets the units.
Done with settings	Closes the shortcut menu.
Reset scaling	Resets the original scale in the calibration curve pane.

Spectra

The Spectra page displays a comparison of the spectra found in the data and the method reference.



❖ **To zoom in on an area**

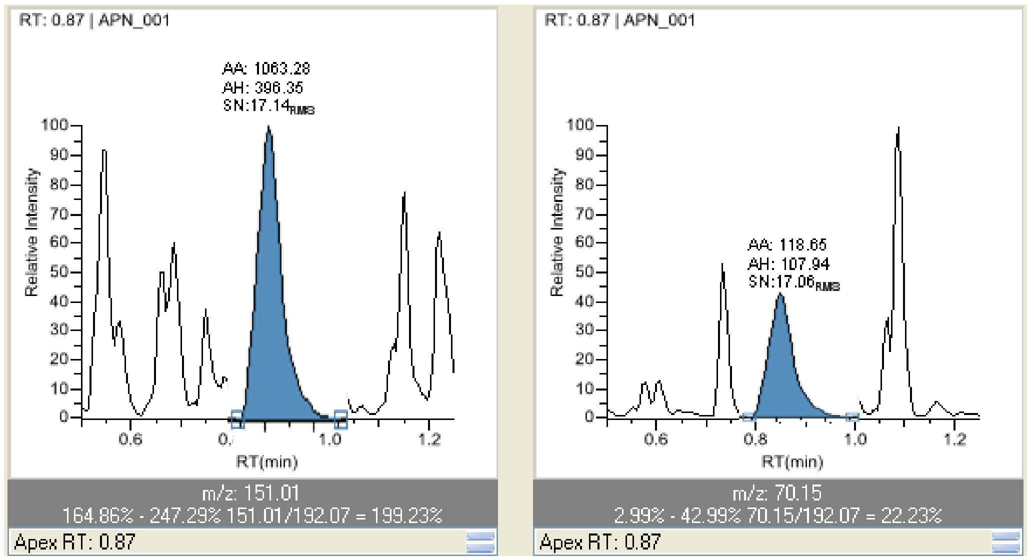
1. Drag the cursor to delineate a rectangle around an area.

   The delineated area expands to fill the view.

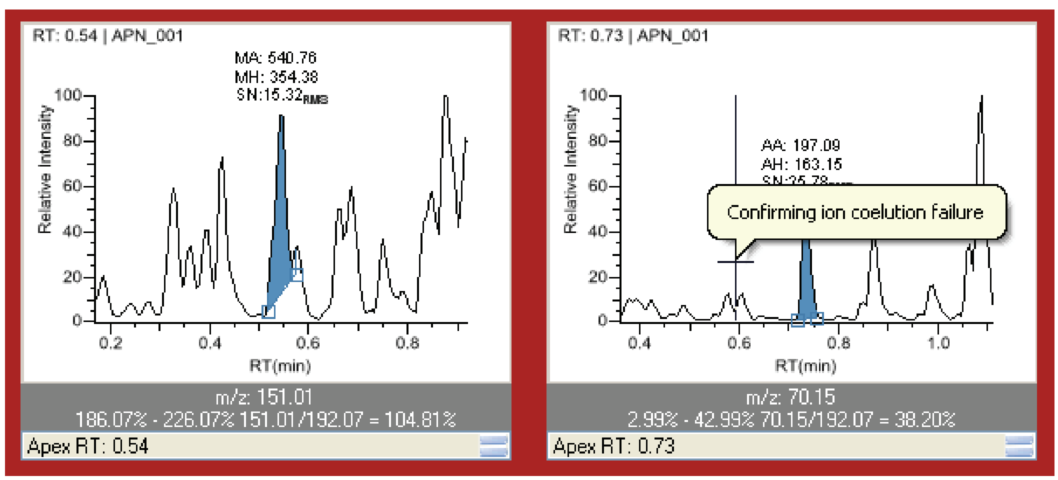
2. To restore the method default view, right-click the spectra plot and choose **Reset Scaling** from the shortcut menu.

Confirming Ions

The Confirming Ions page displays a graphical view of all qualifying/confirming ions for the selected sample and compound and displays calculated ion ratios and ion ratio acceptance windows. A red border indicates that an ion ratio is outside of its window. Depending on the method option settings, another ion view is available on the Ion Overlay page. See “Ion Overlay” on page 228.



A red border indicates that an ion ratio is outside of its window.



Follow these procedures:

- To manually add a peak
- To remove a manually created peak
- To zoom in on a peak
- To change the displayed information for detected peaks
- To display the peak information window

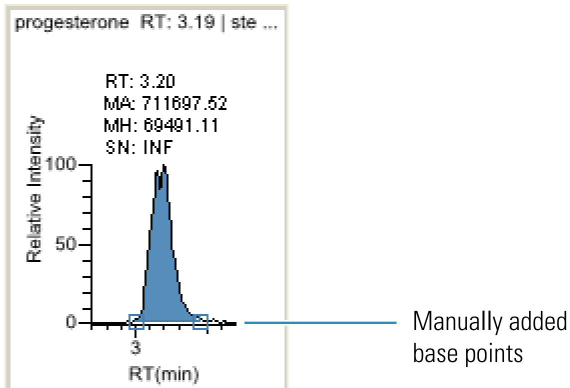
❖ To manually add a peak

1. Right-click the chromatogram plot and select **Add Peak** from the shortcut menu.

   If a peak is already detected, the Add Peak command is not enabled.

2. Click to indicate the left and right base points for the peak.

   The EnviroLab Forms application places the peak delimiter tags at these locations and automatically updates the peak values (area, height, and so forth) in the result set.



❖ To remove a manually created peak

Right-click the chromatogram plot, and choose **Remove Peak** from the shortcut menu.

The EnviroLab Forms application removes the manually added peak.

❖ To zoom in on a peak

1. In the chromatogram plot, drag the cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view to help you examine the peak limits for enhanced review and confirmation.

2. To restore the method default view, right-click the chromatogram plot and choose **Reset Scaling** from the shortcut menu.

❖ To change the displayed information for detected peaks

1. Right-click the chromatogram plot and pause the cursor over **Peak Labels**.

2. Choose to display labels for the peak retention time, peak height, peak area, or signal to noise.

   The label types in the list are selected for displayed labels and cleared for labels that are not displayed.

3. To remove a label, select the label type again and clear it.

   Label settings are globally applied to quan peaks, confirming peaks, and internal standard peaks.

> **Note** The labels do not always update on all peak displays. To update all labels, select a different compound, then reselect the compound whose labels you changed.

❖ To display the peak information window

1. Right-click the quantification and confirming ion chromatogram plots.
2. Choose **Show Peak Info** from the shortcut menu.

   Information in this window includes the data stream processed for this ion, consisting of a particular detector, filter (if applicable), and trace. For example, an MS detector might show a filter of "+ c Full ms [35.00-500.00]" and a Mass Range trace.

   This window also shows the peak area and height, along with the retention times of the peak integration and the peak apex.

Table 56. Confirming Ions shortcut menu (Sheet 1 of 2)

Command	Description
Method integration settings	Displays method integration settings.
Manual integration settings	Displays manual integration settings.
Add peak - Remove peak - Cancel add peak	Adds a peak, removes a manually added peak, or cancels an add peak operation in progress.
Range Calc method: Manual	Selects the method used to calculate the ion ratio range windows: Manual, Average, Weighted Average, or Level
Range calc level	Specifies the range based on the calibration level.
Target ratio:	Specifies the theoretical ratio of the confirming ion's response to the quantification ion's response.
Window type:	Specifies the Absolute or Relative calculation approach for determining the acceptable ion ratio range.
Window: %	Specifies the acceptable ion ratio range.
Peak labels	Displays or hides the peak labels (Label Area, Label Retention Time, Label Height, or Label Signal to Noise).
Show peak info	Displays peak information for the selected compound. For example:

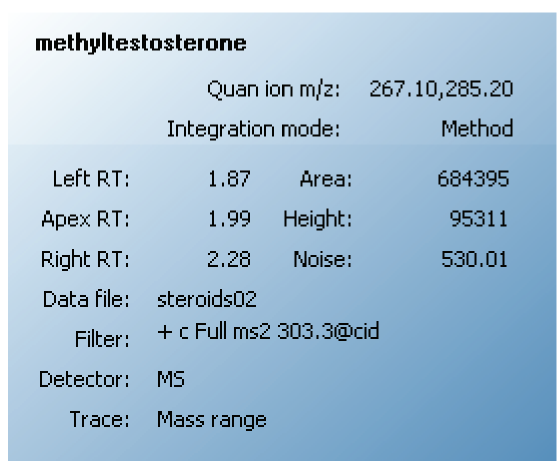
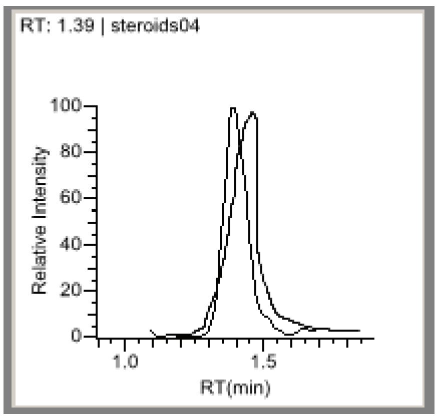


Table 56. Confirming Ions shortcut menu (Sheet 2 of 2)

Command	Description
Reset scaling	Resets the original scaling after a zoom operation.
Peak detection settings	Opens the Peak Detection Settings dialog box for the selected compound. See "Peak Detection Settings" on page 222.

Ion Overlay

The Ion Overlay page represents an overlay of the entire ion set—quantification and qualifying/confirming—for the selected sample and compound. Use this page to graphically review the peak apex alignment and co-eluting peak profiles.



❖ **To zoom in on a peak**

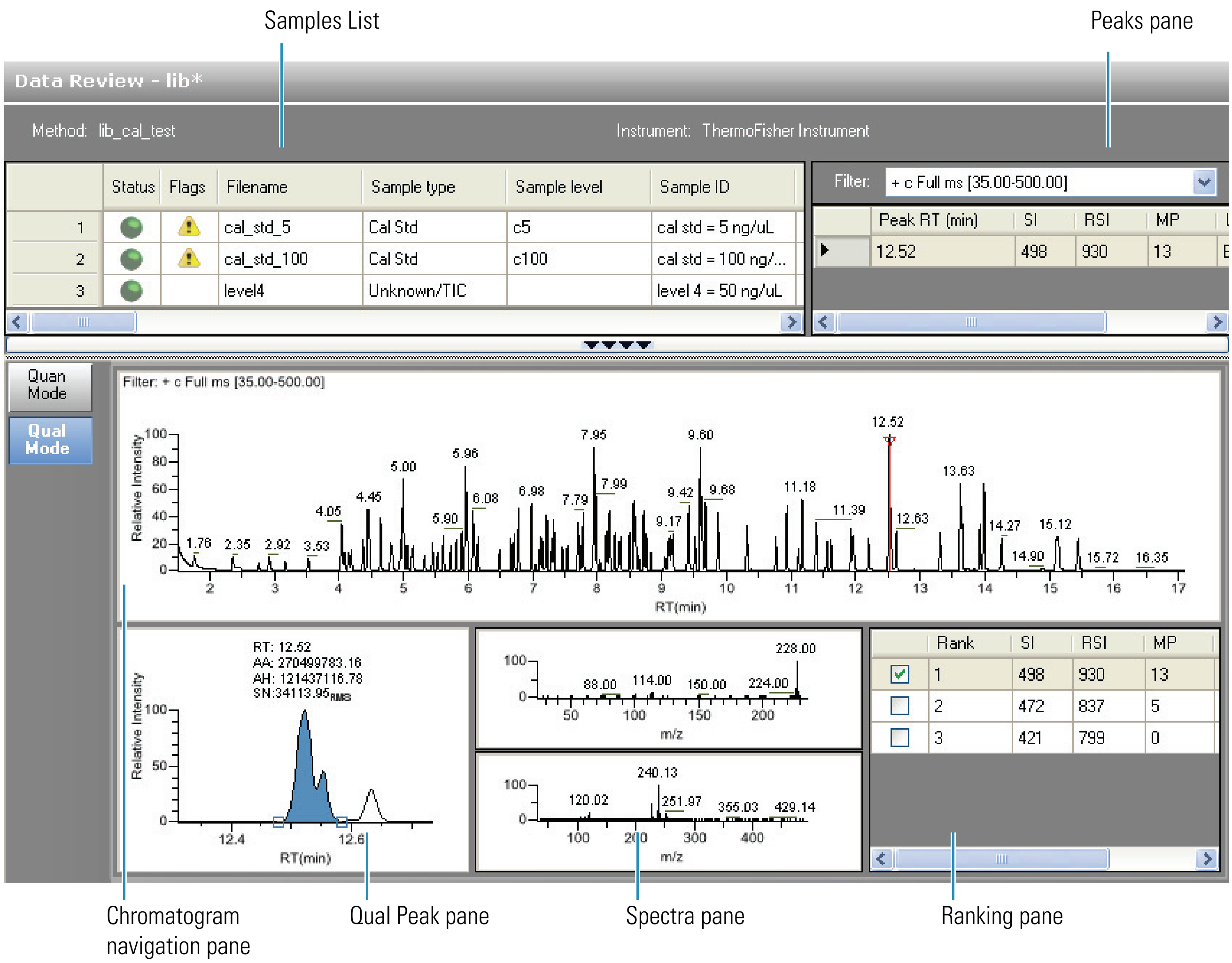
1. Drag the cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view.

2. To restore the method default view, right-click the chromatogram plot and choose **Reset Scaling** from the shortcut menu.

Qual Mode

The Qual Mode displays detected peaks for the selected sample and lets you manually add peaks.



Tip To resize the panes, drag the separators that divide the panes.

In addition to the Samples List, the Qual Mode view displays data in the following panes:

- Peaks Pane
- Chromatogram Navigation Pane
- Qual Peak Pane
- Spectra Pane (reference and selected)
- Ranking Pane

Peaks Pane

The Peaks pane works with the Samples list to display graphical values for a unique sample and peak combination.

❖ To display peaks for a specific compound

1. From the Samples list, select a sample.

> **Note** When you choose a calibration sample, the EnviroLab Forms application returns you to Quan Mode. The Peaks pane is not displayed in Quan Mode.

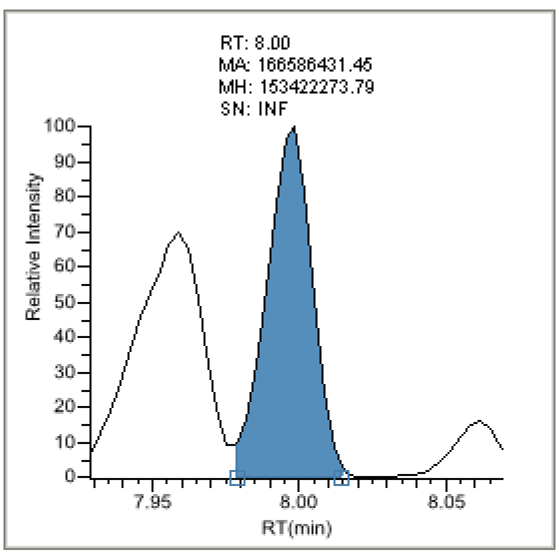
The Peaks pane lists the retention time for peaks identified in the selected sample, the values for the best match methods for each peak, and the compound match.

The number of peaks that are listed is specified in the method. You can change the number of identified peaks in the Method Template Editor. See “Identify the peaks” on page 153.

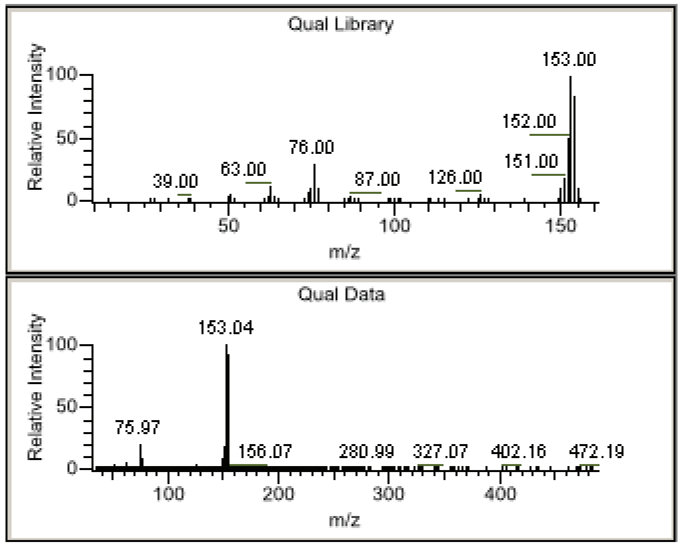
2. From the Peaks pane, select a peak in the sample.

	Peak RT (min)	SI	RSI	MP	Library entry
	5.01	844	847	33	o-Toluidine
	5.46	892	894	98	2-Cyclohexen-1-one, 3,5,5-trimethyl-
▶	8.00	937	937	80	Acenaphthene
	8.84	259	549	0	Naphthalene, 1-methyl-
	10.94	942	943	53	Fluoranthene

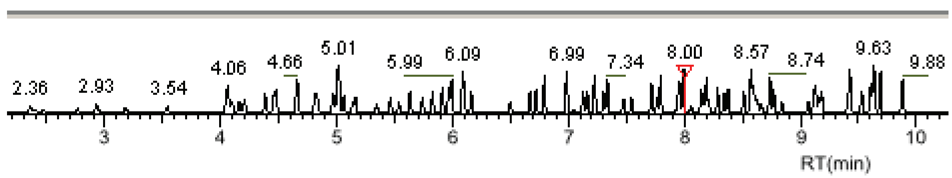
The EnviroLab Forms application displays the selected peak in the Qual Peak pane.



The EnviroLab Forms application displays the spectra data for the peak and the reference spectra for the identified library compound in the Spectra pane.



The EnviroLab Forms application locates the selected peak in the navigation chromatogram.



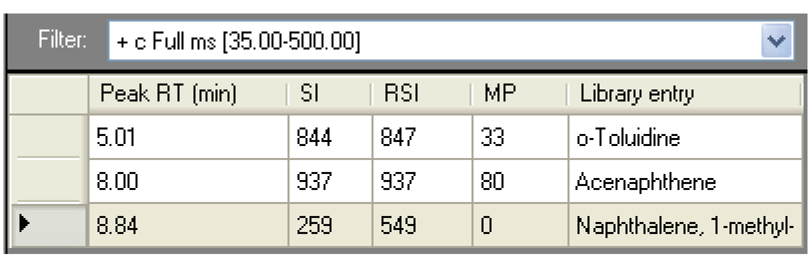
❖ To remove a peak

1. Select a peak in the Peaks pane.
2. Right-click and choose **Remove Selected Peak** from the shortcut menu.

   The EnviroLab Forms application removes the selected peak from the peaks list.

> **Note** There is no undo for this action, but you can manually add a peak to redefine a removed peak. See "Chromatogram Navigation Pane" on page 232.

Figure 54. Peaks pane



Filter: + c Full ms [35.00-500.00]

	Peak RT (min)	SI	RSI	MP	Library entry
	5.01	844	847	33	o-Toluidine
	8.00	937	937	80	Acenaphthene
▶	8.84	259	549	0	Naphthalene, 1-methyl-

Table 57. Peaks pane parameters

Command	Description
Filter	Filter used to identify the peaks. Specified in the raw data file or the master method.
Peak RT (min)	Peak retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
SI	Search index method used to search the NIST library.
RSI	Reverse search index method used to search the NIST library.
MP	Match probability.
Library entry	Library compound that matches the identified peak.
Remove selected peak	Shortcut menu command that removes the selected peak from the peaks list.

Chromatogram Navigation Pane

The chromatogram navigation pane displays all peaks in the selected sample. The peak selected in the Peaks pane is indicated with a red marker.

Follow these procedures:

- To zoom in on a peak
- To manually add a peak

❖ To zoom in on a peak

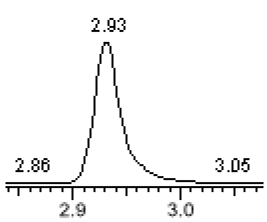
1. In the chromatogram navigation pane, drag the cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view to help you examine the peak limits for enhanced review and confirmation.

2. To restore the default view, right-click the chromatogram navigation pane and choose **Reset Scaling** from the shortcut menu.

❖ To manually add a peak

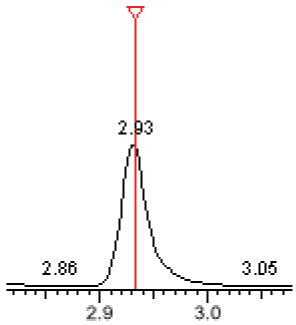
1. Zoom in to make it easier to identify the peak you want to add to the results set.



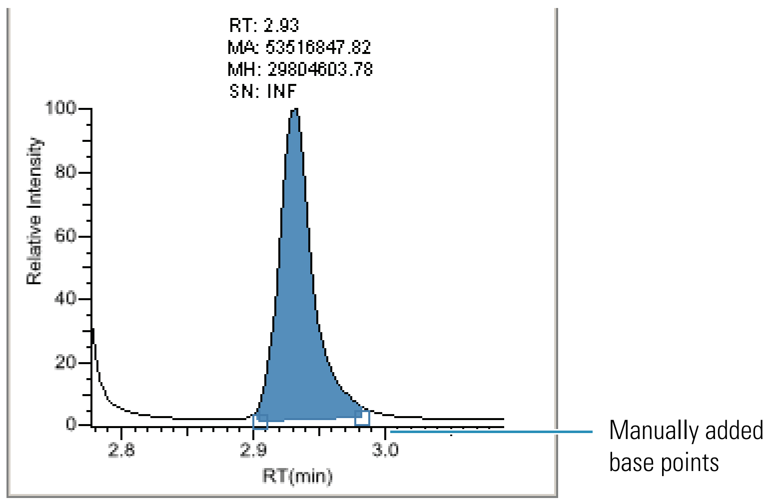
2. Right-click the chromatogram navigation pane, and choose **Add Peak** from the shortcut menu.

3. Click to indicate the left and right base points for the peak.

   The EnviroLab Forms application marks the peak in the chromatogram navigation pane.



   The EnviroLab Forms application places the peak delimiter tags at the base point locations and automatically updates the peak values in the Peaks pane and Qual Peak pane.



	Peak RT (min)	SI	RSI	MP	Library entry
▶	2.93	930	933	94	Phenol, 2-fluoro-
	3.18	834	845	96	Ethanamine, N-ethyl-N-nitroso-
	5.01	800	903	5	Phenol, 3-methyl-

Figure 55. Navigation Chromatogram pane

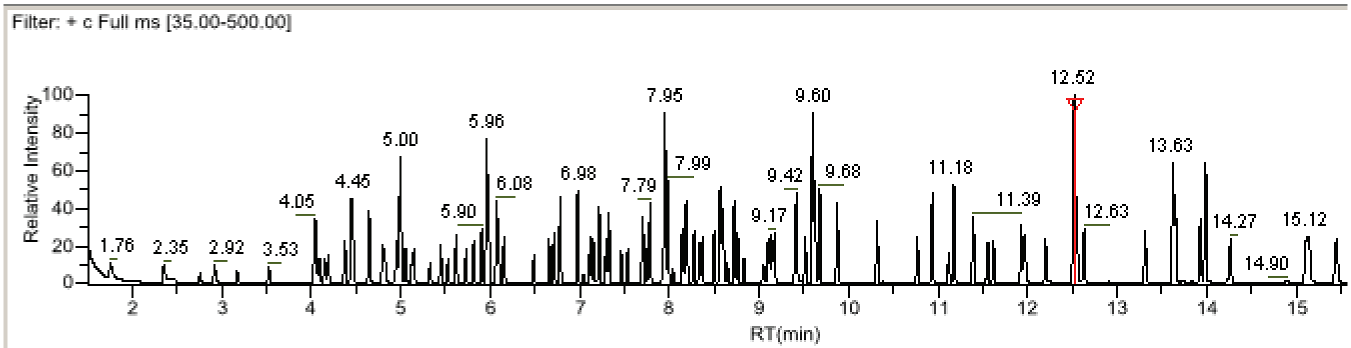


Table 58. Navigation Chromatogram shortcut menu

Command	Description
Add peak	Lets you manually add a peak.
Reset scaling	Resets the original scaling after a zoom operation.

Qual Peak Pane

The Qual Peak pane displays the selected peak.

Follow these procedures:

- To zoom in on a peak
- To manually add a peak
- To remove a peak
- To switch between method and manual integration modes
- To change the displayed information for detected peaks

❖ To zoom in on a peak

1. In the chromatogram plot, drag the cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view to help you examine the peak limits for enhanced review and confirmation.

2. To restore the default view, right-click the chromatogram plot and choose **Reset Scaling** from the shortcut menu.

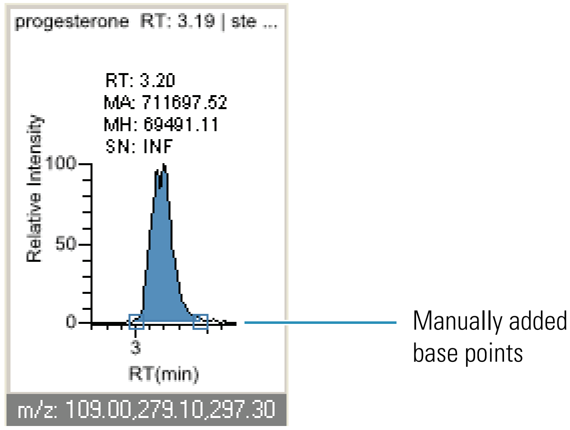
❖ To manually add a peak

1. Right-click anywhere in the Qual Peak pane, and choose **Add Peak** from the shortcut menu.

   If a peak is already detected, the Add Peak command is not enabled.

2. Click to indicate the left and right base points for the peak.

The EnviroLab Forms application places the peak delimiter tags at these locations and automatically updates the peak values (area, height, and so forth) in the result set.



❖ To remove a peak

Right-click the chromatogram plot, and choose **Remove Peak** from the shortcut menu.

The EnviroLab Forms application removes the peak displayed in the Qual Peak pane. All data for this peak is removed from the Qual Mode panes.

❖ To switch between method and manual integration modes

Right-click the chromatogram view and choose **Method Integration** or **Manual Integration** from the shortcut menu.

Initially, the method and manual integration settings that are stored for a compound and file are identical and when you select one mode it does not affect the saved result set. However, when manual data are available, the chromatogram plots and the result set update as you switch between method and manual modes.

As you switch between modes, the changes are reflected in each pane. The generated reports for this data identify the manual modifications.

❖ To change the displayed information for detected peaks

1. Right-click the chromatogram plot and pause the cursor over **Peak Labels**.
2. Choose to display labels for the peak retention time, peak height, peak area, or signal to noise.

   The label types in the list are selected for displayed labels and cleared for labels that are not displayed.

3. To remove a label, select the label type again and clear it.

   Label settings are globally applied to qual peaks, confirming peaks, and internal standard peaks.

> **Note** The labels do not always update on all peak displays. To update all labels, select a different compound, and then reselect the compound whose labels you changed.

Table 59. Qual peak shortcut menu

Command	Description
Reset scaling	Resets the original scaling after a zoom operation.
Method integration	Displays method integration settings.
Manual integration	Displays manual integration settings.
Peak labels	Displays or hides the peak labels (Label Area, Label Retention Time, Label Height, or Label Signal to Noise).
Remove peak	Removes the peak displayed in the Qual pane.

Spectra Pane (reference and selected)

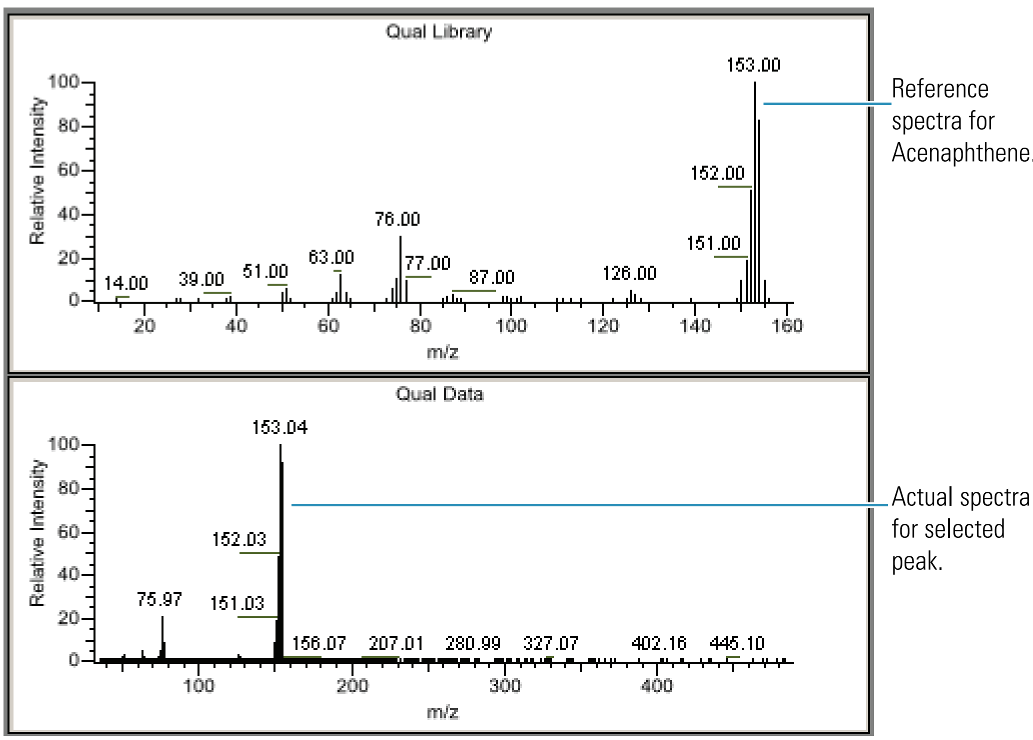
The Spectra pane displays the reference spectra and the spectra for the selected sample. The top pane displays the reference spectra for the identified compound from the library; the bottom pane displays the spectra for the selected peak.

❖ To zoom in on a peak

1. In the spectra plot, drag the cursor to delineate a rectangle around the peak.

   The delineated area expands to fill the view to help you examine the peak limits for enhanced review and confirmation.

2. To restore the default view, right-click the chromatogram plot and choose **Reset Scaling** from the shortcut menu.



	Peak RT (min)	SI	RSI	MP	Library entry
	5.01	844	847	33	o-Toluidine
	5.46	892	894	98	2-Cyclohexen-1-one, 3,5,5-trimethyl-
▶	8.00	937	937	80	Acenaphthene
	8.84	259	549	0	Naphthalene, 1-methyl-
	10.94	942	943	53	Fluoranthene

Ranking Pane

This pane displays the three best library matches for the selected peak. Use this pane to select a different library entry for the peak.

❖ To change the library entry for a selected peak

1. In the Ranking pane, select the check box for the library entry you want to use to identify the selected peak.

    - In the Spectra pane, the reference spectra changes to show the spectra for the selected library entry.
    - In the Peaks pane, the SI, RSI, MP, and Library Entry values update to reflect the selected library entry.

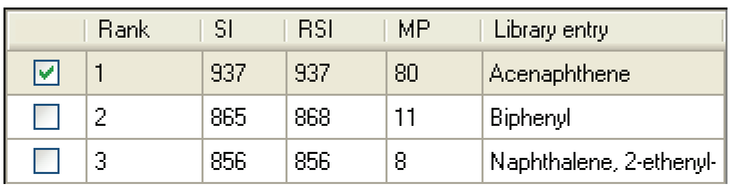


Table 60. Ranking pane parameters

Command	Description
<Check box column>	Lets you choose a library entry for the selected peak.
Rank	Indicates the order of best matches between the selected peak and library entries.
SI	Search index method used to search the NIST library.
RSI	Reverse search index method used to search the NIST library.
MP	Match probability.
Library entry	Library compound that matches the identified peak.

Working in Report View

Use the Report View to display the reports for the batch currently selected in the Data Review view or to display the Active View for the reports.

❖ To open the Report View

1. Click **Production** from the dashboard or the navigation pane.

   The Production navigation pane opens.

2. From the Production navigation pane, click **Report View**.

   From the Report View, you can access the following pages:

   - Displaying the Report View Page
   - Displaying the Active View Page

Displaying the Report View Page

Use the Report View page to select a report and navigate the report display.

❖ To display the Report View page

Click the **Report View** tab.

The Report View page is the default page.

❖ To display a report

1. Select a report type from the Select a Report list.

   Only the report types created for the current batch are displayed in the list.

2. (Optional) When the report type includes separate reports for each sample, select a sample file.

Note All report types create separate reports for each sample except the standard Batch Report and custom reports that are specified as batch-level reports. See "Custom Reports" on page 44.

❖ To print a report

1. Select the report you want to print from the Select a Report list.
2. Do one of the following:

   Choose **File > Print Batch** from the main menu.

   The EnviroLab Forms application immediately sends all reports for the batch to your default printer. There is no dialog box or confirmation message.

   –Or–

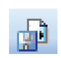
   a. Click the **Print Report** icon, .

      The Print dialog box for your default printer opens.

   b. Follow the typical procedure to print from your printer.

      Landscape reports are automatically rotated to fit the paper.

❖ To export a report

1. Select the report you want to print from the Select a Report list.
2. Click the **Export Report** icon, .

   The Export Report dialog box opens.

3. Locate the folder where you want to write the report file and click **Save**.

   The EnviroLab Forms application writes the Crystal Reports (.rpt) or custom reports file to the specified folder.

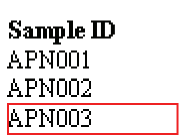
❖ To search for text in a report

1. Select a report from the Select a Report list.
2. Click the **Find Text** icon, .

   The Find Text dialog box opens.

3. Enter your text and click **Find Next**.

   When the EnviroLab Forms application locates the text, it encloses the text in a red box.



❖ To enlarge the report text

1. Select a report from the Select a Report list.
2. Click the **Zoom** icon, , and select a zoom scale.

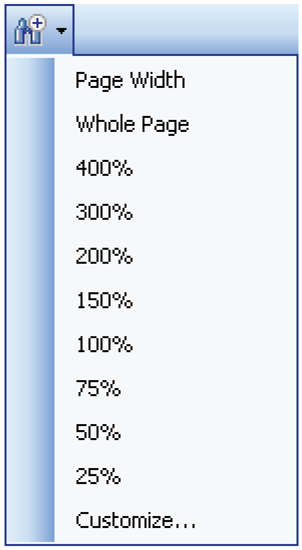


Figure 56. Report View page

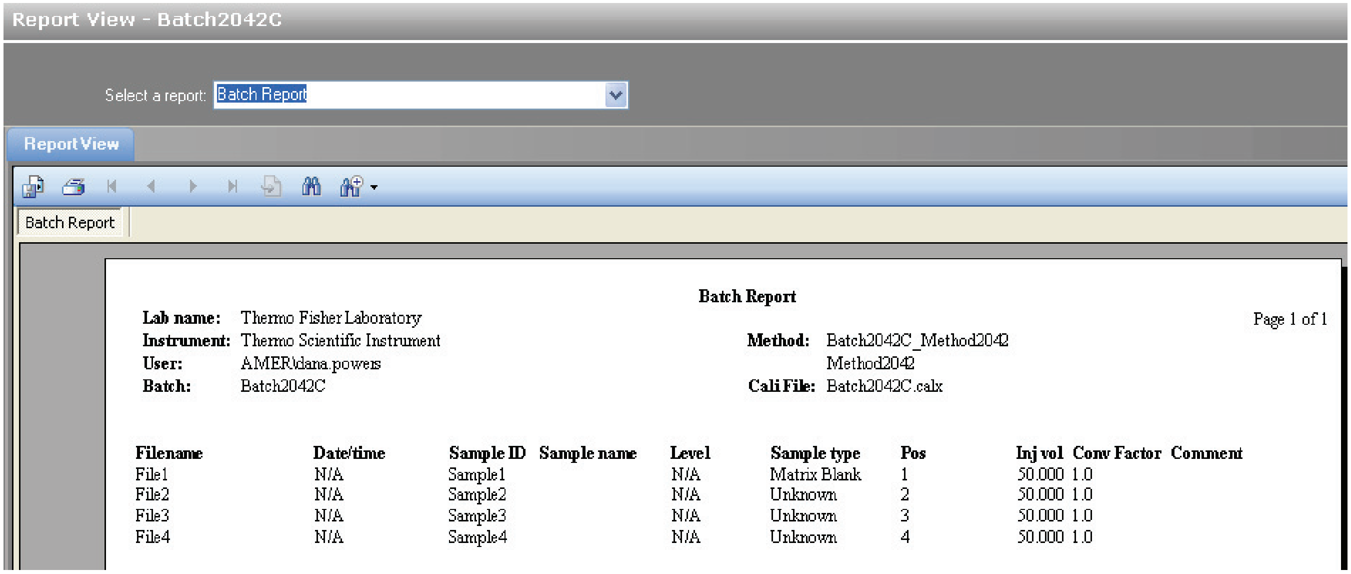


Table 61. Report View parameters

Command	Description
Select a report	Displays the report types created for the current batch.
Export Report 	Writes the Crystal Reports (.rpt) or custom reports file to a specified folder.
Print Report 	Sends all reports for the batch to your default printer. There is no dialog box or confirmation message.
Find Text 	Locates the specified text and encloses the text in a red box.
Zoom 	Enlarges the report text by the specified scale factor.

Displaying the Active View Page

Use the Active View page to view quantitative data for each sample in a report. Data in Active View are labeled with flag information. These flags are based on a comparison of the batch data to criteria defined in the master method.

❖ To display the Active View page

Click the **Active View** tab.

The Active View page displays quantitative data and QAQC error flags for each sample. See "Active View page" on page 244.

❖ To display a report

1. Select a report type from the Select a Report list.

   Only the report types created for the current batch are displayed in the list.

2. (Optional) When the report type includes separate reports for each sample, select a sample file.

❖ To filter which compounds to display

Toggle the **Showing** button to display either all compounds or only compounds that are flagged for failing a QAQC test.

Figure 57. Active View page

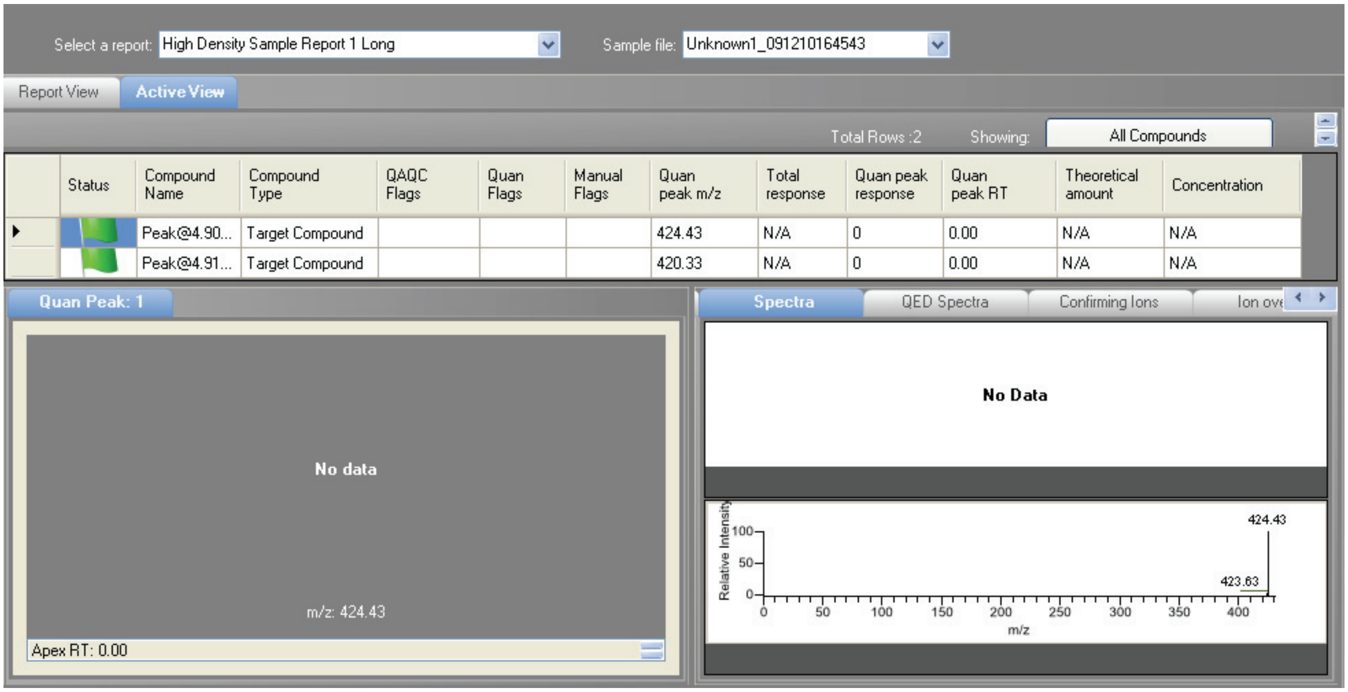


Table 62. Active View parameters (Sheet 1 of 4)

Parameter	Description
Display selection	
Select a report	Displays the report types created for the current batch.
Sample file	Used when the report type includes separate reports for each sample.
Showing	Lists the available compound types to display in Active View: Quan, Non quan, Target, Internal Standards, or Surrogates.

Table 62. Active View parameters (Sheet 2 of 4)

Parameter	Description
Column headings	
Status	The status of the reported compound. • A yellow warning flag indicates one of the following conditions: – The compound was manually integrated – Any of the confirming peaks was manually integrated. – The compound has quan flags. • A red warning flag indicates that the QAQC checks failed. • A green flag indicates that none of these conditions exist. When the compound is an internal standard, warning flags are displayed only on the internal standard report. The Status column is blank for Manual Integration reports.
Compound Name	Alphanumeric name assigned to the compound.
Compound Type	Target Compound, Internal Standard, or Surrogate.
QAQC Flags	Indicates that the QAQC check for the sample failed. The QAQC column is not used for Manual Integration reports.
Quan Flags	Quantification flags include: • Limit of Detection (LOD) • Limit of Quantitation (LOQ) • Limit of Reporting (LOR) • Values between the limit of detection and the limit of quantitation, known as the J flag • Upper Limit of Linearity (ULOL) Quan flags do not apply to the following sample types: Cal Std, Chk Std, Matrix Blank, or Solvent. The Quan Flag column is not used for Manual Integration reports.
Manual Flags	Indicates manually integrated peaks. • M indicates a manually integrated quan peak. • m indicates a manually integrated confirming peak.
Depending on the selected report, the active view page contains any or all of the following parameters:	
Quan peak m/z	Mass-to-charge ratio for the selected quantitation peak.
Total response	The sum of all Quan Peak Response values for the compound.
Quan peak response	Response of the quan peak.

Table 62. Active View parameters (Sheet 3 of 4)

Parameter	Description
Quan peak RT	Retention time for the quan peak.
Theoretical amount	Theoretical amount of the compound. Reports N/A when not applicable.
Concentration	
Confirming *n* Mass	Mass of the confirming peak.
Confirming *n* Response	Response of the confirming peak.
Confirming *n* Manual Flag	Indicates a manually integrated confirming peak.
Confirming *n* Ion Ratio Flag	Indicates that the ion ratio is out of range.
Confirming *n* Ion Ratio	Actual ratio of the confirming ion response to the quan ion response.
Confirming *n* Range	Acceptable range for the confirming ion.
Retention Time	The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Quan mass	The mass-to-charge ratio used to determine the peak area and peak height of the compound.
Response	Sum of all Quan Peak Response values for the compound.
Injection concentration	Calculated amount as the sample was injected, with no conversion applied.
Injection Units	Injection units specified on the Calibration page in Method Development mode. See "Calibration" on page 111.
Sample Concentration	The injected concentration multiplied by the conversion factor.
Sample Units	Sample units specified on the Calibration page in Method Development mode. See "Calibration" on page 111.
QIon	Mass range for the quan peak.
RT	Retention time. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Manual Integration reports	
m/z	Mass-to-charge ratio for the quan peak.
Method RT	Apex retention time for the method-integrated peak.
Method Peak Height	Height of the method-integrated peak.

Table 62. Active View parameters (Sheet 4 of 4)

Parameter	Description
Method Peak Area	Area of the method-integrated peak.
Manual RT	Apex retention time for the manually integrated peak.
Manual Peak Height	Height of the manually integrated peak.
Manual Peak Area	Area of the manually integrated peak.
Internal Standard reports	
Std Response	Average of the internal standard's response as found in the calibration file.
Minimum Response	Minimum response time as specified on the ISTD page in Method Development mode. See "ISTD" on page 127.
Maximum Response	Maximum response time as specified on the ISTD page in Method Development mode. See "ISTD" on page 127.
Sample Response	Area found in the sample.
Std RT	Average retention time as found in the calibration file.
Min RT	Minimum retention time as specified on the ISTD page in Method Development mode. See "ISTD" on page 127.
Max RT	Maximum retention time as specified on the ISTD page in Method Development mode. See "ISTD" on page 127.
Sample RT	Retention time found in the sample.
Graphical data	
Quan Peak 1	
Calibration curve	Displays a graphical view of the calibration curve for the selected compound and key statistical values for evaluating the quality of the calibration.
Spectra	Displays a comparison of the spectra found in the data and the method reference.
Confirming Ions	Displays a graphical view of all qualifying/confirming ions for the selected sample and compound and displays calculated ion ratios and ion ratio acceptance windows.

Active View Report Contents

Each standard report that uses the Active View displays values that are common to all reports:

- Common Active View report values

In addition to the common values, the following reports display additional active view features:

- Blank Report Active View values
- High Density 1 and High Density 1 Long Report Active View values
- High Density 2 and High Density 2 Long Report Active View values
- High Density 3 and High Density 3 Long Report Active View values
- Internal Standard Report Active View values
- Ion Ratio Failure Report Active View values
- LCSLCSD Report Active View values
- Manual Integration Report Active View values
- Method Detection Limit Report Active View values
- Method Validation Report Active View values
- MSMSD Report Active View values
- QC Report Active View values
- Quantitation Report Active View values
- Sample Report and Sample Report Long Active View values
- Solvent Blank Report Active View values

Table 63. Common Active View report values

Column	Description
Status	The status of the reported compound. • A yellow caution sign indicates one of the following conditions: – The compound was manually integrated – Any of the confirming peaks was manually integrated. – The compound has quan flags. – The compound has a QAQC failure. • A green check mark indicates that none of these conditions exist. When the compound is an internal standard, warning flags are displayed only on the internal standard report.
Compound name	Alphanumeric name assigned to the compound.
Compound type	Target Compound, Internal Standard, or Surrogate.
QAQC flags	Indicates that the QAQC check for the sample failed. This column is not included on the Method Validation and MDL reports.
Quan flags	• Quan flags include Limit of Detection (LOD) • Limit of Quantitation (LOQ) • Limit of Reporting (LOR) • Values between the limit of detection and the limit of quantitation, known as the J flag • Upper Limit of Linearity (ULOL) Quan flags do not apply to the following sample types: Cal Std, Chk Std, Matrix Blank, or Solvent. This column is not included on the Calibration report. This column is not included on the Method Validation, Method Detection Limit, or LCSLCSD reports.
Manual flags	Indicates manually integrated peaks. • M indicates a manually integrated quan peak. • m indicates a manually integrated confirming peak.

Table 64. Blank Report Active View values

Column	Description
Retention Time	Retention time for the quan mass. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Quan Mass	Mass range for the quan peak.
Response	Sum of all Quan Peak Response values for the compound.
Inj Conc	Calculated amount as the sample was injected, with no conversion applied.
Inj Units	Injection units specified on the Calibration page in Method Development mode. See "Calibration" on page 111.
Sample Conc	Calculated amount multiplied by the conversion factor.
Sample Units	Sample units specified on the Calibration page in Method Development mode. See "Calibration" on page 111.

Table 66. High Density 1 and High Density 1 Long Report Active View values

Column	Description
m/z	Mass-to-charge ratio for the quan peak.
Total Response	The sum of all Quan Peak Response values for the compound.
Quan Peak Response	Response of the quan peak.
Quan Peak RT	Retention time for the quan peak.
T Amount	Theoretical amount of the compound. Reports N/A when not applicable.
Conc	Calculated (injected) amount.

Table 67. High Density 2 and High Density 2 Long Report Active View values

Column	Description
m/z	Mass-to-charge ratio for the quan peak.
Total Response	Sum of all Quan Peak Response values for the compound.
Quan Peak Response	Response of the quan peak.
Quan Peak RT	Retention time for the quan peak.
T Amount	Theoretical amount of the compound. Reports N/A when not applicable.
Conc	Calculated (injected) amount.
Confirming 1 Mass	Mass of the confirming peak.

Table 67. High Density 2 and High Density 2 Long Report Active View values

Column	Description
Confirming 1 Response	Response of the confirming peak.
Confirming 1 Manual Flag	Indicates a manually integrated confirming peak.
Confirming 1 Ion Ratio Flag	Indicates that the ion ratio is out of range.
Confirming 1 Ion Ratio	Actual ratio of the confirming ion response to the quan ion response.
Confirming 1 Range	Acceptable range for the confirming ion.

Table 68. High Density 3 and High Density 3 Long Report Active View values

Column	Description
m/z	Mass-to-charge ratio for the quan peak.
Total Response	Sum of all Quan Peak Response values for the compound.
Quan Peak Response	Response of the quan peak.
Quan Peak RT	Retention time for the quan peak.
T Amount	Theoretical amount of the compound. Reports N/A when not applicable.
Conc	Calculated (injected) amount.
Confirming 1 Mass	Mass of the confirming peak.
Confirming 1 Response	Response of the confirming peak.
Confirming 1 Manual Flag	Indicates a manually integrated confirming peak.
Confirming 1 Ion Ratio Flag	Indicates that the ion ratio is out of range.
Confirming 1 Ion Ratio	Actual ratio of the confirming ion response to the quan ion response.
Confirming 1 Range	Acceptable range for the confirming ion.
Confirming 2 Mass	Mass of the confirming peak.
Confirming 2 Response	Response of the confirming peak.
Confirming 2 Manual Flag	Indicates a manually integrated confirming peak.
Confirming 2 Ion Ratio Flag	Indicates that the ion ratio is out of range.
Confirming 2 Ion Ratio	Actual ratio of the confirming ion response to the quan ion response.
Confirming 2 Range	Acceptable range for the confirming ion.

Table 69. Internal Standard Report Active View values

Column	Description
Std Response	Average of the internal standard's response as found in the calibration file.
Minimum Response	Minimum response time as specified on the ISTD page in Method Development mode. See "ISTD" on page 127.
Maximum Response	Maximum response time as specified on the ISTD page in Method Development mode. See "ISTD" on page 127.
Sample Response	Area found in the sample.
Std RT	Average retention time as found in the calibration file.
Min RT	Minimum retention time as specified on the ISTD page in Method Development mode. See "ISTD" on page 127.
Max RT	Maximum retention time as specified on the ISTD page in Method Development mode. See "ISTD" on page 127.
Sample RT	Retention time found in the sample.

Table 70. Ion Ratio Failure Report Active View values

Column	Description
Quan Ion	The ion for quan peak.
Qual Ion	The ion for the confirming peak.
Quan Ion Response	Response of the quan ion.
Qual Ion Response	Response of the qual ion.
Ratio	The ratio of the confirming ion response to the quan ion response.
Range	The acceptable range.

Table 71. LCSLCSD Report Active View values

Column	Description
Spike Amount	Lab control theoretical concentration.
LCS Concentration	Lab control spike concentration.
LCS % Received	Lab control concentration percentage.
Lower Limit %	Recovery lower limit as specified in the master method. See the Limits section in "Editing the QAQC Page" on page 117.

Table 71. LCSLCSD Report Active View values

Column	Description
Upper Limit %	Recovery upper limit as specified in the master method. See the Limits section in "Editing the QAQC Page" on page 117.
LCSD Concentration	Lab control spike duplicate concentration
LCSD % Received	Lab control duplicate concentration percentage
RPD	Lab control relative percentage difference
Max RPD	Lab control spike maximum relative percentage difference (set in method)
Number of Rec Failures	Number of recovery failures for lab control spike concentration and lab control spike concentration duplicate.
Number of RPD Failures	Number of relative percentage difference failures for lab control spike concentration and lab control spike concentration duplicate.

Note For LCSLCSD batch reports, the active view peak graphics are shown only when you click a field pertaining to a sample, such as LCS or LCSD concentration fields.

Table 72. Manual Integration Report Active View values

Column	Description
m/z	Mass-to-charge ratio for the quan peak.
Method RT	Apex retention time for the method-integrated peak.
Method Peak Height	Height for the method-integrated peak.
Method Peak Area	Area for the method-integrated peak.
Manual RT	Apex retention time for the manually integrated peak.
Manual Peak Height	Height of the manually integrated peak.
Manual Peak Area	Area of the manually integrated peak.

Table 73. Method Detection Limit Report Active View values

Column	Description
Avg Conc	The average of the concentration for the compound across all samples.
Std Dev	The standard deviation of the concentration.
t-stat	The t-statistic value defined as the ratio of a coefficient to its standard error.
% RSD	%RSD of concentrations
MDL	Method detection limits. The calculated limit of detection.

Note For Method Detection Limit batch reports, the active view peak graphics are shown only when you click a field pertaining to a sample. These numbered fields are to the right of the MDL column.

Table 74. Method Validation Report Active View values

Column	Description
Avg Conc	The average of the concentration for the compound across all samples.
Theo Conc	Values for each compound that represent the expected theoretical concentration of that compound in the sample as defined in the master method. See the Meth Val section in "Editing the QAQC Page" on page 117.
% Diff	The percentage difference calculated as ((MethodValidationMeanValue minus the Theo Conc) divided by the Theo Conc) multiplied by 100.
Min Conc	Calculated by (Min recovery percent * Theo Conc) divided by 100.
Max Conc	Calculated by (Max recovery percent * Theo Conc) divided by 100.
% RSD	%RSD of concentrations
Max % RSD	The maximum relative standard deviation (RSD) of the set of observed concentrations for a component across the set of method validation samples (when in average RF mode) as defined in the master method. See the Meth Val section in "Editing the QAQC Page" on page 117.
Calculated Amount <*Sample Name*>	This field will be reproduced for every Method Val sample.

Table 75. MSMSD Report Active View values

Column	Description
Unknown Concentration	Concentration of the unknown sample.
Spike Amount	Matrix spike theoretical concentration.
MS Concentration	Matrix spike concentration.
MS % Received	Matrix spike concentration percentage.
Lower Limit %	Recovery lower limit as specified in the master method. See the Limits section in "Editing the QAQC Page" on page 117.
Upper Limit %	Recovery upper limit as specified in the master method. See the Limits section in "Editing the QAQC Page" on page 117.
MSD Concentration	Matrix spike duplicate concentration.
MSD % Received	Matrix spike duplicate concentration percentage.
RPD	Matrix spike relative percentage difference.
Max RPD	Maximum relative percentage difference as specified in the master method. See the Lab Control section in "Editing the QAQC Page" on page 117.
Number of Rec Failures	Number of matrix spike and matrix spike duplicate failures.
Number of RPD Failures	Number of relative percentage difference failures.

Note For MSMSD batch reports, the active view peak graphics are shown only when you click a field pertaining to a sample, such as Unknown, MS, or MSD concentration fields.

Table 76. QC Report Active View values (Sheet 1 of 2)

Column	Description
Curve Type	L - Linear A - Average RF Q - Quadratic
Daily RF	The response factor value for Average RF curve types. For all other curve types, this column is blank.
Mean RF	The average response factor as found in the calibration file. Displayed for Average RF curve types. For all other curve types, this column is blank.
Min RF	Minimum QC response factor as found on the QC Check page in the method.

Table 76. QC Report Active View values (Sheet 2 of 2)

Column	Description
RF % D	Percent difference between daily and average response factor.
Max RF Diff (%)	Maximum QC response factor as found on the QC Check page in the method.
QC Amount	The amount defined by the level for the compound.
Calculated Amount	Reportable amount of concentration.
Amount % Difference	Percentage difference between the calculated amount and the QC amount. Use the injected concentration to calculate this value.
Max Amount % Difference	Maximum allowed percentage difference between the calculated amount and the QC amount.

Table 77. Quantitation Report Active View values (Sheet 1 of 2)

Column	Description
RT	Retention time for the peak. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
QIon	Mass range for the quan peak.
Response	Sum of all quan peak response values for the compound.
Injected Concentration (DE2999)	Calculated amount as the sample was injected, with no conversion applied. **Note:** As each additional sample is processed, calibration data changes; therefore, except for the final sample in a batch, a report in active view or report view will show different values from a physical (PDF, XML, or printed) report created at the end of processing. To avoid this discrepancy, do one of the following: • For the standard Quantitation Report or Quantitation Report - 2, observe the active or report view for only the last sample in the batch. • For the custom Quantitation Report, make the report a batch-level report.
Injected units	Injection units specified on the Calibration page in Method Development mode. See “Calibration” on page 111.

Table 77. Quantitation Report Active View values (Sheet 2 of 2)

Column	Description
Sample Conc	Calculated injection amount multiplied by the conversion factor. Refer to the note in the Injected Concentration description.
Sample units	Sample units specified on the Calibration page in Method Development mode. See "Calibration" on page 111.

Table 78. Sample Report and Sample Report Long Active View values

Column	Description
RT	Retention time for the peak. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
Ion Mass	The mass range for the ion.
Response	The total response time (the sum of all quan peak response times for the compound).
Calibration Amount	
Target Range	
Ratio	The ratio of the confirming ion response to the quan ion response.

Table 79. Solvent Blank Report Active View values

Column	Description
RT	Retention time for the quan peak. The time after injection at which the compound elutes. The total time that the compound is retained on the GC column.
QIon	Mass range for the quan peak.
Response	Sum of all Quan Peak Response values for the compound.
Method	Method of evaluation defined in the method.
Upper Limit	Defined in the method.

Working in the Local Method View

A local method is a copy of a master method associated with a batch. From the Local Method View, you can edit a local method or create a method template.

Follow these procedures:

- To open the Local Method View
- To create a method template

❖ To open the Local Method View

1. Click **Production** from the dashboard or the navigation pane.

   The Production navigation pane opens.

2. From the Production navigation pane, click **Local Method**.

   The Local Method View for the currently selected batch opens. Local methods are named *BatchName_MasterMethodName*.

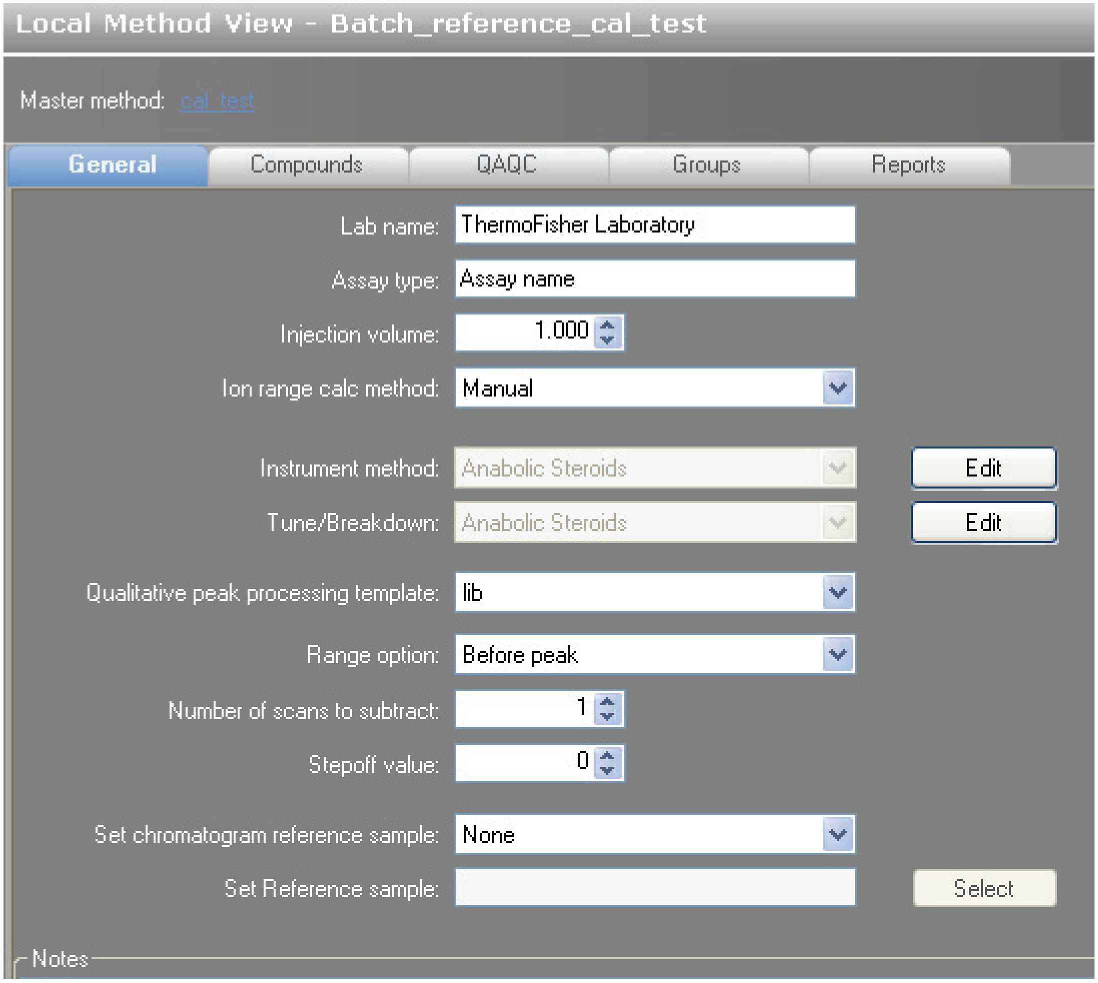
   You can edit many of the method parameters in a local method just as you would edit a master method. See "Editing a Master Method" on page 68.

3. Enter any local changes to the method.

4. Choose **File > Save**.

5. To process the batch or create new reports with the edited local method, return to the Batch View and submit the batch.

Figure 58. Local Method View page



❖ To create a method template

1. Click **Production** from the dashboard or the navigation pane.

   The Production navigation pane opens.

2. From the Production navigation pane, click **Local Method**.

   The Local Method View for the currently selected batch opens. Local methods are named *BatchName_MasterMethodName*.

3. From the main menu, choose **File > New > Method Template**.

   The Method Template Editor opens.

   Beginning with Step 3, follow the instructions "To create a method template" on page 147.

A

Reports

This appendix contains information about standard and custom reports.

Contents

The report engine can generate several different types of reports designed to meet the needs of the laboratory, the laboratory's customers, and key regulatory agencies that might review the results. The following types of reports meet the requirements of various methods and worldwide regulatory agencies and are designed to help track the performance of the system and method. The EnviroLab Forms application can produce both standard reports and custom reports.

Specifying Reports

As an IT Administrator or Manager, you can configure a list of reports that are available for Method Development or Production modes.

For detailed information about configuring reports in the Configuration mode, see "Specifying the Reports Configuration" on page 40.

For detailed information about specifying reports when you create a method in the Method Development mode, see "Editing the Reports Page" on page 138.

For detailed information about viewing batch reports in the Production mode, see "Working in Report View" on page 239.

Standard Reports

For each standard report you generate, you can create a hardcopy print, a PDF (.pdf), or an XML (.xml) output format. In addition to the report type, you can specify a report title for each of your reports. The default report title is the report name.

The EnviroLab Forms application can generate the following types of standard reports:

- Batch Report
- Blank Report
- Breakdown Report
- Calibration Report
- Check Standard Report
- Chromatogram Report
- Compound Calibration Report
- Confirmation Report
- Confirmation Report 2
- High Density Internal Standard Report
- High Density Internal Standard Report Long
- High Density Sample Report 1
- High Density Sample Report 1 Long
- High Density Sample Report 2
- High Density Sample Report 2 Long
- High Density Sample Report 3
- High Density Sample Report 3 Long
- Internal Standard Summary Report
- Ion Ratio Failure Report
- LCSLCSD Report
- Manual Integration Report
- Method Detection Limit Report
- Method Report
- Method Validation Report
- MSMSD Report
- Quantitation Report
- Quantitation Report - 2
- Solvent Blank Report
- Surrogate Recovery Report
- TIC Report
- TIC Summary Report
- Tune Report

To view an example of each type of standard report, see “Sample Standard Reports” on page 266.

Example PDFs of standard report formats are also located in the following folder:

C:\Thermo\Shared\ExampleReports

Custom Reports

For each custom report you generate, you can create a hardcopy printout or an XLS (.xlsm) output file. The default report title is the report name.

A user in the role of IT Administrator or Manager can configure custom reports to generate a single report for an entire batch or to create separate reports for each sample. Rather than creating separate reports for each sample, this method uses data from only the last sample to create a single report for the entire batch.

The EnviroLab Forms application includes the following custom reports:

- AltCalibrationReport
- BatchReport
- BlankReport
- CalibrationDensityReport
- CalibrationReport
- CheckStandardReport
- CompoundCalibrationReport
- ConfirmationReport
- ConfirmationReport2
- HighDensitySampleReport1Long
- HighDensitySampleReport2Long
- HighDensitySampleReport3Long
- QuantitationReport

Report Flags

When generating or viewing a report, you might see one of the following quantification or calibration flags listed on the page.

Table 80. Quantification flags

Flag	Definition
b	Compound was observed at a concentration in a Matrix Blank sample above the specified limit.
s	Compound was observed at a response in a solvent blank sample above the specified limit.
J	Compound was observed at a concentration above the limit of detection, but below the limit of quantitation.
I or *	Confirming/qualifying ion ratio for a compound was observed outside the target ratio range or the coelution between quantification and confirming/qualifying ion was larger than acceptable limit.
C	Compound was observed at a concentration above the specified carryover limit.
?	Compound was observed at a concentration above the specified linearity limit.
D	Compound was observed at a concentration below the specified limit of detection.
Q	Compound was observed at a concentration below the specified limit of quantitation.
POS	Compound was observed at a concentration above the specified cutoff.

Table 81. Calibration flags

Flag	Definition
D	Calibration for this compound exceeded the specified maximum percent relative standard deviation (%RSD).
F	Response factor for this compound was below the specified minimum response factor (Min RF).
R	Calibration for this compound was below the specified minimum correlation coefficient (r^2).
A	Back calculation of the calibration points for this compound exceeded the specified maximum percent difference (Max %D).
X	Calibration point for this compound was excluded from the overall calibration by manual selection.
X(ISNF)	Calibration point for this compound was excluded from the overall calibration because its associated internal standard was not found.

A QAQC failure is identified by an asterisk (*), a shaded row, or the word Fail.

Values on a report that are the result of a manual integration will use an uppercase M to signify a manually integrated quantification ion and a lowercase m to signify a manually integrated qualifying/confirming ion. On alternative reports, manual integration are signified by a black box around the value.

Sample Standard Reports

This section shows samples of the following standard report types:

- Batch Report
- Blank Report
- Breakdown Report
- Calibration Report
- Check Standard Report
- Chromatogram Report
- Compound Calibration Report
- Confirmation Report
- Confirmation Report 2
- High Density Calibration Report
- High Density Internal Standard Report
- High Density Internal Standard Report Long
- High Density Sample Report 1
- High Density Sample Report 1 Long
- High Density Sample Report 2
- High Density Sample Report 2 Long
- High Density Sample Report 3
- High Density Sample Report 3 Long
- Internal Standard Summary Report
- Ion Ratio Failure Report
- LCSLCSD Report
- Manual Integration Report
- Method Detection Limit Report
- Method Report
- Method Validation Report
- MSMSD Report
- Quantitation Report
- Quantitation Report - 2
- Solvent Blank Report
- Surrogate Recovery Report
- TIC Report
- TIC Summary Report
- Tune Report

Tip To easily view reports in landscape format, choose **View > Rotate View > Clockwise** from the Adobe Acrobat viewer menu.

Batch Report

Batch Report

Page 1 of 1

Lab name:	Thermo Fisher Laboratory		
Instrument:	ThermoFisher Instrument	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	March48270B_8level_342010_a	**Cali File:**	EC25B_8level_322010_a_March48270B_8level_342010_a.calx

Filename	Date/time	Sample ID	Sample name	Level	Sample type	Vial Pos	Inj vol	Conv Factor	Comment
342010_a001	3/4/2010 11:13:17 AM	DFTPP		N/A	Tune	1	1.000	1.0	
342010_a002	3/4/2010 11:39:33 AM	blk		N/A	Matrix Blank	2	1.000	1.0	
342010_a003	3/4/2010 12:03:15 PM	check std 50 ng		4	Chk Std	3	1.000	1.0	
342010_a004	3/4/2010 12:33:49 PM	5% diesel		N/A	Unknown	4	1.000	1.0	
342010_a005	3/4/2010 1:00:57 PM	5% diesel		N/A	Unknown	5	1.000	1.0	
342010_a006	3/4/2010 1:29:57 PM	5% diesel		N/A	Unknown	6	1.000	1.0	
342010_a007	3/4/2010 1:58:59 PM	5% diesel		N/A	Unknown	7	1.000	1.0	
342010_a008	3/4/2010 2:28:07 PM	5% diesel		N/A	Unknown	8	1.000	1.0	
342010_a009	3/4/2010 2:57:17 PM	5% diesel		N/A	Unknown	9	1.000	1.0	
342010_a010	3/4/2010 3:26:33 PM	5% diesel		N/A	Unknown	10	1.000	1.0	
342010_a011	3/4/2010 3:55:49 PM	5% diesel		N/A	Unknown	11	1.000	1.0	
342010_a012	3/4/2010 4:25:07 PM	5% diesel		N/A	Unknown	12	1.000	1.0	
342010_a013	3/4/2010 4:54:25 PM	5% diesel		N/A	Unknown	13	1.000	1.0	
342010_a014	3/4/2010 5:23:43 PM	5% diesel		N/A	Unknown	14	1.000	1.0	
342010_a015	3/4/2010 5:52:57 PM	5% diesel		N/A	Unknown	15	1.000	1.0	
342010_a016	3/4/2010 6:22:17 PM	5% diesel		N/A	Unknown	16	1.000	1.0	
342010_a017	3/4/2010 6:51:59 PM	5% diesel		N/A	Unknown	17	1.000	1.0	
342010_a018	3/4/2010 7:21:43 PM	5% diesel		N/A	Unknown	18	1.000	1.0	
342010_a019	3/4/2010 7:51:27 PM	5% diesel		N/A	Unknown	19	1.000	1.0	
342010_a020	3/4/2010 8:21:09 PM	5% diesel		N/A	Unknown	20	1.000	1.0	
342010_a021	3/4/2010 8:50:51 PM	5% diesel		N/A	Unknown	21	1.000	1.0	
342010_a022	3/4/2010 9:20:35 PM	5% diesel		N/A	Unknown	22	1.000	1.0	
342010_a023	3/4/2010 9:50:15 PM	5% diesel		N/A	Unknown	23	1.000	1.0	

* = Samples run outside of a 12 hour period since the Tune sample or samples acquired before tune sample acquisition.

Blank Report

Blank Report

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Lab name:	Thermo Fisher Laboratory	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8level
Instrument	ThermoFisher Instrument		EPAMethod8270B_8level
User:	AMER\jessie.butler		
Batch:	March48270B_8level_342010_a	**Cali File**	EC25B_8level_322010_a_March48270B_8level_342010_a.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	blk	342010_a002	N/A		3/4/2010 11:39:33 AM	

Internal Standards	RT	QIon	Response	Curve Type	Average RF/ Response	Injected Conc	Units	Calculated Conc	Units	Flags
1,4-DICHLOROBENZENE-D4_(IS)	5.57	152.00	2450326	Average RF	0.000	40.000	ng/uL	40.000	ng/uL	
NAPHTHALENE-D8_(IS)	7.05	136.00	8603918	Average RF	0.000	40.000	ng/uL	40.000	ng/uL	
ACENAPHTHENE-D10_(IS)	9.06	164.00	5426894	Average RF	0.000	40.000	ng/uL	40.000	ng/uL	
PHENANTHRENE_D10	10.75	188.00	8670698	Average RF	0.000	40.000	ng/uL	40.000	ng/uL	
CHRYSENE-D12_(IS)	13.75	240.00	3514767	Average RF	0.000	40.000	ng/uL	40.000	ng/uL	
PERYLENE-D12_(IS)	15.59	264.00	3058380	Average RF	0.000	40.000	ng/uL	40.000	ng/uL	

Surrogates	RT	QIon	Response	Curve Type	Average RF/ Response	Injected Conc	Units	Calculated Conc	Units	Max Conc	Flags
phenol-d5(sur)	5.10	99.00	4515414	Average RF	1.843	37.664	ng/uL	37.664	ng/uL	60.000	Pass
nitrobenzene-d5(sur)	6.21	82.00	3000349	Average RF	0.349	40.858	ng/uL	40.858	ng/uL	60.000	Pass
2,4,6-tribromophenol(sur)	9.95	330.00	396341	Average RF	0.073	36.308	ng/uL	36.308	ng/uL	60.000	Pass
p-terphenyl-d14(sur)	12.55	244.00	3010429	Average RF	0.857	40.157	ng/uL	40.157	ng/uL	60.000	Pass

Target Compounds	RT	QIon	Response	Curve Type	Average RF/ Response	Injected Conc	Units	Calculated Conc	Units	Max Conc	Flags
Pyridine_RCRA	2.61	79.00	213	Average RF	0.000	0.002	ng/uL	0.002	ng/uL	0.500	Pass I
2-Picoline	3.38	93.00	73	Average RF	0.000	0.001	ng/uL	0.001	ng/uL	0.500	Pass I
N-Nitrosomethylethylamine_APP9	3.47	88.00	2213	Average RF	0.001	0.049	ng/uL	0.049	ng/uL	0.500	Pass I
Methyl_methanesulfonate	4.01	80.00	16178	Average RF	0.007	0.610	ng/uL	0.610	ng/uL	0.500	Fail I,b
2-fluorophenol(sur)	4.01	112.00	3487653	Average RF	1.423	39.648	ng/uL	39.648	ng/uL	60.000	Pass
N-Nitrosodiethylamine_APP9	4.27	102.00	82	Average RF	0.000	0.002	ng/uL	0.002	ng/uL	0.500	Pass I
Ethyl_methanesulfonate	4.61	79.00	133	Average RF	0.000	0.002	ng/uL	0.002	ng/uL	0.500	Pass I
Phenol(CCC)	5.12	94.00	1314	Average RF	0.001	0.010	ng/uL	0.010	ng/uL	0.500	Pass I
Bis(2-chloroethyl)ether	5.38	93.00	83	Average RF	0.000	0.001	ng/uL	0.001	ng/uL	0.500	Pass I

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

Manually integrated

Breakdown Report

Breakdown Report

Lab name:	Thermo Fisher Laboratory			Page 1 of 1
Instrument:	ThermoFisher Instrument	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8level	
User:	AMER\jessie.butler		EPAMethod8270B_8level	
Batch:	March48270B_8level_342010_a	**Cali File:**	EC25B_8level_322010_a_March48270B_8level_342010_a.calx	

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
1	DFTPP	342010_a001	N/A		3/4/2010 11:13:17 AM	

Group name	Type	Response	% Breakdown	Max % Breakdown	Results
DDT Breakdown			0.07%	20.00%	Pass
p,p'-DDTs	Native	1626098			
4,4'-DDE	Breakdown	1147			
4,4'-DDD	Breakdown	0			

Calibration Report

Calibration Report

Lab name:	Thermo Fisher Laboratory			Page 1 of 7
Instrument:	ThermoFisher Instrument	**Method:**	EC25B_8level_322010_a_EPAMethod8270B_8level	
User:	AMER\jessie.butler		EPAMethod8270B_8level	
Batch:	EC25B_8level_322010_a	**Cali File:**	EC25B_8level_322010_a.calx	

Compound	1	2	3	4	5	6	7	Type	RRF	%RSD	R^2	Flag
N-Nitrosodimethylamine	0.643	0.659	0.638	0.687	0.658	0.644	0.719	A	0.675	6.05		
Pyridine_RCRA	1.225	1.306	1.374	1.439	1.457	1.627	1.574	A	1.446	9.72		
2-Picoline	1.448	1.579	1.713	1.802	1.613	1.827	1.982	A	1.742	10.91		
N-Nitrosomethylethylamine_APP9	0.765	0.737	0.746	0.692	0.637	0.714	0.778	A	0.733	6.91		
Methyl_methanesulfonate	0.369	0.357	0.385	0.392	0.457	0.582	0.453	A	0.433	17.08		A
2-fluorophenol(sur)	1.435	1.441	1.549	1.304	1.379	1.434	1.546	A	1.436	5.70		
N-Nitrosodiethylamine_APP9	0.656	0.642	0.766	0.685	0.629	0.745	0.822	A	0.721	10.89		
Ethyl_methanesulfonate	1.009	1.041	1.094	1.080	0.943	1.099	1.270	A	1.097	10.02		
phenol-d5(sur)	1.977	1.942	1.980	1.946	1.836	2.009	1.939	A	1.957	2.98		
Phenol(CCC)	2.032	2.179	2.084	2.182	1.891	2.147	2.378	A	2.161	7.79		
Aniline	2.596	2.622	2.862	2.841	2.597	2.703	2.924	A	2.747	4.82		
Bis(2-chloroethyl)ether	1.490	1.341	1.456	1.482	1.348	1.432	1.588	A	1.479	7.99		
Pentachloroethane	0.563	0.553	0.468	0.496	0.487	0.506	0.548	A	0.520	6.79		
2-chlorophenol	1.565	1.576	1.699	1.760	1.627	1.822	1.991	A	1.746	9.10		
1,3-Dichlorobenzene	1.529	1.484	1.627	1.555	1.547	1.584	1.628	A	1.576	3.64		
1,4-DICHLOROBENZENE-D4_(IS)	3012531	3099422	3125886	3396342	3303584	3122591	2917955	I		5.98		
1,4-Dichlorobenzene(CCC)	1.496	1.434	1.613	1.409	1.419	1.737	1.821	A	1.584	10.52		
Benzyl_alcohol	0.927	1.000	1.188	1.228	1.131	1.235	1.330	A	1.166	11.96		A
1,2-Dichlorobenzene	1.570	1.502	1.396	1.476	1.425	1.531	1.626	A	1.531	7.03		
2-methylphenol	1.011	1.168	1.148	1.184	1.116	1.234	1.416	A	1.208	11.19		
Bis(2-chloroisopropyl)ether	3.577	3.430	3.638	3.485	3.072	3.150	3.382	A	3.372	5.98		
N-Nitrosopyrrolidine_APP9	0.754	0.797	0.857	0.890	0.765	0.873	0.926	A	0.853	8.79		
3-Methylphenol&4-methylphenol	0.388	0.798	1.630	4.464	6.494	9.844	14.041	L			0.9937	A
Acetophenone	0.563	0.550	0.561	0.583	0.576	0.564	0.617	A	0.579	4.44		
N-Nitroso-di-N-propylamine(SPCC)	0.646	0.629	0.675	0.631	0.594	0.588	0.668	A	0.636	5.00		
o-toluidine_APP9	0.683	0.584	0.738	0.744	0.728	0.721	0.748	A	0.716	8.40		
Hexachloroethane	0.658	0.604	0.627	0.584	0.602	0.654	0.693	A	0.635	5.79		
nitrobenzene-d5(sur)	0.330	0.317	0.350	0.336	0.350	0.343	0.347	A	0.341	3.87		
Nitrobenzene	0.240	0.226	0.251	0.255	0.257	0.252	0.275	A	0.254	6.65		
N-Nitrosopiperidine	0.210	0.214	0.218	0.238	0.220	0.233	0.268	A	0.234	10.17		
Isophorone	0.623	0.657	0.672	0.712	0.704	0.713	0.795	A	0.708	8.38		
2-Nitrophenol(CCC)	0.016	0.030	0.079	0.229	0.381	0.588	0.940	L			0.9914	A
2,4-Dimethylphenol	0.420	0.437	0.447	0.499	0.484	0.478	0.570	A	0.482	10.13		
Bis(2-chloroethoxy)methane	0.446	0.435	0.503	0.517	0.518	0.453	0.575	A	0.498	9.86		
2,4-Dichlorophenol(CCC)	0.249	0.235	0.275	0.310	0.325	0.320	0.384	A	0.306	16.61		A
1,2,4-Trichlorobenzene	0.337	0.312	0.348	0.324	0.355	0.353	0.376	A	0.350	7.77		
NAPHTHALENE-D8_(IS)	10960489	11752571	11247438	12030489	11003294	10994382	10301966	I		5.81		
Naphthalene	1.494	1.356	1.554	1.440	1.522	1.535	1.629	A	1.513	5.56		
p-Chloroaniline	0.604	0.582	0.682	0.669	0.690	0.658	0.698	A	0.660	6.76		
2,6-Dichlorophenol	0.268	0.270	0.295	0.335	0.327	0.336	0.360	A	0.321	12.28		
Hexachloropropene_APP9	0.208	0.194	0.186	0.202	0.207	0.210	0.230	A	0.208	7.34		

Curve Type: A=Average RF; L=Linear; Q=Quadratic;I=Internal standard; Note: Amounts displayed for internal standards represent the ISTD Response.

Calibration flags: D=RSD; F=Response factor; R=R^2; A=Amount;X=Excluded; X(ISNF)=Excluded because ISTD wasn't found.

Manually integrated

Calibration Report

Lab name:	Thermo Fisher Laboratory		Page 7 of 7
Instrument:	ThermoFisher Instrument	**Method:**	EC25B_8level_322010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	EC25B_8level_322010_a	**Cali File:**	EC25B_8level_322010_a.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
3	5ng	run03	1		3/1/2010 1:09:00 PM	
4	10ng	run04	2		3/1/2010 1:37:46 PM	
5	20ng	run05	3		3/1/2010 2:06:38 PM	
6	50ng	run06	4		3/1/2010 2:35:42 PM	
7	80ng	run07	5		3/1/2010 3:04:38 PM	
8	120ng	run08	6		3/1/2010 3:33:32 PM	
9	160ng	run09	7		3/1/2010 4:02:28 PM	
10	200ng	run10	8		3/1/2010 4:31:24 PM	

Curve Type: A=Average RF; L=Linear; Q=Quadratic;I=Internal standard; Note: Amounts displayed for internal standards represent the ISTD Response.

Calibration flags: D=RSD; F=Response factor; R=R^2; A=Amount;X=Excluded; X(ISNF)=Excluded because ISTD wasn't found.

Manually integrated

Check Standard Report

Check Standard Report

Lab name:	Thermo Fisher Laboratory		Page 1 of 4
Instrument:	ThermoFisher Instrument	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	March48270B_8level_342010_a	**Cali File:**	EC25B_8level_322010_a_March48270B_8level_342010_a.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
3	check std 50 ng	342010_a003	4		3/4/2010 12:03:15 PM	

Compound	Curve Type	Daily RF	Mean RF	Min RF	RF %D	Max RF % D	QC amt	Calc amt	Amt %D	Max Amt %D	Flag
N-Nitrosodimethylamine	A	0.708	0.675	0.000	4.94	20.00					Pass
Pyridine_RCRA	A	1.566	1.446	0.000	8.25	20.00					Pass
2-Picoline	A	1.929	1.742	0.000	10.72	20.00					Pass
N-Nitrosomethylethylamine_APP9	A	0.800	0.733	0.000	9.24	20.00					Pass
Methyl_methanesulfonate	A	0.446	0.433	0.000	3.03	20.00					Pass
2-fluorophenol(sur)	A	1.533	1.436	0.000	6.78	20.00					Pass
N-Nitrosodiethylamine_APP9	A	0.776	0.721	0.000	7.69	20.00					Pass
Ethyl_methanesulfonate	A	1.276	1.097	0.000	16.39	20.00					Pass
phenol-d5(sur)	A	2.030	1.957	0.000	3.74	20.00					Pass
Phenol(CCC)	A	2.329	2.161	0.000	7.76	20.00					Pass
Aniline	A	3.004	2.747	0.000	9.35	20.00					Pass
Bis(2-chloroethyl)ether	A	1.629	1.479	0.000	10.15	20.00					Pass
Pentachloroethane	A	0.581	0.520	0.000	11.61	20.00					Pass
2-chlorophenol	A	1.800	1.746	0.000	3.08	20.00					Pass
1,3-Dichlorobenzene	A	1.597	1.576	0.000	1.37	20.00					Pass
1,4-Dichlorobenzene(CCC)	A	1.707	1.584	0.000	7.72	20.00					Pass
Benzyl_alcohol	A	1.281	1.166	0.000	9.89	20.00					Pass
1,2-Dichlorobenzene	A	1.611	1.531	0.000	5.22	20.00					Pass
2-methylphenol	A	1.330	1.208	0.000	10.14	20.00					Pass
Bis(2-chloroisopropyl)ether	A	3.918	3.372	0.000	16.20	20.00					Pass
N-Nitrosopyrrolidine_APP9	A	0.974	0.853	0.000	14.27	20.00					Pass
3-Methylphenol&4-methylphenol	L			0.000			100.000	110.648	10.65	20.00	Pass
Acetophenone	A	0.646	0.579	0.000	11.55	20.00					Pass
N-Nitroso-di-N-propylamine(SPCC)	A	0.701	0.636	0.050	10.21	20.00					Pass
o-toluidine_APP9	A	0.748	0.716	0.000	4.57	20.00					Pass
Hexachloroethane	A	0.685	0.635	0.000	7.94	20.00					Pass
nitrobenzene-d5(sur)	A	0.385	0.341	0.000	12.80	20.00					Pass
Nitrobenzene	A	0.287	0.254	0.000	12.84	20.00					Pass
N-Nitrosopiperidine	A	0.242	0.234	0.000	3.63	20.00					Pass
Isophorone	A	0.769	0.708	0.000	8.59	20.00					Pass
2-Nitrophenol(CCC)	L			0.000			50.000	48.062	-3.88	20.00	Pass
2,4-Dimethylphenol	A	0.526	0.482	0.000	9.12	20.00					Pass

Manually integrated *** = Fail;Curve Type: A=Average RF; L=Linear; Q=Quadratic;R=Recovery limits exceeded**

Check Standard Report

Lab name:	Thermo Fisher Laboratory		Page 4 of 4
Instrument:	ThermoFisher Instrument	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	March48270B_8level_342010_a	**Cali File:**	EC25B_8level_322010_a_March48270B_8level_342010_a.calx

Compound	Curve Type	Daily RF	Mean RF	Min RF	RF %D	Max RF % D	QC amt	Calc amt	Amt %D	Max Amt %D	Flag
2-Acetylaminofluorene_APP9	L			0.000			50.000	49.463	-1.07	20.00	Pass
3,3'-Dichlorobenzidine_APP9	A	0.494	0.460	0.000	7.35	20.00					Pass
Bis(2-ethylhexyl)phthalate	A	1.468	1.377	0.000	6.62	20.00					Pass
Chrysene	A	1.308	1.229	0.000	6.43	20.00					Pass
Benz(a)anthracene	A	1.196	1.224	0.000	-2.26	20.00					Pass
Di-n-octylphthalate(CCC)	L			0.000			50.000	47.882	-4.24	20.00	Pass
7,12-Dimethylbenz(a)anthracene	A	0.623	0.611	0.000	1.90	20.00					Pass
Benzo(b)fluoranthene	A	1.603	1.429	0.000	12.16	20.00					Pass
Benzo(k)fluoranthene	A	1.625	1.485	0.000	9.45	20.00					Pass
Benzo(a)pyrene(CCC)	A	1.480	1.313	0.000	12.69	20.00					Pass
3-Methylcholanthrene	A	0.677	0.665	0.000	1.81	20.00					Pass
Indeno(1,2,3-c,d)pyrene	A	1.428	1.372	0.000	4.11	20.00					Pass
Dibenz(a,h)anthracene	A	1.483	1.377	0.000	7.66	20.00					Pass
Benzo(g,h,i)perylene	A	1.518	1.415	0.000	7.32	20.00					Pass

Internal standard summary:

Compound	Std Response	Min	Max	Sample Response
1,4-DICHLOROBENZENE-D4_(IS)	3101746	1550873(50.00%)	4652619(150.00%)	2709445
NAPHTHALENE-D8_(IS)	11054301	5527150(50.00%)	16581451(150.00%)	9787201
ACENAPHTHENE-D10_(IS)	7115215	3557608(50.00%)	10672823(150.00%)	6364717
PHENANTHRENE_D10	10557810	5278905(50.00%)	15836716(150.00%)	10160713
CHRYSENE-D12_(IS)	3911156	1955578(50.00%)	5866733(150.00%)	3604358
PERYLENE-D12_(IS)	3302593	1651297(50.00%)	4953890(150.00%)	2868444

	Std RT	Min	Max	Sample RT
1,4-DICHLOROBENZENE-D4_(IS)	5.57	5.32(-0.25)	5.82(+0.25)	5.57
NAPHTHALENE-D8_(IS)	7.05	6.80(-0.25)	7.30(+0.25)	7.05
ACENAPHTHENE-D10_(IS)	9.06	8.81(-0.25)	9.31(+0.25)	9.06
PHENANTHRENE_D10	10.75	10.50(-0.25)	11.00(+0.25)	10.75
CHRYSENE-D12_(IS)	13.75	13.50(-0.25)	14.00(+0.25)	13.75
PERYLENE-D12_(IS)	15.59	15.34(-0.25)	15.84(+0.25)	15.59

Surrogate recovery:

Compound	Conc added	Conc recovered	% Recovered	Limits
phenol-d5(sur)	40.000	41.497	103.74	70.00 - 130.00
nitrobenzene-d5(sur)	40.000	45.118	112.80	70.00 - 130.00
2,4,6-tribromophenol(sur)	40.000	42.291	105.73	70.00 - 130.00
p-terphenyl-d14(sur)	40.000	41.924	104.81	70.00 - 130.00

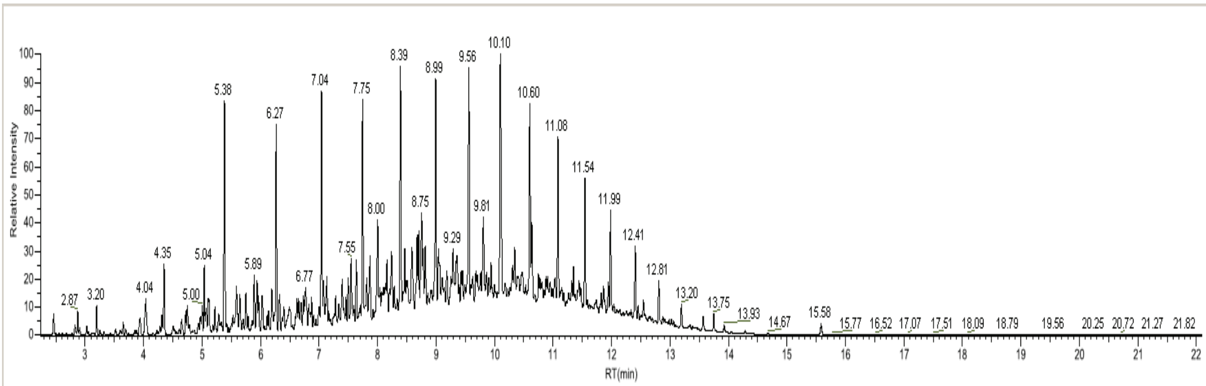
Manually integrated ☐ *** = Fail;Curve Type: A=Average RF; L=Linear; Q=Quadratic;R=Recovery limits exceeded**

Chromatogram Report

Chromatogram Report

Lab name:	Thermo Fisher Laboratory		Page 1 of 1
Instrument:	ThermoFisher Instrument	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	March48270B_8level_342010_a	**Cali File:**	EC25B_8level_322010_a_March48270B_8level_342010_a.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	5% diesel	342010_a004	N/A		3/4/2010 12:33:49 PM	



Compound Calibration Report

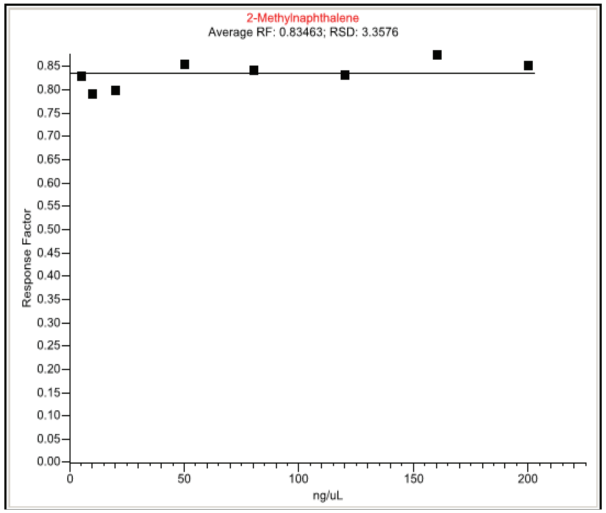
Page 1 of 2

Compound Calibration Report

Lab name: Thermo Fisher Laboratory
Instrument: ThermoFisher Instrument
User: AMER\jessie.butler
Batch: EC25B_8level_322010_a

Method: EC25B_8level_322010_a_EPAMethod8270B_8level
EPAMethod8270B_8level
Cali File: EC25B_8level_322010_a.calx

Compound Name: 2-Methylnaphthalene



Average RF
Pass

Level	Std Amount	Std Area	IS Amount	IS Area	Response factor	Calc amt	Units
1	5.000	1138290	40.000	10960489	0.831	4.977	ng/uL
2	10.000	2323857	40.000	11752571	0.791	9.476	ng/uL
3	20.000	4498791	40.000	11247438	0.800	19.169	ng/uL
4	50.000	12852385	40.000	12030489	0.855	51.200	ng/uL
5	80.000	18533247	40.000	11003294	0.842	80.723	ng/uL
6	120.000	27435115	40.000	10994382	0.832	119.592	ng/uL
7	160.000	36043723	40.000	10301966	0.875	167.678	ng/uL
8	200.000	43212130	40.000	10143779	0.852	204.161	ng/uL

Manually Integrated: **Calibration flags: D =RSD, F = Response factor, R = R Squared, A = Amount**

Compound Calibration Report

Page 2 of 2

Lab name:	Thermo Fisher Laboratory		
Instrument:	ThermoFisher Instrument	**Method:**	EC25B_8level_322010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	EC25B_8level_322010_a	**Cali File:**	EC25B_8level_322010_a.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
3	5ng	run03	1		3/1/2010 1:09:00 PM	
4	10ng	run04	2		3/1/2010 1:37:46 PM	
5	20ng	run05	3		3/1/2010 2:06:38 PM	
6	50ng	run06	4		3/1/2010 2:35:42 PM	
7	80ng	run07	5		3/1/2010 3:04:38 PM	
8	120ng	run08	6		3/1/2010 3:33:32 PM	
9	160ng	run09	7		3/1/2010 4:02:28 PM	
10	200ng	run10	8		3/1/2010 4:31:24 PM	

Manually Integrated:

Calibration flags: D =RSD, F = Response factor, R = R Squared, A = Amount

Confirmation Report

Confirmation Report

Lab name:	Thermo Fisher Laboratory			Page 1 of 1
Instrument:	ThermoFisher Instrument	**Method:**	EC25B_8level_322010_a_EPAMethod8270B_8level	
User:	AMER\jessie.butler		EPAMethod8270B_8level	
Batch:	EC25B_8level_322010_a	**Cali file:**	EC25B_8level_322010_a.calx	

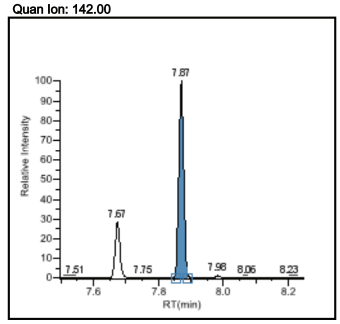
Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	10ng	run04	2		3/1/2010 1:37:46 PM	

2-Methylnaphthalene

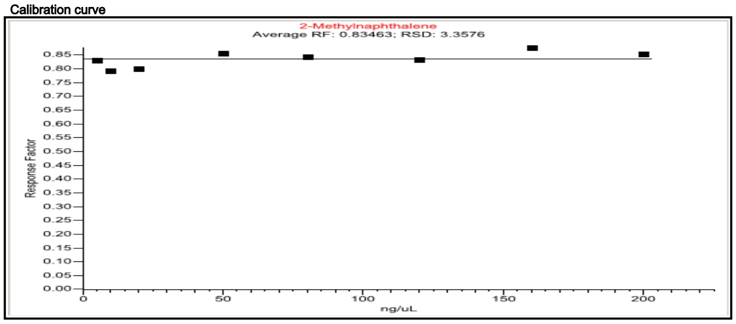
	Injected	Sample
Conc:	9.476 ng/uL	9.476 ng/uL

Retention time:	7.87
Area:	2323857
Height:	2341443

Quan Ion: 142.00

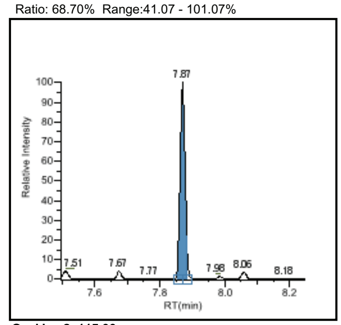


Calibration curve

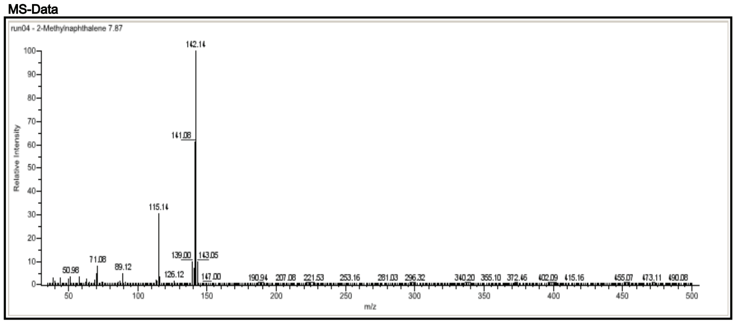


Qual Ion 1: 141.00

Ratio: 68.70% Range:41.07 - 101.07%

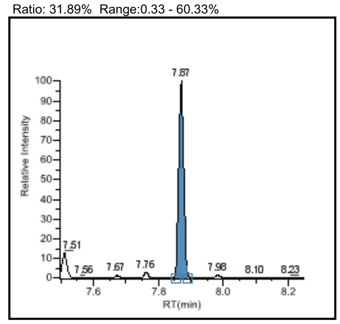


MS-Data



Qual Ion 2: 115.00

Ratio: 31.89% Range:0.33 - 60.33%



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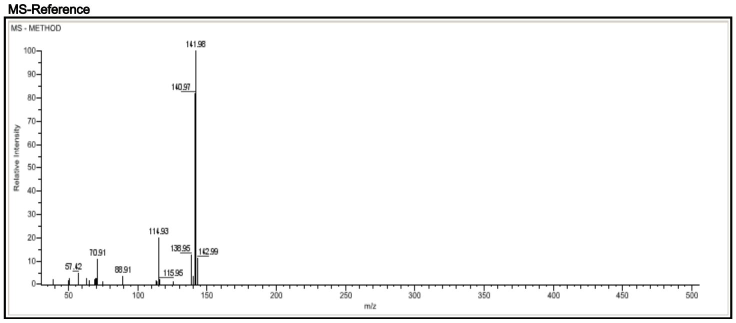

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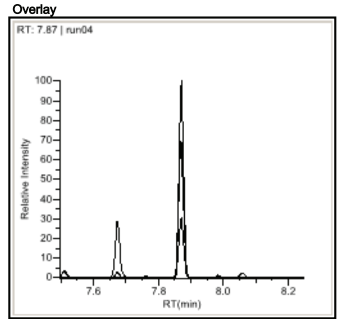


Confirmation Report 2

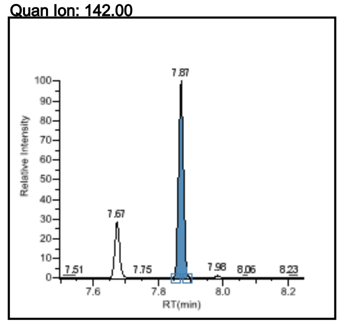
Confirmation Report 2

Lab name:	Thermo Fisher Laboratory		Page 1 of 1
Instrument:	ThermoFisher Instrument	**Method:**	EC25B_8level_322010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	EC25B_8level_322010_a	**Cali file:**	EC25B_8level_322010_a.calx

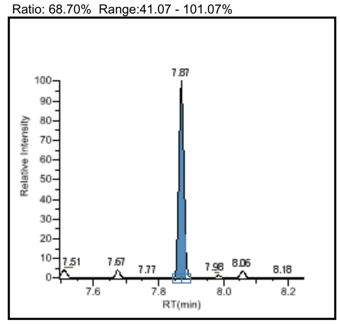
Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	10ng	run04	2		3/1/2010 1:37:46 PM	

Compound Name:	2-Methylnaphthalene
Injected Conc:	9.476 ng/uL
Sample Conc:	9.476 ng/uL
Retention time:	7.87
Area (Quan):	2323857
Height (Quan):	2341443
Qual ratio 1:	Pass
Qual ratio 2:	Pass

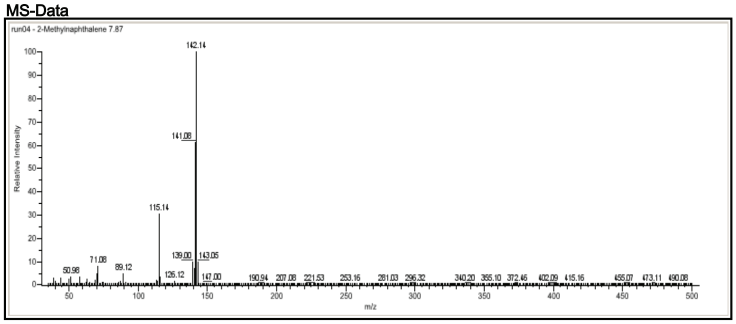
Quan Ion: 142.00



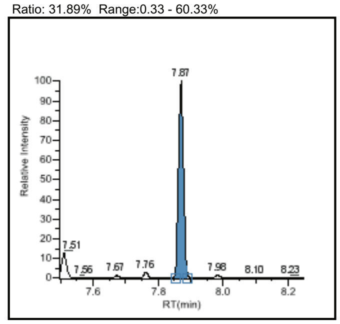
Qual Ion 1: 141.00
Ratio: 68.70% Range:41.07 - 101.07%



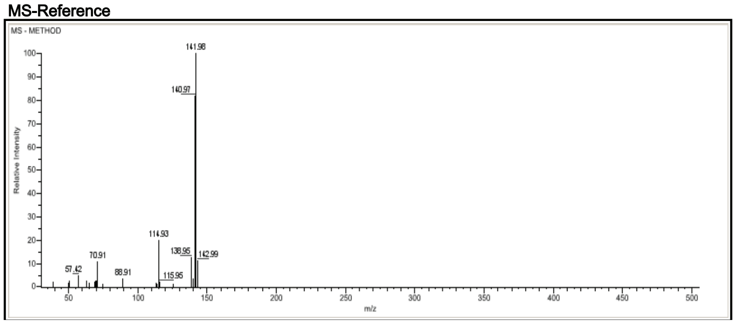
MS-Data



Qual Ion 2: 115.00
Ratio: 31.89% Range:0.33 - 60.33%



MS-Reference



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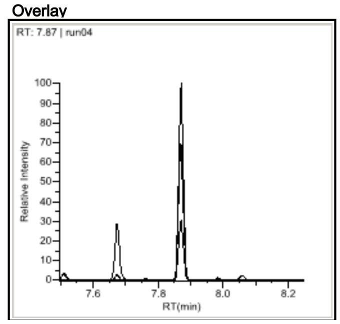
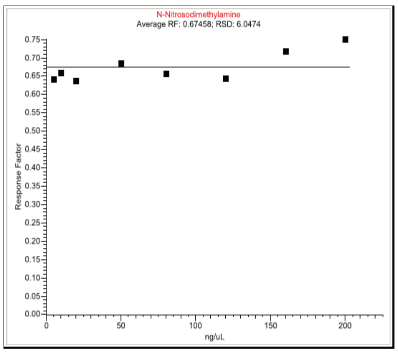
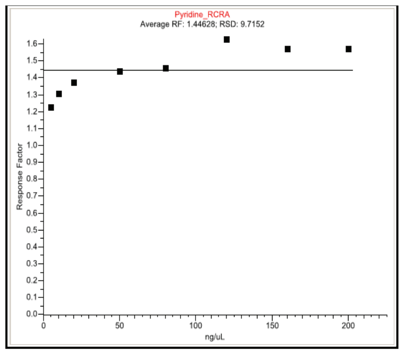


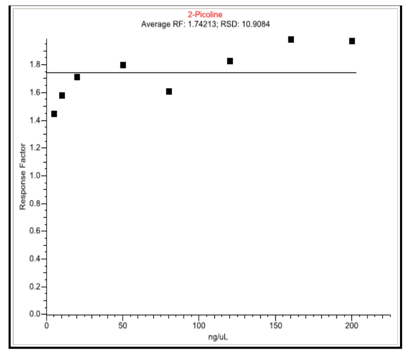
High Density Calibration Report

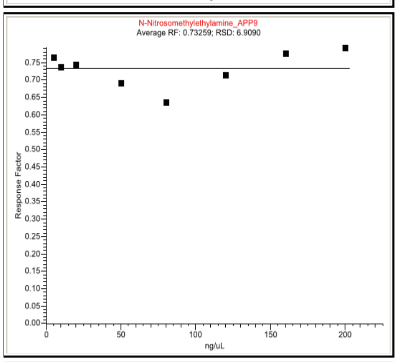
High Density Calibration Report

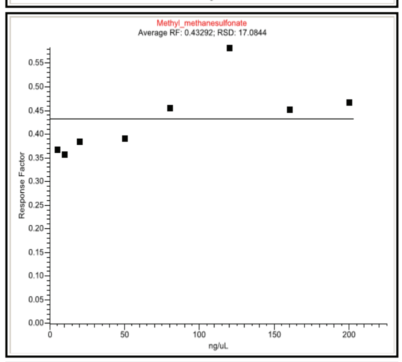
Lab name:	Thermo Fisher Laboratory		Page 1 of 10
Instrument:	ThermoFisher Instrument	**Method:**	EC25B_8level_322010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	EC25B_8level_322010_a	**Cali File:**	EC25B_8level_322010_a.calx

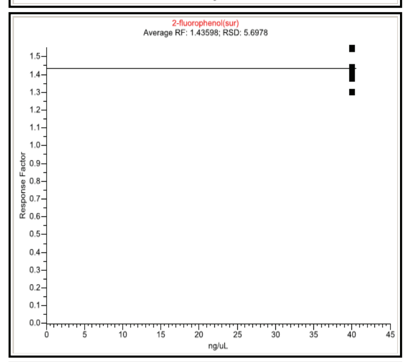


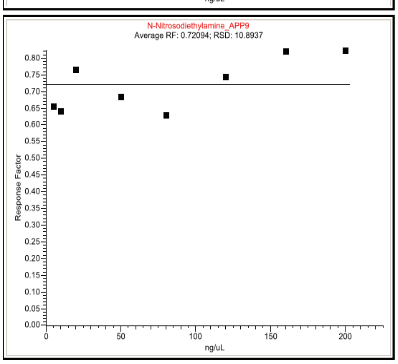


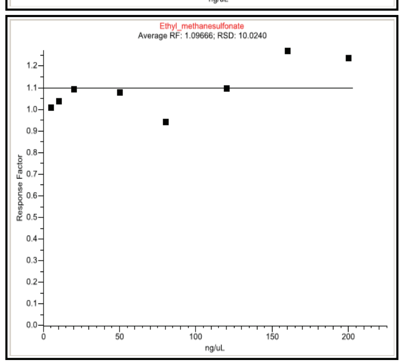


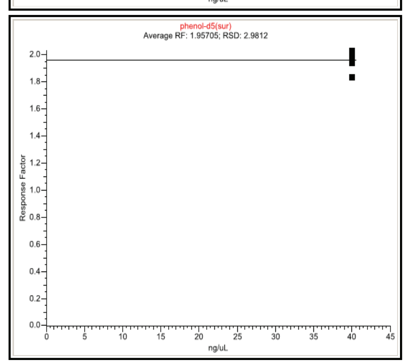


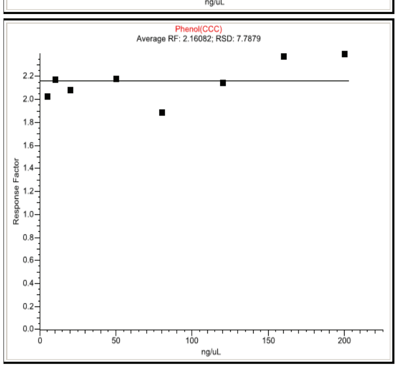


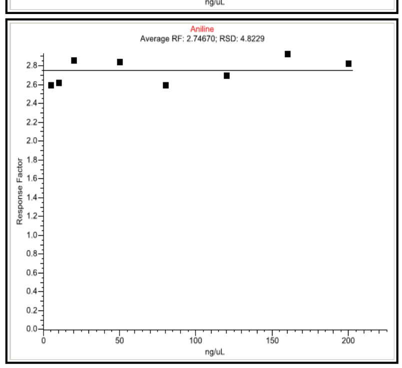


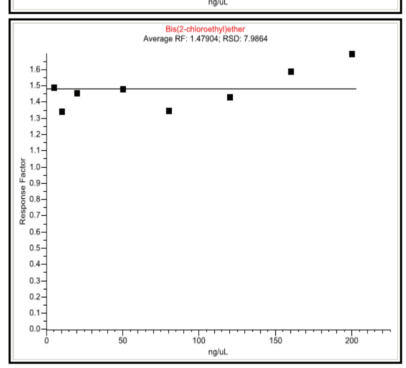












High Density Internal Standard Report

High Density Internal Standard Report

Lab name: Thermo Fisher Laboratory — Page 1 of 20

Instrument: ThermoFisher Instrument — **Method:** EC25B_8level_322010_a_EPAMethod8270B_8level

User: AMER\jessie.butler — EPAMethod8270B_8level

Batch: EC25B_8level_322010_a — **Cali File:** EC25B_8level_322010_a.calx

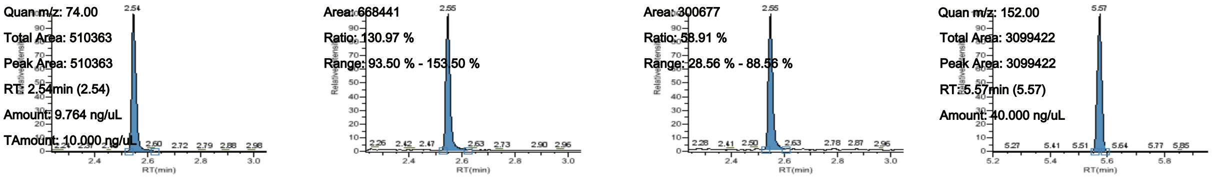
Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	10ng	run04	2		3/1/2010 1:37:46 PM	

N-Nitrosodimethylamine
Quan m/z: 74.00
Total Area: 510363
Peak Area: 510363
RT: 2.54min (2.54)
Amount: 9.764 ng/uL
TAmount: 10.000 ng/uL

Qual m/z: 42.00
Area: 668441
Ratio: 130.97 %
Range: 93.50 % - 153.50 %

Qual m/z: 43.00
Area: 300677
Ratio: 58.91 %
Range: 28.56 % - 88.56 %

1,4-DICHLOROBENZENE-D4_(IS)
Quan m/z: 152.00
Total Area: 3099422
Peak Area: 3099422
RT: 5.57min (5.57)
Amount: 40.000 ng/uL

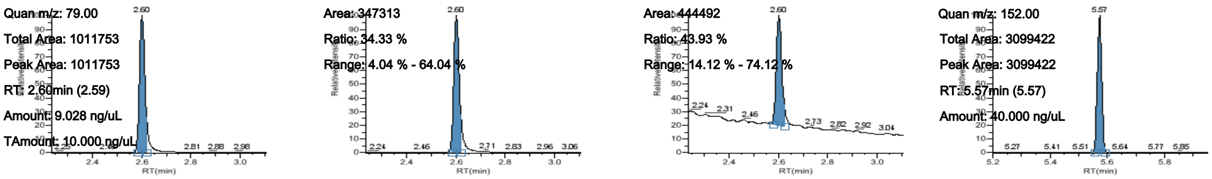


Pyridine_RCRA
Quan m/z: 79.00
Total Area: 1011753
Peak Area: 1011753
RT: 2.60min (2.59)
Amount: 9.028 ng/uL
TAmount: 10.000 ng/uL

Qual m/z: 52.00
Area: 347313
Ratio: 34.33 %
Range: 4.04 % - 64.04 %

Qual m/z: 51.00
Area: 444492
Ratio: 43.93 %
Range: 14.12 % - 74.12 %

1,4-DICHLOROBENZENE-D4_(IS)
Quan m/z: 152.00
Total Area: 3099422
Peak Area: 3099422
RT: 5.57min (5.57)
Amount: 40.000 ng/uL

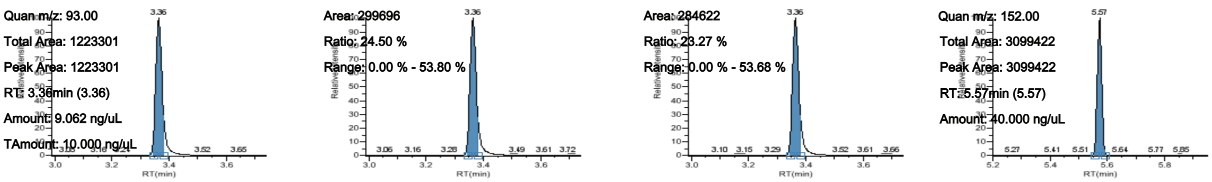


2-Picoline
Quan m/z: 93.00
Total Area: 1223301
Peak Area: 1223301
RT: 3.36min (3.36)
Amount: 9.062 ng/uL
TAmount: 10.000 ng/uL

Qual m/z: 66.00
Area: 299696
Ratio: 24.50 %
Range: 0.00 % - 53.80 %

Qual m/z: 92.00
Area: 284622
Ratio: 23.27 %
Range: 0.00 % - 53.68 %

1,4-DICHLOROBENZENE-D4_(IS)
Quan m/z: 152.00
Total Area: 3099422
Peak Area: 3099422
RT: 5.57min (5.57)
Amount: 40.000 ng/uL

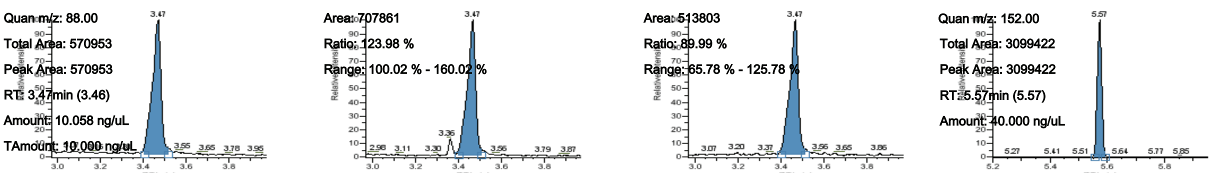


N-Nitrosomethylethylamine_APP9
Quan m/z: 88.00
Total Area: 570953
Peak Area: 570953
RT: 3.47min (3.46)
Amount: 10.058 ng/uL
TAmount: 10.000 ng/uL

Qual m/z: 42.00
Area: 707861
Ratio: 123.98 %
Range: 100.02 % - 160.02 %

Qual m/z: 43.00
Area: 513803
Ratio: 89.99 %
Range: 65.78 % - 125.78 %

1,4-DICHLOROBENZENE-D4_(IS)
Quan m/z: 152.00
Total Area: 3099422
Peak Area: 3099422
RT: 5.57min (5.57)
Amount: 40.000 ng/uL

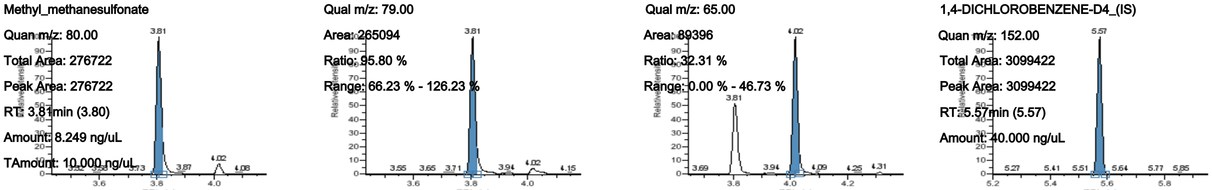


Methyl_methanesulfonate
Quan m/z: 80.00
Total Area: 276722
Peak Area: 276722
RT: 3.81min (3.80)
Amount: 8.249 ng/uL
TAmount: 10.000 ng/uL

Qual m/z: 79.00
Area: 265094
Ratio: 95.80 %
Range: 66.23 % - 126.23 %

Qual m/z: 65.00
Area: 89396
Ratio: 32.31 %
Range: 0.00 % - 46.73 %

1,4-DICHLOROBENZENE-D4_(IS)
Quan m/z: 152.00
Total Area: 3099422
Peak Area: 3099422
RT: 5.57min (5.57)
Amount: 40.000 ng/uL

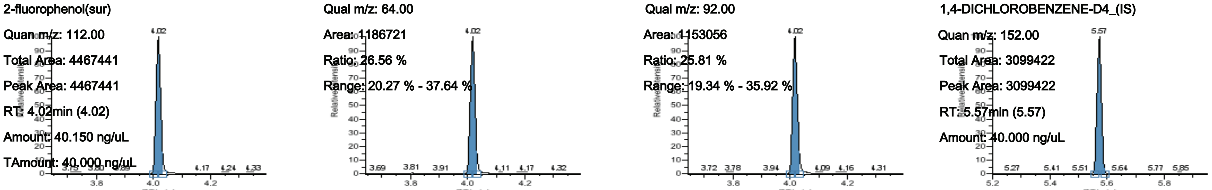


2-fluorophenol(sur)
Quan m/z: 112.00
Total Area: 4467441
Peak Area: 4467441
RT: 4.02min (4.02)
Amount: 40.150 ng/uL
TAmount: 40.000 ng/uL

Qual m/z: 64.00
Area: 1186721
Ratio: 26.56 %
Range: 20.27 % - 37.64 %

Qual m/z: 92.00
Area: 1153056
Ratio: 25.81 %
Range: 19.34 % - 35.92 %

1,4-DICHLOROBENZENE-D4_(IS)
Quan m/z: 152.00
Total Area: 3099422
Peak Area: 3099422
RT: 5.57min (5.57)
Amount: 40.000 ng/uL



Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

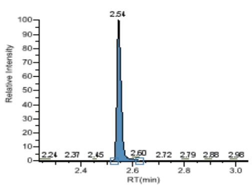
High Density Internal Standard Report Long

High Density Internal Standard Report Long

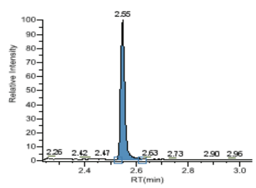
Page 1 of 39

Lab name:	Thermo Fisher Laboratory		
Instrument:	ThermoFisher Instrument	**Method:**	EC25B_8level_322010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	EC25B_8level_322010_a	**Cali File:**	EC25B_8level_322010_a.calx

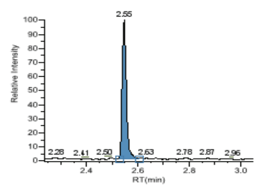
Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	10ng	run04	2		3/1/2010 1:37:46 PM	



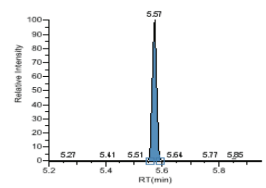
N-Nitrosodimethylamine
Quan m/z: 74.00
Total Area: 510363
Peak Area: 510363
RT: 2.54min (2.54)
Amount: 9.764 ng/uL
TAmount: 10.000 ng/uL



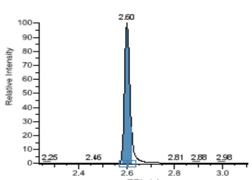
Qual m/z: 42.00
Area: 668441
Ratio: 130.97 %
Range: 93.50 % - 153.50 %



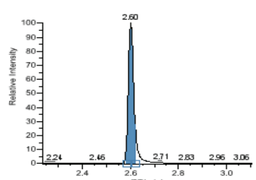
Qual m/z: 43.00
Area: 300677
Ratio: 58.91 %
Range: 28.56 % - 88.56 %



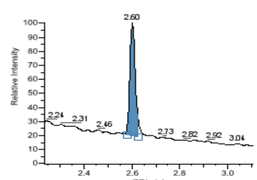
1,4-DICHLOROBENZENE-D4_(IS)
Quan m/z: 152.00
Total Area: 3099422
Peak Area: 3099422
RT: 5.57min (5.57)
Amount: 40.000 ng/uL



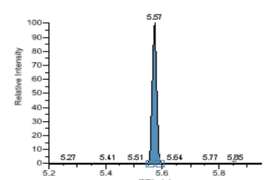
Pyridine_RCRA
Quan m/z: 79.00
Total Area: 1011753
Peak Area: 1011753
RT: 2.60min (2.59)
Amount: 9.028 ng/uL
TAmount: 10.000 ng/uL



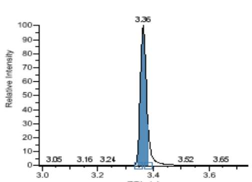
Qual m/z: 52.00
Area: 347313
Ratio: 34.33 %
Range: 4.04 % - 64.04 %



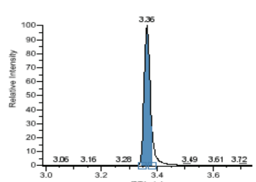
Qual m/z: 51.00
Area: 444492
Ratio: 43.93 %
Range: 14.12 % - 74.12 %



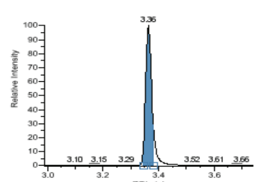
1,4-DICHLOROBENZENE-D4_(IS)
Quan m/z: 152.00
Total Area: 3099422
Peak Area: 3099422
RT: 5.57min (5.57)
Amount: 40.000 ng/uL



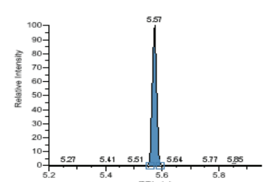
2-Picoline
Quan m/z: 93.00
Total Area: 1223301
Peak Area: 1223301
RT: 3.36min (3.36)
Amount: 9.062 ng/uL
TAmount: 10.000 ng/uL



Qual m/z: 66.00
Area: 299696
Ratio: 24.50 %
Range: 0.00 % - 53.80 %



Qual m/z: 92.00
Area: 284622
Ratio: 23.27 %
Range: 0.00 % - 53.68 %



1,4-DICHLOROBENZENE-D4_(IS)
Quan m/z: 152.00
Total Area: 3099422
Peak Area: 3099422
RT: 5.57min (5.57)
Amount: 40.000 ng/uL

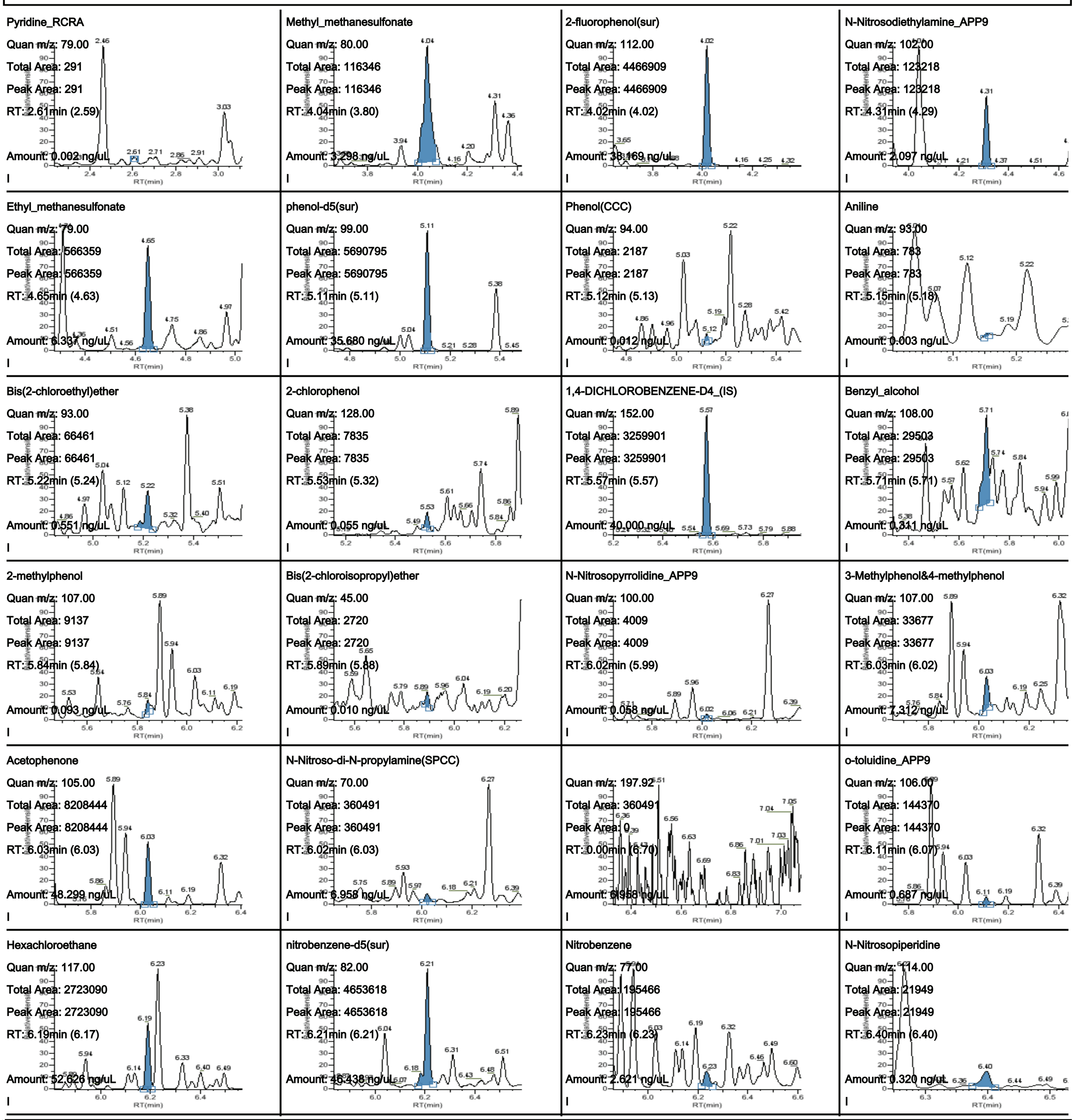
Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

High Density Sample Report 1

High Density Sample Report 1

Lab name:	Thermo Fisher Laboratory		Page 1 of 5
Instrument:	ThermoFisher Instrument	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	March48270B_8level_342010_a	**Cali File:**	EC25B_8level_322010_a_March48270B_8level_342010_a.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	5% diesel	342010_a004	N/A		3/4/2010 12:33:49 PM	



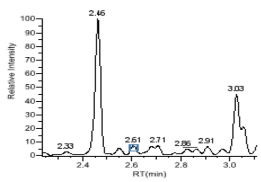
Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

High Density Sample Report 1 Long

High Density Sample Report 1 Long

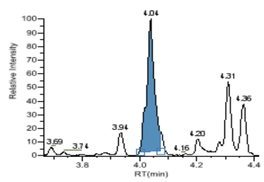
Lab name:	Thermo Fisher Laboratory			Page 1 of 9
Instrument:	ThermoFisher Instrument	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8level	
User:	AMER\jessie.butler		EPAMethod8270B_8level	
Batch:	March48270B_8level_342010_a	**Cali File:**	EC25B_8level_322010_a_March48270B_8level_342010_a.calx	

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	5% diesel	342010_a004	N/A		3/4/2010 12:33:49 PM	



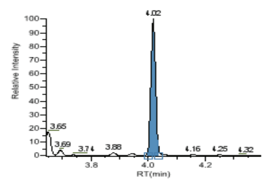
Pyridine_RCRA
Quan m/z: 79.00
Total Area: 291
Peak Area: 291
RT: 2.61min (2.59)

Amount: 0.002 ng/uL
I



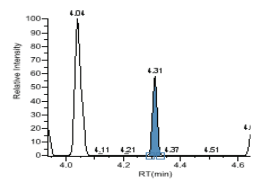
Methyl_methanesulfonate
Quan m/z: 80.00
Total Area: 116346
Peak Area: 116346
RT: 4.04min (3.80)

Amount: 3.298 ng/uL
I



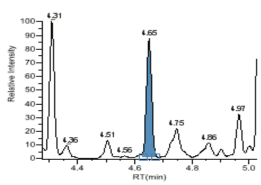
2-fluorophenol(sur)
Quan m/z: 112.00
Total Area: 4466909
Peak Area: 4466909
RT: 4.02min (4.02)

Amount: 38.169 ng/uL
I



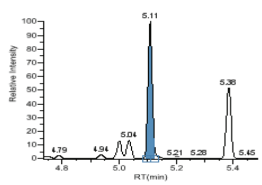
N-Nitrosodiethylamine_APP9
Quan m/z: 102.00
Total Area: 123218
Peak Area: 123218
RT: 4.31min (4.29)

Amount: 2.097 ng/uL
I



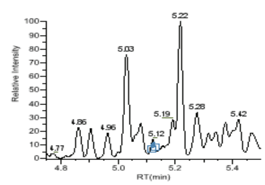
Ethyl_methanesulfonate
Quan m/z: 79.00
Total Area: 566359
Peak Area: 566359
RT: 4.65min (4.63)

Amount: 6.337 ng/uL
I



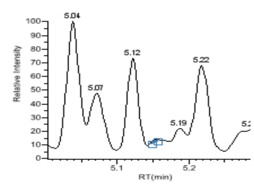
phenol-d5(sur)
Quan m/z: 99.00
Total Area: 5690795
Peak Area: 5690795
RT: 5.11min (5.11)

Amount: 35.680 ng/uL
I



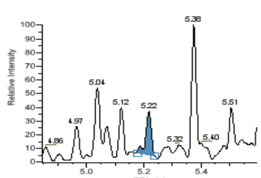
Phenol(CCC)
Quan m/z: 94.00
Total Area: 2187
Peak Area: 2187
RT: 5.12min (5.13)

Amount: 0.012 ng/uL
I



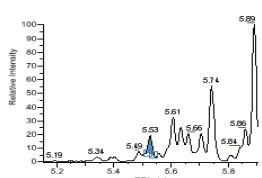
Aniline
Quan m/z: 93.00
Total Area: 783
Peak Area: 783
RT: 5.15min (5.18)

Amount: 0.003 ng/uL
I



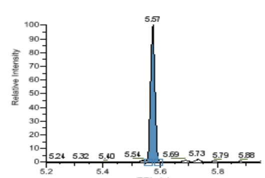
Bis(2-chloroethyl)ether
Quan m/z: 93.00
Total Area: 66461
Peak Area: 66461
RT: 5.22min (5.24)

Amount: 0.551 ng/uL
I



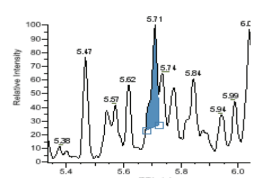
2-chlorophenol
Quan m/z: 128.00
Total Area: 7835
Peak Area: 7835
RT: 5.53min (5.32)

Amount: 0.055 ng/uL
I



1,4-DICHLOROBENZENE-D4_(IS)
Quan m/z: 152.00
Total Area: 3259901
Peak Area: 3259901
RT: 5.57min (5.57)

Amount: 40.000 ng/uL



Benzyl_alcohol
Quan m/z: 108.00
Total Area: 29503
Peak Area: 29503
RT: 5.71min (5.71)

Amount: 0.311 ng/uL
I

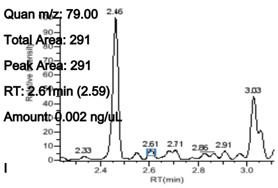
High Density Sample Report 2

High Density Sample Report 2

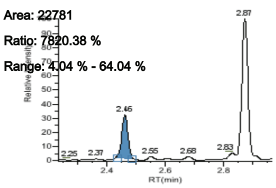
Lab name:	Thermo Fisher Laboratory		Page 1 of 9
Instrument:	ThermoFisher Instrument	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	March48270B_8level_342010_a	**Cali File:**	EC25B_8level_322010_a_March48270B_8level_342010_a.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	5% diesel	342010_a004	N/A		3/4/2010 12:33:49 PM	

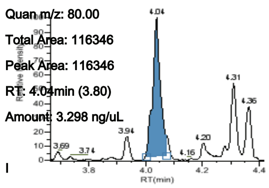
Pyridine_RCRA
Quan m/z: 79.00
Total Area: 291
Peak Area: 291
RT: 2.61min (2.59)
Amount: 0.002 ng/uL
I



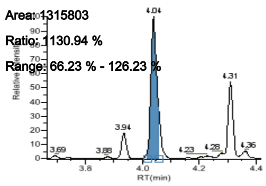
Qual m/z: 52.00
Area: 22781
Ratio: 7820.38 %
Range: 4.04 % - 64.04 %



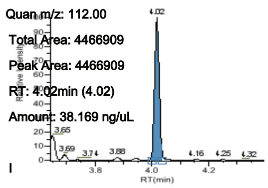
Methyl_methanesulfonate
Quan m/z: 80.00
Total Area: 116346
Peak Area: 116346
RT: 4.04min (3.80)
Amount: 3.298 ng/uL
I



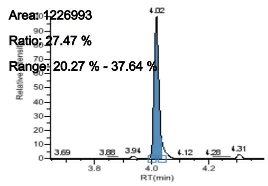
Qual m/z: 79.00
Area: 1315803
Ratio: 1130.94 %
Range: 66.23 % - 126.23 %



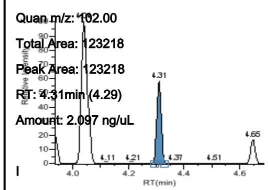
2-fluorophenol(sur)
Quan m/z: 112.00
Total Area: 4466909
Peak Area: 4466909
RT: 4.02min (4.02)
Amount: 38.169 ng/uL
I



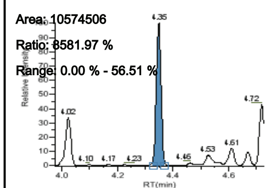
Qual m/z: 64.00
Area: 1226993
Ratio: 27.47 %
Range: 20.27 % - 37.64 %



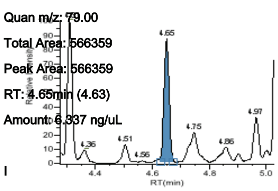
N-Nitrosodiethylamine_APP9
Quan m/z: 102.00
Total Area: 123218
Peak Area: 123218
RT: 4.31min (4.29)
Amount: 2.097 ng/uL
I



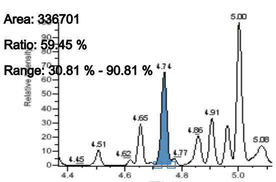
Qual m/z: 57.00
Area: 10574506
Ratio: 8581.97 %
Range: 0.00 % - 56.51 %



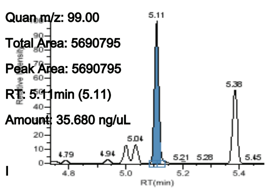
Ethyl_methanesulfonate
Quan m/z: 79.00
Total Area: 566359
Peak Area: 566359
RT: 4.65min (4.63)
Amount: 6.337 ng/uL
I



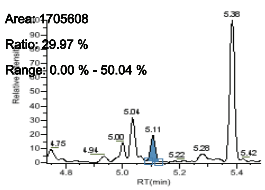
Qual m/z: 109.00
Area: 336701
Ratio: 59.45 %
Range: 30.81 % - 90.81 %



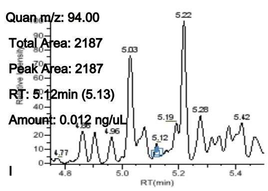
phenol-d5(sur)
Quan m/z: 99.00
Total Area: 5690795
Peak Area: 5690795
RT: 5.11min (5.11)
Amount: 35.680 ng/uL
I



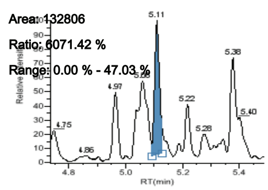
Qual m/z: 42.00
Area: 1705608
Ratio: 29.97 %
Range: 0.00 % - 50.04 %



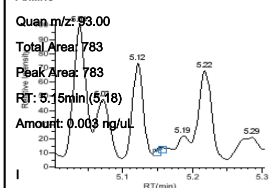
Phenol(CCC)
Quan m/z: 94.00
Total Area: 2187
Peak Area: 2187
RT: 5.12min (5.13)
Amount: 0.012 ng/uL
I



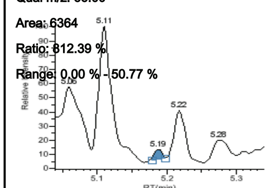
Qual m/z: 66.00
Area: 132806
Ratio: 6071.42 %
Range: 0.00 % - 47.03 %



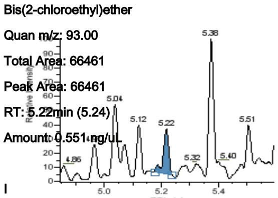
Aniline
Quan m/z: 93.00
Total Area: 783
Peak Area: 783
RT: 5.15min (5.18)
Amount: 0.003 ng/uL
I



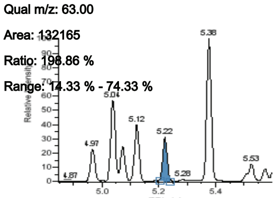
Qual m/z: 66.00
Area: 6364
Ratio: 812.39 %
Range: 0.00 % - 50.77 %



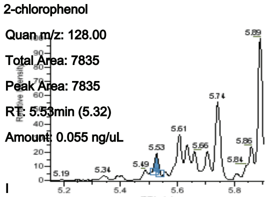
Bis(2-chloroethyl)ether
Quan m/z: 93.00
Total Area: 66461
Peak Area: 66461
RT: 5.22min (5.24)
Amount: 0.551 ng/uL
I



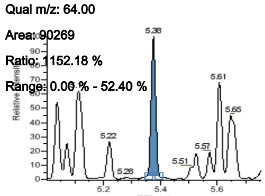
Qual m/z: 63.00
Area: 132165
Ratio: 198.86 %
Range: 14.33 % - 74.33 %



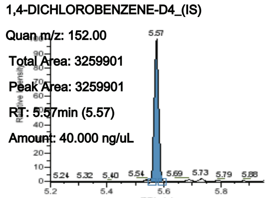
2-chlorophenol
Quan m/z: 128.00
Total Area: 7835
Peak Area: 7835
RT: 5.53min (5.32)
Amount: 0.055 ng/uL
I



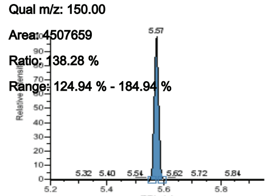
Qual m/z: 64.00
Area: 90269
Ratio: 1152.18 %
Range: 0.00 % - 52.40 %



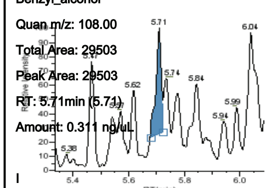
1,4-DICHLOROBENZENE-D4_(IS)
Quan m/z: 152.00
Total Area: 3259901
Peak Area: 3259901
RT: 5.57min (5.57)
Amount: 40.000 ng/uL



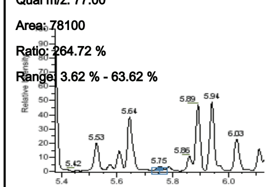
Qual m/z: 150.00
Area: 4507659
Ratio: 138.28 %
Range: 124.94 % - 184.94 %



Benzyl_alcohol
Quan m/z: 108.00
Total Area: 29503
Peak Area: 29503
RT: 5.71min (5.71)
Amount: 0.311 ng/uL
I



Qual m/z: 77.00
Area: 78100
Ratio: 264.72 %
Range: 3.62 % - 63.62 %



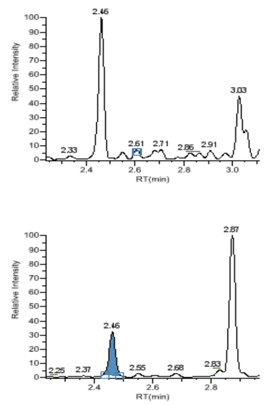
Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent

High Density Sample Report 2 Long

High Density Sample Report 2 Long

Lab name:	Thermo Fisher Laboratory		Page 1 of 18
Instrument:	ThermoFisher Instrument	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	March48270B_8level_342010_a	**Cali File:**	EC25B_8level_322010_a_March48270B_8level_342010_a.calx

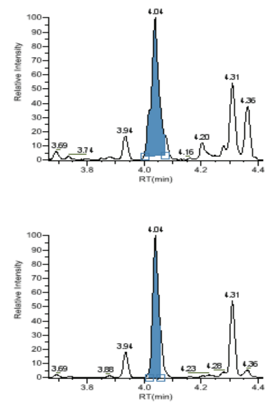
Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	5% diesel	342010_a004	N/A		3/4/2010 12:33:49 PM	



Pyridine_RCRA
Quan m/z: 79.00
Total Area: 291
Peak Area: 291
RT: 2.61min (2.59)
Amount: 0.002 ng/uL

I

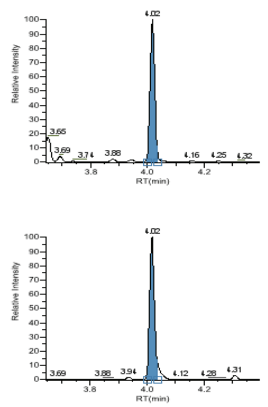
Qual m/z: 52.00
Area: 22781
Ratio: 7820.38 %
Range: 4.04 % - 64.04 %



Methyl_methanesulfonate
Quan m/z: 80.00
Total Area: 116346
Peak Area: 116346
RT: 4.04min (3.80)
Amount: 3.298 ng/uL

I

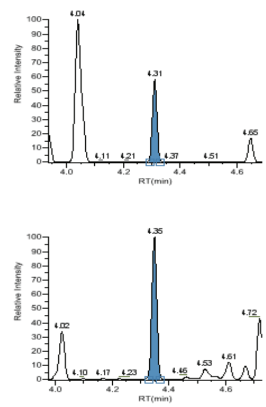
Qual m/z: 79.00
Area: 1315803
Ratio: 1130.94 %
Range: 66.23 % - 126.23 %



2-fluorophenol(sur)
Quan m/z: 112.00
Total Area: 4466909
Peak Area: 4466909
RT: 4.02min (4.02)
Amount: 38.169 ng/uL

I

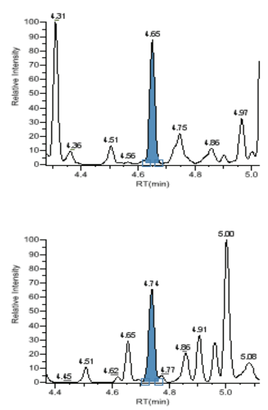
Qual m/z: 64.00
Area: 1226993
Ratio: 27.47 %
Range: 20.27 % - 37.64 %



N-Nitrosodiethylamine_APP9
Quan m/z: 102.00
Total Area: 123218
Peak Area: 123218
RT: 4.31min (4.29)
Amount: 2.097 ng/uL

I

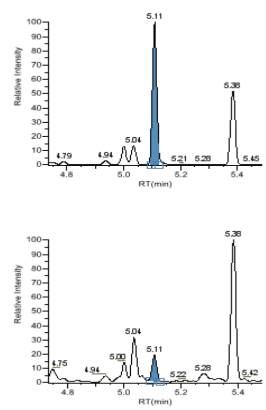
Qual m/z: 57.00
Area: 10574506
Ratio: 8581.97 %
Range: 0.00 % - 56.51 %



Ethyl_methanesulfonate
Quan m/z: 79.00
Total Area: 566359
Peak Area: 566359
RT: 4.65min (4.63)
Amount: 6.337 ng/uL

I

Qual m/z: 109.00
Area: 336701
Ratio: 59.45 %
Range: 30.81 % - 90.81 %



phenol-d5(sur)
Quan m/z: 99.00
Total Area: 5690795
Peak Area: 5690795
RT: 5.11min (5.11)
Amount: 35.680 ng/uL

I

Qual m/z: 42.00
Area: 1705608
Ratio: 29.97 %
Range: 0.00 % - 50.04 %

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

High Density Sample Report 3

High Density Sample Report 3

Lab name: Thermo Fisher Laboratory

Page 1 of 18

Instrument: ThermoFisher Instrument

User: AMER\jessie.butler

Batch: March48270B_8level_342010_a

Method: March48270B_8level_342010_a_EPAMethod8270B_8level
EPAMethod8270B_8level

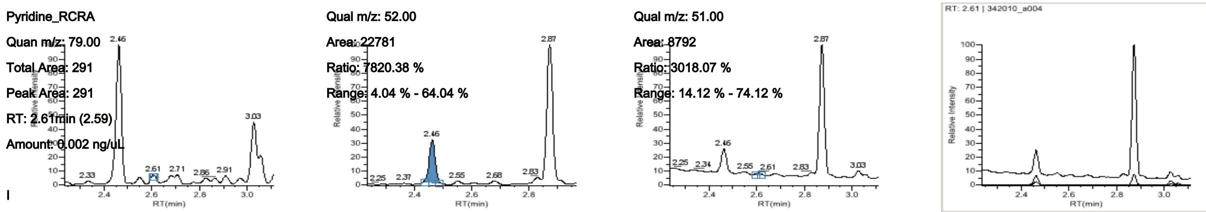
Cali File: EC25B_8level_322010_a_March48270B_8level_342010_a.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	5% diesel	342010_a004	N/A		3/4/2010 12:33:49 PM	

Pyridine_RCRA
Quan m/z: 79.00
Total Area: 291
Peak Area: 291
RT: 2.61 min (2.59)
Amount: 0.002 ng/uL

Qual m/z: 52.00
Area: 22781
Ratio: 7820.38 %
Range: 4.04 % - 64.04 %

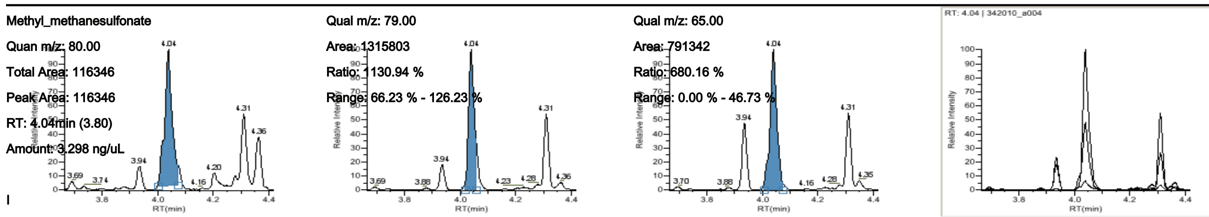
Qual m/z: 51.00
Area: 8792
Ratio: 3018.07 %
Range: 14.12 % - 74.12 %



Methyl_methanesulfonate
Quan m/z: 80.00
Total Area: 116346
Peak Area: 116346
RT: 4.04 min (3.80)
Amount: 3.298 ng/uL

Qual m/z: 79.00
Area: 1315803
Ratio: 1130.94 %
Range: 66.23 % - 126.23 %

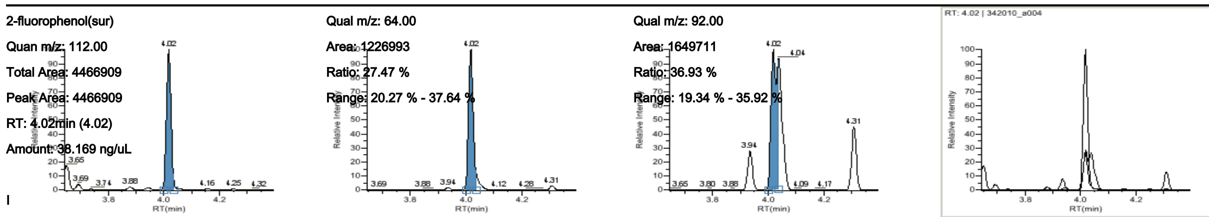
Qual m/z: 65.00
Area: 791342
Ratio: 680.16 %
Range: 0.00 % - 46.73 %



2-fluorophenol(sur)
Quan m/z: 112.00
Total Area: 4466909
Peak Area: 4466909
RT: 4.02 min (4.02)
Amount: 38.169 ng/uL

Qual m/z: 64.00
Area: 1226993
Ratio: 27.47 %
Range: 20.27 % - 37.64 %

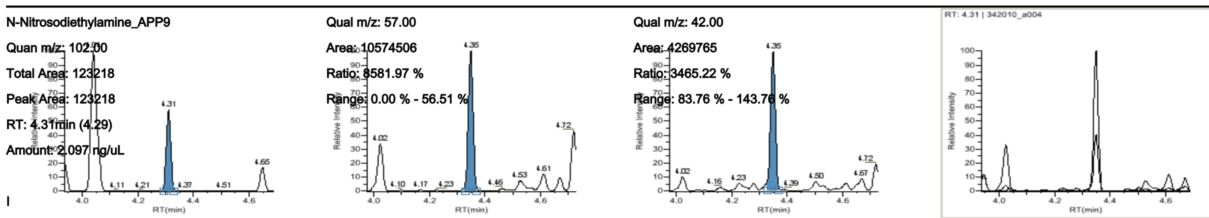
Qual m/z: 92.00
Area: 1649711
Ratio: 36.93 %
Range: 19.34 % - 35.92 %



N-Nitrosodiethylamine_APP9
Quan m/z: 102.00
Total Area: 123218
Peak Area: 123218
RT: 4.31 min (4.29)
Amount: 2.097 ng/uL

Qual m/z: 57.00
Area: 10574506
Ratio: 8581.97 %
Range: 0.00 % - 56.51 %

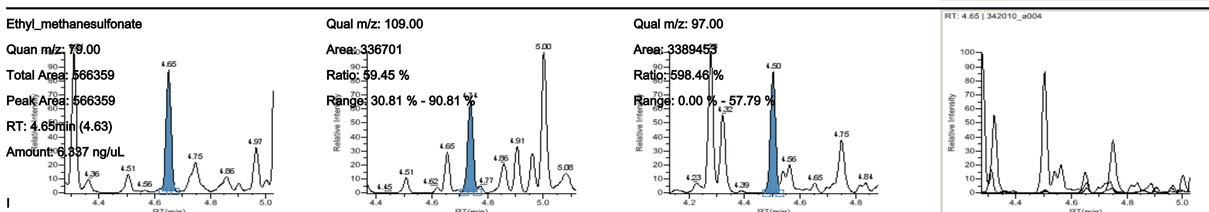
Qual m/z: 42.00
Area: 4269765
Ratio: 3465.22 %
Range: 83.76 % - 143.76 %



Ethyl_methanesulfonate
Quan m/z: 79.00
Total Area: 566359
Peak Area: 566359
RT: 4.65 min (4.63)
Amount: 6.337 ng/uL

Qual m/z: 109.00
Area: 336701
Ratio: 59.45 %
Range: 30.81 % - 90.81 %

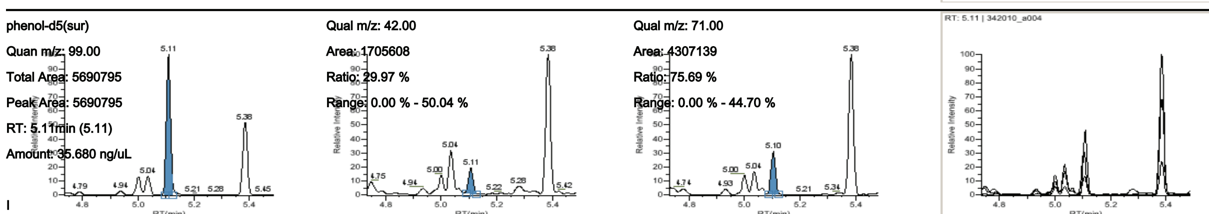
Qual m/z: 97.00
Area: 3389453
Ratio: 598.46 %
Range: 0.00 % - 57.79 %



phenol-d5(sur)
Quan m/z: 99.00
Total Area: 5690795
Peak Area: 5690795
RT: 5.11 min (5.11)
Amount: 35.680 ng/uL

Qual m/z: 42.00
Area: 1705608
Ratio: 29.97 %
Range: 0.00 % - 50.04 %

Qual m/z: 71.00
Area: 4307139
Ratio: 75.69 %
Range: 0.00 % - 44.70 %

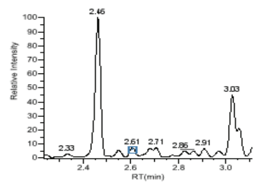
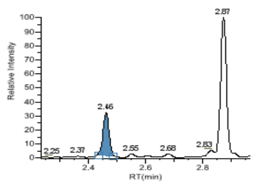
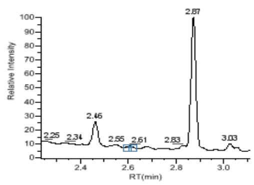
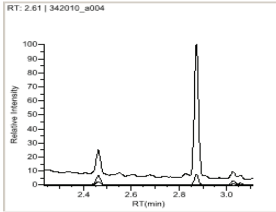


High Density Sample Report 3 Long

High Density Sample Report 3 Long

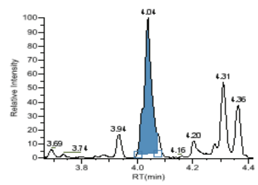
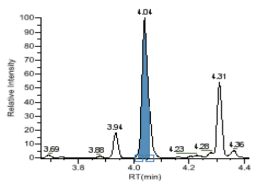
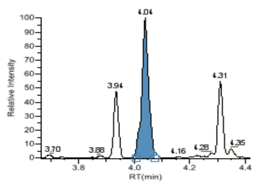
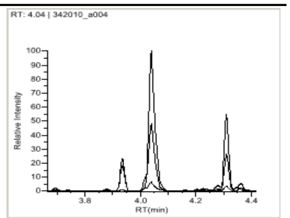
Lab name:	Thermo Fisher Laboratory		Page 1 of 35
Instrument:	ThermoFisher Instrument	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	March48270B_8level_342010_a	**Cali File:**	EC25B_8level_322010_a_March48270B_8level_342010_a.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	5% diesel	342010_a004	N/A		3/4/2010 12:33:49 PM	

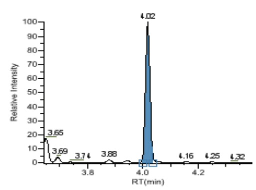
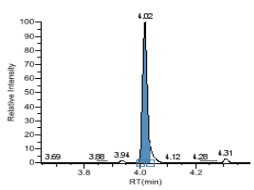
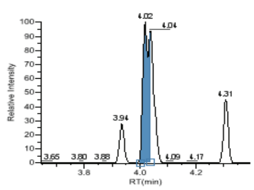
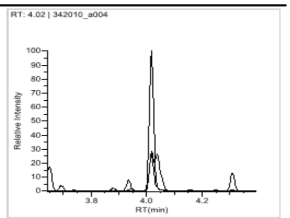
Pyridine_RCRA	**Qual m/z: 52.00**	**Qual m/z: 51.00**
Quan m/z: 79.00	**Area: 22781**	**Area: 8792**
Total Area: 291	**Ratio: 7820.38 %**	**Ratio: 3018.07 %**
Peak Area: 291	**Range: 4.04 % - 64.04 %**	**Range: 14.12 % - 74.12 %**
RT: 2.61min (2.59)		
Amount: 0.002 ng/uL		

I

Methyl_methanesulfonate	**Qual m/z: 79.00**	**Qual m/z: 65.00**
Quan m/z: 80.00	**Area: 1315803**	**Area: 791342**
Total Area: 116346	**Ratio: 1130.94 %**	**Ratio: 680.16 %**
Peak Area: 116346	**Range: 66.23 % - 126.23 %**	**Range: 0.00 % - 46.73 %**
RT: 4.04min (3.80)		
Amount: 3.298 ng/uL		

I

2-fluorophenol(sur)	**Qual m/z: 64.00**	**Qual m/z: 92.00**
Quan m/z: 112.00	**Area: 1226993**	**Area: 1649711**
Total Area: 4466909	**Ratio: 27.47 %**	**Ratio: 36.93 %**
Peak Area: 4466909	**Range: 20.27 % - 37.64 %**	**Range: 19.34 % - 35.92 %**
RT: 4.02min (4.02)		
Amount: 38.169 ng/uL		

I

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

Internal Standard Summary Report

Internal Standard Summary Report

Page 1 of 1

Lab name: Thermo Fisher Laboratory
Instrument: ThermoFisher Instrument
User: AMER\jessie.butler
Batch: March48270B_8level_342010_a

Method: March48270B_8level_342010_a_EPAMethod8270B_8level
EPAMethod8270B_8level
Cali File: EC25B_8level_322010_a_March48270B_8level_342010_a.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	5% diesel	342010_a004	N/A		3/4/2010 12:33:49 PM	

Compound	Std Response	Min	Max	Sample Response
1,4-DICHLOROBENZENE-D4_(IS)	3101746	1550873(50.00%)	4652619(150.00%)	3259901
NAPHTHALENE-D8_(IS)	11054301	5527150(50.00%)	16581451(150.00%)	11741455
ACENAPHTHENE-D10_(IS)	7115215	3557608(50.00%)	10672823(150.00%)	7312176
PHENANTHRENE_D10	10557810	5278905(50.00%)	15836716(150.00%)	10527013
CHRYSENE-D12_(IS)	3911156	1955578(50.00%)	5866733(150.00%)	4162955
PERYLENE-D12_(IS)	3302593	1651297(50.00%)	4953890(150.00%)	3256621
	Std RT	**Min**	**Max**	**Sample RT**
1,4-DICHLOROBENZENE-D4_(IS)	5.57	5.32(-0.25)	5.82(+0.25)	5.57
NAPHTHALENE-D8_(IS)	7.05	6.80(-0.25)	7.30(+0.25)	7.05
ACENAPHTHENE-D10_(IS)	9.06	8.81(-0.25)	9.31(+0.25)	9.06
PHENANTHRENE_D10	10.75	10.50(-0.25)	11.00(+0.25)	10.75
CHRYSENE-D12_(IS)	13.75	13.50(-0.25)	14.00(+0.25)	13.75
PERYLENE-D12_(IS)	15.59	15.34(-0.25)	15.84(+0.25)	15.58

Ion Ratio Failure Report

Ion Ratio Failure Report

Page 1 of 5

Lab name:	Thermo Fisher Laboratory	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8level
Instrument:	ThermoFisher Instrument		EPAMethod8270B_8level
User:	AMER\jessie.butler	**Cali File:**	EC25B_8level_322010_a_March48270B_8level_342010_a.calx
Batch:	March48270B_8level_342010_a		

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	5% diesel	342010_a004	N/A		3/4/2010 12:33:49 PM	

Compound	Response	Quan Ion	Quan Response	Qual Ion	Qual Response	Ratio	Range
Pyridine_RCRA	Area	79.00	291	52.00	22781	7820.38	4.04-64.04
	Area	79.00	291	51.00	8792	3018.07	14.12-74.12
	Area	79.00	291	50.00	4198	1441.05	3.78-63.78
Methyl_methanesulfonate	Area	80.00	116346	79.00	1315803	1130.94	66.23-126.23
	Area	80.00	116346	65.00	791342	680.16	0.00-46.73
2-fluorophenol(sur)	Area	112.00	4466909	92.00	1649711	36.93	19.34-35.92
N-Nitrosodiethylamine_APP9	Area	102.00	123218	57.00	10574506	8581.97	0.00-56.51
	Area	102.00	123218	42.00	4269765	3465.22	83.76-143.76
	Area	102.00	123218	44.00	1003635	814.52	83.93-143.93
Ethyl_methanesulfonate	Area	79.00	566359	97.00	3389453	598.46	0.00-57.79
phenol-d5(sur)	Area	99.00	5690795	71.00	4307139	75.69	0.00-44.70
Phenol(CCC)	Area	94.00	2187	66.00	132806	6071.42	0.00-47.03
	Area	94.00	2187	65.00	253812	11603.33	0.00-41.31
Aniline	Area	93.00	783	66.00	6364	812.39	0.00-50.77
	Area	93.00	783	65.00	261357	33363.80	0.00-39.28
Bis(2-chloroethyl)ether	Area	93.00	66461	63.00	132165	198.86	14.33-74.33
	Area	93.00	66461	95.00	1553489	2337.44	10.48-70.48
2-chlorophenol	Area	128.00	7835	64.00	90269	1152.18	0.00-52.40
	Area	128.00	7835	130.00	0	0.00	7.19-67.19
Benzyl_alcohol	Area	108.00	29503	77.00	78100	264.72	3.62-63.62
	Area	108.00	29503	79.00	80829	273.96	68.13-128.13
	Area	108.00	29503	107.00	3276	11.11	27.90-87.90
2-methylphenol	Area	107.00	9137	108.00	9336	102.18	112.40-172.40
	Area	107.00	9137	79.00	1723254	18859.33	10.34-70.34
Bis(2-chloroisopropyl)ether	Area	45.00	2720	121.00	2829	104.02	0.00-43.73
	Area	45.00	2720	41.00	3422212	125813.08	0.00-59.30
N-Nitrosopyrrolidine_APP9	Area	100.00	4009	41.00	4709758	117477.54	57.91-117.91
	Area	100.00	4009	42.00	2493220	62189.47	19.15-79.15
3-Methylphenol&4-methylphenol	Area	107.00	33677	77.00	527985	1567.78	10.68-70.68
Acetophenone	Area	105.00	8208444	51.00	464948	5.66	27.32-87.32

Manually integrated

LCSLCSD Report

IMPORTANT When the Sample ID is the same for an unknown sample and an LCS or LCSD sample, the unknown sample is included in the LCSLCSD report. The report information for the unknown sample displays as zeros.

LCSLCSD Report

Lab name:	Thermo Fisher Laboratory			Page 1 of 3
Instrument:	ThermoFisher Instrument	**Method:**	EPAMethod8270B_8level_3192010_d_EPAMethod8270B_8level	
User:	AMER\jessie.butler		EPAMethod8270B_8level	
Batch:	EPAMethod8270B_8level_3192010_d	**Cali File:**	EC25B_8level_322010_a_EPAMethod8270B_8level_3192010_d.calx	

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	QC	342010_a002	N/A	QC	3/4/2010 11:39:33 AM	
3	QC	342010_a003	N/A	QC	3/4/2010 12:03:15 PM	
3	QC	352010_a004	N/A	QC	3/5/2010 11:46:24 AM	

QC

Compound	Spike Amt	LCS Conc	% Rec	Lower Limit %	Upper Limit %	LCSD Conc	% Rec	RPD	Max RPD	Rec Fails	RPD Fails
N-Nitrosodimethylamine	50.000	52.470	104.94	80.00	120.00	48.109	0.00	0.00	20.00	0	0
Pyridine_RCRA	50.000	54.126	108.25	80.00	120.00	49.824	0.00	0.00	20.00	0	0
2-Picoline	50.000	55.362	110.72	80.00	120.00	49.123	0.00	0.00	20.00	0	0
N-Nitrosomethylethylamine_APP9	50.000	54.618	109.24	80.00	120.00	48.625	0.00	0.00	20.00	0	0
Methyl_methanesulfonate	50.000	51.515	103.03	80.00	120.00	47.343	0.00	0.00	20.00	0	0
2-fluorophenol(sur)	40.000	42.714	106.78	80.00	120.00	40.370	0.00	0.00	20.00	0	0
N-Nitrosodiethylamine_APP9	50.000	53.846	107.69	80.00	120.00	50.048	0.00	0.00	20.00	0	0
Ethyl_methanesulfonate	50.000	58.196	116.39	80.00	120.00	50.402	0.00	0.00	20.00	0	0
phenol-d5(sur)	40.000	41.497	103.74	80.00	120.00	38.246	0.00	0.00	20.00	0	0
Phenol(CCC)	50.000	53.881	107.76	80.00	120.00	6.253	0.00	0.00	20.00	0	0
Aniline	50.000	54.677	109.35	80.00	120.00	49.783	0.00	0.00	20.00	0	0
Bis(2-chloroethyl)ether	50.000	55.074	110.15	80.00	120.00	48.114	0.00	0.00	20.00	0	0
Pentachloroethane	50.000	55.805	111.61	80.00	120.00	55.431	0.00	0.00	20.00	0	0
2-chlorophenol	50.000	51.542	103.08	80.00	120.00	49.303	0.00	0.00	20.00	0	0
1,3-Dichlorobenzene	50.000	50.683	101.37	80.00	120.00	53.464	0.00	0.00	20.00	0	0
1,4-Dichlorobenzene(CCC)	50.000	53.862	107.72	80.00	120.00	52.303	0.00	0.00	20.00	0	0
Benzyl_alcohol	50.000	54.944	109.89	80.00	120.00	51.102	0.00	0.00	20.00	0	0
1,2-Dichlorobenzene	50.000	52.612	105.22	80.00	120.00	52.981	0.00	0.00	20.00	0	0
2-methylphenol	50.000	55.068	110.14	80.00	120.00	52.087	0.00	0.00	20.00	0	0
Bis(2-chloroisopropyl)ether	50.000	58.101	116.20	80.00	120.00	52.973	0.00	0.00	20.00	0	0
N-Nitrosopyrrolidine_APP9	50.000	57.133	114.27	80.00	120.00	51.010	0.00	0.00	20.00	0	0
3-Methylphenol&4-methylphenol	100.000	110.648	110.65	80.00	120.00	104.217	0.00	0.00	20.00	0	0
Acetophenone	50.000	55.777	111.55	80.00	120.00	52.279	0.00	0.00	20.00	0	0
N-Nitroso-di-N-propylamine(SPCC)	50.000	55.106	110.21	80.00	120.00	48.024	0.00	0.00	20.00	0	0
o-toluidine_APP9	50.000	52.285	104.57	80.00	120.00	52.016	0.00	0.00	20.00	0	0
Hexachloroethane	50.000	53.969	107.94	80.00	120.00	49.931	0.00	0.00	20.00	0	0
nitrobenzene-d5(sur)	40.000	45.118	112.80	80.00	120.00	41.423	0.00	0.00	20.00	0	0
Nitrobenzene	50.000	56.422	112.84	80.00	120.00	50.909	0.00	0.00	20.00	0	0
N-Nitrosopiperidine	50.000	51.817	103.63	80.00	120.00	46.436	0.00	0.00	20.00	0	0
Isophorone	50.000	54.297	108.59	80.00	120.00	54.030	0.00	0.00	20.00	0	0
2-Nitrophenol(CCC)	50.000	48.062	96.12	80.00	120.00	47.032	0.00	0.00	20.00	0	0
2,4-Dimethylphenol	50.000	54.562	109.12	80.00	120.00	51.701	0.00	0.00	20.00	0	0
Bis(2-chloroethoxy)methane	50.000	54.092	108.18	80.00	120.00	53.458	0.00	0.00	20.00	0	0
2,4-Dichlorophenol(CCC)	50.000	55.580	111.16	80.00	120.00	54.251	0.00	0.00	20.00	0	0
1,2,4-Trichlorobenzene	50.000	57.998	116.00	80.00	120.00	53.342	0.00	0.00	20.00	0	0
Naphthalene	50.000	52.884	105.77	80.00	120.00	51.910	0.00	0.00	20.00	0	0
p-Chloroaniline	50.000	50.866	101.73	80.00	120.00	51.242	0.00	0.00	20.00	0	0

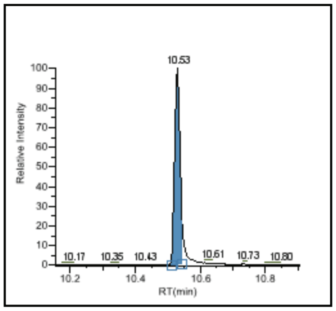
Manual Integration Report

Manual Integration Report

Lab name: Thermo Fisher Laboratory — Page 1 of 1
Instrument: ThermoFisher Instrument — **Method:** EC25B_8level_322010_a_EPAMethod8270B_8level
User: AMER\jessie.butler — EPAMethod8270B_8level
Batch: EC25B_8level_322010_a — **Cali File:** EC25B_8level_322010_a.calx

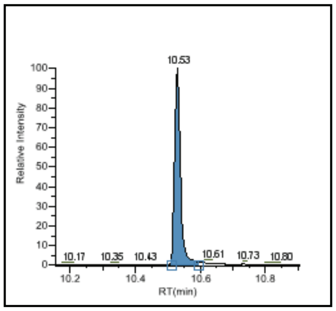
Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	10ng	run04	2		3/1/2010 1:37:46 PM	

Pentachlorophenol(CCC)
m/z: 266.00



Method integration

Apex RT:	10.53
Height:	113493
Area:	124704



Manual integration

Apex RT:	10.53
Height:	114006
Area:	142357

Method Detection Limit Report

Method Detection Limit Report

Lab name:	Thermo Fisher Laboratory		
Instrument:	ThermoFisher Instrument	**Method:**	EPAMethod8270L_JB_2192010_b_EPAMethod8270L_JB
User:	AMER\jessie.butler		EPAMethod8270L_JB
Batch:	EPAMethod8270L_JB_2192010_b	**Cali File:**	EPAMethod8270L_JB_2192010_b.calx

Method Detection Limit Summary

Compound	Avg Conc	Std Dev	t-stat	% RSD	MDL	
N-Nitrosodimethylamine	0.449	0.029	2.998	6.36	0.086	<<<
Pyridine_RCRA	0.403	0.013	2.998	3.11	0.038	<<<
2-Picoline	0.379	0.017	2.998	4.37	0.050	<<<
N-Nitrosomethylethylamine_APP9	0.511	0.125	2.998	24.42	0.374	<<<
Methyl_methanesulfonate	0.363	0.034	2.998	9.28	0.101	<<<
2-fluorophenol(sur)	39.978	1.244	2.998	3.11	3.731	
N-Nitrosodiethylamine_APP9	0.391	0.027	2.998	6.94	0.081	<<<
Ethyl_methanesulfonate	0.370	0.028	2.998	7.68	0.085	<<<
phenol-d5(sur)	39.300	0.704	2.998	1.79	2.112	
Phenol(CCC)	0.426	0.144	2.998	33.72	0.431	<<<
Aniline	0.454	0.024	2.998	5.26	0.072	<<<
Bis(2-chloroethyl)ether	0.485	0.022	2.998	4.57	0.066	<<<
Pentachloroethane	0.495	0.031	2.998	6.25	0.093	<<<
2-chlorophenol	0.451	0.022	2.998	4.97	0.067	<<<
1,3-Dichlorobenzene	0.486	0.018	2.998	3.68	0.054	<<<
1,4-DICHLOROBENZENE-D4_(IS)	2609592	58805		2.25		IS
1,4-Dichlorobenzene(CCC)	0.516	0.007	2.998	1.43	0.022	<<<
Benzyl_alcohol	0.301	0.023	2.998	7.55	0.068	<<<
1,2-Dichlorobenzene	0.484	0.022	2.998	4.49	0.065	<<<
2-methylphenol	0.402	0.040	2.998	9.87	0.119	<<<
Bis(2-chloroisopropyl)ether	0.476	0.018	2.998	3.80	0.054	<<<
N-Nitrosopyrrolidine_APP9	0.363	0.024	2.998	6.48	0.071	<<<
3-Methylphenol&4-methylphenol	0.371	0.011	2.998	2.96	0.033	<<<
Acetophenone	0.467	0.028	2.998	6.02	0.084	<<<
N-Nitroso-di-N-propylamine(SPCC)	0.434	0.023	2.998	5.32	0.069	<<<
o-toluidine_APP9	0.479	0.028	2.998	5.76	0.083	<<<
Hexachloroethane	0.501	0.034	2.998	6.70	0.101	<<<
nitrobenzene-d5(sur)	39.503	1.946	2.998	4.93	5.833	
Nitrobenzene	0.566	0.028	2.998	4.93	0.084	<<<
N-Nitrosopiperidine	0.432	0.030	2.998	7.04	0.091	<<<
Isophorone	0.421	0.021	2.998	5.05	0.064	<<<
2-Nitrophenol(CCC)	0.330	0.022	2.998	6.60	0.065	<<<
2,4-Dimethylphenol	0.378	0.015	2.998	3.95	0.045	<<<
Bis(2-chloroethoxy)methane	0.446	0.011	2.998	2.41	0.032	<<<
2,4-Dichlorophenol(CCC)	0.363	0.027	2.998	7.49	0.082	<<<
1,2,4-Trichlorobenzene	0.512	0.024	2.998	4.74	0.073	<<<
NAPHTHALENE-D8_(IS)	9245585	360030		3.89		IS
Naphthalene	0.480	0.019	2.998	3.89	0.056	<<<
p-Chloroaniline	0.360	0.025	2.998	6.87	0.074	<<<
2,6-Dichlorophenol	0.359	0.026	2.998	7.24	0.078	<<<
Hexachloropropene_APP9	0.449	0.046	2.998	10.23	0.138	<<<
Hexachlorobutadiene(CCC)	0.517	0.032	2.998	6.27	0.097	<<<
N-Nitroso-di-N-butylamine	0.371	0.033	2.998	8.95	0.100	<<<
4-Chloro-3-methylphenol(CCC)	0.306	0.024	2.998	7.98	0.073	<<<
Safrole_APP9	0.405	0.016	2.998	4.01	0.049	<<<
2-Methylnaphthalene	0.440	0.022	2.998	4.89	0.064	<<<
Hexachlorocyclopentadiene(SPCC)	0.427	0.015	2.998	3.53	0.045	<<<
1,2,4,5-Tetrachlorobenzene	0.547	0.035	2.998	6.31	0.103	<<<
2,4,5-Trichlorophenol	0.352	0.025	2.998	7.03	0.074	<<<
2,4,6-Trichlorophenol(CCC)	0.337	0.030	2.998	8.78	0.089	<<<

Manually integrated

Method Detection Limit Report

Lab name:	Thermo Fisher Laboratory			Page 7 of 7
Instrument:	ThermoFisher Instrument	**Method:**	EPAMethod8270L_JB_2192010_b_EPAMethod8270L_JB	
User:	AMER\jessie.butler		EPAMethod8270L_JB	
Batch:	EPAMethod8270L_JB_2192010_b	**Cali File:**	EPAMethod8270L_JB_2192010_b.calx	

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	0.5ng1	test17	N/A		2/18/2010 12:43:19 PM	
5	0.5ng2	test18	N/A		2/18/2010 1:12:09 PM	
6	0.5ng3	test19	N/A		2/18/2010 1:40:55 PM	
7	0.5ng4	test20	N/A		2/18/2010 2:09:43 PM	
8	0.5ng5	test21	N/A		2/18/2010 2:38:31 PM	
9	0.5ng6	test22	N/A		2/18/2010 3:07:23 PM	
10	0.5ng7	test23	N/A		2/18/2010 3:36:14 PM	
11	0.5ng8	test24	N/A		2/18/2010 4:05:09 PM	

Manually integrated

Method Report

Method Report

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level			**Page number:**	Page 1 of 36
Master method name:	EPAMethod8270B_8level				
Current calibration file:	EC25B_8level_322010_a.calx				
Assay type:	Robustness	**Ion range calc method:**	Level	4	
Inj vol:	1.000				
Instrument method:	TargetsSplit				
Tune/Breakdown method	DFTPPSplit				

Compound identification:

Compound	Quan mass	RT	Window	View Width	Use as reference	Reference compound
N-Nitrosodimethylamine	74.00	2.54	30.00	1.00	No	1,4-DICHLOROBENZENE-D4_(IS)
Pyridine_RCRA	79.00	2.59	30.00	1.00	No	1,4-DICHLOROBENZENE-D4_(IS)
2-Picoline	93.00	3.36	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
N-Nitrosomethylethylamine_APP9	88.00	3.46	30.00	1.00	No	1,4-DICHLOROBENZENE-D4_(IS)
Methyl_methanesulfonate	80.00	3.80	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
2-fluorophenol(sur)	112.00	4.02	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
N-Nitrosodiethylamine_APP9	102.00	4.29	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
Ethyl_methanesulfonate	79.00	4.63	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
phenol-d5(sur)	99.00	5.11	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
Phenol(CCC)	94.00	5.13	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
Aniline	93.00	5.18	30.00	0.30	No	1,4-DICHLOROBENZENE-D4_(IS)
Bis(2-chloroethyl)ether	93.00	5.24	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
Pentachloroethane	167.00	5.24	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
2-chlorophenol	128.00	5.32	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
1,3-Dichlorobenzene	146.00	5.51	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
1,4-DICHLOROBENZENE-D4_(IS)	152.00	5.57	30.00	0.75	Yes	
1,4-Dichlorobenzene(CCC)	146.00	5.59	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
Benzyl_alcohol	108.00	5.71	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
1,2-Dichlorobenzene	146.00	5.77	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
2-methylphenol	107.00	5.84	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
Bis(2-chloroisopropyl)ether	45.00	5.88	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
N-Nitrosopyrrolidine_APP9	100.00	5.99	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
3-Methylphenol&4-methylphenol	107.00	6.02	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
Acetophenone	105.00	6.03	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
N-Nitroso-di-N-propylamine(SPCC)	70.00	6.03	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
o-toluidine_APP9	106.00	6.07	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
Hexachloroethane	117.00	6.17	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
nitrobenzene-d5(sur)	82.00	6.21	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
Nitrobenzene	77.00	6.23	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
N-Nitrosopiperidine	114.00	6.40	30.00	0.30	No	1,4-DICHLOROBENZENE-D4_(IS)
Isophorone	82.00	6.50	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
Phenol, pentachloro-	265.75	6.52	30.00	0.75	No	
2-Nitrophenol(CCC)	139.00	6.61	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
2,4-Dimethylphenol	122.00	6.64	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
Bis(2-chloroethoxy)methane	93.00	6.75	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
DFTPP	197.92	6.75	30.00	0.75	No	
2,4-Dichlorophenol(CCC)	162.00	6.88	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
1,2,4-Trichlorobenzene	180.00	6.98	30.00	0.75	No	1,4-DICHLOROBENZENE-D4_(IS)
NAPHTHALENE-D8_(IS)	136.00	7.05	30.00	0.75	Yes	
Naphthalene	128.00	7.08	30.00	0.75	No	NAPHTHALENE-D8_(IS)
p-Chloroaniline	127.00	7.13	30.00	0.75	No	NAPHTHALENE-D8_(IS)
2,6-Dichlorophenol	162.00	7.14	30.00	0.75	No	NAPHTHALENE-D8_(IS)
Hexachloropropene_APP9	213.00	7.19	30.00	0.75	No	NAPHTHALENE-D8_(IS)
Hexachlorobutadiene(CCC)	225.00	7.23	30.00	0.75	No	NAPHTHALENE-D8_(IS)
Benzidineperf	184.14	7.51	30.00	0.75	No	
N-Nitroso-di-N-butylamine	84.00	7.51	30.00	0.75	No	NAPHTHALENE-D8_(IS)
4,4'-DDE	246.00	7.54	30.00	0.75	No	
4-Chloro-3-methylphenol(CCC)	107.00	7.68	30.00	0.75	No	NAPHTHALENE-D8_(IS)
Safrole_APP9	162.00	7.76	30.00	0.75	No	NAPHTHALENE-D8_(IS)

Method Report

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level			**Page number:**	Page 4 of 36
Master method name:	EPAMethod8270B_8level				
Current calibration file:	EC25B_8level_322010_a.calx				
Assay type:	Robustness	**Ion range calc method:**	Level	4	
Inj vol:	1.000				
Instrument method:	TargetsSplit				
Tune/Breakdown method	DFTPPSplit				

Compound calibration:

Compound	Response	Calibration	Curve type	Weighting	Origin	Units	ISTD Name	ISTD Units
N-Nitrosodimethylamine	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
Pyridine_RCRA	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
2-Picoline	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
N-Nitrosomethylethylamine_APP9	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
Methyl_methanesulfonate	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
2-fluorophenol(sur)	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
N-Nitrosodiethylamine_APP9	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
Ethyl_methanesulfonate	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
phenol-d5(sur)	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
Phenol(CCC)	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
Aniline	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
Bis(2-chloroethyl)ether	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
Pentachloroethane	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
2-chlorophenol	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
1,3-Dichlorobenzene	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
1,4-Dichlorobenzene(CCC)	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
Benzyl_alcohol	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
1,2-Dichlorobenzene	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
2-methylphenol	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
Bis(2-chloroisopropyl)ether	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
N-Nitrosopyrrolidine_APP9	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
3-Methylphenol&4-methylphenol	Area	Internal	Linear	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
Acetophenone	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
N-Nitroso-di-N-propylamine(SPCC)	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
o-toluidine_APP9	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
Hexachloroethane	Area	Internal	Average RF	Equal	Ignore	ng/uL	1,4-DICHLOROBENZENE-D4_(IS)	ng/uL
nitrobenzene-d5(sur)	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
Nitrobenzene	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
N-Nitrosopiperidine	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
Isophorone	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
2-Nitrophenol(CCC)	Area	Internal	Linear	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
2,4-Dimethylphenol	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
Bis(2-chloroethoxy)methane	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
2,4-Dichlorophenol(CCC)	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
1,2,4-Trichlorobenzene	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
Naphthalene	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
p-Chloroaniline	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
2,6-Dichlorophenol	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
Hexachloropropene_APP9	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
Hexachlorobutadiene(CCC)	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
N-Nitroso-di-N-butylamine	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
4-Chloro-3-methylphenol(CCC)	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
Safrole_APP9	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
2-Methylnaphthalene	Area	Internal	Average RF	Equal	Ignore	ng/uL	NAPHTHALENE-D8_(IS)	ng/uL
Hexachlorocyclopentadiene(SPCC)	Area	Internal	Average RF	Equal	Ignore	ng/uL	ACENAPHTHENE-D10_(IS)	ng/uL
1,2,4,5-Tetrachlorobenzene	Area	Internal	Average RF	Equal	Ignore	ng/uL	ACENAPHTHENE-D10_(IS)	ng/uL
2,4,5-Trichlorophenol	Area	Internal	Average RF	Equal	Ignore	ng/uL	ACENAPHTHENE-D10_(IS)	ng/uL
2,4,6-Trichlorophenol(CCC)	Area	Internal	Average RF	Equal	Ignore	ng/uL	ACENAPHTHENE-D10_(IS)	ng/uL
2-fluorobiphenyl(sur)	Area	Internal	Average RF	Equal	Ignore	ng/uL	ACENAPHTHENE-D10_(IS)	ng/uL
Isosafrole_APP9	Area	Internal	Average RF	Equal	Ignore	ng/uL	ACENAPHTHENE-D10_(IS)	ng/uL
2-Chloronaphthalene	Area	Internal	Average RF	Equal	Ignore	ng/uL	ACENAPHTHENE-D10_(IS)	ng/uL

Method Report

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level			**Page number:**	Page 7 of 36
Master method name:	EPAMethod8270B_8level				
Current calibration file:	EC25B_8level_322010_a.calx				
Assay type:	Robustness	**Ion range calc method:**	Level	4	
Inj vol:	1.000				
Instrument method:	TargetsSplit				
Tune/Breakdown method	DFTPPSplit				

QAQC Limits:

Compound	LOD	LOQ	LOR	ULOL	Carryover
N-Nitrosodimethylamine	0.500	1.000	1.000	160.000	0.500
Pyridine_RCRA	0.500	1.000	1.000	160.000	0.500
2-Picoline	0.500	1.000	1.000	160.000	0.500
N-Nitrosomethylethylamine_APP9	0.500	1.000	1.000	160.000	0.500
Methyl_methanesulfonate	0.500	1.000	1.000	160.000	0.500
2-fluorophenol(sur)	0.500	1.000	1.000	160.000	0.500
N-Nitrosodiethylamine_APP9	0.500	1.000	1.000	160.000	0.500
Ethyl_methanesulfonate	0.500	1.000	1.000	160.000	0.500
phenol-d5(sur)	0.500	1.000	1.000	160.000	0.500
Phenol(CCC)	0.500	1.000	1.000	160.000	0.500
Aniline	0.500	1.000	1.000	160.000	0.500
Bis(2-chloroethyl)ether	0.500	1.000	1.000	160.000	0.500
Pentachloroethane	0.500	1.000	1.000	160.000	0.500
2-chlorophenol	0.500	1.000	1.000	160.000	0.500
1,3-Dichlorobenzene	0.500	1.000	1.000	160.000	0.500
1,4-Dichlorobenzene(CCC)	0.500	1.000	1.000	160.000	0.500
Benzyl_alcohol	0.500	1.000	1.000	160.000	0.500
1,2-Dichlorobenzene	0.500	1.000	1.000	160.000	0.500
2-methylphenol	0.500	1.000	1.000	160.000	0.500
Bis(2-chloroisopropyl)ether	0.500	1.000	1.000	160.000	0.500
N-Nitrosopyrrolidine_APP9	0.500	1.000	1.000	160.000	0.500
3-Methylphenol&4-methylphenol	0.500	1.000	1.000	160.000	0.500
Acetophenone	0.500	1.000	1.000	160.000	0.500
N-Nitroso-di-N-propylamine(SPCC)	0.500	1.000	1.000	160.000	0.500
o-toluidine_APP9	0.500	1.000	1.000	160.000	0.500
Hexachloroethane	0.500	1.000	1.000	160.000	0.500
nitrobenzene-d5(sur)	0.500	1.000	1.000	160.000	0.500
Nitrobenzene	0.500	1.000	1.000	160.000	0.500
N-Nitrosopiperidine	0.500	1.000	1.000	160.000	0.500
Isophorone	0.500	1.000	1.000	160.000	0.500
2-Nitrophenol(CCC)	0.500	1.000	1.000	160.000	0.500
2,4-Dimethylphenol	0.500	1.000	1.000	160.000	0.500
Bis(2-chloroethoxy)methane	0.500	1.000	1.000	160.000	0.500
2,4-Dichlorophenol(CCC)	0.500	1.000	1.000	160.000	0.500
1,2,4-Trichlorobenzene	0.500	1.000	1.000	160.000	0.500
Naphthalene	0.500	1.000	1.000	160.000	0.500
p-Chloroaniline	0.500	1.000	1.000	160.000	0.500
2,6-Dichlorophenol	0.500	1.000	1.000	160.000	0.500
Hexachloropropene_APP9	0.500	1.000	1.000	160.000	0.500
Hexachlorobutadiene(CCC)	0.500	1.000	1.000	160.000	0.500
N-Nitroso-di-N-butylamine	0.500	1.000	1.000	160.000	0.500
4-Chloro-3-methylphenol(CCC)	0.500	1.000	1.000	160.000	0.500
Safrole_APP9	0.500	1.000	1.000	160.000	0.500
2-Methylnaphthalene	0.500	1.000	1.000	160.000	0.500
Hexachlorocyclopentadiene(SPCC)	0.500	1.000	1.000	160.000	0.500
1,2,4,5-Tetrachlorobenzene	0.500	1.000	1.000	160.000	0.500
2,4,5-Trichlorophenol	0.500	1.000	1.000	160.000	0.500
2,4,6-Trichlorophenol(CCC)	0.500	1.000	1.000	160.000	0.500
2-fluorobiphenyl(sur)	0.500	1.000	1.000	160.000	0.500
Isosafrole_APP9	0.500	1.000	1.000	160.000	0.500
2-Chloronaphthalene	0.500	1.000	1.000	160.000	0.500

Method Report

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level			**Page number:**	Page 10 of 36
Master method name:	EPAMethod8270B_8level				
Current calibration file:	EC25B_8level_322010_a.calx				
Assay type:	Robustness	**Ion range calc method:**	Level	4	
Inj vol:	1.000				
Instrument method:	TargetsSplit				
Tune/Breakdown method	DFTPPSplit				

Groups:

DDT Breakdown

4,4'-DDE
4,4'-DDD
p,p'-DDTs

Method Report

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level			**Page number:**	Page 11 of 36
Master method name:	EPAMethod8270B_8level				
Current calibration file:	EC25B_8level_322010_a.calx				
Assay type:	Robustness	**Ion range calc method:**	Level	4	
Inj vol:	1.000				
Instrument method:	TargetsSplit				
Tune/Breakdown method	DFTPPSplit				

Report options:

Quan report options

Report concentration:	Always
Decimal places to be reported:	3
Show chromatogram on Quantitation report:	True
Display valid compound only:	True

Qual options

Sort Qual results by:	Reverse Search Index
Enable limiting peaks:	True
Limit Peaks to :	Top 10 by Height

User interface options

Shade row when sample is outside of evaluation criteria:	True
Separate ion overlay display :	True
Use alternative calibration report format:	True
Show quan flags and legend:	True

EnviroLab Forms settings

Quan flags

Flag values below LOD:	False
Flag values below LOQ:	False
Flag values above LOR:	False
Flag values above ULOL:	False
Flag values above Carryover:	False
Flag values between LOD and LOQ:	True

Correct for surrogates option

Correct for surrogates:	False

Method Report

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level			**Page number:**	Page 12 of 36
Master method name:	EPAMethod8270B_8level				
Current calibration file:	EC25B_8level_322010_a.calx				
Assay type:	Robustness	**Ion range calc method:**	Level	4	
Inj vol:	1.000				
Instrument method:	TargetsSplit				
Tune/Breakdown method	DFTPPSplit				

QAQC Calibration:

Compound	Max RSD (%)	Min RF	R^2 threshold	Max amt diff (%)
N-Nitrosodimethylamine	20.00	0.00	0.990	20.000
Pyridine_RCRA	20.00	0.00	0.990	20.000
2-Picoline	20.00	0.00	0.990	20.000
N-Nitrosomethylethylamine_APP9	20.00	0.00	0.990	20.000
Methyl_methanesulfonate	20.00	0.00	0.990	20.000
2-fluorophenol(sur)	20.00	0.00	0.990	20.000
N-Nitrosodiethylamine_APP9	20.00	0.00	0.990	20.000
Ethyl_methanesulfonate	20.00	0.00	0.990	20.000
phenol-d5(sur)	20.00	0.00	0.990	20.000
Phenol(CCC)	20.00	0.80	0.990	20.000
Aniline	20.00	0.00	0.990	20.000
Bis(2-chloroethyl)ether	20.00	0.70	0.990	20.000
Pentachloroethane	20.00	0.00	0.990	20.000
2-chlorophenol	20.00	0.80	0.990	20.000
1,3-Dichlorobenzene	20.00	0.00	0.990	20.000
1,4-Dichlorobenzene(CCC)	20.00	0.00	0.990	20.000
Benzyl_alcohol	20.00	0.00	0.990	20.000
1,2-Dichlorobenzene	20.00	0.00	0.990	20.000
2-methylphenol	20.00	0.70	0.990	20.000
Bis(2-chloroisopropyl)ether	20.00	0.00	0.990	20.000
N-Nitrosopyrrolidine_APP9	20.00	0.00	0.990	20.000
3-Methylphenol&4-methylphenol	20.00	0.60	0.990	20.000
Acetophenone	20.00	0.01	0.990	20.000
N-Nitroso-di-N-propylamine(SPCC)	20.00	0.50	0.990	20.000
o-toluidine_APP9	20.00	0.00	0.990	20.000
Hexachloroethane	20.00	0.30	0.990	20.000
nitrobenzene-d5(sur)	20.00	0.00	0.990	20.000
Nitrobenzene	20.00	0.20	0.990	20.000
N-Nitrosopiperidine	20.00	0.00	0.990	20.000
Isophorone	20.00	0.40	0.990	20.000
2-Nitrophenol(CCC)	20.00	0.10	0.990	20.000
2,4-Dimethylphenol	20.00	0.20	0.990	20.000
Bis(2-chloroethoxy)methane	20.00	0.30	0.990	20.000
2,4-Dichlorophenol(CCC)	20.00	0.20	0.990	20.000
1,2,4-Trichlorobenzene	20.00	0.00	0.990	20.000
Naphthalene	20.00	0.70	0.990	20.000
p-Chloroaniline	20.00	0.01	0.990	20.000
2,6-Dichlorophenol	20.00	0.00	0.990	20.000
Hexachloropropene_APP9	20.00	0.00	0.990	20.000
Hexachlorobutadiene(CCC)	20.00	0.01	0.990	20.000
N-Nitroso-di-N-butylamine	20.00	0.00	0.990	20.000
4-Chloro-3-methylphenol(CCC)	20.00	0.20	0.990	20.000
Safrole_APP9	20.00	0.00	0.990	20.000
2-Methylnaphthalene	20.00	0.40	0.990	20.000
Hexachlorocyclopentadiene(SPCC)	20.00	0.05	0.990	20.000
1,2,4,5-Tetrachlorobenzene	20.00	0.01	0.990	20.000
2,4,5-Trichlorophenol	20.00	0.20	0.990	20.000
2,4,6-Trichlorophenol(CCC)	20.00	0.20	0.990	20.000
2-fluorobiphenyl(sur)	20.00	0.00	0.990	20.000
Isosafrole_APP9	20.00	0.00	0.990	20.000
2-Chloronaphthalene	20.00	0.80	0.990	20.000

Method Report

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level			**Page number:**	Page 15 of 36
Master method name:	EPAMethod8270B_8level				
Current calibration file:	EC25B_8level_322010_a.calx				
Assay type:	Robustness	**Ion range calc method:**	Level	4	
Inj vol:	1.000				
Instrument method:	TargetsSplit				
Tune/Breakdown method	DFTPPSplit				

QAQC Check Standard:

Compound	Max RF diff (%)	Min RF	Max amt diff (%)
N-Nitrosodimethylamine	20.00	0.000	20.000
Pyridine_RCRA	20.00	0.000	20.000
2-Picoline	20.00	0.000	20.000
N-Nitrosomethylethylamine_APP9	20.00	0.000	20.000
Methyl_methanesulfonate	20.00	0.000	20.000
2-fluorophenol(sur)	20.00	0.000	20.000
N-Nitrosodiethylamine_APP9	20.00	0.000	20.000
Ethyl_methanesulfonate	20.00	0.000	20.000
phenol-d5(sur)	20.00	0.000	20.000
Phenol(CCC)	20.00	0.000	20.000
Aniline	20.00	0.000	20.000
Bis(2-chloroethyl)ether	20.00	0.000	20.000
Pentachloroethane	20.00	0.000	20.000
2-chlorophenol	20.00	0.000	20.000
1,3-Dichlorobenzene	20.00	0.000	20.000
1,4-Dichlorobenzene(CCC)	20.00	0.000	20.000
Benzyl_alcohol	20.00	0.000	20.000
1,2-Dichlorobenzene	20.00	0.000	20.000
2-methylphenol	20.00	0.000	20.000
Bis(2-chloroisopropyl)ether	20.00	0.000	20.000
N-Nitrosopyrrolidine_APP9	20.00	0.000	20.000
3-Methylphenol&4-methylphenol	20.00	0.000	20.000
Acetophenone	20.00	0.000	20.000
N-Nitroso-di-N-propylamine(SPCC)	20.00	0.050	20.000
o-toluidine_APP9	20.00	0.000	20.000
Hexachloroethane	20.00	0.000	20.000
nitrobenzene-d5(sur)	20.00	0.000	20.000
Nitrobenzene	20.00	0.000	20.000
N-Nitrosopiperidine	20.00	0.000	20.000
Isophorone	20.00	0.000	20.000
2-Nitrophenol(CCC)	20.00	0.000	20.000
2,4-Dimethylphenol	20.00	0.000	20.000
Bis(2-chloroethoxy)methane	20.00	0.000	20.000
2,4-Dichlorophenol(CCC)	20.00	0.000	20.000
1,2,4-Trichlorobenzene	20.00	0.000	20.000
Naphthalene	20.00	0.000	20.000
p-Chloroaniline	20.00	0.000	20.000
2,6-Dichlorophenol	20.00	0.000	20.000
Hexachloropropene_APP9	20.00	0.000	20.000
Hexachlorobutadiene(CCC)	20.00	0.000	20.000
N-Nitroso-di-N-butylamine	20.00	0.000	20.000
4-Chloro-3-methylphenol(CCC)	20.00	0.000	20.000
Safrole_APP9	20.00	0.000	20.000
2-Methylnaphthalene	20.00	0.000	20.000
Hexachlorocyclopentadiene(SPCC)	20.00	0.050	20.000
1,2,4,5-Tetrachlorobenzene	20.00	0.000	20.000
2,4,5-Trichlorophenol	20.00	0.000	20.000
2,4,6-Trichlorophenol(CCC)	20.00	0.000	20.000
2-fluorobiphenyl(sur)	20.00	0.000	20.000
Isosafrole_APP9	20.00	0.000	20.000
2-Chloronaphthalene	20.00	0.000	20.000

Method Report

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level			**Page number:**	Page 18 of 36
Master method name:	EPAMethod8270B_8level				
Current calibration file:	EC25B_8level_322010_a.calx				
Assay type:	Robustness	**Ion range calc method:**	Level	4	
Inj vol:	1.000				
Instrument method:	TargetsSplit				
Tune/Breakdown method	DFTPPSplit				

QAQC Blank

Compound	Criterion	Max value
N-Nitrosodimethylamine	Concentration	0.500
Pyridine_RCRA	Concentration	0.500
2-Picoline	Concentration	0.500
N-Nitrosomethylethylamine_APP9	Concentration	0.500
Methyl_methanesulfonate	Concentration	0.500
2-fluorophenol(sur)	Concentration	60.000
N-Nitrosodiethylamine_APP9	Concentration	0.500
Ethyl_methanesulfonate	Concentration	0.500
phenol-d5(sur)	Concentration	60.000
Phenol(CCC)	Concentration	0.500
Aniline	Concentration	0.500
Bis(2-chloroethyl)ether	Concentration	0.500
Pentachloroethane	Concentration	0.500
2-chlorophenol	Concentration	0.500
1,3-Dichlorobenzene	Concentration	0.500
1,4-Dichlorobenzene(CCC)	Concentration	0.500
Benzyl_alcohol	Concentration	0.500
1,2-Dichlorobenzene	Concentration	0.500
2-methylphenol	Concentration	0.500
Bis(2-chloroisopropyl)ether	Concentration	0.500
N-Nitrosopyrrolidine_APP9	Concentration	0.500
3-Methylphenol&4-methylphenol	Concentration	0.500
Acetophenone	Concentration	0.500
N-Nitroso-di-N-propylamine(SPCC)	Concentration	0.500
o-toluidine_APP9	Concentration	0.500
Hexachloroethane	Concentration	0.500
nitrobenzene-d5(sur)	Concentration	60.000
Nitrobenzene	Concentration	0.500
N-Nitrosopiperidine	Concentration	0.500
Isophorone	Concentration	0.500
2-Nitrophenol(CCC)	Concentration	0.500
2,4-Dimethylphenol	Concentration	0.500
Bis(2-chloroethoxy)methane	Concentration	0.500
2,4-Dichlorophenol(CCC)	Concentration	0.500
1,2,4-Trichlorobenzene	Concentration	0.500
Naphthalene	Concentration	0.500
p-Chloroaniline	Concentration	0.500
2,6-Dichlorophenol	Concentration	0.500
Hexachloropropene_APP9	Concentration	0.500
Hexachlorobutadiene(CCC)	Concentration	0.500
N-Nitroso-di-N-butylamine	Concentration	0.500
4-Chloro-3-methylphenol(CCC)	Concentration	0.500
Safrole_APP9	Concentration	0.500
2-Methylnaphthalene	Concentration	0.500
Hexachlorocyclopentadiene(SPCC)	Concentration	0.500
1,2,4,5-Tetrachlorobenzene	Concentration	0.500
2,4,5-Trichlorophenol	Concentration	0.500
2,4,6-Trichlorophenol(CCC)	Concentration	0.500
2-fluorobiphenyl(sur)	Concentration	60.000
Isosafrole_APP9	Concentration	0.500
2-Chloronaphthalene	Concentration	0.500
2-Nitroaniline	Concentration	0.500
1,4-Naphthoquinone_APP9	Concentration	0.500
Dimethyl_phthalate	Concentration	0.500
1,3-Dinitrobenzene_app9	Concentration	0.500

Method Report

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level			**Page number:**	Page 21 of 36
Master method name:	EPAMethod8270B_8level				
Current calibration file:	EC25B_8level_322010_a.calx				
Assay type:	Robustness	**Ion range calc method:**	Level	4	
Inj vol:	1.000				
Instrument method:	TargetsSplit				
Tune/Breakdown method	DFTPPSplit				

QAQC ISTD:

Compound	Min recovery (%)	Max recovery (%)	Min RT (-min)	Max RT (+min)
1,4-DICHLOROBENZENE-D4_(IS)	50.00	150.00	0.25	0.25
NAPHTHALENE-D8_(IS)	50.00	150.00	0.25	0.25
ACENAPHTHENE-D10_(IS)	50.00	150.00	0.25	0.25
PHENANTHRENE_D10	50.00	150.00	0.25	0.25
CHRYSENE-D12_(IS)	50.00	150.00	0.25	0.25
PERYLENE-D12_(IS)	50.00	150.00	0.25	0.25

Method Report

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level			**Page number:**	Page 22 of 36
Master method name:	EPAMethod8270B_8level				
Current calibration file:	EC25B_8level_322010_a.calx				
Assay type:	Robustness	**Ion range calc method:**	Level	4	
Inj vol:	1.000				
Instrument method:	TargetsSplit				
Tune/Breakdown method	DFTPPSplit				

QAQC Solvent Blank:

Compound	Method	Upper Limit %
N-Nitrosodimethylamine	None	
Pyridine_RCRA	None	
2-Picoline	None	
N-Nitrosomethylethylamine_APP9	None	
Methyl_methanesulfonate	None	
2-fluorophenol(sur)	None	
N-Nitrosodiethylamine_APP9	None	
Ethyl_methanesulfonate	None	
phenol-d5(sur)	None	
Phenol(CCC)	None	
Aniline	None	
Bis(2-chloroethyl)ether	None	
Pentachloroethane	None	
2-chlorophenol	None	
1,3-Dichlorobenzene	None	
1,4-DICHLOROBENZENE-D4_(IS)	None	
1,4-Dichlorobenzene(CCC)	None	
Benzyl_alcohol	None	
1,2-Dichlorobenzene	None	
2-methylphenol	None	
Bis(2-chloroisopropyl)ether	None	
N-Nitrosopyrrolidine_APP9	None	
3-Methylphenol&4-methylphenol	None	
Acetophenone	None	
N-Nitroso-di-N-propylamine(SPCC)	None	
o-toluidine_APP9	None	
Hexachloroethane	None	
nitrobenzene-d5(sur)	None	
Nitrobenzene	None	
N-Nitrosopiperidine	None	
Isophorone	None	
2-Nitrophenol(CCC)	None	
2,4-Dimethylphenol	None	
Bis(2-chloroethoxy)methane	None	
2,4-Dichlorophenol(CCC)	None	
1,2,4-Trichlorobenzene	None	
NAPHTHALENE-D8_(IS)	None	
Naphthalene	None	
p-Chloroaniline	None	
2,6-Dichlorophenol	None	
Hexachloropropene_APP9	None	
Hexachlorobutadiene(CCC)	None	
N-Nitroso-di-N-butylamine	None	
4-Chloro-3-methylphenol(CCC)	None	
Safrole_APP9	None	
2-Methylnaphthalene	None	
Hexachlorocyclopentadiene(SPCC)	None	
1,2,4,5-Tetrachlorobenzene	None	
2,4,5-Trichlorophenol	None	
2,4,6-Trichlorophenol(CCC)	None	
2-fluorobiphenyl(sur)	None	
Isosafrole_APP9	None	
2-Chloronaphthalene	None	
2-Nitroaniline	None	
1,4-Naphthoquinone_APP9	None	

.

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level			**Page number:**	Page 25 of 36
Master method name:	EPAMethod8270B_8level				
Current calibration file:	EC25B_8level_322010_a.calx				
Assay type:	Robustness	**Ion range calc method:**	Level	4	
Inj vol:	1.000				
Instrument method:	TargetsSplit				
Tune/Breakdown method	DFTPPSplit				

QAQC Surrogates:

Compound	Theo Conc	Min Recovery (%)	Max Recovery (%)
phenol-d5(sur)	40.000	70.00	130.00
nitrobenzene-d5(sur)	40.000	70.00	130.00
2,4,6-tribromophenol(sur)	40.000	70.00	130.00
p-terphenyl-d14(sur)	40.000	70.00	130.00

Method Report

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level			**Page number:**	Page 26 of 36
Master method name:	EPAMethod8270B_8level				
Current calibration file:	EC25B_8level_322010_a.calx				
Assay type:	Robustness	**Ion range calc method:**	Level	4	
Inj vol:	1.000				
Instrument method:	TargetsSplit				
Tune/Breakdown method	DFTPPSplit				

QAQC Matrix Spike:

Compound	Theo Conc	Min Recovery (%)	Max Recovery (%)	Max RPD
N-Nitrosodimethylamine	0.000	0.00	0.00	0.00
Pyridine_RCRA	0.000	0.00	0.00	0.00
2-Picoline	0.000	0.00	0.00	0.00
N-Nitrosomethylethylamine_APP9	0.000	0.00	0.00	0.00
Methyl_methanesulfonate	0.000	0.00	0.00	0.00
2-fluorophenol(sur)	0.000	0.00	0.00	0.00
N-Nitrosodiethylamine_APP9	0.000	0.00	0.00	0.00
Ethyl_methanesulfonate	0.000	0.00	0.00	0.00
phenol-d5(sur)	0.000	0.00	0.00	0.00
Phenol(CCC)	0.000	0.00	0.00	0.00
Aniline	0.000	0.00	0.00	0.00
Bis(2-chloroethyl)ether	0.000	0.00	0.00	0.00
Pentachloroethane	0.000	0.00	0.00	0.00
2-chlorophenol	0.000	0.00	0.00	0.00
1,3-Dichlorobenzene	0.000	0.00	0.00	0.00
1,4-Dichlorobenzene(CCC)	0.000	0.00	0.00	0.00
Benzyl_alcohol	0.000	0.00	0.00	0.00
1,2-Dichlorobenzene	0.000	0.00	0.00	0.00
2-methylphenol	0.000	0.00	0.00	0.00
Bis(2-chloroisopropyl)ether	0.000	0.00	0.00	0.00
N-Nitrosopyrrolidine_APP9	0.000	0.00	0.00	0.00
3-Methylphenol&4-methylphenol	0.000	0.00	0.00	0.00
Acetophenone	0.000	0.00	0.00	0.00
N-Nitroso-di-N-propylamine(SPCC)	0.000	0.00	0.00	0.00
o-toluidine_APP9	0.000	0.00	0.00	0.00
Hexachloroethane	0.000	0.00	0.00	0.00
nitrobenzene-d5(sur)	0.000	0.00	0.00	0.00
Nitrobenzene	0.000	0.00	0.00	0.00
N-Nitrosopiperidine	0.000	0.00	0.00	0.00
Isophorone	0.000	0.00	0.00	0.00
2-Nitrophenol(CCC)	0.000	0.00	0.00	0.00
2,4-Dimethylphenol	0.000	0.00	0.00	0.00
Bis(2-chloroethoxy)methane	0.000	0.00	0.00	0.00
2,4-Dichlorophenol(CCC)	0.000	0.00	0.00	0.00
1,2,4-Trichlorobenzene	0.000	0.00	0.00	0.00
Naphthalene	0.000	0.00	0.00	0.00
p-Chloroaniline	0.000	0.00	0.00	0.00
2,6-Dichlorophenol	0.000	0.00	0.00	0.00
Hexachloropropene_APP9	0.000	0.00	0.00	0.00
Hexachlorobutadiene(CCC)	0.000	0.00	0.00	0.00
N-Nitroso-di-N-butylamine	0.000	0.00	0.00	0.00
4-Chloro-3-methylphenol(CCC)	0.000	0.00	0.00	0.00
Safrole_APP9	0.000	0.00	0.00	0.00
2-Methylnaphthalene	0.000	0.00	0.00	0.00
Hexachlorocyclopentadiene(SPCC)	0.000	0.00	0.00	0.00
1,2,4,5-Tetrachlorobenzene	0.000	0.00	0.00	0.00
2,4,5-Trichlorophenol	0.000	0.00	0.00	0.00
2,4,6-Trichlorophenol(CCC)	0.000	0.00	0.00	0.00
2-fluorobiphenyl(sur)	0.000	0.00	0.00	0.00
Isosafrole_APP9	0.000	0.00	0.00	0.00
2-Chloronaphthalene	0.000	0.00	0.00	0.00
2-Nitroaniline	0.000	0.00	0.00	0.00
1,4-Naphthoquinone_APP9	0.000	0.00	0.00	0.00
Dimethyl_phthalate	0.000	0.00	0.00	0.00
1,3-Dinitrobenzene_app9	0.000	0.00	0.00	0.00
2,6-Dinitrotoluene	0.000	0.00	0.00	0.00

Method Report

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level		**Page number:**	Page 29 of 36
Master method name:	EPAMethod8270B_8level			
Current calibration file:	EC25B_8level_322010_a.calx			
Assay type:	Robustness	**Ion range calc method:**	Level	4
Inj vol:	1.000			
Instrument method:	TargetsSplit			
Tune/Breakdown method	DFTPPSplit			

QAQC Lab Control:

Compound	Theo Conc	Min Recovery (%)	Max Recovery (%)	Max RPD
N-Nitrosodimethylamine	0.000	0.00	0.00	0.00
Pyridine_RCRA	0.000	0.00	0.00	0.00
2-Picoline	0.000	0.00	0.00	0.00
N-Nitrosomethylethylamine_APP9	0.000	0.00	0.00	0.00
Methyl_methanesulfonate	0.000	0.00	0.00	0.00
2-fluorophenol(sur)	0.000	0.00	0.00	0.00
N-Nitrosodiethylamine_APP9	0.000	0.00	0.00	0.00
Ethyl_methanesulfonate	0.000	0.00	0.00	0.00
phenol-d5(sur)	0.000	0.00	0.00	0.00
Phenol(CCC)	0.000	0.00	0.00	0.00
Aniline	0.000	0.00	0.00	0.00
Bis(2-chloroethyl)ether	0.000	0.00	0.00	0.00
Pentachloroethane	0.000	0.00	0.00	0.00
2-chlorophenol	0.000	0.00	0.00	0.00
1,3-Dichlorobenzene	0.000	0.00	0.00	0.00
1,4-Dichlorobenzene(CCC)	0.000	0.00	0.00	0.00
Benzyl_alcohol	0.000	0.00	0.00	0.00
1,2-Dichlorobenzene	0.000	0.00	0.00	0.00
2-methylphenol	0.000	0.00	0.00	0.00
Bis(2-chloroisopropyl)ether	0.000	0.00	0.00	0.00
N-Nitrosopyrrolidine_APP9	0.000	0.00	0.00	0.00
3-Methylphenol&4-methylphenol	0.000	0.00	0.00	0.00
Acetophenone	0.000	0.00	0.00	0.00
N-Nitroso-di-N-propylamine(SPCC)	0.000	0.00	0.00	0.00
o-toluidine_APP9	0.000	0.00	0.00	0.00
Hexachloroethane	0.000	0.00	0.00	0.00
nitrobenzene-d5(sur)	0.000	0.00	0.00	0.00
Nitrobenzene	0.000	0.00	0.00	0.00
N-Nitrosopiperidine	0.000	0.00	0.00	0.00
Isophorone	0.000	0.00	0.00	0.00
2-Nitrophenol(CCC)	0.000	0.00	0.00	0.00
2,4-Dimethylphenol	0.000	0.00	0.00	0.00
Bis(2-chloroethoxy)methane	0.000	0.00	0.00	0.00
2,4-Dichlorophenol(CCC)	0.000	0.00	0.00	0.00
1,2,4-Trichlorobenzene	0.000	0.00	0.00	0.00
Naphthalene	0.000	0.00	0.00	0.00
p-Chloroaniline	0.000	0.00	0.00	0.00
2,6-Dichlorophenol	0.000	0.00	0.00	0.00
Hexachloropropene_APP9	0.000	0.00	0.00	0.00
Hexachlorobutadiene(CCC)	0.000	0.00	0.00	0.00
N-Nitroso-di-N-butylamine	0.000	0.00	0.00	0.00
4-Chloro-3-methylphenol(CCC)	0.000	0.00	0.00	0.00
Safrole_APP9	0.000	0.00	0.00	0.00
2-Methylnaphthalene	0.000	0.00	0.00	0.00
Hexachlorocyclopentadiene(SPCC)	0.000	0.00	0.00	0.00
1,2,4,5-Tetrachlorobenzene	0.000	0.00	0.00	0.00
2,4,5-Trichlorophenol	0.000	0.00	0.00	0.00
2,4,6-Trichlorophenol(CCC)	0.000	0.00	0.00	0.00
2-fluorobiphenyl(sur)	0.000	0.00	0.00	0.00
Isosafrole_APP9	0.000	0.00	0.00	0.00
2-Chloronaphthalene	0.000	0.00	0.00	0.00
2-Nitroaniline	0.000	0.00	0.00	0.00
1,4-Naphthoquinone_APP9	0.000	0.00	0.00	0.00
Dimethyl_phthalate	0.000	0.00	0.00	0.00
1,3-Dinitrobenzene_app9	0.000	0.00	0.00	0.00
2,6-Dinitrotoluene	0.000	0.00	0.00	0.00

Method Report

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level			**Page number:**	Page 32 of 36
Master method name:	EPAMethod8270B_8level				
Current calibration file:	EC25B_8level_322010_a.calx				
Assay type:	Robustness	**Ion range calc method:**	Level	4	
Inj vol:	1.000				
Instrument method:	TargetsSplit				
Tune/Breakdown method	DFTPPSplit				

QAQC Method Validation:

Compound	Theo Conc	Min Recovery (%)	Max Recovery (%)	Max RSD
N-Nitrosodimethylamine	40.000	80.00	120.00	20.00
Pyridine_RCRA	40.000	80.00	120.00	20.00
2-Picoline	40.000	80.00	120.00	20.00
N-Nitrosomethylethylamine_APP9	40.000	80.00	120.00	20.00
Methyl_methanesulfonate	40.000	80.00	120.00	20.00
2-fluorophenol(sur)	40.000	80.00	120.00	20.00
N-Nitrosodiethylamine_APP9	40.000	80.00	120.00	20.00
Ethyl_methanesulfonate	40.000	80.00	120.00	20.00
phenol-d5(sur)	40.000	80.00	120.00	20.00
Phenol(CCC)	40.000	80.00	120.00	20.00
Aniline	40.000	80.00	120.00	20.00
Bis(2-chloroethyl)ether	40.000	80.00	120.00	20.00
Pentachloroethane	40.000	80.00	120.00	20.00
2-chlorophenol	40.000	80.00	120.00	20.00
1,3-Dichlorobenzene	40.000	80.00	120.00	20.00
1,4-Dichlorobenzene(CCC)	40.000	80.00	120.00	20.00
Benzyl_alcohol	40.000	80.00	120.00	20.00
1,2-Dichlorobenzene	40.000	80.00	120.00	20.00
2-methylphenol	40.000	80.00	120.00	20.00
Bis(2-chloroisopropyl)ether	40.000	80.00	120.00	20.00
N-Nitrosopyrrolidine_APP9	40.000	80.00	120.00	20.00
3-Methylphenol&4-methylphenol	40.000	80.00	120.00	20.00
Acetophenone	40.000	80.00	120.00	20.00
N-Nitroso-di-N-propylamine(SPCC)	40.000	80.00	120.00	20.00
o-toluidine_APP9	40.000	80.00	120.00	20.00
Hexachloroethane	40.000	80.00	120.00	20.00
nitrobenzene-d5(sur)	40.000	80.00	120.00	20.00
Nitrobenzene	40.000	80.00	120.00	20.00
N-Nitrosopiperidine	40.000	80.00	120.00	20.00
Isophorone	40.000	80.00	120.00	20.00
2-Nitrophenol(CCC)	40.000	80.00	120.00	20.00
2,4-Dimethylphenol	40.000	80.00	120.00	20.00
Bis(2-chloroethoxy)methane	40.000	80.00	120.00	20.00
2,4-Dichlorophenol(CCC)	40.000	80.00	120.00	20.00
1,2,4-Trichlorobenzene	40.000	80.00	120.00	20.00
Naphthalene	40.000	80.00	120.00	20.00
p-Chloroaniline	40.000	80.00	120.00	20.00
2,6-Dichlorophenol	40.000	80.00	120.00	20.00
Hexachloropropene_APP9	40.000	80.00	120.00	20.00
Hexachlorobutadiene(CCC)	40.000	80.00	120.00	20.00
N-Nitroso-di-N-butylamine	40.000	80.00	120.00	20.00
4-Chloro-3-methylphenol(CCC)	40.000	80.00	120.00	20.00
Safrole_APP9	40.000	80.00	120.00	20.00
2-Methylnaphthalene	40.000	80.00	120.00	20.00
Hexachlorocyclopentadiene(SPCC)	40.000	80.00	120.00	20.00
1,2,4,5-Tetrachlorobenzene	40.000	80.00	120.00	20.00
2,4,5-Trichlorophenol	40.000	80.00	120.00	20.00
2,4,6-Trichlorophenol(CCC)	40.000	80.00	120.00	20.00
2-fluorobiphenyl(sur)	40.000	80.00	120.00	20.00
Isosafrole_APP9	40.000	80.00	120.00	20.00
2-Chloronaphthalene	40.000	80.00	120.00	20.00

Method Report

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level			**Page number:**	Page 35 of 36
Master method name:	EPAMethod8270B_8level				
Current calibration file:	EC25B_8level_322010_a.calx				
Assay type:	Robustness	**Ion range calc method:**	Level	4	
Inj vol:	1.000				
Instrument method:	TargetsSplit				
Tune/Breakdown method	DFTPPSplit				

Breakdown Groups

GroupName	**Max % breakdown**
DDT Breakdown	20.00

Members

4,4'-DDE
4,4'-DDD
p,p'-DDTs

Method Report

Method name:	EC25B_8level_322010_a_EPAMethod8270B_8level			**Page number:**	Page 36 of 36
Master method name:	EPAMethod8270B_8level				
Current calibration file:	EC25B_8level_322010_a.calx				
Assay type:	Robustness	**Ion range calc method:**	Level	4	
Inj vol:	1.000				
Instrument method:	TargetsSplit				
Tune/Breakdown method	DFTPPSplit				

QAQC Tune:

Tune compound:	DFTPP
Tune method:	8270D
Use selected method only:	True
Require background subtraction:	True
Step off:	20

Eval mass	Base peak?	Low Op	Low Limit (%)	High Op	High Limit (%)	Relative To
51		>=	10.00	<=	80.00	Base peak
68				<	2.00	69
70				<	2.00	69
127		>=	10.00	<=	80.00	Base peak
197				<	2.00	198
198	True	>	50.00	<=	100.00	Base peak
199		>=	5.00	<=	9.00	198
275		>=	10.00	<=	60.00	Base peak
365		>	1.00			198
441		>	0.00	<	24.00	442
442	True	>	50.00	<=	100.00	Base peak
443		>=	15.00	<=	24.00	442

Method Validation Report

Method Validation Report

Lab name:	Thermo Fisher Laboratory		Page 1 of 7
Instrument:	ThermoFisher Instrument	**Method:**	EPAMethod8270B_3192010_a_EPAMethod8270B
User:	AMER\jessie.butler		EPAMethod8270B
Batch:	EPAMethod8270B_3192010_a	**Cali File:**	HotNeedleCurve8270B_2162010_a_EPAMethod8270B_3192010_a.calx

Method Validation Summary

Compound	Avg Conc	Theo Conc	% Diff	Min Conc	Max Conc	% RSD	Max % RSD	
N-Nitrosodimethylamine	4.625	5.000	-7.49	4.000	6.000	2.76	20.00	
Pyridine_RCRA	4.026	5.000	-19.47	4.000	6.000	2.95	20.00	
2-Picoline	3.939	5.000	-21.22	4.000	6.000	4.00	20.00	<<<
N-Nitrosomethylethylamine_APP9	4.848	5.000	-3.03	4.000	6.000	2.22	20.00	
Methyl_methanesulfonate	4.047	5.000	-19.05	4.000	6.000	4.33	20.00	
2-fluorophenol(sur)	37.610	40.000	-5.98	32.000	48.000	3.38	20.00	
N-Nitrosodiethylamine_APP9	4.214	5.000	-15.71	4.000	6.000	6.89	20.00	
Ethyl_methanesulfonate	4.243	5.000	-15.15	4.000	6.000	4.22	20.00	
phenol-d5(sur)	38.014	40.000	-4.97	32.000	48.000	3.48	20.00	
Phenol(CCC)	2.540	5.000	-49.21	4.000	6.000	97.37	20.00	<<<
Aniline	4.464	5.000	-10.72	4.000	6.000	1.36	20.00	
Bis(2-chloroethyl)ether	4.554	5.000	-8.92	4.000	6.000	3.34	20.00	
Pentachloroethane	4.555	5.000	-8.90	4.000	6.000	2.88	20.00	
2-chlorophenol	4.043	5.000	-19.14	4.000	6.000	4.51	20.00	
1,3-Dichlorobenzene	4.274	5.000	-14.52	4.000	6.000	2.61	20.00	
1,4-DICHLOROBENZENE-D4_(IS)	2353314					2.95	IS	
1,4-Dichlorobenzene(CCC)	4.231	5.000	-15.38	4.000	6.000	4.04	20.00	
Benzyl_alcohol	3.950	5.000	-21.00	4.000	6.000	2.19	20.00	<<<
1,2-Dichlorobenzene	4.357	5.000	-12.86	4.000	6.000	4.41	20.00	
2-methylphenol	4.036	5.000	-19.27	4.000	6.000	6.12	20.00	
Bis(2-chloroisopropyl)ether	4.716	5.000	-5.67	4.000	6.000	4.34	20.00	
N-Nitrosopyrrolidine_APP9	4.274	5.000	-14.53	4.000	6.000	4.47	20.00	
3-Methylphenol&4-methylphenol	4.016	10.000	-59.84	8.000	12.000	2.27	20.00	<<<
Acetophenone	4.429	5.000	-11.43	4.000	6.000	2.70	20.00	
N-Nitroso-di-N-propylamine(SPCC)	4.536	5.000	-9.29	4.000	6.000	3.70	20.00	
o-toluidine_APP9	4.435	5.000	-11.29	4.000	6.000	2.95	20.00	
Hexachloroethane	4.793	5.000	-4.13	4.000	6.000	3.57	20.00	
nitrobenzene-d5(sur)	37.878	40.000	-5.31	32.000	48.000	3.44	20.00	
Nitrobenzene	4.537	5.000	-9.25	4.000	6.000	3.81	20.00	
N-Nitrosopiperidine	4.512	5.000	-9.76	4.000	6.000	3.30	20.00	
Isophorone	4.370	5.000	-12.59	4.000	6.000	2.24	20.00	
2-Nitrophenol(CCC)	3.829	5.000	-23.43	4.000	6.000	5.25	20.00	<<<
2,4-Dimethylphenol	4.154	5.000	-16.92	4.000	6.000	3.60	20.00	
Bis(2-chloroethoxy)methane	4.425	5.000	-11.50	4.000	6.000	4.76	20.00	
2,4-Dichlorophenol(CCC)	3.680	5.000	-26.39	4.000	6.000	2.20	20.00	<<<
1,2,4-Trichlorobenzene	4.327	5.000	-13.46	4.000	6.000	3.64	20.00	
NAPHTHALENE-D8_(IS)	8392934					3.21	IS	
Naphthalene	4.513	5.000	-9.74	4.000	6.000	3.26	20.00	
p-Chloroaniline	4.100	5.000	-18.00	4.000	6.000	2.47	20.00	
2,6-Dichlorophenol	3.760	5.000	-24.81	4.000	6.000	4.56	20.00	<<<
Hexachloropropene_APP9	0.000	5.000	-100.00	4.000	6.000	0.00	20.00	<<<
Hexachlorobutadiene(CCC)	4.540	5.000	-9.20	4.000	6.000	3.68	20.00	
N-Nitroso-di-N-butylamine	4.223	5.000	-15.54	4.000	6.000	4.59	20.00	
4-Chloro-3-methylphenol(CCC)	3.796	5.000	-24.08	4.000	6.000	2.68	20.00	<<<
Safrole_APP9	4.381	5.000	-12.37	4.000	6.000	2.60	20.00	
2-Methylnaphthalene	4.459	5.000	-10.81	4.000	6.000	5.07	20.00	
Hexachlorocyclopentadiene(SPCC)	4.087	5.000	-18.27	4.000	6.000	6.79	20.00	
1,2,4,5-Tetrachlorobenzene	4.869	5.000	-2.62	4.000	6.000	4.77	20.00	
2,4,5-Trichlorophenol	3.530	5.000	-29.41	4.000	6.000	3.54	20.00	<<<
2,4,6-Trichlorophenol(CCC)	3.788	5.000	-24.24	4.000	6.000	4.98	20.00	<<<

Manually integrated

<<< = Failure

Method Validation Report

Lab name:	Thermo Fisher Laboratory			Page 4 of 7
Instrument:	ThermoFisher Instrument	**Method:**	EPAMethod8270B_3192010_a_EPAMethod8270B	
User:	AMER\jessie.butler		EPAMethod8270B	
Batch:	EPAMethod8270B_3192010_a	**Cali File:**	HotNeedleCurve8270B_2162010_a_EPAMethod8270B_3192010_a.calx	

Method Validation Report Data

Compound	1	2	3	4	5	6	7	8
N-Nitrosodimethylamine	4.410	4.813	4.740	4.655	4.532	4.541	4.677	4.636
Pyridine_RCRA	4.055	4.089	4.189	3.952	3.800	3.993	4.123	4.010
2-Picoline	3.847	4.007	4.046	3.991	3.640	3.944	4.168	3.868
N-Nitrosomethylethylamine_APP9	4.786	4.870	4.790	4.849	4.663	4.940	5.022	4.866
Methyl_methanesulfonate	3.889	4.013	3.961	4.133	3.974	3.880	4.417	4.112
2-fluorophenol(sur)	35.816	38.876	37.888	38.069	35.761	37.882	39.230	37.356
N-Nitrosodiethylamine_APP9	3.794	4.162	4.367	4.375	3.941	4.203	4.743	4.131
Ethyl_methanesulfonate	4.532	4.142	4.222	4.295	3.945	4.131	4.269	4.404
phenol-d5(sur)	35.696	38.838	38.731	39.525	37.297	38.548	38.838	36.636
Phenol(CCC)	0.789	0.877	5.489	0.709	0.710	0.659	5.586	5.499
Aniline	4.370	4.440	4.499	4.571	4.465	4.460	4.494	4.413
Bis(2-chloroethyl)ether	4.527	4.640	4.804	4.602	4.381	4.352	4.659	4.468
Pentachloroethane	4.479	4.489	4.417	4.684	4.592	4.708	4.693	4.379
2-chlorophenol	4.034	3.775	4.401	4.116	4.097	4.052	3.920	3.949
1,3-Dichlorobenzene	4.436	4.154	4.188	4.437	4.305	4.242	4.255	4.173
1,4-DICHLOROBENZENE-D4_(IS)	2371553	2274428	2281292	2325935	2453155	2380010	2299718	2440419
1,4-Dichlorobenzene(CCC)	3.922	4.057	4.150	4.385	4.336	4.287	4.310	4.398
Benzyl_alcohol	3.919	3.907	3.959	4.062	3.951	4.088	3.862	3.849
1,2-Dichlorobenzene	4.002	4.334	4.624	4.412	4.416	4.280	4.545	4.242
2-methylphenol	3.607	4.309	3.831	4.131	3.928	4.099	4.029	4.356
Bis(2-chloroisopropyl)ether	4.851	4.828	4.817	4.689	4.243	4.840	4.806	4.656
N-Nitrosopyrrolidine_APP9	4.083	4.194	4.419	4.482	4.456	4.341	4.274	3.941
3-Methylphenol&4-methylphenol	3.914	3.945	4.081	4.154	3.897	4.023	4.088	4.024
Acetophenone	4.487	4.426	4.570	4.287	4.603	4.304	4.327	4.424
N-Nitroso-di-N-propylamine(SPCC)	4.406	4.495	4.655	4.394	4.338	4.675	4.826	4.498
o-toluidine_APP9	4.389	4.591	4.629	4.287	4.483	4.424	4.258	4.422
Hexachloroethane	4.568	4.782	4.857	4.810	4.543	4.875	5.074	4.839
nitrobenzene-d5(sur)	37.711	38.852	40.144	38.715	36.496	36.580	37.867	36.655
Nitrobenzene	4.476	4.582	4.854	4.432	4.375	4.364	4.496	4.722
N-Nitrosopiperidine	4.288	4.390	4.789	4.573	4.546	4.432	4.528	4.550
Isophorone	4.293	4.326	4.481	4.273	4.238	4.433	4.469	4.449
2-Nitrophenol(CCC)	3.704	3.722	4.242	3.664	3.895	3.619	3.922	3.861
2,4-Dimethylphenol	4.089	4.202	4.263	3.924	4.252	3.947	4.242	4.312
Bis(2-chloroethoxy)methane	4.393	4.530	4.637	4.379	4.366	4.088	4.254	4.750
2,4-Dichlorophenol(CCC)	3.631	3.677	3.707	3.685	3.833	3.638	3.553	3.718
1,2,4-Trichlorobenzene	4.170	4.495	4.559	4.086	4.312	4.256	4.371	4.366
NAPHTHALENE-D8_(IS)	8412838	8059419	7906637	8500152	8601128	8585401	8428072	8649826
Naphthalene	4.474	4.444	4.670	4.499	4.315	4.452	4.786	4.464
p-Chloroaniline	4.001	4.109	4.253	4.181	4.188	3.973	4.082	4.013
2,6-Dichlorophenol	4.015	3.969	3.631	3.611	3.737	3.528	3.821	3.765
Hexachloropropene_APP9	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Hexachlorobutadiene(CCC)	4.485	4.288	4.783	4.367	4.550	4.722	4.616	4.511
N-Nitroso-di-N-butylamine	4.030	4.443	4.309	4.218	4.290	3.874	4.430	4.190
4-Chloro-3-methylphenol(CCC)	3.684	3.751	3.909	3.817	3.646	3.912	3.766	3.885

Manually integrated

<<< = Failure

Method Validation Report

Lab name:	Thermo Fisher Laboratory		Page 7 of 7
Instrument:	ThermoFisher Instrument	**Method:**	EPAMethod8270B_3192010_a_EPAMethod8270B
User:	AMER\jessie.butler		EPAMethod8270B
Batch:	EPAMethod8270B_3192010_a	**Cali File:**	HotNeedleCurve8270B_2162010_a_EPAMethod8270B_3192010_a.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
1	5ng01	sample35a	N/A		2/17/2010 10:40:26 AM	
2	5ng02	sample36a	N/A		2/17/2010 11:09:21 AM	
3	5ng03	sample37	N/A		2/17/2010 11:38:23 AM	
4	5ng04	sample38	N/A		2/17/2010 12:07:09 PM	
5	5ng05	sample39	N/A		2/17/2010 12:35:59 PM	
6	5ng06	sample40	N/A		2/17/2010 1:04:45 PM	
7	5ng07	sample41	N/A		2/17/2010 1:33:31 PM	
8	5ng08	sample42	N/A		2/17/2010 2:02:17 PM	

Manually integrated

<<< = Failure

MSMSD Report

MSMSD Report

Lab name:	Thermo Fisher Laboratory		Page 1 of 3
Instrument:	ThermoFisher Instrument	**Method:**	EPAMethod8270B_8level_3192010_d_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	EPAMethod8270B_8level_3192010_d	**Cali File:**	EC25B_8level_322010_a_EPAMethod8270B_8level_3192010_d.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	QC	342010_a002	N/A	QC	3/4/2010 11:39:33 AM	
3	QC	342010_a003	N/A	QC	3/4/2010 12:03:15 PM	
3	QC	352010_a004	N/A	QC	3/5/2010 11:46:24 AM	

QC

Compound	Unknown Conc	Spike Amt	MS Conc	% Rec	Recovery % Min	Max	MSD Conc	% Rec	RPD	Max RPD	Rec Fails	RPD Fails
N-Nitrosodimethylamine	0.000	50.000	52.470	104.94	80.00	120.00	48.109	96.22	8.67	20.00	0	0
Pyridine_RCRA	0.002	50.000	54.126	108.25	80.00	120.00	49.824	99.64	8.28	20.00	0	0
2-Picoline	0.001	50.000	55.362	110.72	80.00	120.00	49.123	98.24	11.94	20.00	0	0
N-Nitrosomethylethylamine_APP9	0.049	50.000	54.618	109.14	80.00	120.00	48.625	97.15	11.62	20.00	0	0
Methyl_methanesulfonate	0.610	50.000	51.515	101.81	80.00	120.00	47.343	93.47	8.54	20.00	0	0
2-fluorophenol(sur)	39.648	40.000	42.714	7.66	80.00	120.00	40.370	1.80	123.78	20.00	2	1
N-Nitrosodiethylamine_APP9	0.002	50.000	53.846	107.69	80.00	120.00	50.048	100.09	7.31	20.00	0	0
Ethyl_methanesulfonate	0.002	50.000	58.196	116.39	80.00	120.00	50.402	100.80	14.35	20.00	0	0
phenol-d5(sur)	37.664	40.000	41.497	9.58	80.00	120.00	38.246	1.46	147.26	20.00	2	1
Phenol(CCC)	0.010	50.000	53.881	107.74	80.00	120.00	6.253	12.49	158.46	20.00	1	1
Aniline	0.000	50.000	54.677	109.35	80.00	120.00	49.783	99.56	9.37	20.00	0	0
Bis(2-chloroethyl)ether	0.001	50.000	55.074	110.15	80.00	120.00	48.114	96.23	13.49	20.00	0	0
Pentachloroethane	0.001	50.000	55.805	111.61	80.00	120.00	55.431	110.86	0.67	20.00	0	0
2-chlorophenol	0.000	50.000	51.542	103.08	80.00	120.00	49.303	98.61	4.44	20.00	0	0
1,3-Dichlorobenzene	0.001	50.000	50.683	101.36	80.00	120.00	53.464	106.93	5.34	20.00	0	0
1,4-Dichlorobenzene(CCC)	0.000	50.000	53.862	107.72	80.00	120.00	52.303	104.61	2.94	20.00	0	0
Benzyl_alcohol	0.079	50.000	54.944	109.73	80.00	120.00	51.102	102.05	7.26	20.00	0	0
1,2-Dichlorobenzene	0.001	50.000	52.612	105.22	80.00	120.00	52.981	105.96	0.70	20.00	0	0
2-methylphenol	0.003	50.000	55.068	110.13	80.00	120.00	52.087	104.17	5.56	20.00	0	0
Bis(2-chloroisopropyl)ether	0.002	50.000	58.101	116.20	80.00	120.00	52.973	105.94	9.23	20.00	0	0
N-Nitrosopyrrolidine_APP9	0.024	50.000	57.133	114.22	80.00	120.00	51.010	101.97	11.33	20.00	0	0
3-Methylphenol&4-methylphenol	7.087	100.000	110.648	103.56	80.00	120.00	104.217	97.13	6.41	20.00	0	0
Acetophenone	0.002	50.000	55.777	111.55	80.00	120.00	52.279	104.55	6.48	20.00	0	0
N-Nitroso-di-N-propylamine(SPCC)	5.963	50.000	55.106	98.29	80.00	120.00	48.024	84.12	15.53	20.00	0	0
o-toluidine_APP9	0.001	50.000	52.285	104.57	80.00	120.00	52.016	104.03	0.52	20.00	0	0
Hexachloroethane	0.002	50.000	53.969	107.93	80.00	120.00	49.931	99.86	7.77	20.00	0	0
nitrobenzene-d5(sur)	40.858	40.000	45.118	10.65	80.00	120.00	41.423	1.41	153.16	20.00	2	1
Nitrobenzene	0.056	50.000	56.422	112.73	80.00	120.00	50.909	101.71	10.28	20.00	0	0
N-Nitrosopiperidine	0.001	50.000	51.817	103.63	80.00	120.00	46.436	92.87	10.95	20.00	0	0
Isophorone	0.011	50.000	54.297	108.57	80.00	120.00	54.030	108.04	0.49	20.00	0	0
2-Nitrophenol(CCC)	7.946	50.000	48.062	80.23	80.00	120.00	47.032	78.17	2.60	20.00	1	0
2,4-Dimethylphenol	0.000	50.000	54.562	109.12	80.00	120.00	51.701	103.40	5.39	20.00	0	0
Bis(2-chloroethoxy)methane	0.001	50.000	54.092	108.18	80.00	120.00	53.458	106.91	1.18	20.00	0	0
2,4-Dichlorophenol(CCC)	0.000	50.000	55.580	111.16	80.00	120.00	54.251	108.50	2.42	20.00	0	0
1,2,4-Trichlorobenzene	0.001	50.000	57.998	116.00	80.00	120.00	53.342	106.68	8.36	20.00	0	0
Naphthalene	0.010	50.000	52.884	105.75	80.00	120.00	51.910	103.80	1.86	20.00	0	0
p-Chloroaniline	0.002	50.000	50.866	101.73	80.00	120.00	51.242	102.48	0.74	20.00	0	0
2,6-Dichlorophenol	0.000	50.000	52.295	104.59	80.00	120.00	54.068	108.14	3.33	20.00	0	0
Hexachloropropene_APP9	0.001	50.000	53.537	107.07	80.00	120.00	52.945	105.89	1.11	20.00	0	0
Hexachlorobutadiene(CCC)	0.001	50.000	57.689	115.38	80.00	120.00	57.135	114.27	0.96	20.00	0	0
N-Nitroso-di-N-butylamine	0.000	50.000	55.296	110.59	80.00	120.00	51.622	103.24	6.87	20.00	0	0

Manually integrated

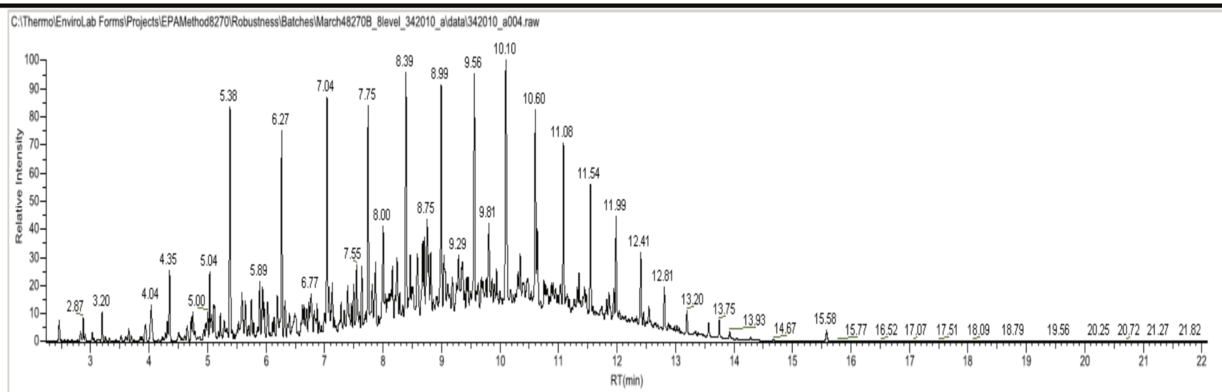
Quantitation Report

Quantitation Report

Page 1 of 6

Lab name:	Thermo Fisher Laboratory		
Instrument	ThermoFisher Instrument	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	March48270B_8level_342010_a	**Cali File**	EC25B_8level_322010_a_March48270B_8level_342010_a.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	5% diesel	342010_a004	N/A		3/4/2010 12:33:49 PM	



Internal Standards	RT	QIon	Response	Curve Type	Average RF/ Response	Injected Conc	Units	Calculated Conc	Units	Flags
1,4-DICHLOROBENZENE-D4_(IS)	5.57	152.00	3259901	Average RF	0.000	40.000	ng/uL	40.000	ng/uL	
NAPHTHALENE-D8_(IS)	7.05	136.00	11741455	Average RF	0.000	40.000	ng/uL	40.000	ng/uL	
ACENAPHTHENE-D10_(IS)	9.06	164.00	7312176	Average RF	0.000	40.000	ng/uL	40.000	ng/uL	
PHENANTHRENE_D10	10.75	188.00	10527013	Average RF	0.000	40.000	ng/uL	40.000	ng/uL	
CHRYSENE-D12_(IS)	13.75	240.00	4162955	Average RF	0.000	40.000	ng/uL	40.000	ng/uL	
PERYLENE-D12_(IS)	15.58	264.00	3256621	Average RF	0.000	40.000	ng/uL	40.000	ng/uL	

Surrogates	RT	QIon	Response	Curve Type	Average RF/ Response	Injected Conc	Units	Calculated Conc	Units	Flags
phenol-d5(sur)	5.11	99.00	5690795	Average RF	1.746	35.680	ng/uL	35.680	ng/uL	I
nitrobenzene-d5(sur)	6.21	82.00	4653618	Average RF	0.396	46.438	ng/uL	46.438	ng/uL	
2,4,6-tribromophenol(sur)	9.96	330.00	509575	Average RF	0.070	34.645	ng/uL	34.645	ng/uL	I
p-terphenyl-d14(sur)	12.55	244.00	3194754	Average RF	0.767	35.980	ng/uL	35.980	ng/uL	

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

Manually integrated

Quantitation Report

Lab name: Thermo Fisher Laboratory
Instrument ThermoFisher Instrument
User: AMER\jessie.butler
Batch: March48270B_8level_342010_a

Method: March48270B_8level_342010_a_EPAMethod8270B_8level
EPAMethod8270B_8level
Cali File EC25B_8level_322010_a_March48270B_8level_342010_a.calx

Target Compounds	RT	QIon	Response	Curve Type	Average RF/ Response	Injected Conc	Units	Calculated Conc	Units	Flags
Pyridine_RCRA	2.61	79.00	291	Average RF	0.000	0.002	ng/uL	0.002	ng/uL	I
Methyl_methanesulfonate	4.04	80.00	116346	Average RF	0.036	3.298	ng/uL	3.298	ng/uL	I
2-fluorophenol(sur)	4.02	112.00	4466909	Average RF	1.370	38.169	ng/uL	38.169	ng/uL	I
N-Nitrosodiethylamine_APP9	4.31	102.00	123218	Average RF	0.038	2.097	ng/uL	2.097	ng/uL	I
Ethyl_methanesulfonate	4.65	79.00	566359	Average RF	0.174	6.337	ng/uL	6.337	ng/uL	I
Phenol(CCC)	5.12	94.00	2187	Average RF	0.001	0.012	ng/uL	0.012	ng/uL	I
Aniline	5.15	93.00	783	Average RF	0.000	0.003	ng/uL	0.003	ng/uL	I
Bis(2-chloroethyl)ether	5.22	93.00	66461	Average RF	0.020	0.551	ng/uL	0.551	ng/uL	I
2-chlorophenol	5.53	128.00	7835	Average RF	0.002	0.055	ng/uL	0.055	ng/uL	I
Benzyl_alcohol	5.71	108.00	29503	Average RF	0.009	0.311	ng/uL	0.311	ng/uL	I
2-methylphenol	5.84	107.00	9137	Average RF	0.003	0.093	ng/uL	0.093	ng/uL	I
Bis(2-chloroisopropyl)ether	5.89	45.00	2720	Average RF	0.001	0.010	ng/uL	0.010	ng/uL	I
N-Nitrosopyrrolidine_APP9	6.02	100.00	4009	Average RF	0.001	0.058	ng/uL	0.058	ng/uL	I
3-Methylphenol&4-methylphenol	6.03	107.00	33677	Linear	0.010	7.312	ng/uL	7.312	ng/uL	I
Acetophenone	6.03	105.00	8208444	Average RF	0.699	48.299	ng/uL	48.299	ng/uL	I
N-Nitroso-di-N-propylamine(SPCC)	6.02,0.00	70.00,197.92	360491	Average RF	0.111	6.958	ng/uL	6.958	ng/uL	I
o-toluidine_APP9	6.11	106.00	144370	Average RF	0.012	0.687	ng/uL	0.687	ng/uL	I
Hexachloroethane	6.19	117.00	2723090	Average RF	0.835	52.626	ng/uL	52.626	ng/uL	I
Nitrobenzene	6.23	77.00	195466	Average RF	0.017	2.621	ng/uL	2.621	ng/uL	I
N-Nitrosopiperidine	6.40	114.00	21949	Average RF	0.002	0.320	ng/uL	0.320	ng/uL	I
Isophorone	6.51	82.00	1178628	Average RF	0.100	5.673	ng/uL	5.673	ng/uL	I
2-Nitrophenol(CCC)	6.62	139.00	60472	Linear	0.005	8.822	ng/uL	8.822	ng/uL	I
2,4-Dimethylphenol	6.66	122.00	262923	Average RF	0.022	1.859	ng/uL	1.859	ng/uL	I

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

Manually integrated

Quantitation Report - 2

Quantitation Report - 2

MS Integ Params:	EPAMethod8270B_8level	**Quant Time:**	3/19/2010 2:23:02 PM
Quant Method:	March48270B_8level_342010_a_EPAMethod8270B_8level	**Data File:**	342010_a004
Title:	Robustness	**Acq on:**	3/4/2010 12:33:49 PM
Last Update:	3/19/2010 2:29:20 PM	**Sample:**	
Data Acq Method:	TargetsSplit	**Comment:**	
Operator:	AMER\jessie.butler	**Vial:**	4
Instr:	ThermoFisher Instrument	**Multiplr:**	1.000
Response Via:	EC25B_8level_322010_a_March48270B_8level_342010_a.calx	**Quant Results File:**	C:\Thermo\EnviroLab Forms\Projects\EPAMethod8270\Robustness\Batches\March48270B_8level_342010_a\Data\342010_a004.rsx

Internal Standards

Compound Name	RT	QIon	Response	Conc	Units	Dev (min)	Flags
16 1,4-DICHLOROBENZENE-D4_(IS)	5.57	152.00	3259901	40.000	ng/uL	0.00	
39 NAPHTHALENE-D8_(IS)	7.05	136.00	11741455	40.000	ng/uL	0.00	
67 ACENAPHTHENE-D10_(IS)	9.06	164.00	7312176	40.000	ng/uL	-0.01	
96 PHENANTHRENE_D10	10.75	188.00	10527013	40.000	ng/uL	0.00	
115 CHRYSENE-D12_(IS)	13.75	240.00	4162955	40.000	ng/uL	-0.01	
122 PERYLENE-D12_(IS)	15.58	264.00	3256621	40.000	ng/uL	-0.01	

Surrogates

Compound Name	RT	QIon	Response	Conc	Units	Dev (min)	Spiked Amt	Recovery	Flags
9 phenol-d5(sur)	5.11	99.00	5690795	35.680	ng/uL	0.00	40	9.2001368662164	I
28 nitrobenzene-d5(sur)	6.21	82.00	4653618	46.438	ng/uL	0.00	40	16.095247854346	
85 2,4,6-tribromophenol(sur)	9.96	330.00	509575	34.645	ng/uL	0.00	40	6.6134684703991	I
105 p-terphenyl-d14(sur)	12.55	244.00	3194754	35.980	ng/uL	0.00	40	9.9499376657474	

Target Compounds

Compound Name	RT	QIon	Response	Conc	Units	Dev (min)	Flags
2 Pyridine_RCRA	2.61	79.00	291	0.002	ng/uL	0.02	I
5 Methyl_methanesulfonate	4.04	80.00	116346	3.298	ng/uL	0.24	I
6 2-fluorophenol(sur)	4.02	112.00	4466909	38.169	ng/uL	0.00	I
7 N-Nitrosodiethylamine_APP9	4.31	102.00	123218	2.097	ng/uL	0.02	I
8 Ethyl_methanesulfonate	4.65	79.00	566359	6.337	ng/uL	0.02	I
10 Phenol(CCC)	5.12	94.00	2187	0.012	ng/uL	-0.01	I
11 Aniline	5.15	93.00	783	0.003	ng/uL	-0.03	I
12 Bis(2-chloroethyl)ether	5.22	93.00	66461	0.551	ng/uL	-0.02	I
14 2-chlorophenol	5.53	128.00	7835	0.055	ng/uL	0.21	I
18 Benzyl_alcohol	5.71	108.00	29503	0.311	ng/uL	0.00	I

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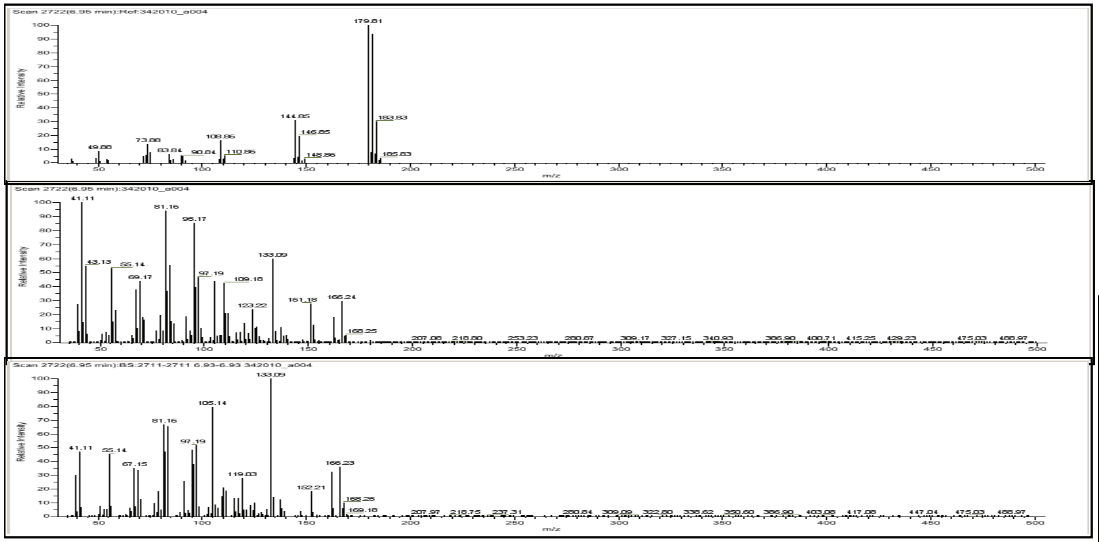
3/19/2010 2:58:53PM

EPAMethod8270B_8level

Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank

Manually integrated

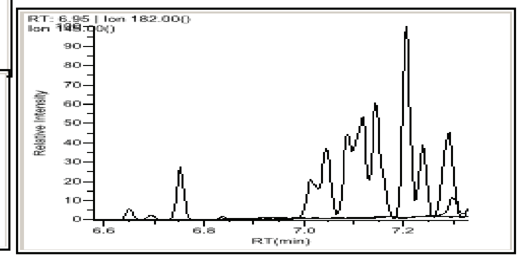
Quantitation Report - 2



38
1,2,4-Trichlorobenzene

Concen:	0.016		
RT:	6.95		Scan# 2722
Delta R.T.:	-0.03		
Lab File:	342010_a004		
Acq:	3/4/2010 12:33:49 PM		
Tgt Ion: 182.00	Resp:	1639	

Ion	Ratio	Lower	Upper
182.00	301.77		
145.00	17393.34	4.50	64.50



Page 5 of 57
3/19/2010 2:58:53PM
EPAMethod8270B_8level
Flag legend: LOD<J<LOQ; I=Ion ratio failure; C=Carryover; ?=Linearity limit ;D=Detection limit; Q=Quan limit; POS=Rpt limit; b=Blank; s=Solvent blank
Manually integrated

Solvent Blank Report

Solvent Blank Report

Page 1 of 3

Lab name:	Thermo Fisher Laboratory		
Instrument:	ThermoFisher Instrument	**Method:**	EPAMethod8270B_8level_3122010_b_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	EPAMethod8270B_8level_3122010_b	**Cali File:**	EC25B_8level_322010_a_EPAMethod8270B_8level_3122010_b.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
2	blk	3122010_b002	N/A		3/12/2010 7:11:20 PM	

Internal Standards	RT	QIon	Response	Method	Upper Limit
1,4-DICHLOROBENZENE-D4_(IS)	5.57	152.00		None	
NAPHTHALENE-D8_(IS)	7.05	136.00		None	
ACENAPHTHENE-D10_(IS)	9.06	164.00		None	
PHENANTHRENE_D10	10.75	188.00		None	
CHRYSENE-D12_(IS)	13.75	240.00		None	
PERYLENE-D12_(IS)	15.58	264.00		None	

Surrogates	RT	QIon	Response	Method	Upper Limit
phenol-d5(sur)	5.10	99.00		None	
nitrobenzene-d5(sur)	6.20	82.00		None	
2,4,6-tribromophenol(sur)	9.95	330.00		None	
p-terphenyl-d14(sur)	12.54	244.00		None	

Target Compounds	RT	QIon	Response	Method	Upper Limit
Pyridine_RCRA	2.57	79.00		None	
N-Nitrosomethylethylamine_APP9	3.47	88.00		None	
Methyl_methanesulfonate	4.01	80.00		None	
2-fluorophenol(sur)	4.01	112.00		None	
N-Nitrosodiethylamine_APP9	4.47	102.00		None	
Ethyl_methanesulfonate	4.58	79.00		None	
Phenol(CCC)	5.13	94.00		None	
2-chlorophenol	5.21	128.00		None	
1,3-Dichlorobenzene	5.59	146.00		None	
1,4-Dichlorobenzene(CCC)	5.59	146.00		None	
Benzyl_alcohol	5.74	108.00		None	
1,2-Dichlorobenzene	5.79	146.00		None	
Bis(2-chloroisopropyl)ether	5.75	45.00		None	
N-Nitrosopyrrolidine_APP9	6.21	100.00		None	
Acetophenone	6.03	105.00		None	
N-Nitroso-di-N-propylamine(SPCC)	6.20,6.45	70.00,197.92		None	
Hexachloroethane	6.13	117.00		None	
Nitrobenzene	6.20	77.00		None	
N-Nitrosopiperidine	6.20	114.00		None	

Manually integrated

Surrogate Recovery Report

Surrogate Recovery Report

Lab name:	Thermo Fisher Laboratory		
Instrument:	ThermoFisher Instrument	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	March48270B_8level_342010_a	**Cali File:**	EC25B_8level_322010_a_March48270B_8level_342010_a.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	5% diesel	342010_a004	N/A		3/4/2010 12:33:49 PM	

Compound	Conc added	Conc recovered	% Recovered	Limits
phenol-d5(sur)	40.000	35.680	89.20	70.00 - 130.00
nitrobenzene-d5(sur)	40.000	46.438	116.10	70.00 - 130.00
2,4,6-tribromophenol(sur)	40.000	34.645	86.61	70.00 - 130.00
p-terphenyl-d14(sur)	40.000	35.980	89.95	70.00 - 130.00

TIC Report

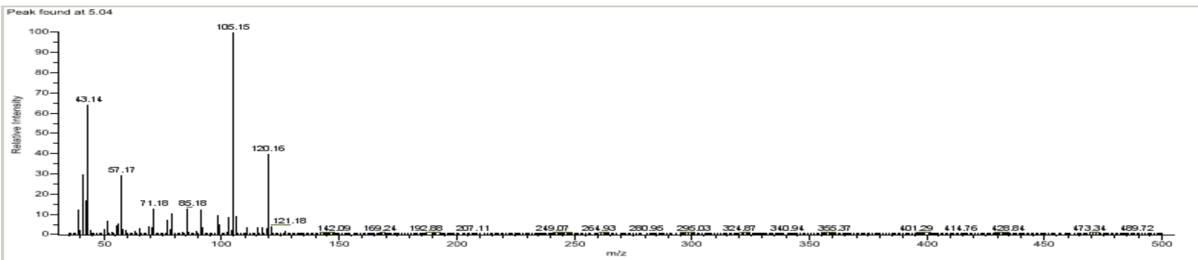
TIC Report Page 1 of 5

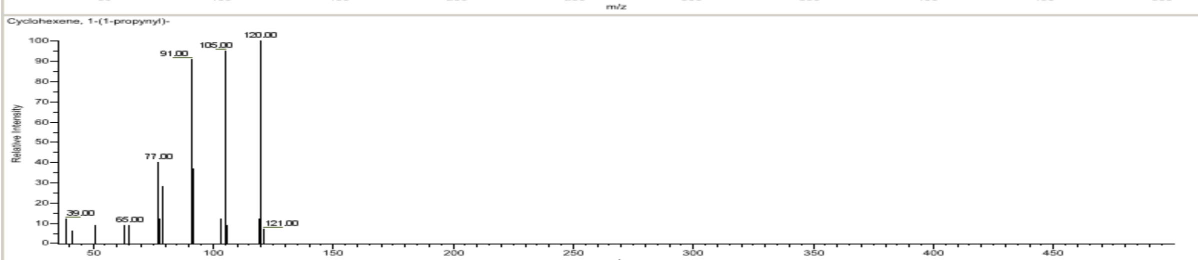
Lab name:	Thermo Fisher Laboratory		
Instrument:	ThermoFisher Instrument	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8le
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	March48270B_8level_342010_a	**Cali File:**	EC25B_8level_322010_a_March48270B_8level_34201(

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	5% diesel	342010_a004	N/A		3/4/2010 12:33:49 PM	

Peak:	Retention time	Area	Height	Inj. estimate	In-sample est.	Flag
Cyclohexene, 1-(1-propynyl)-	5.04	243538856	71816093	104.902	104.902	

Compound	CAS number	Library	Entry	Match prob.	Search index	Rev. search index	Formula	Weight
Cyclohexene, 1-(1-propynyl)-	1655056	mainlib	82371	0	623	845	C9H12	120





Manually integrated

Flag legend: P = Library entry selected manually

TIC Summary Report

TIC Summary Report

Lab name:	Thermo Fisher Laboratory		Page 1 of 1
Instrument:	ThermoFisher Instrument	**Method:**	March48270B_8level_342010_a_EPAMethod8270B_8level
User:	AMER\jessie.butler		EPAMethod8270B_8level
Batch:	March48270B_8level_342010_a	**Cali File:**	EC25B_8level_322010_a_March48270B_8level_342010_a.calx

Vial Pos	Sample ID	Filename	Level	Sample Name	File Date	Comment
4	5% diesel	342010_a004	N/A		3/4/2010 12:33:49 PM	

Internal standards

Internal standard	ISTD#	RT	Response	Injected Conc	Injected Units	Sample Conc	Sample Units
1,4-DICHLOROBENZENE-D4_(IS)	1	5.59	92863341	40.000	ng/uL	40.000	ng/uL
NAPHTHALENE-D8_(IS)	2	7.04	305413673	40.000	ng/uL	40.000	ng/uL

Qualitatively-identified compounds

Compound	Uses ISTD#	RT	Response	Injected Conc	Injected Units	Sample Conc	Sample Units	Flag
Cyclohexene, 1-(1-propynyl)-	1	5.04	243538856	104.902	ng/uL	104.902	ng/uL	
Decane	1	5.38	307929153	132.638	ng/uL	132.638	ng/uL	
Undecane	1	6.27	231391187	99.670	ng/uL	99.670	ng/uL	
2,6-Dimethyldecane	2	8.39	309626174	40.552	ng/uL	40.552	ng/uL	
Eicosane	2	11.08	391448222	51.268	ng/uL	51.268	ng/uL	

Manually integrated

Flag legend: P = Library entry selected manually

Tune Report

Tune Report

Lab name: Thermo Fisher Laboratory
Page 1 of 1

Instrument: ThermoFisher Instrument
Method: EC25B_8level_322010_a_EPAMethod8270B_8level (EPAMethod8270B_8level)

User: AMER\jessie.butler

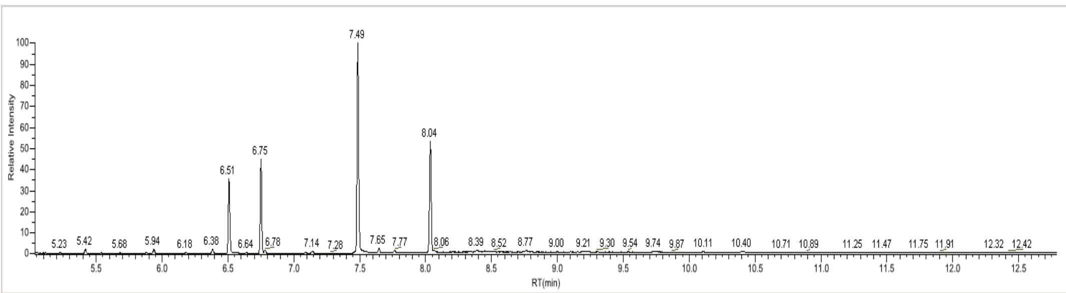
Batch: EC25B_8level_322010_a

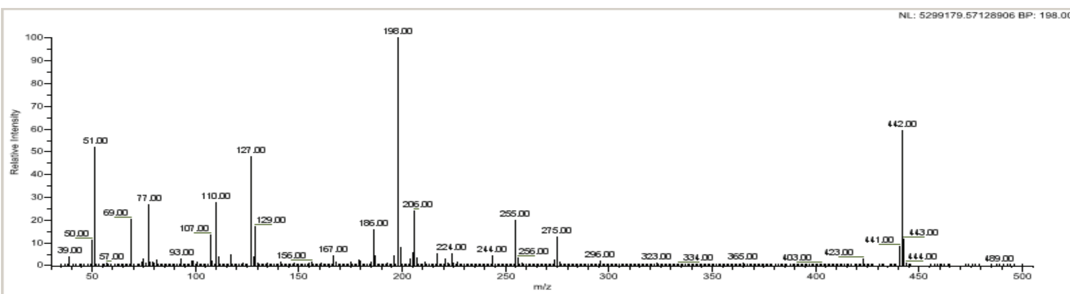
EPA Method: 8270D

Data File: C:\Thermo\EnviroLab Forms\Projects\EPAMethod8270\Robustness\Batches\EC25B_8level_322010_a\Data\run01.raw

Acquisition Date: 3/1/2010 11:50:03 AM

Mass Spectrum Data: Scan#: 990 - 992 RT: 6.75 - 6.75 SB: Scan 980 @ 6.73 min





m/z	Ion abundance criteria	% Relative abundance	Pass/fail
51	greater than or equal to 10% AND less than or equal to 80% of Base Peak	52.2	Pass
68	less than 2% of m/z 69	0.9	Pass
70	less than 2% of m/z 69	0.5	Pass
127	greater than or equal to 10% AND less than or equal to 80% of Base Peak	48.1	Pass
197	less than 2% of m/z 198	0.5	Pass
198	greater than 50% AND less than or equal to 100% of Base Peak	100.0	Pass
199	greater than or equal to 5% AND less than or equal to 9% of m/z 198	7.8	Pass
275	greater than or equal to 10% AND less than or equal to 60% of Base Peak	12.7	Pass
365	greater than 1% of m/z 198	1.1	Pass
441	greater than 0% AND less than 24% of m/z 442	14.7	Pass
442	greater than 50% AND less than or equal to 100% of Base Peak	59.3	Pass
443	greater than or equal to 15% AND less than or equal to 24% of m/z 442	19.8	Pass

Determined base peak: 198 m/z

8270D passed

Using Copy Down and Fill Down

This appendix describes the Copy Down and Fill Down commands that you can use to make entering column values easier.

You can use the Fill Down command for the Sample Name, Sample ID, Vial Position, and Sample Level columns.

You can use the Copy Down command for the Sample Type, Vial Position, Injection Volume, Conv Factor, and Sample Level columns.

Follow these procedures

- To automatically enter sequential column values
- To automatically copy column values
- To use Copy Down or Fill Down for a range of samples

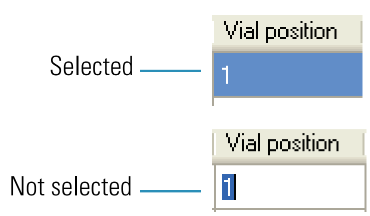
❖ To automatically enter sequential column values

1. Enter a value for the first row of the fill down sequence.

   This does not have to be the first sample row. You can begin the fill down procedure from any row in the sequence.

2. Select the cell whose value is the first in the fill down sequence.

   Observe that this cell is selected.



   You can repeatedly use the **Fill Down** command to create multiple sequences. See "Example 1" on page 325.

3. Right-click and choose **Fill Down** from the shortcut menu.

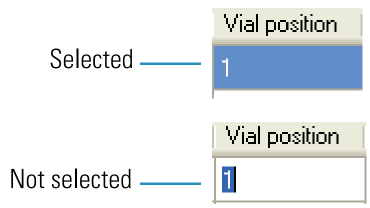
   The application enters sequential column values starting with the value in the selected row and ending with the last row in the column.

> **Note** If you use the Fill Down command for the Vial Position column and you have an autosampler configured, the EnviroLab Forms application knows the number of vial positions configured in your autosampler and numbers the positions accordingly. See "Example 2" on page 325.

❖ To automatically copy column values

1. Select the cell whose value you want to copy to all cells below it.

   Observe that this cell is selected.



2. Right-click and choose **Copy Down** from the shortcut menu.

   The value is copied to all rows below the selected row.

❖ To use Copy Down or Fill Down for a range of samples

1. To select a range of sample values, do one of the following:

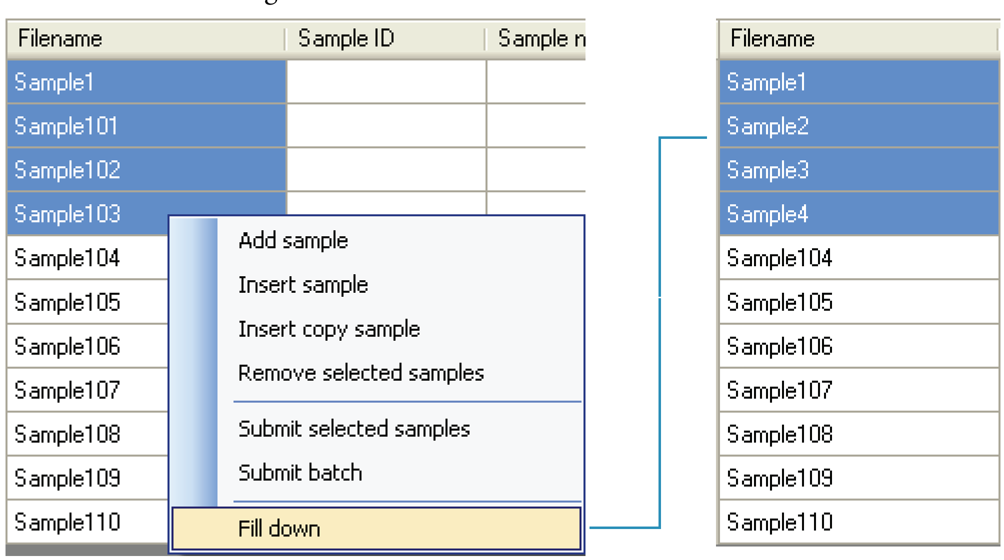
   - Drag your cursor to select a contiguous group of sample values.

     –Or–

   - Hold down the SHIFT key to select a contiguous group of sample values.

2. Right-click and choose the appropriate command from the shortcut menu.

   The column values are copied or entered sequentially starting with the value in the first selected row and ending with the last selected row.



Example 1

You can repeatedly use the Fill Down command to create multiple sequences.

Vial position
A:A1
A:A2
A:A1
A:A2
A:A1
A:A2
A:A3
A:A4

Example 2

The EnviroLab Forms application knows the number of vial positions configured in your autosampler and numbers the positions accordingly.

Vial position
A:A1
A:A2
A:A3
A:A4
A:A5
A:A6
A:A7
A:A8
A:A9
A:A10
A:A11
A:A12
A:B1
A:B2
A:B3
A:B4
A:B5
A:B6

Using Filter Criteria

The filter criteria tool is available from the compound datastore in the Configuration mode and the acquisition list in the Method Development mode.

❖ To filter the compound list

1. To display only a filtered list of compounds, click the funnel icon, , in the column header.

   For each column, a list of filterable criteria is displayed. On all columns, your filter choice are All, Blanks, and NonBlanks. Other filter criteria is specific to the individual columns.

2. To create a custom filter based on compound values in a specific column, choose **Custom** from the column list box.

   The Enter Filter Criteria dialog box opens. See "Enter Filter Criteria" on page 328.

3. From the Operator list box, select an operator.

4. From the Operand list box, select an operand.

5. When all conditions are defined, click **OK**.

   The complete filter string is displayed at the bottom of the dialog box. For example:

   ```
   chemical formula = Blanks
   ```

Enter Filter Criteria

The Enter Filter Criteria dialog box is specifically named for the column on which you are filtering. In this example, the selected column is the Compound Name column.

Figure 59. Enter Filter Criteria dialog box

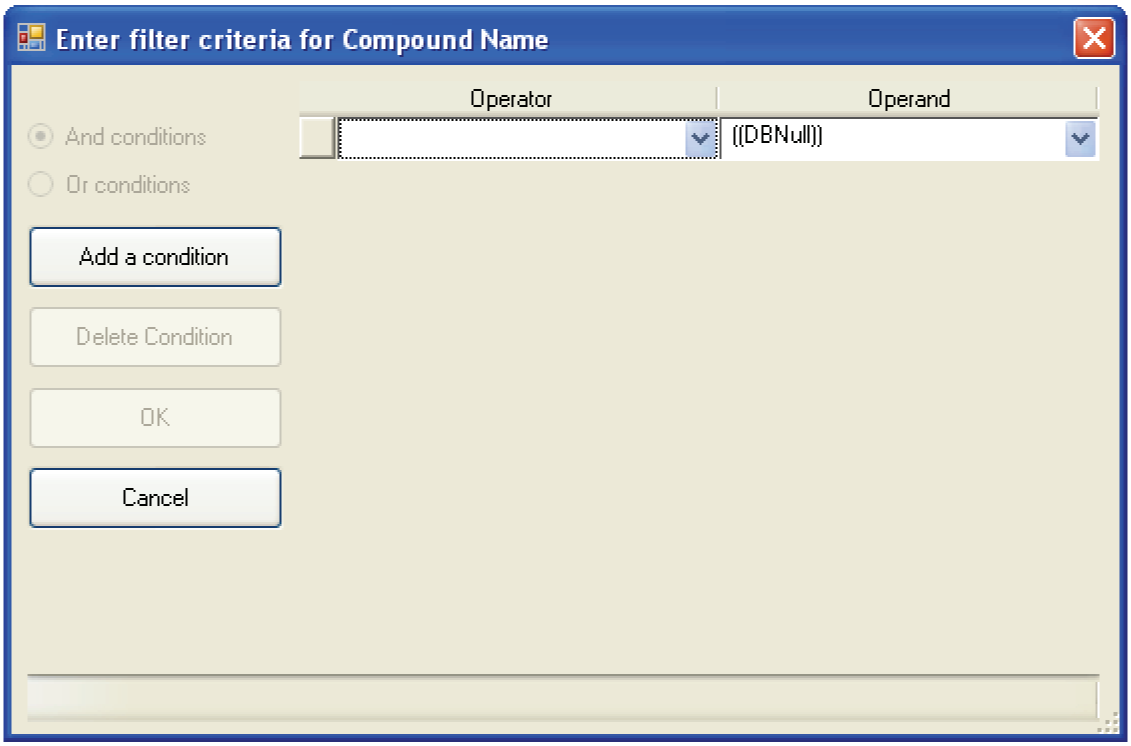


Table 82. Enter Filter Criteria parameters

Parameter	Description
And conditions	Requires that all filter criteria must be met.
Or conditions	Requires that any of the specified filter criteria be met.
Add a condition	Adds a new, empty condition to the filter criteria.
Delete condition	Deletes the selected condition. Click the box at the left of the row to select the condition.
Operator	The mathematical function applied to the operand.
Operand	The arguments to which the operator is applied.

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