

# **SYNGISTIX FOR AA**



## **Software Guide**



# **Syngistix for AA Software Guide**

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## Release History

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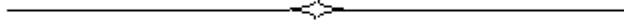
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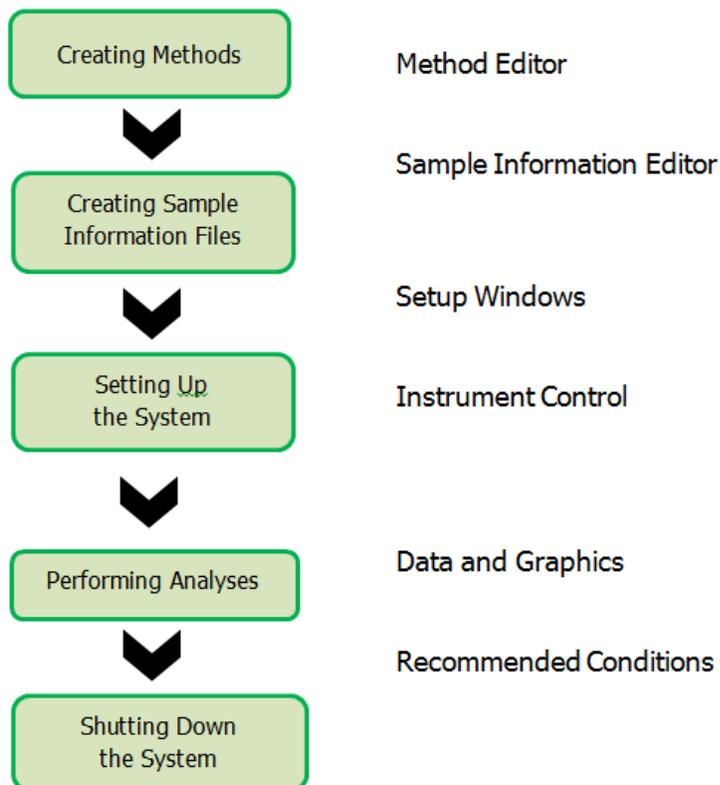


# **Introduction**

## ***Introduction to Syngistix***

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The following diagram shows an overview of the workflow.



## ***Important Features of the Syngistix Software***

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- This highly usable product was developed by a team of application experts, laboratory managers, graphic designers, cognitive psychologists, and users from all over the world. Sample analysis, scheduling, and data reporting can be handled easily and efficiently.
- Operation is simplified. Based on the familiar Microsoft Windows ribbon and graphics, the software has easy-to-use graphics and familiar menus.
- Complete system controls and useful online information are at the user's fingertips, making procedures simple and routine, even for new operators with minimal training in AA lab procedures. Less training is required and time can be saved, hence increasing lab productivity.
- The automation of many routine tasks not only saves time, but also avoids expensive, time-consuming errors.
- Comprehensive data reprocessing and reporting capabilities include: built-in QC automation routines; full data reprocessing from stored spectra; methods and data stored in a commercial database; and easy generation of customized reports using off-the-shelf word processor or spreadsheet programs.
- The flexibility of Syngistix should allow you to comply with all the various quality control protocols and regulatory procedures associated with Good Laboratory Practice (GLP) and Good Automated Laboratory Practice (GALP) requirements.

### ***Related Applications***

In addition to the Syngistix software, PerkinElmer provides:

- **The Data Manager software application** lets you archive, copy, delete, and rename the data sets created by Syngistix. Within this application, you can select a subset of the data from a results data set and save it in a file format that can be read by many off-the-shelf applications, including spreadsheet and database management programs. In addition, you can create printed reports of data where you control the design of and the information included in the report.
- **Syngistix Offline** is a second copy of the Syngistix application that does not control the instrument. You can use Syngistix to edit methods, enter sample information, examine data, build IEC or MSF models, or reprocess data in the software without operating the instrument. This is useful when you wish to work with methods and data while an analysis is in progress.

### ***Related Documentation***

The following documentation is available for Syngistix:

- **Syngistix Data Manager OnLine Help.** The Data Manager Help file is available online from the Data Manager application. Press the F1 function key to display information for the window that is currently on screen.
- **Syngistix User Setup OnLine Help**
- **Mobile Setup OnLine Help**
- **Syngistix Document Pack**

## ***Important Prerequisites***

Before you use Syngistix software, you should:

- **Understand AA principles and practices.** If you need background information, you should consult one of the many textbooks available.
- **Know how to use a personal computer.** If you need further information, consult your computer manual.
- **Understand Windows fundamentals.** If you have questions, refer to manuals, books, CD-ROM, or online tutorials on Microsoft Windows.

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## Workspaces

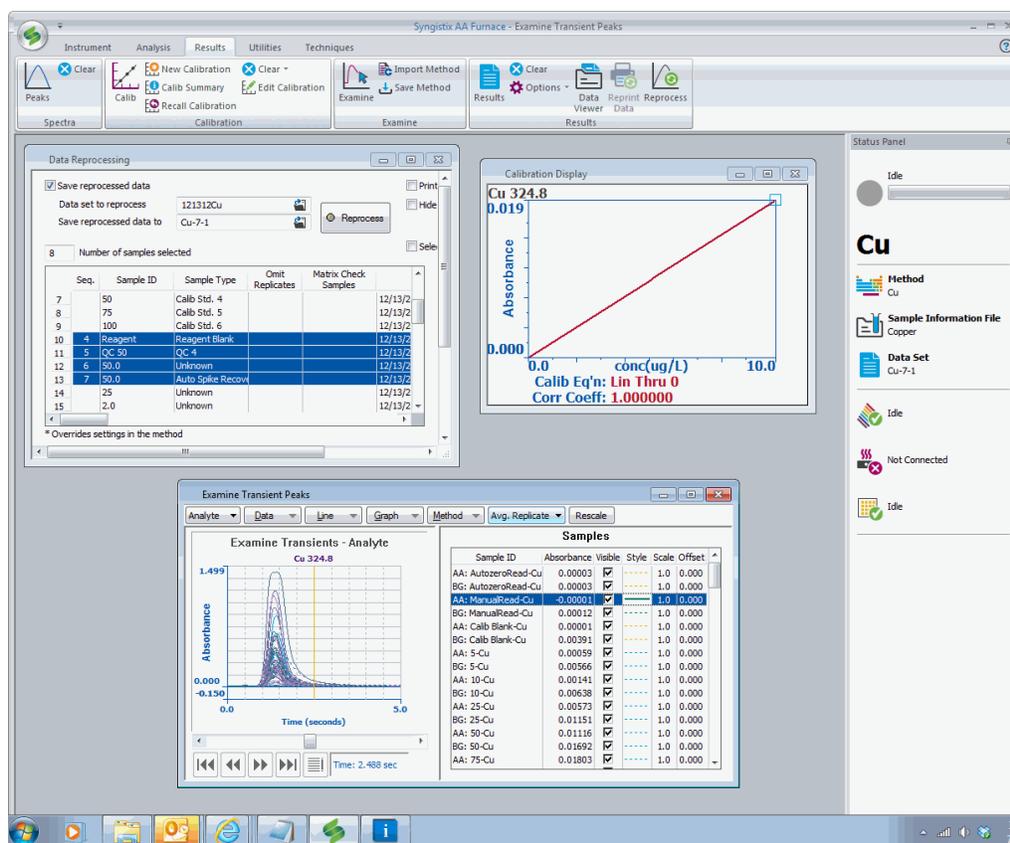
Workspaces let you store a group of selected windows for later use. The workspace saves all of the entries you have made in the windows for your methods and analyses. It also saves the location of each window on the screen. The workspace is saved in a workspace file, which has the extension .ifsx. Using workspaces, you can fill in and arrange windows once, saving time whenever you set up methods or perform analyses.

Entries that you can save using a workspace include the names of the method and sample information file, information contained in the Automated Analysis window (Set Up page), and any information concerning multi-method analysis. It also saves decisions that you have made for your analysis, such as if data is to be saved and where, if it is to be printed, and if the method in memory is to be used.

**Note:** When you close Syngistix, the current Workspace is automatically saved and will redisplay when you restart Syngistix.

To create a workspace:

1. Open the desired windows, fill in the entries for your methods and analyses and arrange the windows on the screen.  
For example, suppose you have run an analysis and arranged the windows as follows:



2. You can save the entire screen with all of the displayed windows and entries in a "Workspace" file to redisplay later.

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3. To save the position of these windows and the entries within them, from the **Application button** , select **Save As** from the **Workspace** menu item.
4. In the dialog that appears, type a name for the workspace and click the **Save** button. For example, suppose you type "analysis".
5. When you wish to view (or use) these windows and their entries again, in the **Application button**, select **Workspace** then **Open**.
6. In the dialog that appears, select a saved file and click on **Open**. The windows with the entries appear exactly as before.

## ***Tips and Hints***

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- You should maintain your results library on a regular basis. Use the Data Manager to archive old data sets, delete them from the library, check the library, and pack the library.
- Analytical results are stored in a Microsoft Access-compatible database. The database structure is described in an electronic document (Results.pdf) included on the Document Pack CD.
- You can analyze a priority sample without stopping the system by clicking on the Priority... button on the Analysis page of the Automated Analysis Control window and entering the autosampler location, sample ID, and other descriptive information.
- If you do not understand how an entry or control is used, pause the mouse pointer over the item for a few seconds and a tip explaining it will be displayed.
- The Recommended Conditions window provides you with suggested parameters to use when determining each element along with remarks that highlight potential problems and solutions to help you perform better analyses.
- You can export data from the results library in a comma delimited format using the Export Data wizard included in the Data Manager.
- You can append samples to the end of the Analysis List while analyzing samples. Enter the descriptive information in the Sample Information Editor, select the samples to be added, and click on the Append to Analysis List... button to append the additional samples to the list.
- Display the Autosampler Load List window after selecting your methods and sample information file for a list of solutions to be placed in each autosampler location.
- You can change the colors of your graphical displays. Right-click in the Calibration Display, Transient Peaks Display, Edit Calibration, or Examine Transient Peaks Options dialogs.
- When analyzing samples with concentrations well above the detection limit, it may be possible to operate the hollow cathode lamp below the recommended current to prolong its life.
- Change the autosampler tray configuration by selecting the Autosampler tab in the Devices dialog, on the Instrument tab and selecting the proper tray file. To use custom trays, create a new autosampler tray file and put it in the directory with the other tray files.
- The Sample Information Editor can be configured to include only the fields you need for your samples. Click on the window with the right mouse button and choose the Parameter List... command to display a dialog where the fields can be selected. Once configured, a template describing the configuration can be saved as a design file for future use.
- Double-click on the header row of most grid-type displays of parameters in the Method and Sample Information editors to display column fill dialogs that help you enter parameters in the columns.
- Status Panel displays information on each of the hardware devices connected to your computer. For more information, double-click on the icon to display the diagnostics window.

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- When hollow cathode lamps become weak near the end of their life, it is sometimes possible to extend their life for a short time by increasing the operating current until a replacement can be purchased.
- A complete list of units that can be selected in the software are contained in a file called units.inix located in the Configuration directory (C:\Users\Public\PerkinElmer Syngistix\AA\ SystemFiles\ Configuration). Edit this file (using Notepad) to rearrange, delete, or add units. Instructions for editing the file are contained in the file.
- The Recommended Conditions window provides you with suggested parameters to use when determining each element along with remarks that highlight potential problems and solutions to help you perform better analyses.
- You can save the layout of windows on the screen and the names of files currently open by selecting Workspace from the Application button then use the Save As.. command. To recall the workspace and arrange the screen as it was saved, use the Workspace Open command.
- Measuring the characteristic mass or characteristic concentration before performing analyses is a good way to check that the instrument system is performing correctly.
- You can check a method for internal consistency by selecting the Check Method command in the Method group on the Analysis tab. Any problems discovered will be reported in a dialog. The same check is automatically performed when the method is saved and before it is used to analyze samples.
- To print an analytical header during a manual analysis, select Analytical Header from the Options drop-down menu in the Results group on the Results tab.
- When performing analyses using the graphite furnace, you will normally observe better results if you deposit the sample on a platform and use the peak area method of measuring the signals.
- You can display information on the instrument hardware components attached to your system by selecting the Diagnostic command in the Utilities group on the Instrument tab. Each component has a page of information showing its status and commands that have been exchanged between computer and hardware.
- The system "signs" the data for each sample when it is stored in the results library. Use the Verify Data Set... command in the Data Manager to check that no changes have been made since the data were collected by the instrument.
- Select Syngistix Offline from the Utilities tab to display a second copy of the application where you can edit methods, enter sample information, examine data, and perform other tasks while analyses are in progress.
- You can display the autosampler locations for all samples, blanks, standards, and quality control samples in the currently selected methods and sample information file using the Autosampler Loading List window.
- It is easy to create additional results libraries by typing in the name of a new library instead of selecting an existing library when entering a new data set name.
- When performing multi-method analyses, use the Autosampler Load List window to display the location of all solutions required by all methods to be sure the locations are compatible.
- You can automatically export your data as a tab or comma delimited text file at the end of analyses. Create the export design using the Data Manager, then select it using the Automatic Export command in the Analyze group on the Analysis tab.

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- See the Syngistix for AA Document Pack CD for application notes, technical papers, and documents that describe specialized features of the system such as a description of the file formats used by the software.
- You must always analyze a calibration blank before the calibration standards. If blank is analyzed after the standards, errors will result.
- You can schedule the instrument to automatically turn off the lamps and/or the flame when analyses are complete.
- Use the New Method command by clicking New in the Method group on the Analysis tab to display the New Method dialog and create a new method. This is the easiest way to create a new method without danger of overwriting an existing method.
- The system automatically performs a series of checks when you begin analyses to detect mistakes or conditions that must be corrected before analyses can proceed.
- If you have occasional samples with high concentrations of analyte, it is possible to schedule an extra wash step following them to minimize carry over to the next sample. Schedule the extra wash step on the Sampler page of the Method Editor.
- Reagent blanks can be used to compensate for contamination of the samples by the reagents used during the sample preparation process. Reagent blanks are selected and scheduled on the Calibration page of the Method Editor.
- If you are only interested in using a small part of the calibration range or if you can not prepare a valid calibration blank for some reason, use the bracketing calibration curve equation option.
- When a method is opened the calibration curve is cleared and a new calibration curve is prepared as blanks and standards are analyzed.
- Quality control samples can be automatically analyzed at periodic intervals. The QC samples are defined on the QC page of the Method Editor. Scheduling can also be defined as part of the method or, alternatively, as part of the sample information file.
- When one or more measured concentrations in a quality control sample is not within predefined limits, the system will automatically perform appropriate actions such as recalibration, recalibration and reanalyzing samples, printing messages, or stopping the analyses.
- The amount of information to be printed on the log during analyses can be selected on the Options page of the Method Editor.
- The individual raw peak profiles can be saved with the other analytical data in the results library. Saving peak profiles allows the data to be examined and used to recalculate the analytical results using different analytical parameters, but requires more disk space. Turning off this option saves disk space.
- You can have the system play sounds at the end of long operations or if problems develop during analyses. Choose the Notifications from the Applications button to turn sounds on or off and to select files containing the sounds you want to hear.
- Use the Sample Information Editor to enter descriptive information about your samples such as sample ID's (names), weight and dilution information, autosampler locations, and descriptive remarks.
- When analyzing samples with concentrations well above the detection limit, it may be possible to operate the hollow cathode lamp below the recommended current to prolong its life.

## ***Upgrading from WinLab - What's New***

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When upgrading from WinLab to Syngistix you will have the same functionality that you have become accustomed to with many new features that provide a simplified workflow. Some of the new features are:

- Ribbon Style Interface - Consolidates the Workflow to 4 tabs with no hidden menus.
- Data Viewer - This is a tabular data view to compliment the classic results view.
- Expandable Windows (specifically Continuous Graphics, as more time/data points are added if you expand horizontally)
- Updated graphics and user interfaces - Provides a clean look to view your data and information.
- INConX - Mobile app to view Syngistix data and control the plasma from an iDevice.
- Consolidated Analysis Window - Combines Automated and Manual analysis with a common run list in one window.
- Status Panel (with quick links) - Provides a quick view of your current status and by double-clicking a graphic to display its associated dialog.
- Right-click Menus for Display Options - Provides easy navigation to functions in dialogs.
- Most Recently Used Mechanism - Displays the last five methods/files opened.
- Combined Devices Window - Puts your devices in one dialog for easy control.
- In Syngistix some files have been changed to include an "x" at the end of the file extension. For example, Sample Information files now use the .sifx file extension instead of the .sif file extension.

The table below lists the file name extensions that have been changed to include an "x".

<b>File Description</b>	<b>New File Extension</b>	<b>Old File Extension</b>
INI Configuration files	.inix	.ini
Autosampler Tray files	.Trayx	.Tray
Configuration files	.configx	.config
Sample Information Definition Files	.sidx	.sid
Sample Information Files	.sifx	.sif
Workspaces	.wspx	.wsp
QC Charting Style files	.chtx	.cht
Report Style files	.repx	.rep
Export Style files	.xptx	.xpt

## ***Libraries and Files In Data Manager***

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### ***Libraries and Data***

The Syngistix Data Manager application uses database technology to organize information in a structured format that is easy to manipulate. This information includes: parameters needed to perform analyses; data collected during analyses; and parameters used by related Syngistix applications.

The data generated before, during, and after analyses is stored in libraries. Each library is a group of related tables and indices that contain data in a structured format.

### ***Data Manager***

The Data Manager is a Syngistix application that helps you organize and manage the data stored in libraries. You can rename, copy, archive, and delete data sets.

***Important Note:*** *Library maintenance should be done periodically to prevent your Results Library from becoming too large. A large Results Library can lead to disk problems. Maintenance procedures include archiving, deleting, and packing data sets. For additional information, please refer to Data Manager Help: What's Important About Managing Data.*

### ***Files***

Not all Syngistix information is stored in database libraries. For example, sample information is stored in ASCII files, so that you can easily create compatible sample information files using off-the-shelf applications such as spreadsheet programs. You can use the Windows Explorer to copy, rename, move, or delete these files.



# **Performing Analyses**

## **Overview**

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This section contains procedures to aid you in setting up Syngistix for the many different types of analysis that you can perform, and then, to start and control the analyses. For most techniques you have the option of operating the instrument in either a manual mode, with or without an autosampler, or in an automated mode with an autosampler.

While you are using a window in Syngistix you can obtain information about the window by pressing the F1 key, or clicking the Help button. The help topics that appear then have links to other topics, such as procedures or topics for other relevant windows.

For information about using specific instruments and accessories, see the users guides supplied with the instruments.

## ***Switching on the System***

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To switch on the system:

1. Make sure that the spectrometer and the other instruments in the system are correctly installed. You may need to install a lamp (HCL) before you switch on the spectrometer. See the user's guides for your system.
2. Switch on the exhaust ventilation system.
3. Turn on the gas supplies and set the pressures to the values recommended in the user's guide for your system.
4. For furnace systems, either turn on the cooling water, or make sure that the cooling system is filled to the MAX mark and the switch on the rear of the cooling system is in the on position.
5. Switch on the computer.
6. If you have changed the configuration of the system, such as installed a different autosampler, or added or removed any accessories, use the Reconfigure utility to reconfigure the software.
7. Switch on the spectrometer. If you need the flow-injection system, the diluter or other accessories, switch these on.
8. Start Syngistix:  
On the Windows desktop, click the Windows **Start** Ball > **All Programs** > **PerkinElmer Syngistix for AA** > **Syngistix for AA**.

## ***Reconfiguring the System***

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You must configure the software to recognize all the components in your analysis system, such as flame and furnace autosamplers, a flow-injection system, or a diluter. When the Syngistix software is first installed, it is configured according to the components in your analysis system at the time of installation. If you install, or remove, an accessory, you must change the software configuration. To do this, you use the **Reconfigure** utility.

To reconfigure the system:

1. Shut down the analysis system and exit Syngistix.
2. Install any new accessories as described in the user's guides for your spectrometer and the accessories.
3. Start the **Reconfigure** utility: On the Windows desktop, click the Windows **Start** Ball > **All Programs** > **PerkinElmer Syngistix for AA** > **Reconfigure**.
4. Follow the instructions on the screen and select the components in the new configuration, for example, a different autosampler, or the diluter.
5. Switch on the system as described in the online help or the user's guide for your spectrometer.

## ***Analyses with Flame and FIAS Techniques***

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To perform an analysis:

1. Read the safety information in the user's guides for your system before you operate the spectrometer.
2. Switch on and set up the spectrometer and accessories.
3. Create or open a Method.
4. Set up the system for the technique you intend to use: Flame, FIAS-MHS, FIAS-Flame.
5. Allow the lamps to warm up for at least 10 minutes.
6. Optimize the analytical conditions, analyze a reference solution, and calculate the characteristic mass.
7. Prepare the samples, QC and check samples and calibration solutions. Also prepare any ancillary solutions that you need, for example carrier solutions and reagents for the FIAS system.
8. Create a Sample Information file. The entries in the sample information file depend on calibration technique that you intend to use.
9. Perform the analysis, automatically, using the autosampler, or using manual sampling.
10. Shut down the analysis system.

## ***Controlling Automated Analyses***

### ***Starting an analysis***

1. Display the windows you need.
2. Set up the **Automated Analysis** window.
3. Load the autosampler.
4. Analyze the samples:
  - **Furnace** technique: Normal analysis using a calibration curve
  - **Furnace** technique: Addition technique
  - or --
  - **Flame and FIAS-MHS** technique: Normal analysis using a calibration curve
  - **Flame and FIAS-MHS** technique: Addition technique

### ***Procedures that you may need during an analysis***

- Analyzing priority samples
- Stopping an analysis
- Restarting an analysis
- Recalibration and Reslope
- Flushing the autosampler

### ***Controlling Manual Analyses***

1. Display the windows you need.
2. Set up the Manual Analysis window.
3. If you need a calibration curve, analyze the calibration solutions.
4. Analyze the samples using one of the techniques below:
  - Calibration curve technique.
  - Analyte addition technique.
  - Additions-calibrate technique.

### ***Procedures that you may need during an analysis***

- Stopping an analysis
- Reslope

### ***When you start an analysis ...***

When you start an analysis, the system first checks for errors in the method and in the sample information file. If the system finds an error, a message appears, and you must correct the error before the system will start the analysis.

When you click on a button to start an analysis, a green indicator appears on the button and the other buttons become inactive. The system uses the analytical conditions in the active method for each replicate. When all the solutions have been analyzed, the green indicator on the button disappears and the other buttons become active.

The progress of the analysis is shown in the **Status Panel**.

# ***Analysis with a Furnace and FIAS-Furnace Techniques***

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## ***Analyses with a Furnace System***

If you intend to use Zeeman background correction:



**Warning: Strong Magnetic Field — Health hazard for wearers of heart pacemakers**

Make sure that anyone wearing a heart pacemaker, or having metallic implants, is at least 0.6 meter (24 inches) away from the furnace — in any direction — while the furnace is operating.

To perform an analysis:

1. Read the safety information in the user's guides for your system before you operate the spectrometer.
2. Switch on and set up the spectrometer and accessories.
3. Create or open a Method.
4. Set up the system for the Technique you intend to use: Furnace or FIAS-Furnace.
5. Allow the lamps to warm up for at least 10 minutes.
6. Optimize the analytical conditions, analyze a reference solution, and calculate the characteristic mass.
7. Prepare the samples, QC and check samples and calibration solutions. Also prepare any ancillary solutions that you need, for example matrix modifiers.
8. Create a Sample Information file. The entries in the sample information file depend on calibration technique that you intend to use.
9. Perform the analysis.
10. Shut down the analysis system.

## ***Controlling Automated Analyses***

### ***Starting an analysis***

1. Display the windows you need
2. Set up the Automated Analysis window
3. Load the autosampler
4. Analyze the samples:
  - **Furnace** technique: Normal analysis using a calibration curve

- **Furnace** technique: Addition technique  
-- or --
- **Flame and FIAS-MHS** technique: Normal analysis using a calibration curve
- **Flame and FIAS-MHS** technique: Addition technique

***Procedures that you may need during an analysis***

- Analyzing priority samples
- Stopping an analysis
- Restarting an analysis
- Recalibration and Reslope
- Flushing the autosampler

***When you start an analysis ...***

When you start an analysis, the system first checks for errors in the method and in the sample information file. If the system finds an error, a message appears, and you must correct the error before the system will start the analysis.

When you click on a button to start an analysis, a green indicator appears on the button and the other buttons become inactive. The system uses the analytical conditions in the active method for each replicate. When all the solutions have been analyzed, the green indicator on the button disappears and the other buttons become active.

The progress of the analysis is shown in the **Status Panel**.

## ***Analyses with MHS Technique***

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To perform an analysis:

1. Read the safety information in the user's guides for your system before you operate the spectrometer.
2. Switch on and set up the spectrometer and accessories.
3. Create or open a Method.
4. Set up the system for the MHS technique.
5. Allow the lamps to warm up for at least 10 minutes.
6. Optimize the analytical conditions, analyze a reference solution, and calculate the characteristic mass.
7. Prepare the samples, QC and check samples and calibration solutions. Also prepare any ancillary solutions that you need, for example reagents for the MHS system.
8. Create a sample information file. The entries in the sample information file depend on calibration technique that you intend to use.
9. Perform the analysis. With an MHS system you must use manual sampling.
10. Shut down the analysis system.

### ***Controlling Analyses with an MHS system***

1. Display the windows you need.
2. Set up the Manual Analysis window.
3. If you need a calibration curve, analyze the calibration solutions.
4. Analyze the samples.

### ***When you start an analysis ...***

When you start an analysis, the system first checks for errors in the method and in the sample information file. If the system finds an error, a message appears, and you must correct the error before the system will start the analysis.

When you click on a button to start an analysis, a green indicator appears on the button and the other buttons become inactive. The system uses the analytical conditions in the active method for each replicate. When all the solutions have been analyzed, the green indicator on the button disappears and the other buttons become active.

The progress of the analysis is shown in the **Status Panel**.

## ***Creating Methods***

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If your spectrometer supports more than one analytical technique, before you create a new method, you must select the correct technique.

1. To change the technique, click on the **Techniques** tab, then click on an analytical technique that you intend to use.
2. On the **Analysis** tab, in the **Method** group, click on **New**. The **New Method** dialog appears.
3. In this dialog, select the element that you intend to determine using the method.
4. Select one of the options that tells the system which parameter values to use as starting values in the new method.
5. In the **Method Editor**, select parameter values that are suitable for the analysis you intend to do.
  - a. Set up the **Spectrometer** pages correctly for the type of measurements that you intend to make.
  - b. Set up the **Sampler** pages correctly for the technique that you intend to use.
  - c. Set up the **Calibration** pages correctly for the calibration technique that you intend to use.
  - d. Make sure you set the correct parameters for the following techniques: emission, diluter, MHS.
6. Save the method with a suitable name, to create a stored, customized method.

When you save a method, the system searches for inconsistent and incompatible parameter values. If there are such problems, the **Check Method** dialog appears containing a list of problems. You must correct the parameter values before you can use the method for an analysis.

## ***Opening a Method***

You must open a method before you use many of the windows in Syngistix and before you can start an analysis. When you open a method it becomes the active method. Methods are stored in two places; in the methods library, and in results data sets.

To open a method stored in the methods library:

1. On the **Analysis** tab, in the **Method** group, click on **Open**. The **Open Method** dialog appears.
2. In this dialog, select the method that you want to open, then click **OK**.

To open a method stored in a results data set:

1. On the **Analysis** tab, in the **Method** group, click on **Import Method**. The **Select results Data Set** dialog appears.
2. Select a **Results** data set where the method was saved and click **OK**. The **Import from Results Library** dialog appears with the available methods for import.
3. Select a method then click **Import**.

## ***Saving a Method***

You must save a method if you want to use it later. When you save a method, the software puts a copy of the method in the methods library. You can save a method either before you use it for an analysis or while you are using it, for example during method development.

The system always saves a copy of the active method that it used to obtain a set of results in the results data set, with the results.

### **To save the method with the original name:**

Use this procedure when you have modified a customized method and you want to save it with the original name.

- On the **Analysis** tab, in the **Method** group, click on the **Save** drop-down and select **Save**.

### **To save the method with a new name:**

Use this procedure when you have created a new method, or have modified a customized method and do not want to overwrite the original method.

1. On the **Analysis** tab, in the **Method** group, click on the **Save** drop-down and select **Save As**.  
The **Save Method As** dialog appears.
2. In this dialog, type a name for the method, then click **OK**.

### **To save the method as a text file:**

Use this procedure to save the information in the method as a text file to use for other purposes, such as with a word processing software.

1. On the **Analysis** tab, in the **Method** group, click on the **Save** drop-down and select **Save As Text**.  
The **Save As** dialog appears.
2. In this dialog, type a name for the method, then click **OK**.

## ***Printing a Method***

You can print the contents of a method directly from Syngistix, or save the method as a text file and then print the information using another software tool. Also, during an analysis, the system prints information about the method along with the results. You select how much information the system prints with the results on the Options page of the Method Editor.

To print the contents of the method directly from Syngistix:

1. On the **Analysis** tab, in the **Method** group, click on **Open**.  
The **Open Method** dialog appears.
2. In this dialog, select the method to open.
3. On the **Analysis** tab, in the **Method** group, click on **Method**.  
The Method Editor opens.
4. From the **Application** button select **Print Preview** from the **Print Active Window** menu.

## ***Method Settings for Flame Emission***

### **Method Editor > Spectrometer > Define Element page**

- For Signal Type, select Flame Emission.

### **Method Editor > Sampler > Autosampler page**

- If you intend to use an autosampler, select the location of the emission setup solution that the system will use to set the signal level.

## ***Method settings for online dilution***

Even if you do not generally want to dilute the samples, you can use the diluter to dilute samples that have an analyte concentration higher than that of the most concentrated calibration standard.

### **Method Editor > Sampler > AutoPrep page**

- Select the **AutpPrep** option, then set the dilution factor and other parameters.

### **Method Editor > Calibration > Standard Concentrations page**

- You can select either to prepare the calibration solutions yourself or to have the diluter prepare them. If the diluter will prepare them, click on Set, then enter the relevant information in the dialog that appears.

### **Method Editor > Checks > Beyond Calibration page**

- For samples that are more concentrated than the most concentrated calibration standard, you can select dilution parameters in the Beyond Calibration dialog.

## ***Method settings for MHS***

### **Method Editor > Spectrometer > Define Element page**

- For **Signal Type**, select **Atomic Absorption**. Do not use background correction.
- For **Signal Measurement**, select **Peak Height**.
- Set **Smoothing** to **19** points.

### **Method Editor > Spectrometer > Settings page**

- Set the **BOC** to **2** seconds.
- Set the **Read Delay** to **0** — zero.
- Set the **Read Time** to be long enough that the signal appears and decays within the time set. As a starting value, set **30** seconds.

### **Method Editor > Spectrometer > Sampler > Flame page**

- Select **Air** as the **Oxidant**. You must use the air-acetylene flame.

## ***Setting Up Lamps***

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### ***Aligning Lamps***

1. Install lamps in the lamp compartment as described in the user's guide for the spectrometer.
2. On the **Instrument** tab, in the **Spectrometer** group, click on **Lamp Setup**.  
The Lamp Setup window appears. Normally, since the lamps are element-coded, the system sets the recommended values for the lamp parameters. However, if you are setting up a multi-element lamp, you may need to select an element other than the first in the list, for example to check the energy.
3. In the **Set Up** column, click on **Lamp #** for the lamp that you want to align.
4. Allow an **EDL** to warm up for 10 to 20 minutes before you align it.
5. If your spectrometer has lamp alignment controls, align each lamp to maximize the energy reaching the detector. The energy is shown by the bar graph and the Energy value.  
Refer to the user's guide for your spectrometer for a description of the controls.
6. Close the **Lamp Setup** window.
7. Close the lamp compartment cover.

### ***Removing Lamps***

**Note:** *Do not unplug and remove lamps while they are switched on.*

1. On the **Instrument** tab in the **Spectrometer** group, click on **Lamp Setup**.  
The Lamp Setup window appears.
2. If the **On** button for the lamp you intend to remove is green, click the button to switch off the lamp.
3. Close the **Lamp Setup** window.
4. Unplug and remove the lamps. For EDLs, remove the coding plugs also.

### ***Tips for Installing Lamps***

- Install the lamps in the lamp compartment as described in the user's guide for the spectrometer.
- Use PerkinElmer lamps; coded or uncoded. You can use both hollow cathode and electrodeless discharge lamps -- HCLs and EDLs.
- Do not touch the front window of the lamp; perspiration or other contamination can reduce the intensity of the radiation.

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- If you install more than one lamp containing a particular element, for example, a single-element copper lamp and a multi-element lamp containing copper, the system will use the lamp in the location with the lower number when you perform determinations of that element. Make sure that you place the preferred lamp in the location with the lower number.
- Connect each lamp plug to the socket that has the same number as the location of the lamp.
- With EDLs, make sure that you use the correct coding plug and connect it to the correct socket. This is the socket with the same number as the location of the lamp in the cassette.
- If you use the wrong coding plug or connect the coding plug to the wrong socket, you will cause the spectrometer to malfunction and may cause irreparable damage to the lamp.

## ***Preparing the Flame System for Analyses***

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### ***Setting up the Flame System***

1. Read the safety information in the users guides for your system before you operate the spectrometer.
2. Make sure that all the instruments are correctly installed. See the users guides for your system.
3. Switch on the instruments.
4. On the **Techniques** tab and select the **Flame** technique.
5. Create or open a Method.  
If you intend to make emission measurements, make sure that you select parameters for emission.
6. If you intend to make absorption measurements, install and align the lamps that you require. For emission measurements, you do not require a lamp.
7. Set up the burner system.
8. Perform the safety checks, then ignite the flame.  
If you have installed a different nebulizer, cleaned the nebulizer, or the settings on the nebulizer have been altered since it was last used, select an air/acetylene flame so that you can set up the nebulizer.
9. If necessary, set up the nebulizer.
10. Align and optimize the burner.
11. When you have finished, calculate the characteristic concentration.

### ***Setting up the Diluter-Flame System***

You use the diluter with the flame technique to dilute the samples automatically. You may either dilute all of the samples, or only those samples that are more concentrated than the most concentrated calibration standard.

1. Read the safety information in the user's guides for your system before you operate the spectrometer.
2. Make sure that all the instruments are correctly installed. Read the user's guides for your system.
3. Switch on the instruments.
4. On the **Techniques** tab and select the **Flame** technique.
5. Create or open a Method.  
Make sure that you select the correct parameters for using the diluter.

If you intend to make emission measurements, make sure that you select parameters for emission.

6. If you intend to make absorption measurements, install and align the lamps that you require  
For emission measurements, you do not require a lamp.
7. Set up the burner system.
8. Perform the safety checks, then ignite the flame.  
If you have installed a different nebulizer, cleaned the nebulizer, or the settings on the nebulizer have been altered since it was last used, select an air/acetylene flame so that you can set up the nebulizer.
9. If necessary, set up the nebulizer.
10. Align and optimize the burner.
11. Measure the nebulizer aspiration rate and enter the value in the Diluter Control window.
12. When you have finished, calculate the characteristic concentration.

## ***Safety Checks for the Flame System***

### ***Make sure that:***

1. The fume ventilation system is switched on.
2. The burner is correctly installed and the end-cap is secured.
3. The correct gaskets are fitted to the burner. Fit the recommended solvent resistant gaskets if you intend to aspirate organic solvents.
4. The correct burner head is fitted.
5. The correct nebulizer is fitted and that it is correctly secured with the clamp.
6. The fuel and oxidant connectors are properly connected to the burner and the nebulizer.
7. The drain system is installed and operating correctly.
8. The door of the atomizer compartment is shut.
9. All the safety interlocks are correctly closed.

On an instrument with automatic gas controls, when the interlocks are closed, the Safety Interlock box in the Flame Control window contains a check mark.

On an instrument with manual gas controls, make sure that the red Ignite button on the spectrometer is not illuminated.

***If the interlocks are not closed:***

One or more of the following may be the cause:

- The drain, nebulizer, or burner head are not correctly installed
- The acetylene or oxidant pressure is too low
- The flame sensor or the flame ignitor is not connected
- The liquid level in the drain siphon is too low.
- The liquid level in the drain vessel is too high.

See the user's guide for your burner system for details about the safety interlocks.

***Igniting the Flame***



**Warning: UV Radiation -- Risk of eye damage**

The flame, especially the nitrous oxide/acetylene flame, may emit UV radiation which can damage your eyes. Always wear UV-absorbing safety glasses when looking at the flame. Keep the burner door closed when the flame is burning.

In an emergency, switch off the spectrometer to safely extinguish the flame and shut down the fuel and oxidant flows.

***Select an air/acetylene flame:***

- If you are setting up the burner.
- If you have installed a different nebulizer, cleaned the nebulizer, or the settings on the nebulizer have been altered since it was last used.
- If you intend to use the flame to heat the quartz tube atomizer, e.g. for the MHS 15.
- On an instrument with manual gas controls, if you intend to use the nitrous oxide/acetylene flame, ignite the flame with air/acetylene, then change over to nitrous oxide/acetylene when the flame is lit.

***Procedure***

For an instrument with manual gas controls, refer to the user's guide for the instrument for instructions on igniting the flame.

1. Set up the burner for the analyses that you intend to perform.
2. Switch on the exhaust ventilation system.
3. Perform the safety checks.
4. Set the burner gas pressures to the values recommended in the user's guide for your system.

5. On the **Instrument** tab, in the **Atomizer** group, click on **Flame Control**. The **Flame Control** window appears.
6. Select the **Oxidant: Air** or **N20**. Always select Air if you need to set up the nebulizer.
7. Ignite the flame: click on **Flame Off/On**.

## ***Aligning and Optimizing the Burner***



### **Warning: Flashback hazard**

Set up the nebulizer using an air/acetylene flame and make small adjustments slowly. Never set up the nebulizer with a nitrous oxide/acetylene flame.

If you intend to make emission measurements, but you need to align the burner, for example for a new burner head, you must change to absorption mode to align the burner, then select emission mode to optimize the burner conditions.

### ***Procedure***

1. Install and align the correct lamp for the element you have selected in the method.
2. On the **Instrument** tab, in the **Atomizer** group, click on **Flame Control**. The **Flame Control** window appears.
3. Click **Align Burner**. The Align Burner Wizard and Continuous Graphics window appear. Use this wizard to align and optimize the burner.
4. When you have finished, calculate the characteristic concentration.

### ***Suggested settings and adjustments for optimizing the burner***

Always aspirate the solutions through the same nebulizer tube that you will use during the analysis. This will ensure that the aspiration rate is the same during the optimization procedure and the subsequent analyses. For example, if you intend to use the diluter, aspirate the solutions through the diluter and diluent feed tube. With a FIAS-Flame system, use the nebulizer feed tube from the FIAS system.

For absorption measurements, use the recommended sensitivity-check solution. For information about this on the **Analysis** tab in the **Method** group, click on **Recommended Conditions**. For emission measurements, use the element that you intend to determine. Use a concentration equal to that of the most concentrated calibration solution that you intend to use.

If you intend to use the impact bead, make sure that it is in front of the nebulizer orifice.

There are a number of burner settings that you must take into account to obtain a well optimized burner system. These settings may interact so you may have to optimize each in turn and repeat the cycle more than once. The list below shows the suggested adjustments and the sequence in which you should perform them.

- The burner position — use the **Align Burner Wizard**;

***Fehler! Verwenden Sie die Registerkarte 'Start', um Heading 1 dem Text zuzuweisen, der hier angezeigt werden soll. . 31***

- The nebulizer aspiration rate — make small adjustments and wait until the signal stabilizes before you make a further adjustment. You should not need to move the regulator very much if the nebulizer is correctly set up;
- The gas flow rates — make small adjustments and wait until the signal stabilizes before you make a further adjustment. Do not set values at the extremes of the allowable ranges;
- Re-optimize the burner position.

## ***Calculating the Characteristic Concentration: Flame***

When you have optimized the analytical conditions and created a suitable method, analyze a reference solution and calculate the characteristic concentration.

### ***Procedure***

For information about the recommended sensitivity-check solution, on the **Analysis** tab, in the **Method** group, click **Recommended Conditions**.

1. Allow the lamps to warm up for at least 10 minutes.
2. Prepare a blank solution and a sensitivity-check solution of the element and place the solutions in the sample tray.
3. Open the correct method and enter a value of 5 for Replicates.
4. On the **Analysis** tab, in the **Analyze** group, click **Analysis**, then click **Automated** tab.
5. Set up the Automated Analysis with the correct method name and the sample tray locations of the blank and the reference solution.
6. In the **Automated** Analysis window, click **Analyze Sample**.
7. On the **Analysis** tab, in the **Analyze** group, click **Characteristic Conc**. The **Calculate Characteristic Concentration** dialog appears.
8. Enter the Sample Concentration of the sensitivity-check solution, then press **Enter**.
9. Enter the readings for the blank and sensitivity-check solutions. The readings are shown in the **Results** window.
10. Press **Enter**. The system calculates the characteristic concentration.

### ***Troubleshooting***

The calculated value should be within 20% of the comparison value. If it is not:

- With the online dilution accessory, there is always a small flow of diluent to the nebulizer which produces a dilution of the measurement solution. This results in characteristic concentration values higher than those for the basic flame technique.
- Make sure that the solutions you used were correctly prepared.
- Re-optimize the burner conditions.



# ***Preparing the Furnace System for Analysis***

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## ***Setting up the Furnace System***

1. Read the safety information in the users guides for your system before you operate the spectrometer.
2. Make sure that all the instruments are correctly installed. See the users guides for your system.
3. Switch on the instruments.
4. On the **Techniques** tab, click on the **Furnace** technique.
5. Create or open a Method.
6. Install and align the lamps that you require
7. If your system has a fume extraction unit, set this up.
8. Install and condition a graphite tube.
9. If necessary, align the furnace.
10. Set up the autosampler.
11. Optimize the conditions to get the best signal.

## ***Setting up the FIAS-Furnace System***

1. Read the safety information in the users guides for your system before you operate the spectrometer.
2. Make sure that all the instruments are correctly installed. See the user's guides for each instrument in your system.
3. Switch on the instruments.
4. On the **Techniques** tab, select the **FIAS-Furnace** technique.
5. Create or open a Method.
6. Install and align the lamps that you require
7. Install, pretreat, and condition a graphite tube.
8. If necessary, align the furnace.
9. Install and align the quartz pipet tip on the furnace autosampler as described in the FIAS-Furnace user's guide.
10. Start the flow-injection system.
11. Set the flow rates of the carrier and reductant.

12. Set up the autosampler.
13. Optimize the conditions to get the best signal.

## ***Setting up the Autosampler***

### ***Summary***

You need to prime the system and align the pipet tip to ensure that the pipet tip correctly takes up the sample solution out of the cup, then injects the sample correctly into the graphite tube.

1. Make sure that the rinsing system components are correctly installed — see the user's guide for the furnace.
2. On the **Instrument** tab, in the **Devices** group, click on **Devices**.
3. Click the **Furnace Autosampler** tab, select the size of the sample tray you intend to use, then click **Apply Settings**.
4. Fill and prime the rinsing system.
5. Align the autosampler — align the autosampler arm and set the depth of the pipet tip in the graphite tube and in the sample cup.

### ***You should check and if necessary correct the alignment:***

- Before you start an analysis.
- After you have moved the autosampler or changed or adjusted any components on the autosampler.
- After you have changed the graphite tube or the contacts, or opened and closed the furnace.
- After you have aligned the graphite furnace.

## ***Optimizing the Analytical Conditions: Furnace***

The procedure for optimizing the analytical conditions and performing method development are very much dependent on the particular application of the analysis and the type of samples you have. Chemical interactions can affect the absorption signal and the analytical conditions that you require may depend on the sample preparation technique that you use.

For more detailed information and procedures, see:

- The sections in the user's guides and techniques guides for the technique you are using, for example the **FIAS-Furnace** technique.
- The Recommended Conditions window.

### ***Suggested procedure***

1. Change only one parameter at a time and wait until the next signal appears before you make a further adjustment. During the optimization procedure, you should make sure that:

- The autosampler is pipetting and injecting the solutions correctly.
  - The furnace program is optimized for the samples and the absorbance signal is a suitable size and shape.
  - The precision of repeated measurements is acceptable.
2. When you have finished, calculate the characteristic mass.
  3. Make sure that you make all the necessary changes to the method that you intend to use for the subsequent analyses.

### ***Validating the procedure***

When you have optimized the conditions, you should

Perform recovery measurements.

- Analyze certified reference materials.
- Compare the results from the calibration curve technique with those from the analyte addition technique.
- Use the features in Syngistix that automate procedures such as recovery measurements, precision calculations, matrix duplicate and recovery calculations, and analyzing QC samples. You select these in the Method Editor on the Checks and QC pages.

### ***Calculating the Characteristic Mass: Furnace***

When you have optimized the analytical conditions and created a suitable method, analyze a reference solution and calculate the characteristic mass.

**If you intend to use Zeeman background correction:**



#### **Warning: Strong Magnetic Field — Health hazard for wearers of heart pacemakers**

Make sure that anyone wearing a heart pacemaker, or having metallic implants, is at least 0.6 meter (24 inches) away from the furnace — in any direction — while the furnace is operating.

### ***Procedure***

For information about the recommended sensitivity-check solution, on the Analysis tab, in the Method group, click Recommended Conditions.

1. Allow the lamps to warm up for at least 10 minutes.
2. Prepare a blank solution, a sensitivity-check solution of the element and if necessary a matrix modifier, and place the solutions in the sample tray.
3. Open the correct method and enter the locations and volumes of the solutions that you require, for example, modifier, diluent sample. Enter a value of 5 for Replicates.
4. On the **Analysis** tab, in the **Analyze** group, click **Analysis**, then click the **Automated** tab.

5. Set up the **Automated** Analysis with the correct method name and the sample tray locations of the blank and the reference solution.
6. In the Automated Analysis window, click **Analyze Sample**.
7. On the **Analysis** tab, in the **Analyze** group, click **Characteristic Conc.** The **Calculate Characteristic Mass** dialog appears.
8. Enter the concentration of the sensitivity-check solution, then press **Enter**.
9. Enter the readings for the blank and sensitivity-check solutions. The readings are shown in the Results window. Use either peak height or peak area depending on the recommendation in the Recommended Conditions window.
10. Press **Enter**. The system calculates the characteristic mass.

### ***Troubleshooting***

The calculated value should be within 20% of the comparison value. If it is not:

- Make sure that the solutions you used were correctly prepared.
- Make sure that the graphite tube and contacts are not contaminated and are correctly installed.
- Re-optimize the analytical conditions.

## ***Preparing the FIAS System for Analysis***

### ***Setting up the FIAS-MHS System***

1. Read the safety information in the user's guides for your system before you operate the spectrometer.
2. Make sure that all the instruments are correctly installed. See the user's guides for your system.
3. Switch on the instruments.
4. On the **Techniques** tab and select the **FIAS-MHS** technique.
5. Create or open a Method.
6. Install and align the lamps that you require.
7. Align the quartz tube.
8. Switch on the heating for the quartz tube.
9. Start the flow-injection system.
10. Set the flow rates of the carrier and reductant.
11. Set the waste flow rate for the gas/liquid separator.
12. Optimize the conditions to get the best signal.

### ***Setting up the FIAS-Flame System***

1. Read the safety information in the users guides for your system before you operate the spectrometer.
2. Make sure that all the instruments are correctly installed. See the user's guides for your system.
3. Switch on the instruments.
4. On the **Techniques** tab and select the **FIAS-Flame** technique.
5. Create or open a Method.  
If you intend to make emission measurements, make sure that you select parameters for emission.
6. If you intend to make absorption measurements, install and align the lamps that you require  
For emission measurements, you do not require a lamp.
7. Set up the burner system.
8. Perform the safety checks, then ignite the flame.  
If you have installed a different nebulizer, cleaned the nebulizer, or the settings on the nebulizer have been altered since it was last used, select an air/acetylene flame so that you can set up the nebulizer.
9. If necessary, set up the nebulizer.
10. Start the flow-injection system.
11. Align and optimize the burner.
12. Set the carrier flow rate.
13. Optimize the conditions to get the best signal.

### ***Aligning the Quartz Tube***

To obtain the best analytical results, the radiation beam from the lamp must pass directly along the center of the furnace or the quartz tube.

You do not need to align the quartz tube before every analysis unless you have altered the quartz tube since it was previously optimized. However, you must align the tube if you have:

- Removed and re-installed the quartz tube or the QT-furnace that holds the tube and heats it.
- Re-installed the end windows of the quartz tube, for example after cleaning them.

***Procedure for aligning the quartz tube***

1. Make sure the correct lamp is installed.
2. Install the QT-furnace and quartz tube as described in the user's guide for the spectrometer or flow-injection system.
3. On the **Instrument** tab, in the **Devices** group, click on **Devices**, then click the **FIAS** tab.  
The **FIAS Control** window appears.
4. Make sure that the quartz tube heating is switched off. In the **FIAS Control** window, make sure that the **Cell On/Off** button is not highlighted.
5. Click **Align FIAS**.  
The **Align Furnace/FIAS Wizard** appears.
6. Use this wizard to align the quartz tube.

## ***Optimizing the Analytical Conditions for FIAS-MHS***

When you have set up the system, analyze some typical solutions and make the adjustments suggested below to optimize the analytical conditions.

For more detailed information and procedures, see:

- The users guides for the spectrometer and flow-injection system.
- The **Recommended Conditions** window.

### ***Suggested procedure***

- Change only one parameter at a time and wait until the next signal appears before you make a further adjustment.
- When you have finished, calculate the characteristic mass.
- Make sure that you make all the necessary changes to the method that you intend to use for the subsequent analyses.

### ***Timing of the peak maximum***

- The signal should reach its maximum value between 5 and 8 seconds after the beginning of the **Read Time**, and the signal should return to the baseline before the end of the Read Time. Set appropriate values for the Read Time and Read Delay on the Instrument page.
- If the peak maximum appears too early, slightly decrease the carrier gas flow. If the peak maximum appears too late, slightly increase the carrier gas flow.

If the carrier gas flow is too high, the mercury or hydride vapor leaves the quartz tube before it can be measured. If the flow is too low, not all of the mercury or hydride vapor has entered the quartz tube when the system makes a measurement. A flow in the range 40 - 70 mL/min is normally correct.

### ***Absorbance of replicates***

- The absorbance values for all the replicates should be similar. If the absorbance for the first replicate is higher than that for the subsequent replicates, lengthen the Fill step on the FIAS page. If the absorbance for the first replicate is lower than that for the subsequent replicates, lengthen the Prefill step on the FIAS page.

### ***Sensitivity***

- The waste flow from the gas/liquid separator can affect the sensitivity. If the waste flow is too high, mercury or hydride vapor may escape through the waste outlet. If the waste flow is too low, liquid may enter the sample transfer tube and the quartz tube. If liquid enters this tube or the tube, you must thoroughly decontaminate and dry these parts; see the user's guide for the flow injection system.
- You may improve the sensitivity by slightly changing the flow rates of the carrier and reductant.

## ***Optimizing the Conditions for FIAS-Flame***

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When you have set up the system, analyze some typical solutions and make the adjustments suggested below to optimize the analytical conditions. For more detailed information and procedures, see:

- The users guides for the spectrometer and flow-injection system.
- The **Recommended Conditions** window.

### ***Suggested procedure***

- Change only one parameter at a time and wait until the next signal appears before you make a further adjustment.
- When you have finished, calculate the characteristic mass or concentration.
- Make sure that you make all the necessary changes to the method that you intend to use for the subsequent analyses.

### ***Adjustments***

- The absorbance values for all the replicates should be similar. If the absorbance for the first replicate is higher than that for the subsequent replicates, lengthen the **Fill** step on the **FIAS** page. If the absorbance for the first replicate is lower than that for the subsequent replicates, lengthen the **Prefill** step on the **FIAS** page.
- The signal must appear and decay within the **Read Time**. Set appropriate values for the **Read Time** and **Read Delay** on the **Instrument** page.
- You may improve the sensitivity by slightly changing the flow rates of the carrier and any reagents.
- The sensitivity depends on the burner and nebulizer settings exactly as for the normal flame technique. make sure that you have optimized the burner.

## ***Calculating the Characteristic Mass: FIAS-MHS***

When you have optimized the analytical conditions and created a suitable method, analyze a reference solution and calculate the characteristic mass.

### ***Procedure***

For information about the recommended sensitivity-check solution, on the Analysis tab, in the Method group, click **Recommended Conditions**.

1. Allow the lamps to warm up for at least 10 minutes.
2. Prepare a blank solution, a sensitivity-check solution of the element and the necessary reagents, and place the solutions in the sample tray.
3. Open the correct **Method** and enter a value of **5** for **Replicates**.

4. On the **Analysis** tab, in the **Analyze** group, click **Analysis**, then click **Automated** tab.
5. Set up the **Automated** Analysis window with the correct method name and the sample tray locations of the blank and the reference solution.
6. Click Analyze Samples.
7. On the Analysis tab, in the Analyze group, click Characteristic Mass. The Calculate Characteristic Mass dialog appears.
8. Enter the concentration of the sensitivity-check solution, then press **Enter**.
9. Enter the readings for the **Blank** and sensitivity-check solutions. The readings are shown in the **Results** window. Use either peak height or peak area depending on the recommendation in the **Recommended Conditions** window.
10. Press **Enter**. The system calculates the characteristic mass.

### ***Troubleshooting***

The calculated value should be within 20% of the comparison value. If it is not:

- Make sure that the solutions you used were correctly prepared.
- Make sure that the sample volume on the **FIAS** page of the **Method Editor** is the same as the volume of the sample loop that you are using.
- Make sure that the tube is clean and correctly aligned.
- Re-optimize the analytical conditions.

### ***Calculating the Characteristic Mass or Concentration: FIAS-Flame***

When you have optimized the analytical conditions and created a suitable method, analyze a reference solution and calculate the characteristic mass or concentration.

There are no recommended characteristic mass or concentration values for the FIAS-flame technique. Use the calculated value as a day-to-day check on the reproducibility of your analytical system.

### ***Procedure***

For information about the recommended sensitivity-check solution, in the on the **Analysis** tab in the **Method** group, click on **Recommended Conditions**.

1. Allow the lamps to warm up for at least 10 minutes.
2. Prepare a blank solution and a sensitivity-check solution of the element and place the solutions in the sample tray.
3. Open the correct **Method** and enter a value of **5** for **Replicates**.
4. On the **Analysis** tab, in the **Analyze** group, click **Analysis**, then click **Automated** tab.
5. Set up the **Automated** Analysis window with the correct method name and the sample tray locations of the blank and the reference solution.

6. In the **Automated** Analysis window, click **Analyze Sample**.
7. On the Analysis tab, in the Analyze group, click Characteristic Conc. The Calculate Characteristic Concentration dialog appears.
8. Enter the concentration of the sensitivity-check solution, then press **Enter**.
9. Enter the readings for the **Blank** and sensitivity-check solutions. The readings are shown in the **Results** window.
10. Press **Enter**. The system calculates the characteristic concentration.

### ***Troubleshooting***

The calculated value should be within 20% of the comparison value. If it is not:

- Make sure that the sample volume on the **FIAS** page of the **Method Editor** is the same as the volume of the sample loop that you are using.
- Make sure that the solutions you used were correctly prepared.
- Re-optimize the analytical conditions.

## ***Preparing the MHS System for Analysis***

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### ***Setting up the MHS System***

1. Read the safety information in the users guides for your system before you operate the spectrometer.
2. Make sure that all the instruments are correctly installed. See the user's guides for your system.
3. Switch on the instruments.
4. On the **Techniques** tab and select the **MHS** technique.
5. Create or open a Method.  
Make sure that you select the correct parameters for the MHS technique.
6. Install and align the lamps that you require.
7. Install the 10 cm air/acetylene burner head, the standard nebulizer, and the QTA mount for the quartz tube. See the user's guides for your system for further information.
8. Perform the safety checks, then ignite the flame.  
You may need to swing the QTA mount away from the burner head to ignite the flame.  
Select an air/acetylene flame for heating the quartz tube. See the users guides for your system for further information.
9. If necessary, set up the nebulizer.
10. Align the quartz tube.

### ***Aligning the Quartz Tube for MHS***

To obtain the best analytical results, the radiation beam from the lamp must pass directly along the center of the furnace or the quartz tube. You do not need to align the quartz tube before every analysis unless you have altered the quartz tube since it was previously optimized. However, you must align the tube if you have:

- Removed and re-installed the quartz tube or the support.
- Re-installed the end windows of the quartz tube, for example after cleaning them.

### ***Procedure for aligning the quartz tube***

1. Install and align the appropriate lamp.
2. Install the quartz tube support and quartz tube as described in the user's guide for the spectrometer or MHS system.
3. On the **Instrument** tab, in the **Atomizer** group, click on **Flame Control**.  
The **Flame Control** window appears.

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4. Make sure that the flame is not burning.
5. Click **Align Cell**. The **Align Furnace/FIAS Wizard** appears. Use this wizard to align the quartz tube.

## ***Shutting Down the System***

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### ***Shutting Down the Furnace System***

It is important that you rinse out the autosampler after every analysis series and before you shut down the system to ensure that the valves are clean and maintain their high precision delivery. Make sure the rinsing solutions are clean and free of particles. Particles can lodge in the valves, causing leaks and non-reproducible results. Use the solutions in the order shown.

1. If you have been using an organic rinsing fluid, use isopropanol or other water-miscible solvent.
2. Dilute nitric acid. This is especially important for elements with a tendency to carryover.
3. Isopropanol.
4. Deionized water.

### ***Shutdown Procedure***

1. Fill the rinse bottle with the first rinsing solution.
2. In the **Furnace Control** window, click on **Flush Sampler** a number of times to fill the rinsing system with the solution and flush all the air out of the system.
3. Repeat the previous step for each rinsing solution.
4. Empty the autosampler waste bottle. Dispose of waste solutions correctly, according to the safety regulations in force in your area.
5. Remove all the samples and reagents from the sample tray. Wipe up any spillages.
6. Switch off the spectrometer.
7. Turn off the gas supplies.
8. If the fume extraction unit needs cleaning, follow the instructions given in the user's guide for the furnace.
9. Exit Syngistix: Click the **Application** button then click **Exit**.
10. If you do not want to use the computer for other tasks, shut down the computer and printer as described in the users guides

### ***Shutting Down the Flame System***

1. With the flame still burning, aspirate the correct rinsing solutions, in the sequence listed below, to rinse the nebulizer and burner. Either aspirate the solutions manually or use the autosampler.

If you used only aqueous solutions during the analysis:

- Aspirate deionized water for five minutes.

If you used organic solvents during the analysis:

- a. Aspirate an organic solvent that is miscible with both the solvent you used during the analysis and water for five minutes.
  - b. Aspirate acetone for five minutes.
  - c. Aspirate 1% nitric acid for five minutes.
  - d. Aspirate deionized water for five minutes.
2. Extinguish the flame and bleed the gas lines using the controls in the Flame Control window.
  3. Exit Syngistix: Click the **Application** button then click **Exit**.
  4. Switch off the spectrometer and any accessories.
  5. If you do not want to use the computer for other tasks, shut down the computer and printer as described in the users guides.
  6. Empty the burner drain vessel. Dispose of waste solutions according to the safety regulations in your area.

### ***Shutting Down the FIAS-MHS System***

1. Rinse the fluid system with the correct rinsing solutions, in the sequence listed below, to remove all traces of the reagents and samples.

If you used only aqueous solutions during the analysis:

- Aspirate deionized water for five minutes.

If you used organic solvents during the analysis:

- a. Aspirate an organic solvent, that is, miscible with both the solvent you used during the analysis and water, for five minutes.
  - b. Aspirate ethanol for five minutes.
  - c. Aspirate 1% nitric acid for five minutes.
  - d. Aspirate deionized water for five minutes.
2. Switch the FIAS pumps off:  
On the **FIAS** tab in the **Devices** window, click the **Pump** button to stop the corresponding pump.
  3. Release the pressure on the pump tubes. Swing the pressure levers away from the pump tube magazines.
  4. Exit Syngistix: Click the **Application** button then click **Exit**.
  5. Turn off the carrier gas supply to the flow-injection system.
  6. Switch off the spectrometer and any accessories.
  7. If you do not want to use the computer for other tasks, shut down the computer and printer as described in the users guides.

8. Empty the waste vessel. Dispose of waste solutions according to the safety regulations in your area.

### ***Shutting Down the FIAS-Flame System***

1. With the flame still burning, rinse the fluid system with the correct rinsing solutions, in the sequence listed below, to rinse the flow system, nebulizer, and burner.

If you used only aqueous solutions during the analysis:

- Aspirate deionized water for five minutes.

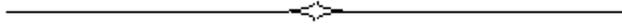
If you used organic solvents during the analysis:

- a. Aspirate an organic solvent, that is miscible with both the solvent you used during the analysis and water, for five minutes.
- b. Aspirate ethanol for five minutes.
- c. Aspirate 1% nitric acid for five minutes.
- d. Aspirate deionized water for five minutes.

2. Extinguish the flame and bleed the gas lines using the controls in the **Flame Control** window.
3. Switch the FIAS pumps off:  
On the **FIAS** tab in the **Devices** window, click the **Pump** button to stop the corresponding pump.
4. Release the pressure on the pump tubes. Swing the pressure levers away from the pump tube magazines.
5. Exit Syngistix: Click the **Application** button then click **Exit**.
6. Turn off the carrier gas supply to the flow-injection system.
7. Switch off the spectrometer and any accessories.
8. If you do not want to use the computer for other tasks, shut down the computer and printer as described in the users guides.
9. Empty the flow system waste bottle and burner drain vessel. Dispose of waste solutions according to the safety regulations in your area.

### ***Shutting Down the Flame-Heated MHS System***

1. Shut down the MHS system as described in the user's guide for this accessory.
2. Extinguish the flame and bleed the gas lines using the controls in the **Flame Control** window.
3. Exit Syngistix: Click the **Application** button then click **Exit**.
4. Switch off the spectrometer and any accessories.
5. If you do not want to use the computer for other tasks, shut down the computer and printer as described in the users guides.



# **Software Overview**

## ***Syngistix Ribbon***

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The Ribbon helps you quickly find the functions and the most frequently used windows you need to complete a task. It consists of an Application button and commands organized by tabs and groups within each tab. The Application button contains a drop-down menu of commands that involve doing something to or with a file that is not directly related to a specific command window. The Ribbon itself contains commands that affect the content a window. Major task are organized into tabs that contain groups of functions to help you perform a specific task.

### ***Application Button***

Clicking on the Application button provides the following commands that are available at all times:

**Workspace:** When you click on Workspace, you can open a previously saved workspace or save the displayed workspace. Clicking Open displays the Open dialog, which lists stored workspaces. To create a new workspace, see Workspaces.

**Notifications:** Display the Sounds Page dialog.

**Arrange Windows:** Select how you want your windows arranged in a workspace; Arrange All, Cascade, Tile Horizontally, Tile Vertically, or Close All Windows.

**Print Active Window:** Select how you want to preview and print the active screen.

**Print Setup:** Use this command to set options for printing, such as printer name, paper size and orientation. (See your Windows manual for further information on printing, if needed.)

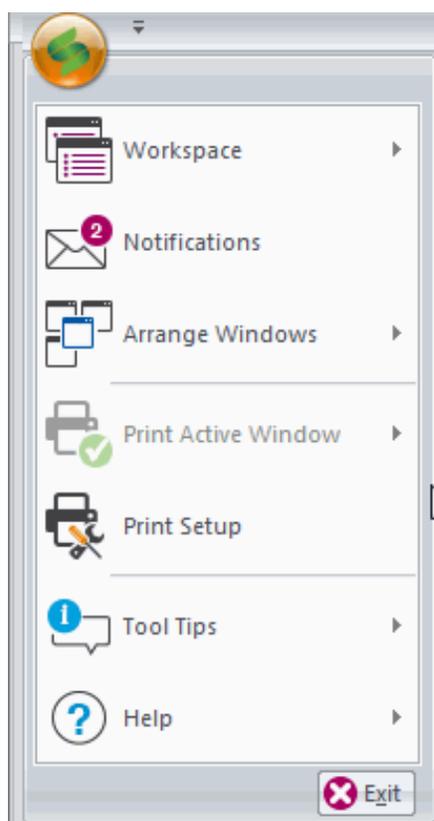
**Tool Tips:** Select the tool tip language and select to show or not show them

**Help:** Select the Help, Consumables Catalog, Support Form, and About Syngistix.

### ***The Ribbon Tabs***

The Ribbon consists of the following tabs.

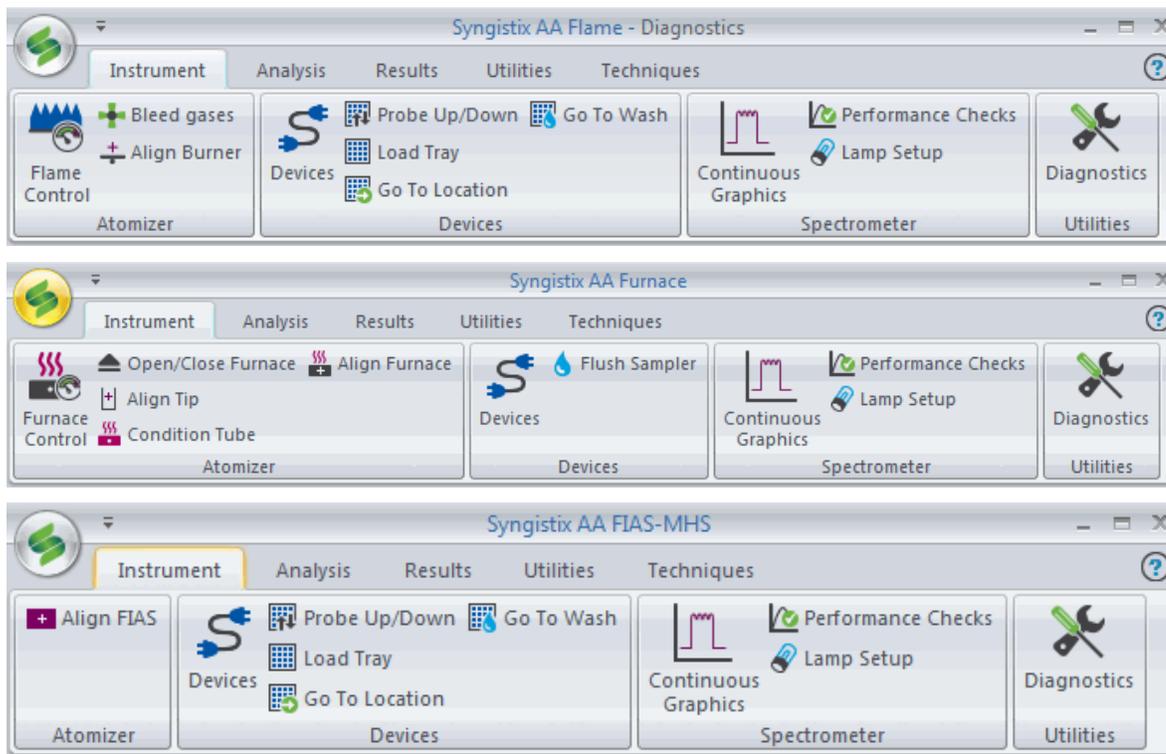
Instrument, Analysis, Results, Utilities, and Techniques.



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## ***Instrument Tab Commands***

The **Instrument** tab is populated with icons relevant to the technique chosen.



### ***Atomizer Group***

**Flame Control:** Click to view the Flame Control window. You use the Flame Control window to control the gas flows, bleed gases, align the burner and turn the flame on and off. You can only use these controls when there is no analysis in progress. The status of the gas flows are shown at the top of this window.

**Furnace Control:** Click to view the Furnace Control window. You use the Furnace Control window to control the furnace, condition the graphite tube and align the autosampler. You can only use these controls when there is no analysis in progress. The status of the furnace and the furnace program are shown at the top of this window.

**Align FIAS:** Click to view the Align FIAS window. You use the FIAS Control window to manually control the FIAS pump module and view the progress of the FIAS program. The status of the FIAS pump module and the FIAS program are shown at the top of this window..

### ***Devices Group***

**Devices:** Click to display the dialog to control your devices; Autosampler, FIAS, etc.

**Probe Up/Down:** Use this command to move the autosampler probe up or down, depending on its current position.

**Load Tray:** Use this command to move the autosampler probe up and then to the back left position. This is the same as clicking on Load Tray in the Automated Analysis Control window.

**Go to Location...:** Use this command to select the location where the autosampler probe will move. When you click on this command, the Go To Location dialog appears.

**Go to Wash:** Use this command to go to the autosampler location of the wash solution. The location of the wash solution is selected in the method on the Sampler: Autosampler Wash page.

## ***Spectrometer Group***

**Continuous Graphics:** Click to display the Continuous Graphics window. Here you view the data for selected analytical wavelengths in a continuous readout mode. Use this command to change the parameters for Settings, Lines, and Colors in the Continuous Graphics display.

**Performance Checks:** Click to display the Spectrometer Control Performance Checks dialog to set detection limits.

**Lamp Setup:** Click to display the Lamp Setup window, used to install, identify, and setup lamps.

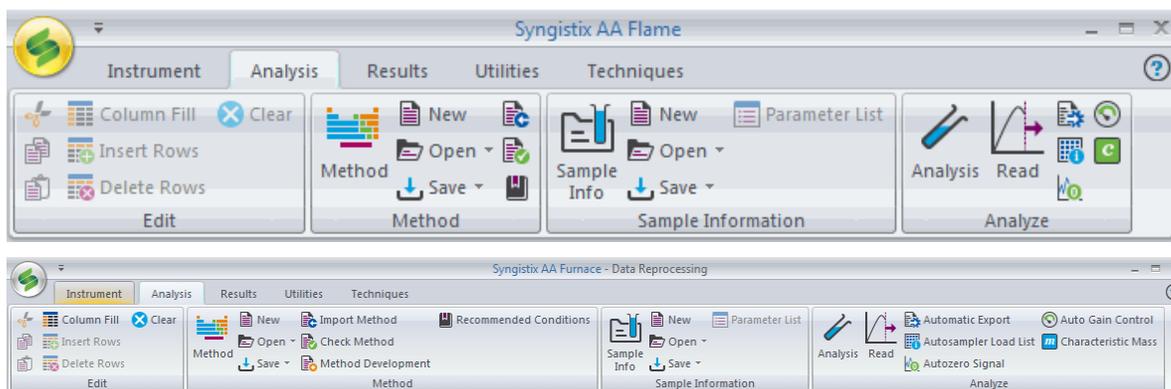
## ***Utilities Group***

**Diagnostics:** Click to displays diagnostic information.

**Tube View:** Click to display the Tube View camera window.

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## ***Analysis Tab Commands***



### ***Edit Group***

**Column Fill..:** Use this command to fill a selected column in the Method Editor or Sample Information Editor. When you click on this command, a dialog appears where you enter values to fill the selected column.

**Insert Rows:** Use this command to insert an empty row into a table of parameters such as those in the Method Editor or Sample Information Editor. Select a position in the line after the one you want to insert and then select the command. A line will be inserted before the line containing the cursor. All entries below the inserted line move down one position.

**Delete Rows:** Use this command to delete selected rows from a table. All entries below move up respectively one position.

**Cut:** Use this command to remove selected text or values in a table and place in the Windows clipboard.

**Clear:** Use this command to remove selected text or values in a table.

### ***Method Group***

**Method:** Click to display the Method Editor window to enter the analytical parameters that the system needs to perform an analysis.

**New:** Use this command to create a new method. The Create New Method dialog appears, where you can select a set of plasma conditions in a new method for different types of analyses, for example, organic or aqueous. Or, you can choose to use a copy of the active method or another stored method as a starting point.

**Open:** Use this command to select a stored method for editing or performing manual analyses. The Open Method dialog appears.

**Save:** Use this command to save changes to the active method. The first time you save a Method, the Save As Method dialog will appear prompting you for a name. Note: If, for any reason, a method is not ready to be saved, a check method dialog will appear.

**Import Method:** Use this command to import a method.

**Check Method:** Use this command to check for any problems or inconsistencies in the method.

**Method Development (Furnace only):** Use this wizard to perform method development for the furnace program automatically. You can analyze various different sample mixtures using the a furnace program you have already developed, or perform temperature studies where the system automatically increments the temperatures of the furnace steps.

**Recommended Conditions:** Use this command to display the Recommended Conditions window, which shows recommended analytical conditions for determining an element.

## ***Sample Information Group***

**Sample Info:** Click to display the Sample Information Editor window to enter information about your samples; for example, the location of the samples in the autosampler, sample IDs, sample weights and sample volumes.

**New:** Use this command to create a new sample information file. The New Sample Information file dialog appears, in which you select the default design (default.sidx) or a design you have created. The design (.sidx) file is a template that contains the sample parameters that you want to use. To create a design file, see Using the Sample Information Editor.

**Open:** Use this command to select a stored sample information file for editing or performing manual analyses. An Open dialog appears, where you can select a sample information file.

**Save:** Use this command to save changes to the active sample information file. The first time you save a sample information file, the Save As Sample Information File dialog will appear prompting you for a name.

**Parameter List:** Use this command to open the Sample Information Parameters dialog , where you can add parameters to a sample information file. Parameters can be common to all samples or they can vary by sample.

## ***Analyze Group***

**Analysis:** Click to open the Manual and Automated analysis window.

**Read:** Use this command to perform an instrument reading using the parameters in the method.

**Automatic Export:** Use this command if you want to automatically export data contained in a results data set and write it into a file that can be read by many other programs, including spreadsheet and database management programs. The Automatic Export dialog appears. The export file contains ASCII data records.

**Automatic Load List:** Use this command to include or exclude an element from your method in an analysis. When you click on this command, the Enable/Disable Elements dialog appears, where you can make your selections.

**Autozero Signal:** Use this command to perform a reading and use the result as a system blank value.

**Auto Gain Control:** Click to set the detector parameters to the optimum values for the active lamp.

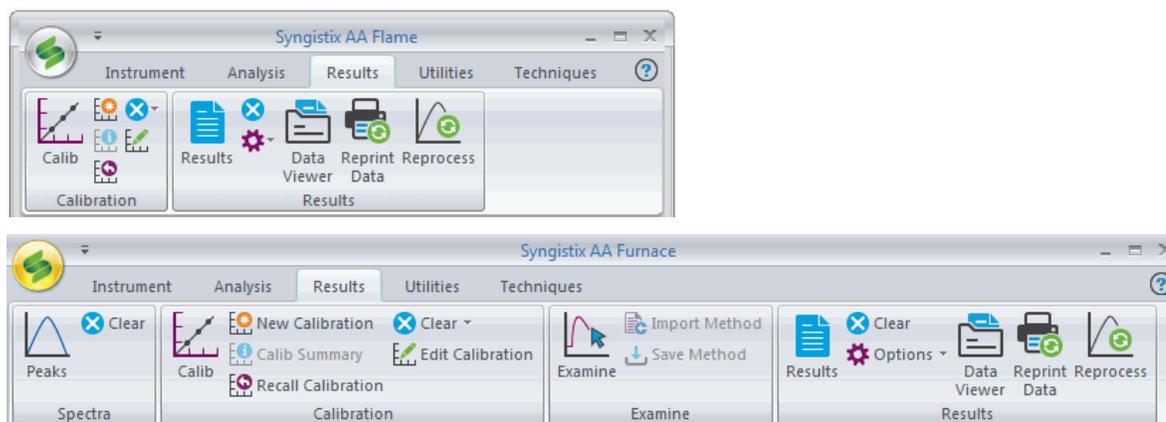
**Characteristic Mass:** Click to display the Characteristic Mass dialog.

or

**Characteristic Concentration:** Click to display the Characteristic Concentration dialog which is used in the **flame technique** when a given concentration of an analyte produces a continuous absorbance.

## Results Tab Commands

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### Spectra Group (Furnace only)

**Peaks:** Click to display the Transient Peaks Display which is used to view transient signals during analyses.

**Clear:** Use this command to clear the display on the Peaks window.

### Calibration Group

**Calibration:** Click to display the Calibration window used to view the active calibration curve.

**New Calibration:** Use this command to clear the existing calibrations from the Calibration Display window. You can generate a new calibration by analyzing the calibration standards.

**Calibration Summary:** When you are performing a Manual Analysis, use this command to view a summary of the calibration data. When you click on this command, a calibration summary is added to the information in the Results Display Window. (In an Automated Analysis, the calibration summary appears automatically in the Results Display Window after the last standard is analyzed, provided that this option is selected on the Options page of the Method Editor.)

**Recall Calibration...:** Use this command to recall a stored calibration from the results library. After you click on this command, select the results data set where the calibration is stored. If several sets of calibrations have been run, the most recent one will be recalled.

**Clear Calibration Blank:** Use this command to clear the calibration blank concentrations from the analysis. If multiple calibration blanks have been analyzed, all calibration blank concentrations are cleared.

### Examine Group

**Examine:** Click to displays the Examine Transients Peak used to view the analyte signal peaks that are saved in the database. You must save the data in order to perform these functions in this window.

**Import Method:** Use this command to import a method.

**Save Method:** Use this command to save a method.

### Results Group

**Results:** Use this command to view the Results Display window, which shows the measurements made on the current sample, the calculated concentration values, and statistical information.

**Clear:** Use this command to clear the display.

### Options

**User Message:** Use this command to print or save a message with your results. The Message dialog appears, where you enter the message.

**Analytical Header:** Displays the Analytical header in the Results window.

**Find:** Displays the Find dialog to search within the Results window.

**Reset Page Numbers:** When information in the Results window is printing, use this command to reset the page number of the next page to be printed to 1. This overrides the usual situation where the page numbers are consecutive when the Results window is printed.

**Skip Line:** In the Results window, use this command to add a blank line after the end of the text. When the Results window is printed, it will contain the added space.

**New Page:** When information in the Results window is printing, use the command to force a page to print, even if the page is only half filled with information. Usually, a page does not print until it is completely filled.

**Data Viewer:** Click to launch the Data Viewer window containing your Results.

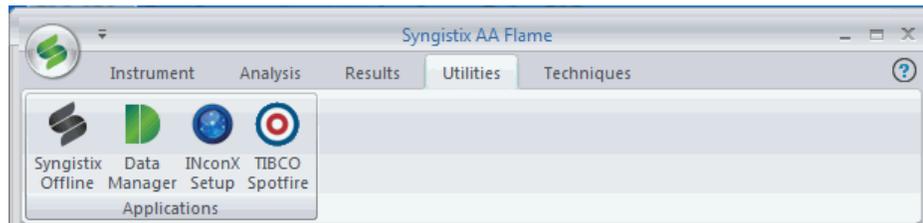
**Reprint Data:** Use this command to view the Reprint Data window. You use this window to specify which results data you want to reprint.

**Reprocess:** Click to view the Data Reprocessing window. You use this window to reprocess existing data.

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## ***Utilities Tab Commands***

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### ***Applications Group***

**Syngistix Offline:** Use this command to run Syngistix Offline without the software controlling the AA. This allows the user to edit methods and reprocess the data.

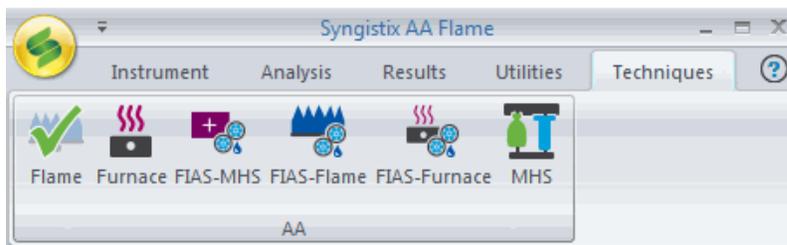
**Data Manager:** Use this command to open Data Manager for reporting, data export, and database maintenance.

**INconX Setup:** Use this command to run the INconX Setup application to connect to an iDevice.

**TIBCO Spotfire:** Use this command to launch the Spotfire application.

## Techniques Commands

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### AA Group

Use this command to change the analysis technique. The system displays only those windows and pages that are necessary for the selected technique. The above example shows six techniques. A green check mark displays over the current technique.

**Flame:** Clicking this icon changes the Syngistix analysis technique to Flame.

**Furnace:** Clicking this icon changes the Syngistix analysis technique to Furnace.

**FIAS-MHS:** Clicking this icon changes the Syngistix analysis technique to FIAS-MHS.

**FIAS-Flame:** Clicking this icon changes the Syngistix analysis technique to FIAS-Flame.

**FIAS Furnace:** Clicking this icon changes the Syngistix analysis technique to FIAS-Furnace.

**MHS:** Clicking this icon changes the Syngistix analysis technique to MHS.

## ***Keyboard Shortcuts***

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The following keyboard shortcuts are available in Syngistix.

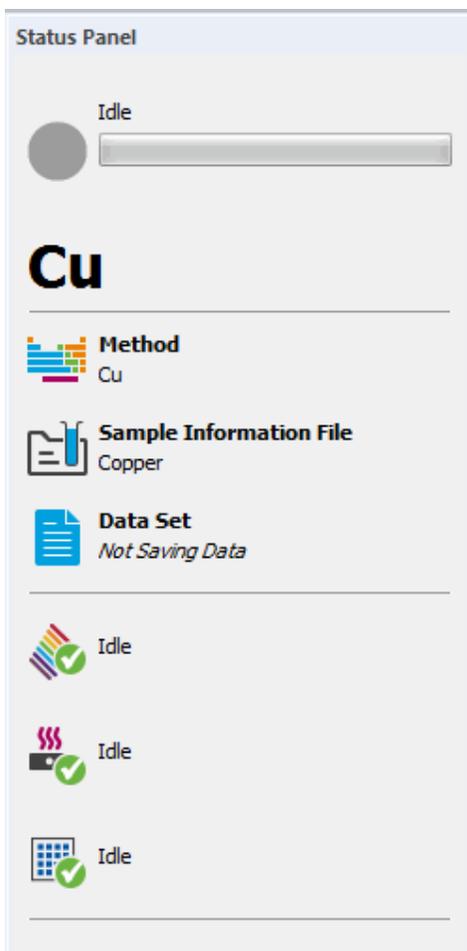
<b>Key</b>	<b>Function</b>
F1 Help	Help
F2	AGC
F3	Autozero
F4	Read
F5	Analyze Blank
F6	Analyze Standard
F7	Analyze Sample
F8	Cancel Analysis
F9	Furnace On/Off
F10	Flame On/Off
Shift-F10	Bleed Gases
F11	Probe Up/Down
Shift-F11	Load Tray



# **Status Panel and Diagnostics**

## Status Panel

The Status Panel monitors the system to check status of the following: Furnace, lamp, Spectrometer, Autosampler, Auto Shutdown/Startup, and mobile application.



The **Status Panel** provides an instant visual so you can see what is happening at that point in time with your system. You can move the Status Panel to any location within the software workspace; however, by default it appears in the upper right-hand portion of the workspace. It is dockable to either the left or right by clicking and holding the mouse and then dragging it. It can also be minimized and/or pinned to the right. For a listing of status types refer to About the Status Display. Double-clicking the Status Panel title bar docks the Status Panel to the right side.

**Note:** When moving the Status Panel, the screen displays non-functional "docking control" arrow buttons.

The upper portion of the Status Panel consists of a System Status (text field), a Progress Bar that corresponds with the System Status, and an additional Detailed Status (text field). This section lists the various statuses that will be displayed.

The Status Panel consists the following elements:

### ***System Status***

This text field displays a high level status of the current operation being performed. The upper portion of the Status Panel consists of a System Status (text field), a Progress Bar that corresponds with the System Status, and an additional Detailed Status (text field). This section lists the various statuses that will be displayed.

### ***Analysis Indicator Light***

This circle changes colors to indicate whether the system is analyzing, idle, or paused. Double-clicking on the Analysis Indicator displays the Analysis window.

**Green** – A green circle indicates the system is successfully analyzing.

**Gray** – A grey circle indicates that the system is idle, but ready.

**Yellow** – A yellow circle indicates that the system is paused.

**Progress Bar** - The progress bar pertains to the System Status currently displayed. The progress bar is only shown when a System Status is being displayed that requires a progress bar.

**Note:** Double-clicking on an icon displays the appropriate screen. For example, double-clicking on the Hardware icon takes you to Diagnostics.

**Detailed Status:** This text field is only displayed when an operation displayed in the System Status requires an additional detailed status.

**Fehler! Verwenden Sie die Registerkarte 'Start', um Heading 1 dem Text zuzuweisen, der hier angezeigt werden soll. . 63**

**Active data files:** Lists the current **Method**, **Sample Information File**, and **Data Set**.

**Diagnostic Status:** The most recent diagnostic status from each piece of hardware configured for the system next to the corresponding appropriate icon. Will also include icon and status for scheduler and INconX when configured.

**Note:** *The element name is displayed above "Method".*

You can drag the panel around the workspace and it will behave like a floating pane. To dock the panel double-click anywhere in the pane and the pane is docked in the right-hand area of the Syngistix workspace.

**Note:** *If Data Storage is off, the Data Set name field will state: "Not saving data." and will appear in italics.*

**Sample Steps** – Sample steps are used as the detailed step for any analyses including automated analyses, manual analyses, align view, and performance checks. Sample steps indicate the operation being performed to perform the analysis. Sample steps include but are not limited to:

Method Delay: (Countdown)

Read Delay: (Countdown)

Opening Shutter: (Countdown)

Reading Replicate X

Processing Replicate X

Wash time: (Countdown)

Moving Autosampler

## ***Status Icons***

By double-clicking on the status icon for the Furnace, Flame, Spectrometer, Diluter, or Autosampler, you can get further information about the system component in the Instrument Diagnostics window. By double-clicking on the status icon for Auto Shutdown/Startup, you open the Automatic Shutdown/Startup dialog.

### **AA Furnace**



### **AA Flame**



### Spectrometer Status Icons



### Diluter Status Icons



### Autosampler Status Icons



### Furnace Autosampler Status Icons



### FIAS Status Icons



### INconX

Only displays if the mobile is enabled.



## ***System Messages***

The System Monitor windows display the most recent messages pertaining to the system component. To view a complete log of messages, refer to the Instrument Diagnostics Window.

## ***Automated Analysis Status***

---

The System Status text displays the high level analysis status. "Analyzing All" when a user selects Analyze All, "Calibrating" when a user selects Calibrate. "Analyzing Samples" when a user selects Analyze Samples.

The progress bar shows how much of the entire analysis (percent complete) has been performed.

The Detailed status text displays the sample step. (Read Time, Opening Shutter, Reading Replicate X, Wash time: X, etc.)

## ***Align View Status***

The System Status displays: "Performing Align View."

The progress bar shows the total progress of the Align View operation.

The Detailed Status displays the current sample step for the Align View operation.

## ***Reprint Status***

The System Status displays: "Reprinting". There is no progress bar or detailed status.

## ***Download Firmware Status***

The System Status displays which firmware is being downloaded. (Spectrometer, Generator, Autosampler, FIAS, Furnace, Flame)

The progress bar shows approximately how much of the current firmware download operation has been completed. There is no Detailed Status.

## ***Manual Analysis Status***

The System Status displays what is currently displayed in the software and includes the wavelength and replicate being analyzed.

The progress bar shows the sample progress (how much/the approximate percentage of the analysis has been completed for the current sample. The Detailed Status displays the sample step.

## ***Reprocessing Status***

The System Status displays: "Reprocessing".

The progress bar shows approximately how much of reprocessing operation has been completed. The Detailed Status displays the status of the reprocessing operations.

## ***Performance Check Status***

The System Status is treated as a normal sample.

The progress bar shows approximately how much of performance check operation has been completed. The Detailed status displays the steps.

## ***Wavelength Calibration Status***

The System Status displays: "Performing a System Wavelength Calibration".

The progress bar shows approximately how much of the wavelength calibration has been completed.

The Detailed Status displays the steps: Read Delay, Measuring replicate 1 .... 5, Hg Lamp warming up with countdown, Measuring replicate 1

## ***Mercury Realignment Status***

The System Status displays: "Performing a Mercury Realignment".

The progress bar shows approximately how much of the Hg realignment operation has been completed.

The Detailed Status displays: Hg lamp warming up 90 .... 1, Measuring replicate 1

## ***Instrument Warm Up Status***

The System Status displays: "Warming up instrument". There is no progress bar or detailed status.

## ***AA Burner Alignment Status***

The System Status displays: "Aligning burner".

The progress bar shows approximately how much of the burner alignment operation has been completed. There is no Detailed Status.

## ***Diagnostic Status***

The bottom half of the status panel displays the current diagnostic status of the hardware the software is configured for. These are the exact same statuses shown in Diagnostics window pertaining to each device.

**Flame AA Autosampler:** The status displays the most recent status displayed in a Flame AA Diagnostics window.

**FIAS:** The status displays the most recent status displayed in the FIAS Diagnostics window.

## ***INconX***

The status panel will only display an icon or status for INconX when the system currently has the Mobile Server enabled through Mobile Setup.

The status will display the number of mobile connections currently connected to software i.e. Connections: 2

The addition of the icon and status panel should happen immediately upon selecting Apply in Mobile setup after enabling Mobile Server. When the user disables the mobile server and presses apply, the icon and status should immediately disappear.

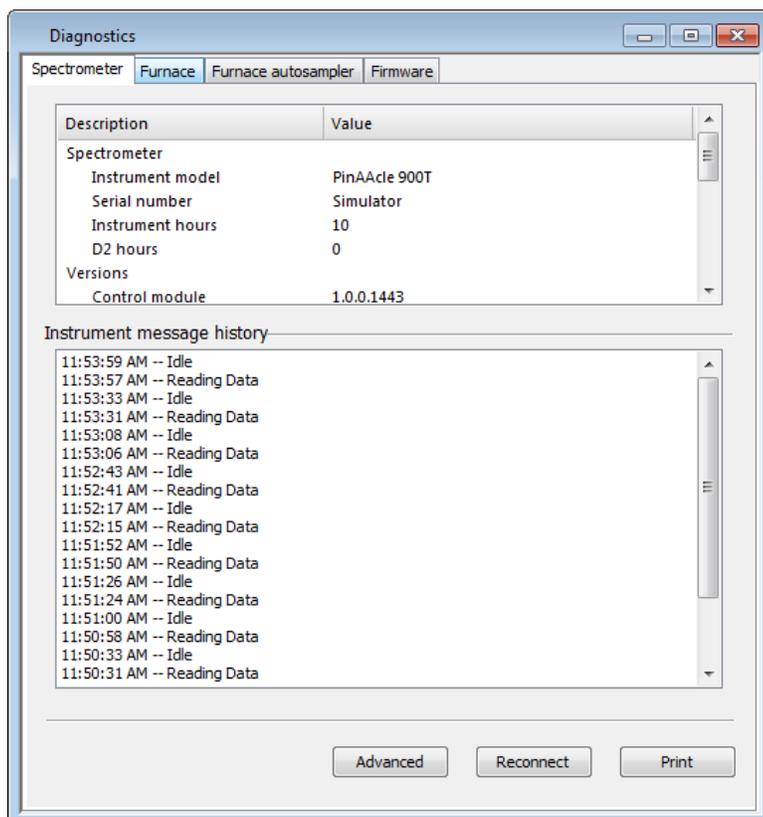
**Fehler! Verwenden Sie die Registerkarte 'Start', um Heading 1 dem Text zuzuweisen, der hier angezeigt werden soll. . 67**

## ***Instrument Diagnostics Window***

You use this window to review the value of parameters for the overall system and the spectrometer, plasma, and autosampler. This window is also used to reset communication between the system components.

To display this window:

- In the **Instrument** tab in the **Utilities** group, click on **Diagnostics**.



### ***Instrument Diagnostics***

The Instrument Diagnostics window contains tabs that provide access to information on each system component, including the status of the component and a log of messages.

- Click on the appropriate tab on the top of the window to select these pages:
  - Spectrometer
  - Flame
  - Furnace
  - FIAS
  - Autosampler
  - Furnace Autosampler
  - AutoPrep-50 Page
  - Firmware

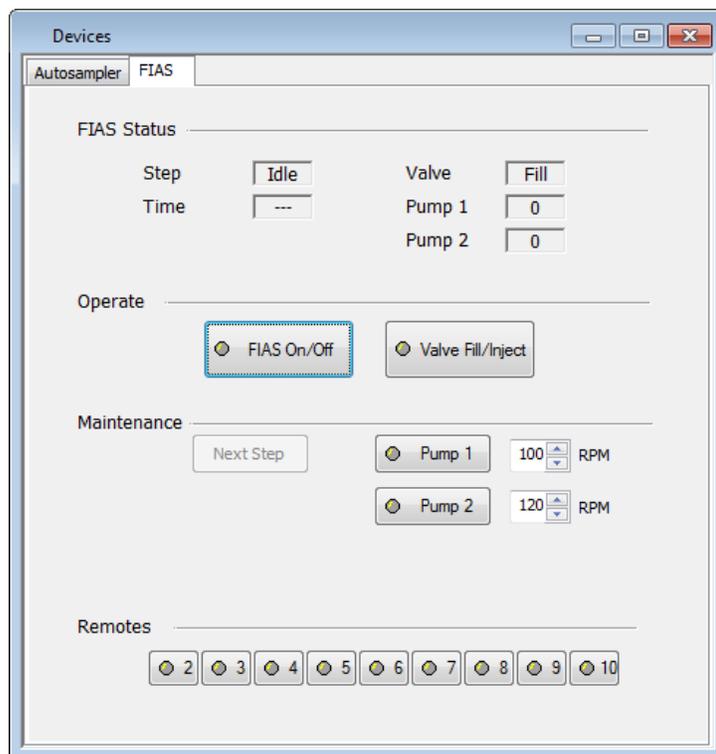


# **Devices**

## FIAS Control

You use the FIAS Control window to manually control the FIAS pump module and view the progress of the FIAS program.

**Note:** You can only use these controls when there is no analysis in progress.



### FIAS Status

The status of the FIAS pump module and the FIAS program is shown in this section. This includes the **Step**, **Time**, **Valve**, **Pump 1**, and **Pump 2** status.

### Operate

**FIAS On/Off:** To start or stop the FIAS program, click on this button. This button is inactive if there is an analysis in progress.

**Valve Fill/Inject:** To change the position of the valve, click on this button.

- Fill -- The sample loop is filled with sample.
- Inject -- The sample in the sample loop is injected into the carrier stream.

### Maintenance

**Next Step:** To skip the remainder of the current step in the FIAS program and continue with the next step in the time-event program, click on this button. If the skipped step contains the read step, the read function will not be performed.

**Fehler! Verwenden Sie die Registerkarte 'Start', um Heading 1 dem Text zuzuweisen, der hier angezeigt werden soll. . 71**

**Cell On/Off:** To turn the quartz cell heater on or off, click on this button. The cell will be heated to the temperature entered in the Method Editor FIAS page. When you turn the cell on, you will not be able to start a FIAS program until the cell has reached the preset temperature.

**Note:** *The Cell On/Off feature is only available in the FIAS-MHS. This feature does not appear if you are running a FIMS 100/400.*

**Pump 1:** To start or stop the pump, click on this button. To the right of the button you can select a value for the speed of Pump 1.

**Pump 2:** To start or stop the pump, click on this button. To the right of the button you can select a value for the speed of Pump 2.

**Note:** *This button does not appear if you are running a FIMS 100.*

## **Remotes**

**Remotes 2 through 10** are switches that you use to control instruments that are connected to the Remote contacts on the rear of the flow-injection unit. Remote 1 is always used to trigger the Read function on the spectrometer. Select the box to switch the remote on; a cross appears in the box. Clear the box to switch off the remote.

**Align FIAS** (This wizard is only available in the FIAS-MHS): To align the FIAS, click on this button. The Align FIAS wizard provides an easy way to align the FIAS. If you select the Cancel button on the wizard, the procedure will stop and the FIAS will not be aligned.

**Note:** *Please note that the Align FIAS feature is only available with the AAnalyst 700/800 and PinAAcle series.*

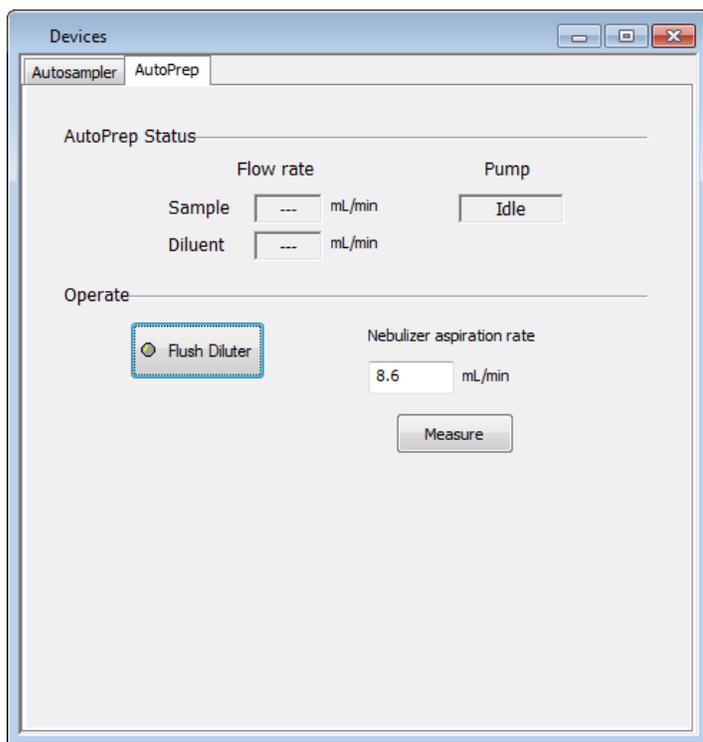
## ***AutoPrep (Diluter) Control***

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In Flame technique this window is used to calculate the dilution factor for samples.

### ***AutoPrep Status***

The status of the diluter is shown in this section. This includes the **Flow rate** of the **Sample** and **Diluent** in mL/min and the **Pump** status.



### ***Operate***

**Flush Diluter:** Press this button to flush out the diluter; for example, at the end of a run.

**Nebulizer aspiration rate (mL/min):** Display the current aspiration rate. To change this rate press the **Measure** button to display the **Measure Uptake Rate** dialog.

## ***Autosampler Configuration***

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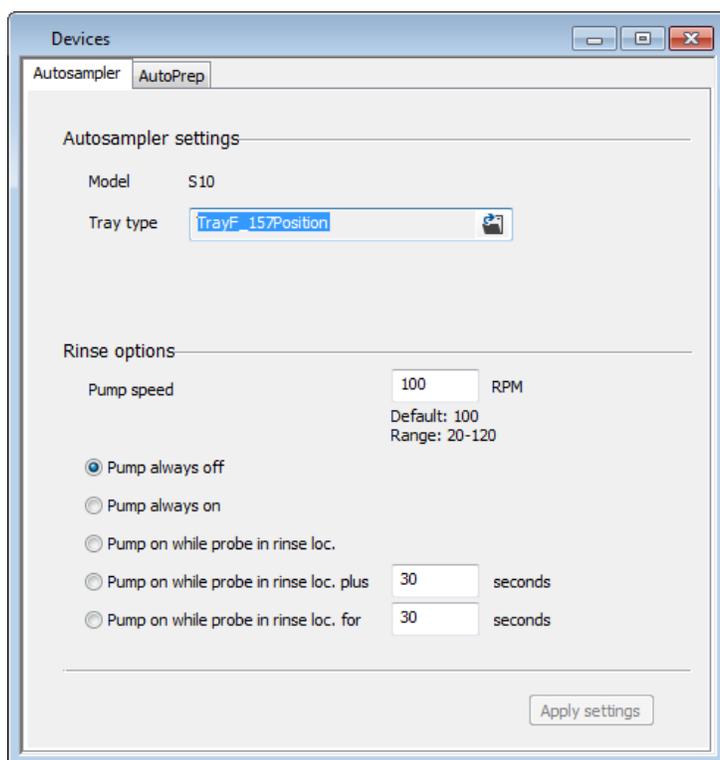
You use this dialog to view the autosampler model and select the tray type that you are using.

To display this dialog:

1. On the **Instrument** tab, in the **Devices** group, click on **Devices**.  
The devices screen appears.
2. Click the **Autosampler** tab.

### ***Using this dialog***

- Select the tray type that corresponds to your autosampler configuration.



### ***Model***

The autosampler model is set to the configuration, which was set up when the software was installed.

- To change the model, exit the software and run the Reconfigure utility. To run the Reconfigure utility, click on **Start ▶ All Programs ▶ PerkinElmer Syngistix for AA ▶ Reconfigure**.

### ***Tray Type***

1. Click on the file icon to browse to select a different autosampler tray.
2. In the dialog that appears, the trays are listed that can be used with the current autosampler configuration.

3. Click on the tray you are using and then click on **Open**.

### ***Rinse Options***

The rinse options display for those autosamplers that have a rinse location used to rinse the sample probe. If you want to change the rinse solution continuously, select one of the options where the pump is switched on. Use a higher **Pump Speed** to change the rinse solution more quickly.

Select from the following rinse options:

**Pump always off:** The rinse pump is always switched off, even when the sampling probe is in the rinse location. When this option is active, other rinse pump options cannot be selected.

**Pump always on:** The rinse pump runs continuously.

**Pump on while probe in rinse loc:** The rinse pump is on for the dwell time that the sampling probe is in the rinse location. The dwell time is preset in the operating software and cannot be changed by the user.

**Pump on while probe in rinse loc. plus xx seconds:** The rinse pump is on for the dwell time that the sampling probe is in the rinse location; it continues to pump for the number of seconds entered in the entry box after the sampling probe has been raised out of the rinse location.

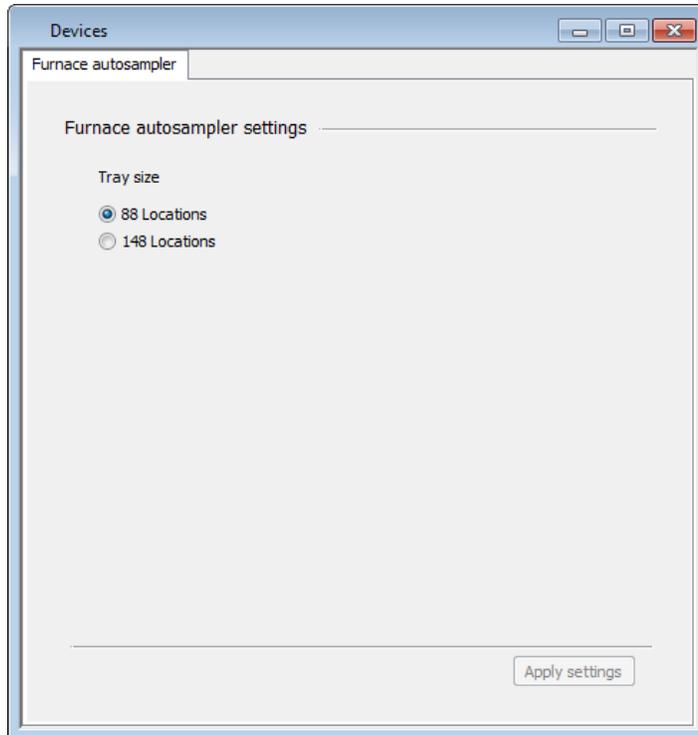
**Pump on when probe in rinse loc. for xx seconds:** The rinse pump starts when the sampling probe enters the rinse location and pumps for the number of seconds entered in the entry box. This time can be longer or shorter than the default dwell time of the probe in the rinse location.

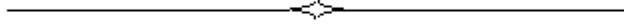
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## ***Furnace Autosampler Options***

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Use this dialog to select the sample tray and the slurry sampler. In this dialog, the numbers show the maximum number of sample locations in the various trays. Select the number that applies to the sample tray that you intend to use.





# **Analysis Control Window**

## ***Analysis Control Windows***

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You can operate the instrument in either a manual mode (with or without an autosampler), or in an automated mode (with an autosampler only). When you operate in manual mode, you define the order and control the analysis. When you operate in automated mode, the application can run Blanks, Standards and Samples in a pre-defined order.

You can also reprocess data stored in the results library using different analytical settings such as signal measurement algorithm, standard concentrations, units of concentration or QC concentrations.

- Select the appropriate analysis control window depending on the task you wish to perform.

### **To do this**

Analyze a few samples manually:  
for, FIAS-MHS , MHS , or Flame Analyses

Analyze many samples using an autosampler.

Recalculate stored data using different analytical conditions.

### **Use**

Manual Analysis Control tab

Automated Analysis Control tab

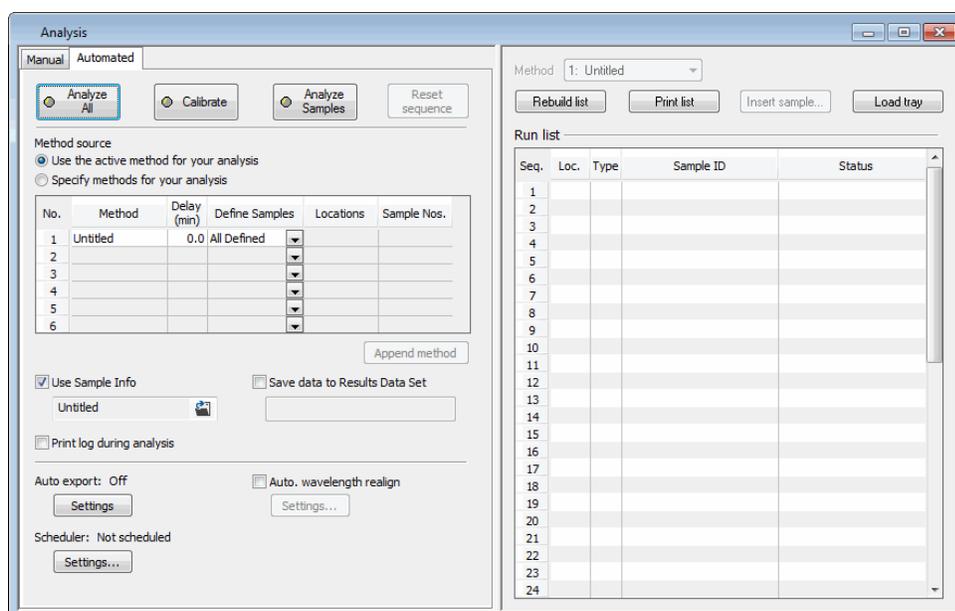
Data Reprocessing window

## Automated Analysis Tab

When you want to perform an automated analysis, (the application runs blanks, standards and samples in a pre-defined order) use this window to control the system and autosampler. Usually, you enter information in the method for analyzing blanks, calibration standards, and QC samples. If, however, you wish to analyze any of the blanks, calibration standards, or QC samples as samples, you must enter their IDs in the sample information file. As a result, they will be treated like samples in addition to the usage specified in the method.

To display this window:

1. On the **Analysis** tab, then in the **Analyze** group, click **Analysis**.
2. Click on the **Automated** tab. The window appears displaying the Automated tab parameters on the left side and the associated automated **Run List** on the right side.



You use this screen to select methods and a Sample Information file. You also can select a results data set to store the data, print an analysis log, and select other actions to occur during an analysis.

**Note:** You can change setup options even after an analysis has begun by returning to this window.

## Window Controls and Entries

### Analyze All

- Click on this button to analyze all of the samples in the **Run List** on the right side of this window.
- To interrupt the analysis sequence, click again on **Analyze All**. The Stopping an Analytical Sequence dialog appears, so that you can select when the analysis will stop.

Usually, **Analyze All** first calibrates the system, then analyzes the samples identified on the this window. If, however, you stopped the automated analysis before all the samples were analyzed (and did not click on **Reset Sequence**), you may resume the analysis at a particular place in the

analytical sequence by clicking again on **Analyze All**. The Continuing an Analytical Sequence dialog appears so that you can select the point where the interrupted analysis will restart.

### **Calibrate**

- Click on this button to start the calibration sequence. The system uses the blank and standards defined in the method.
- To interrupt the calibration sequence, click again on **Calibrate**. The Stopping an Analytical Sequence dialog appears so that you can select when the blank and standard analysis will stop. If you stopped the blank and standard analysis, (and you did not click on **Reset Sequence**), you may resume at a particular place in the calibration sequence by clicking again on **Calibrate**. The Continuing an Analytical Sequence dialog appears so that you can select the point where the interrupted analysis will restart.

When calibration is complete, you may want to examine the calibration curves in the Calibration window before analyzing samples.

### **Analyze Samples**

- Click on this button to start analyzing samples after the instrument has been calibrated.
- Click on the button a second time to stop the analyses. The Stopping an Analytical Sequence dialog appears, so that you can select when the sample analysis will stop.

The analysis usually starts at the beginning of the sequence that is shown on this window. If, however, you stopped the automated analysis before all samples were analyzed, (and you did not click on **Reset Sequence**), you may resume the analysis at a particular place in the analytical sequence by clicking again on **Analyze Samples**. The Continuing an Analytical Sequence dialog appears so that you can select the point where the interrupted analysis will restart.

**Note:** *If you schedule one or more **After Initial Calib QC** samples in the method, **Analyze Samples** will analyze the QC as part of the sample list. This is useful if you wish to use an existing calibration curve, analyze the **After Initial Calib QC** sample as a check (without reanalyzing your calibration standards), then take action based on the pass or fail status of the QC. For more information on QCs see the Method Editor: QC Pages.*

### **Reset Sequence**

This button resets the analytical sequence back to the beginning.

- Click on this button to reset the analytical sequence to 1. The next time you click on Analyze All, Analyze Samples or Calibrate, the sequence will be rebuilt and the system will start with the first item in the list.

### **Method Source**

- Choose **Use the Active Method for your Analysis** which uses the active method already in memory to analyze samples. (This is the normal choice when using a single method to analyze samples.)  
or
- Choose **Specify methods for your analysis** which opens methods in the list to analyze samples. (Use this option when you want to analyze samples using several methods in a sequence.)

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## **Analytical Sequence Table**

This sequence of method and sample information works with the **Run List**.

**Method:** You use this entry field to select the method(s) for the Automated analysis.

- Double-click on an entry field in the **Method** column. In the **Open Method** dialog that appears, select a method.

**Note:** To select more than one method, you must first select the Method source. This option is located below the Methods and Sample Locations table. You can select up to 50 methods.

**Delay (min):** This is the time, in minutes, that the system waits before it starts the method. This allows the lamp to warm up and the flame to stabilize if appropriate before the system makes measurements. (Maximum of 99 minutes)

**Define Samples:** By selecting samples from a **Sample Information** file, information you have supplied about the samples (for example, sample weights or dilutions) is used in the analysis. Use this column to specify the samples you want to use from a Sample Information file.

1. Open a **Sample Information** file.
2. Select the check box for **Use Sample Info** below the name of the sample information file. Three options appear in the Sample Info File column in a drop-down list.
3. Select **All Defined** if you want to analyze all of the samples in the sample information file.
4. Select **Locations**, if you want to select only certain autosampler locations.
5. Select **Sample Nos**, if you want to select samples by the sample numbers listed in the sample information file.

**Locations:** If you do not want to analyze all of the samples in the Sample Information file, use this entry field to select only the autosampler locations of the samples that you want to analyze. If you have selected **All Defined** or **Sample Nos** in the **Define Samples** file drop-down list, you cannot enter locations here. If you have not selected the check box for **Use Sample Info**, the locations do not apply to a Sample Information file.

- Type individual locations or a range of locations. Use commas to separate the locations and ranges. It is not necessary to enter the locations of blanks, QC's, check or calibration solutions. Enter locations for these if you want them to be treated as a sample within the analysis. Example: **10-15,18,20,22,25-30**.

**Sample Nos:** If you do not want to analyze all the samples in the Sample Information file, use this entry field to select only the sample numbers that you want to analyze. If you have selected **All Defined** or **Locations** from the **Define Samples** drop-down list, you cannot enter sample numbers here.

**Example:** If you only want to analyze #s 1, 3, 4, and 5, but not #2, in the **Sample Info File** column, select **Sample Nos**. This opens the Sample

numbers field so that the sample numbers can be entered.

**Append Method:** This button is only enabled during an analysis. Click on this button to display the Append Method dialog from where you can add methods to the run list after an analysis has started.

## ***Use Sample Info***

Select this check box to use the information specified in the Sample Information file (initial weight, dilution, volume, etc.) during the analysis. The software uses the information to calculate corrections for final results.

A Sample Information file stores information about the samples. The system uses this file to label the data from your samples and often needs it to calculate final concentrations. The sample information file also specifies the autosampler locations of the samples. This field shows the Sample Information file that describes the sample sequence.

- To select a **Sample Information** file, click on the folder icon in the field box. In the Open Sample Information dialog that appears, select an existing sample information file. If you wish to create a new file, use the Sample Information Editor.

**Note:** *If a Sample Information file is not entered, the "Untitled" sample information file that is currently open in the editor is listed.*

## ***Save data to Results Data Set***

This shows the name of the Results Data Set where the analysis results will be stored.

- Clicking the **Save data to Results Data Set** check box opens the **Select a Results Data Set** dialog. To select options for the type of data to be saved and for the type of results to be displayed and printed, use the **Options** page in the **Method Editor**.
- To save data, select a **Results Data Set** name where the data will be stored by clicking on the folder icon in the field box and in the **Select Results Data Set** dialog that appears, type a new data set name, or select an existing one.
- If you do not want to save data, do not specify a Results Data Set name, or click on the **Save data to Results Data Set** check box to clear the check mark, gray out the field, and remove the folder icon.

**Note:** *For information on the amount of disk storage space that is required for your results, see Equation for Calculating Disk Storage for Results.*

## ***Additional Options***

**Print Log During Analyses:** Select this box to print a log of signals, analytical results, and other information about the analysis. The log includes an analytical header and, for each sample, a sample header and the data that is shown in the Results Display window as selected in the Options page of the Method Editor. Look at the selections on the Method Editor Window Options page to get an overview of the selected analytical results that will appear in the printout.

**Fehler! Verwenden Sie die Registerkarte 'Start', um Heading 1 dem Text zuzuweisen, der hier angezeigt werden soll.. 83**

**Auto Export:** To automatically export data and write it into a file that can be read by many other programs, including spreadsheet and database management programs, select this box and click on Settings button to select one or two export designs. For more information, see the Data Manager Help.

**Lamps Off At End Of Analysis:** Select this option to have the lamps automatically shut off at the end of the analysis for **Analyze All** and **Analyze Samples**.

**Pre-light lamps:** When Pre-Light Lamps is enabled for a single method run, the system warms up the lamp for the specified amount of time prior to analyzing samples. For multi-method runs, the Pre-Light Lamps feature turns on the lamp corresponding to the element in the next method prior to the end of the previous method.

When this option is checked you can click on the **Set...** button to change the warm up times. Click here for more information on changing the warm up times.

**Flame Off At The End Of An Analysis (Flame only):** Select this option to have the Flame turned off at the end of the analysis for **Analyze All** and **Analyze Samples**.

**Flame/Pumps Off At End Of Analysis (FIAS-Flame only):** Select this option to have the Flame and FIAS pumps turned off at the end of the analysis for **Analyze All** and **Analyze Samples**.

**Cell/Pumps Off At End Of Analysis (FIAS-MHS only):** Select this option to have the cell and FIAS pumps turned off at the end of the analysis for **Analyze All** and **Analyze Samples**.

**Note:** *If more than one method is listed, you can view which method is being used for the current analysis. The methods are numbered, type in, or click the arrow, to choose the Method number.*

## ***Run List***

The **Run List** on the right half of the window displays the samples associated with the method and order in which they will be run.

**Rebuild List:** To refresh the display (to show changes you have made to the method or sample information file), click on this button.

**Print List:** To print the sequence, location, sample type, ID, and status information shown, click on this button. The printed report also shows the current date and time as well as the method name.

**Insert Sample:** To insert a new sample into the sequence (only during an analysis), click on this button and in the Priority Sample dialog that appears, enter new sample information.

**Select Loc.:** To select samples for an analysis click on this button, the Select Samples dialog appears. From this dialog you can select samples for an analysis.

## ***Progress Bar (in the Status Panel)***

The status of the analysis is shown in the Status Panel. The **Progress Bar** shows how much (the approximate percentage) of the analysis has been completed for the current sample.

The current operation being performed is shown below the Progress Bar.

## Manual Analysis Tab

You use this window to set up and perform an analysis manually.

To display this window:

- On the **Analysis** tab, then in the **Analyze** group, click **Analysis**. The window appears displaying the Manual analysis tab parameters and the associated **Manual Analysis Run List**.

### Window Controls and Entries

#### Analyze Blank

- Click on this button to analyze the calibration or reagent blank solution shown in the entry field. When you do this, you are defining the calibration or reagent blank for the analysis. To interrupt the blank analysis, click again on **Analyze Blank**.
- To change the blank shown in the entry field, select an option from the drop-down list. Only the blanks that you have defined in the Calib: IDs and Locations page in the active method appear here.

#### Analyze Standard

- Click on this button to analyze the calibration standard shown in the entry field. The results of this analysis are used to set up a calibration. To interrupt the standard analysis, click again on **Analyze Standard** button.
- To change the standard shown in the entry field, select one from the drop-down list. The list shows all of the standards, including reslope, that you defined in the active method. A calibration curve is created after all blanks and standards defined in the method are run. To view a calibration curve, on the **Results** tab, in the **Calibration** group, click on the **Calib** button.

**Fehler! Verwenden Sie die Registerkarte 'Start', um Heading 1 dem Text zuzuweisen, der hier angezeigt werden soll.. 85**

- To check the concentration values that were entered for the standard in the method, click the **Conc...** button. In the View Standard/QC Concentrations dialog that appears, the concentrations and units of each standard are shown. To change the concentration of a standard, use the Method Editor > Calibration-Calib Units and Concentration.

### **Analyze Sample**

- Click on this button to analyze the sample indicated by the No: (Number) entry field. To interrupt the analysis, click again on **Analyze Sample**.

#### **Sample No.**

This shows the sample number of the current sample in the Sample Information file.

- Enter a different sample number, if needed. The Sample ID entry field shows the ID of the sample you selected.

#### **Sample ID**

This identifies the sample that you are currently analyzing. If you are using a Sample Information file, the ID shown in the file appears here. Enter a different ID, if needed.

- To add or change dilution or other data for the sample, click the **Details...** button. In the Sample Details dialog that appears, change the appropriate entries by replacing the existing text or selecting an item from a drop-down list. For example, type a new Batch ID, then make a selection in the list of Volume Units.

### **Analyze QC**

- Click on this button to analyze the Quality Control sample in the entry field. To interrupt the standard analysis, click again on **Analyze QC**.
- To change the standard shown in the entry field, select one from the drop-down list. The list shows the QC samples currently defined in method.
- To check the concentration values that were entered for the QC in the method, click the **Conc...** button. In the View Standard/QC Concentrations dialog that appears, the concentrations and units of each are shown.

**Note:** *When QC Samples are run from the Manual Analysis window the following information is used from the active method: QC Sample ID, Count as Sample, Subtract Reagent Blank, the content from the Concentrations and Limits tab page. Information defined on the Schedule QCs tab and both Action tab pages of the Method Editor are ignored for QCs run in Manual Mode.*

#### **Go to A/S Loc.**

- Click on this button to move the autosampler probe to the selected autosampler location shown in the entry field. The autosampler location are the sites of the testing solution (blank, standards, or samples) that you want to analyze manually. You can only select one autosampler location at a time for Manual Analysis. The Auto Sampler Monitor reflects the change. If no autosampler is configured this button will be grayed out and you will not be able to select it. The **Status Panel** reflects this change.

### **Override Method**

When using the **Read Delay** process, this check box controls whether the instrument will use the values in the active method or the changes you make in this window. If it is left blank, the values in the active method are used. If the Override Method box is checked, the values entered in this page are used. The values entered in the method are not changed.

### **Go to Wash**

- Click on this button to move the autosampler probe to the wash location. The Autosampler Monitor reflects the change.

### **Read Delay (sec)**

This is the time, in seconds, that the system waits after it receives an analyze command before it starts to measure the signal. This delay allows the sample to reach the plasma before measurement begins. If the method contains a flush time that is greater than zero, the system will perform a sample flush before beginning the read delay. By default, the read delay from the method will be used.

- To use a read delay that is different than that shown in the method, select the Override Method box and enter a new read delay value.

### **Sample Information file**

This field shows the Sample Information file that describes the sample sequence.

- To select a Sample Information file, click on the folder icon in the field box. In the **Open Sample Information** dialog that appears, select an existing sample information file. If you wish to create a new file, use the Sample Information Editor.

**Note:** *The sample information file should contain entries for samples only. All other solutions, such as blanks and standards, are defined in the Method Editor.*

### **Save Data to Results Data Set**

This shows the name of the results data set where the analysis results will be stored. Saving data is optional.

- To save data, select a results data set name where the data will be stored by clicking on the folder icon in the field box and in the **Select Results Data Set** dialog that appears, type a new data set name or select an existing one. A check mark appears in the **Save Data** box next to During Analysis, confirming that data will be saved.
- If you do not want to save data, disable Save Data, or do not specify a results data set name.

**Note:** *To be able to reprocess data, it must be saved.*

**Note:** *For information on the amount of disk storage space that is required for your results, see Equation for Calculating Disk Storage for Results.*

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### ***Print Log During Analyses***

Select the Print Log box to print a log of signals, analytical results, and other information about the analysis. The log includes an analytical header and, for each sample, a sample header and the data that is shown in the Results Display window. Look at all of the selections on the Method Editor Window Options page to get an overview of the selected analytical results that will appear in the printout.

### ***Run List***

The **Run List** on the right half of the window displays the corresponding sample information and order in which they will be run.

**Clear List:** To clear the display click on this button.

**Print List:** To print the sequence, location, sample type, ID, and status information shown, click on this button. The printed report also shows the current date and time as well as the method name.

**Insert Sample:** To insert a new sample into the sequence (only during an analysis), click on this button and in the Priority Sample dialog that appears, enter new sample information.

**Select Loc.:** To select samples for an analysis click on this button, the Select Samples dialog appears. From this dialog you can select samples for an analysis.

### ***Progress Bar (in the Status Panel)***

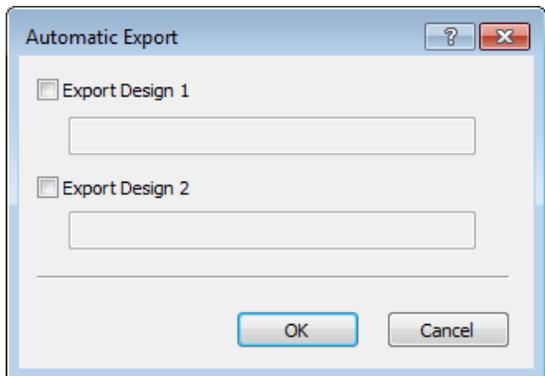
The status of the analysis is shown in the Status Panel. The **Progress Bar** shows how much (the approximate percentage) of the analysis has been completed for the current sample.

The current operation being performed is shown below the Progress Bar.

## Automatic Export

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You use this dialog if you want the software to automatically export data contained in a results data set and write it into a file that can be read by many other third-party software packages, including spreadsheet and database management programs. The export file contains data records.



To automatically reformat data:

**Note:** You must first create the Export Design(s) in the Data Manager. An export design defines a subset of data items that you want to export from a data set. For more information, refer to Data Manager Help. When exporting data, you have the ability to select two of your designs as Export Design 1 and Export Design 2. You may want to do this if you want different information to be exported or you want the data to be exported to two separate file locations. Remember, in each Export Design created you assign the directory path where you want your results stored.

1. In the **Export Design 1** entry field type the name of the design you created in the Data Manager or click on Browse... next to the entry field and when the dialog appears select the name of the design (\*.xptx) and click on OK.
2. Repeat step 1 if an **Export Design 2** was created in the Data Manager.
3. Click on **OK**.

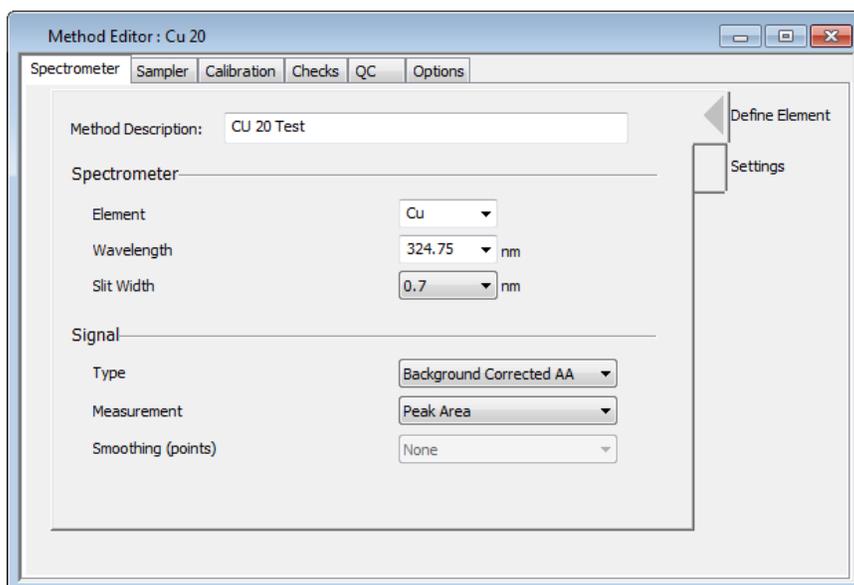
A check-mark appears in the Auto Export check-box indicating that for each analysis you perform, data will be exported automatically. To stop exporting data in this manner, click on the check-box to clear the check-mark.

# **Method Editor**

## Method Editor Window

You use the Method Editor to create a new method or to modify the parameters in an existing method. You must use one or more methods to perform an analysis.

If your spectrometer supports more than one analytical technique, for example furnace and flow-injection, you must select the analytical technique that you are interested in so that the system will display the correct pages and parameters.



### The Pages of the Method Editor

The Method Editor window has tabs along the top that give you access to the main sections of the Method Editor, most of which consist of more than one page.

Tab/Pages	Use to...
Spectrometer	Set up the spectrometer to measure the signal correctly.
Sampler	Set the specific parameters for the atomizer you intend to use and the associated accessories (Flame, Furnace, FIAS) such as an autosampler or diluter.
Calibration	Select the calibration technique, define the calibration solutions, and select the concentration units that the system uses to report the results.
Checks	Select the type of analytical tests that you want the system to perform during an analysis, such as precision tests and recovery measurements.
QC	Select the locations of quality control solutions and give instructions for performing quality control procedures.
Options	Enter remarks about the method and select options for the results display, printed log, and results data set.

### Useful Conventions

Within the tables located in the Method Editor, entries that are in a normal font can be modified in that table. Entries that are in a bold font are for view only and cannot be modified from within that table.

## ***Introduction to Methods***

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### ***What is a method?***

All the analytical information needed by the system to perform an analysis and report the results of an analysis is contained in a method (and a sample information file, if it is used). You can use an existing method as it is, modify an existing method to suit the purposes of your application, or create a new method. You must use a method to perform an analysis.

### ***The Active Method***

When you open a method it becomes the active method, and the name of the method is displayed in the toolbar. Only one method can be active at any one time. When you start an analysis, the system uses the analytical conditions in the active method for the analysis. If the system finds inconsistent or incompatible parameter values in the method, you must correct the parameter values before the system will start the analysis.

### ***Customized methods — Methods Library***

To create a customized method for a particular analysis, you use the Method Editor. When you save a customized method, the system stores it in the Methods Library. You can modify, save, recall and rename customized methods. As a basis for a customized method, you can use either the recommended conditions or a method you have previously saved in the Methods Library or in a results library.

### ***Recommended conditions***

Syngistix contains recommended parameter values for different types of analyses. You can use these as they are, or as the basis for customized methods.

### ***Methods in the Results Library***

You can save a copy of the method that you used to perform an analyses in the as part of the results data set. You might want to do this so that you can recall a method to use for another analysis later, or to save information about the analytical parameters you used for analyzing particular samples.

### ***The Method Editor***

You use the Method Editor to create a new customized method or modify a stored customized method.

### ***To Delete, Copy, and Rename Methods***

On the **Utilities** tab in the **Applications** group, click **Data Manager** and use that application to perform these tasks. For additional information, please refer to the Data Manager Help.

## Spectrometer Pages

You use these two pages to define the parameters that control how the system measures the signals and collects data.

**Define Element:** Use this page to set up the instrument to measure the signal at the correct wavelength.

The screenshot shows the 'Define Element' page within the Spectrometer software. The interface includes a tabbed menu at the top with 'Spectrometer', 'Sampler', 'Calibration', 'Checks', 'QC', and 'Options'. The 'Spectrometer' tab is active. On the right side, there are two buttons: 'Define Element' and 'Settings'. The main area contains the following settings:

- Method Description: CU 20 Test
- Spectrometer:
  - Element: CU
  - Wavelength: 324.75 nm
  - Slit Width: 0.7 nm
- Signal:
  - Type: Background Corrected AA
  - Measurement: Peak Area
  - Smoothing (points): None

**Settings:** Use this page to set up the instrument to measure the signal at the correct time.

The screenshot shows the 'Settings' page within the Spectrometer software. The interface includes the same tabbed menu as the 'Define Element' page. On the right side, there are two buttons: 'Define Element' and 'Settings'. The 'Settings' button is active. The main area contains the following settings:

- Read parameters:
  - Time: 5.0 sec
  - Delay time: 0.0 sec
  - BOC time: 2 sec
  - Replicates:
    - Same for all samples: 3
    - Vary by sample: Set...
- Lamp current:
  - Use value entered in Lamp Setup window
  - Use current: 0 mA

## ***Sampler - Flame and FIAS Pages***

---

These pages only appear if you have selected a flame or flow-injection technique and the correct accessories in the system configuration.

### ***Flame***

Use this page to set the parameters for the correct flame characteristics for the element you intend to determine.

### ***FIAS***

Use this page to enter the event versus time program that controls the flow injection system.

### ***Autosampler***

You use this page to tell the system how and when to wash the autosampler sample tube and sample probe. You can make the wash procedure dependent on the concentration of the analyte in the solution. You also select the autosampler location of the emission setup solution when you are using the flame emission technique.

You select the autosampler tray on the **Instrument** tab, in the **Devices** group, click on **Devices**, then click the **Autosampler** tab.

### ***AutoPrep***

Use this page to select online dilution for the flame technique. If this page appears, make sure that the diluter is switched on even if you do not intend to use the diluter, otherwise the system will report communication errors.

## ***Sampler - Furnace***

These pages only appear if you have selected the furnace technique.

### ***Furnace Program***

Use the program page to set up the temperature-versus-time program that controls the graphite furnace.

The screenshot shows the 'Furnace program' configuration window. It includes tabs for Spectrometer, Sampler, Calibration, Checks, QC, and Options. The 'Furnace program' section contains a 'Read step' dropdown set to 4, an 'Injection temperature' of 50 °C, and an 'Extra furnace cleanout' checkbox. A 'Default program' button is also present. Below these controls is a table with the following data:

Step #	Temp (°C)	Ramp Time (sec)	Hold Time (sec)	Internal Flow (mL/min)	GasType
1	110	1	15	250	Normal
2	130	5	20	250	Normal
3	900	10	15	250	Normal
->4	1900	0	5	0	Normal
5	2450	1	3	250	Normal
6					
7					
8					

On the right side of the window, there is a vertical navigation pane with buttons for 'Furnace Program', 'Autosampler', and 'Sequence'. The 'Furnace Program' button is currently selected.

### ***Autosampler***

You use this page to enter the sample tray locations of the modifiers and diluent, and to enter the volumes of sample, diluent, and modifier to pipet into the graphite tube.

You select the autosampler tray from the **Instrument** tab, in the **Devices** group, click **Devices** then click the Furnace Autosampler tab.

The screenshot shows the 'Autosampler' configuration window. It includes tabs for Spectrometer, Sampler, Calibration, Checks, QC, and Options. The 'Sample' section contains 'Volume' (20 µL), 'Diluent volume' (0 µL), and 'Diluent location' (1). The 'Matrix modifiers' section contains two entries, '#1 volume' and '#2 volume', both set to 0 µL and location 1. Each entry has two checkboxes: 'Add to calibration blank and standards' and 'Add to reagent blank and samples', both of which are checked.

On the right side of the window, there is a vertical navigation pane with buttons for 'Furnace Program', 'Autosampler', and 'Sequence'. The 'Autosampler' button is currently selected.

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## ***Sequence***

Use this page to set up a sequence of steps to coordinate the operation of the autosampler and the furnace program.

The screenshot shows a software window titled "Autosampler and furnace sequence" with several tabs: Spectrometer, Sampler, Calibration, Checks, QC, and Options. The main content area is a table with two columns: "Step" and "Actions and Parameters".

Step	Actions and Parameters
A	Pipet diluent + modifier 1 + spike + sample/std
B	Run furnace steps 1 to end
C	
D	
E	
F	
G	
H	
I	

Below the table, there are two buttons: "Simple..." and "Custom...".

At the bottom of the window, there are settings for "Pipet speed":

- Take up: 100 %
- Dispensing: 100 %

On the right side of the window, there are three stacked buttons: "Furnace Program", "Autosampler", and "Sequence". The "Sequence" button is currently selected, indicated by a grey arrow pointing to it from the left.

## Calibration Pages Overview

**Equation and Units:** Use this page to select the calibration equation and parameters for reporting the results.

Spectrometer | Sampler | Calibration | Checks | QC | Options

Calibration Equation

Equation: Nonlinear Through Zero

Maximum decimal places: 3

Maximum significant figures: 4

Additions:  System-prepared  Analyst-prepared

Units

Calibration: mg/L

Sample: mg/L

Equation and Units  
Standard Concentrations  
Initial Calibration  
Calibration Check  
Recalibration

**Standard Concentrations:** Use this page to enter IDs, locations, and concentrations for the calibration standards.

Spectrometer | Sampler | Calibration | Checks | QC | Options

Standard concentrations

	ID	Conc	A/S Loc.	Stock (uL)	Dil. (uL)
Calib Blank	Calib Blank 1		1	20	0
Reslope Std.					
Reagent Blank					
Standard 1	Calib Std 1	10	2	10	10
Standard 2	Calib Std 2	20	2	20	0
Standard 3					
Standard 4					
Standard 5					
Standard 6					
Standard 7					
Standard 8					

Calculate standard volumes...

Equation and Units  
Standard Concentrations  
Initial Calibration  
Calibration Check  
Recalibration

**Initial Calibration:** Use this page to select exactly which calibration curve to use when the system first uses the method for an analysis.

**Fehler! Verwenden Sie die Registerkarte 'Start', um Heading 1 dem Text zuzuweisen, der hier angezeigt werden soll.. 97**

The screenshot shows the 'Initial calibration options' dialog box. At the top, there are tabs for 'Spectrometer', 'Sampler', 'Calibration', 'Checks', 'QC', and 'Options'. The 'Calibration' tab is active. The dialog is divided into two sections: 'When opening this method manually' and 'When using this method in a multimethod sequence'. In the first section, there is a checkbox 'Load the calibration curve set selected below' with an empty text box. In the second section, there are three radio buttons: 'Start by constructing new calibration curves' (which is selected), 'Start using the stored calibration curve set selected below' (with an empty text box), and an unselected one. On the right side, there is a vertical navigation pane with buttons for 'Equation and Units', 'Standard Concentrations', 'Initial Calibration', 'Calibration Check', and 'Recalibration'. The 'Initial Calibration' button is highlighted.

**Calibration Check (Correlation Coefficient):** Use this page to set the minimum acceptable value for the correlation coefficient for the calibration curve. You also select the actions that the system will perform if the correlation coefficient falls below this value.

The screenshot shows the 'Calibration check' dialog box. It has the same tabs as the previous dialog. The 'Checks' tab is active. The dialog is titled 'Calibration check' and has a checked checkbox. It contains a 'Minimum correlation coefficient' field with the value '0.995000'. Below this, there are two numbered sections: '1. Repeat calibration' with a dropdown set to '0' and the text 'times and continue if OK', and '2. If still not OK' with four radio button options: 'Print message and continue' (selected), 'Use nonlinear calibration and continue', 'Go to next method', and 'Stop'. The right-side navigation pane is the same as in the previous dialog, with the 'Calibration Check' button highlighted.

**Recalibration:** Use this page to set up recalibrations periodically during the analysis.

The screenshot shows the 'Periodic recalibration' dialog box. It has the same tabs. The 'QC' tab is active. The dialog is titled 'Periodic recalibration' and has a checked checkbox. It contains a 'Recalibration type' dropdown menu with options 'Complete Recalibration', 'Reslope', and 'Blank Only'. Below this is a 'Frequency' section with two radio buttons: 'Every' (selected) with a dropdown set to '1' and the text 'samples', and 'Before samples in autosampler locations' with an empty text box. At the bottom, there is a checkbox 'Analyze standards at end' and a note: '\*Note that standards will be analyzed as samples following any "at end" QCs. This only applies to automated analyses started with the Analyze All or Analyze Samples commands.' The right-side navigation pane is the same as in the previous dialog, with the 'Recalibration' button highlighted.

## Checks Pages Overview

**Precision:** Use this page to calculate the precision of the results for samples, calibration standards, recovery samples and QC samples.

The screenshot shows the 'Precision' configuration page. At the top, there are tabs for 'Spectrometer', 'Sampler', 'Calibration', 'Checks', 'QC', and 'Options'. The 'Checks' tab is active. The main area is titled 'Precision check' and contains several sections:

- Precision check:** Includes checkboxes for 'Samples' (checked), 'Calibration standards', 'Recovery samples', and 'QC samples'.
- Limits:** Features a dropdown menu for 'Precision check signal' set to 'Concentration (Calibration units)'. Below it is a 'Signal limit' input field with the value '0' and the unit 'ug/L'. There are two conditional action checkboxes: 'If signal > limit and RSD > 0.000 %, then action' and 'If signal <= limit and SD > 0 then action'.
- Out of Limit Actions:** Includes a radio button for 'Reanalyze' (selected) with a spinner set to '1' times, and a radio button for 'Print message only'. There is also a checkbox for 'If spike outside of limit, also reanalyze sample'.

On the right side, a vertical navigation pane shows a list of pages: 'Precision' (selected with a left-pointing arrow), 'Beyond Calibration', 'Matrix Recovery', 'Automatic Recovery 1', 'Automatic Recovery 2', and 'Sample Limits'.

**Beyond Calibration Range:** Use this page to select the action to perform on measurement solutions that have an analyte concentration higher than that of the most concentrated calibration standard.

The screenshot shows the 'Beyond calibration range' configuration page. At the top, there are tabs for 'Spectrometer', 'Sampler', 'Calibration', 'Checks', 'QC', and 'Options'. The 'Checks' tab is active. The main area is titled 'Beyond calibration range' and contains several sections:

- Check range on:** Includes checkboxes for 'Samples' (checked) and 'Recovery samples'.
- Overall limit:** A spinner input field set to '110' with the label '% of calibration range'.
- Dilute and reanalyze after:** Includes radio buttons for '1 replicate' (selected) and 'All replicates'.
- Alternate sample volumes (µL):** Five spinner input fields, all set to '0'.
- Use alternate volume blanks:** A checkbox that is currently unchecked.
- If spike > overcal limit, also reanalyze sample:** A checkbox that is currently unchecked.

On the right side, a vertical navigation pane shows a list of pages: 'Precision', 'Beyond Calibration' (selected with a left-pointing arrow), 'Matrix Recovery', 'Automatic Recovery 1', 'Automatic Recovery 2', and 'Sample Limits'.

**Matrix Recovery:** Use this page to set up recovery calculations on selected samples that were spiked during the sample preparation procedure.

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Spectrometer | Sampler | Calibration | Checks | QC | Options

Matrix recovery

Concentration units  Calibration  Sample

	Added Analyte Concentration
Recovery Set 1	
Recovery Set 2	
Recovery Set 3	
Recovery Set 4	
Recovery Set 5	
Recovery Set 6	

Note that the autosampler positions of the matrix recovery sample sets are defined in the sample information file. Add the Matrix Check Samples column to the Parameters That Vary By Sample section. Double click on the location in that column for the spiked sample to display a dialog where you can define the recovery set to be used and the Reference Location containing the unspiked sample.

Precision  
Beyond Calibration  
Matrix Recovery  
Automatic Recovery 1  
Automatic Recovery 2  
Sample Limits

**Automatic Recovery 1:** Use this page to define the properties of the spike solution that you intend to use for the automatic recovery measurements. This feature is for the furnace technique.

Spectrometer | Sampler | Calibration | Checks | QC | Options

Automatic recovery 1

Concentration units  Calibration  Sample

Spike standard Autosampler location 1

Volume 0  $\mu\text{L}$

Concentration 0  $\text{ug/L}$

Expected concentration increase 0.000  $\text{ug/L}$

Recovery limits Lower 85 %  
Upper 115 %

If sample concentration < 0  $\text{ug/L}$   
then set sample concentration to 0 when performing recovery calculations

Precision  
Beyond Calibration  
Matrix Recovery  
Automatic Recovery 1  
Automatic Recovery 2  
Sample Limits

**Automatic Recovery 2:** Use this page to select exactly when the system will perform recovery measurements and the actions to take when the calculated recovery is outside the limits you select. This feature is for the furnace technique.

Spectrometer | Sampler | Calibration | Checks | **QC** | Options

Automatic recovery 2

Frequency

All samples

Every 1

Samples with concs between 0 and 0 ug/L

Samples in AS locations

Add recovery standard to "count as sample" QC samples

Add recovery standard to all QC samples

Failure actions

1. Dilute and rerun sample using alternate volumes below (uL)

0 0 0 0 0

Use alternate volume blanks

2. Rerun sample using

Precision

Beyond Calibration

Matrix Recovery

Automatic Recovery 1

Automatic Recovery 2

Sample Limits

**Sample Limits:** Use this page to quickly and easily set up sample limit checks. When a sample result falls above or below a specified range, a message is displayed in the Results window to indicate the failure.

Spectrometer | Sampler | Calibration | Checks | **QC** | Options

Sample limits

Concentration units:  Calibration  Sample

Calculate Limits...

Show sample limit range along with out of limit remark

	Analyte	Units	Conc	Lower	Upper
1	Cu 324.75	ug/L			

Precision

Beyond Calibration

Matrix Recovery

Automatic Recovery 1

Automatic Recovery 2

Sample Limits

**Fehler! Verwenden Sie die Registerkarte 'Start', um Heading 1 dem Text zuzuweisen, der hier angezeigt werden soll.. 101**

## ***QC Pages Overview***

You use the QC pages to enter parameters that describe quality control samples and set up QC analysis procedures to perform runtime checks of instrument performance and validation of the analytical results.

To perform tests on the normal samples and calibration solutions, use the **Checks** pages.

**QC Sample Definition:** Use this page to enter the names and autosampler locations for the QC samples.

The screenshot shows the 'QC Sample Definition' page. At the top, there are tabs for 'Spectrometer', 'Sampler', 'Calibration', 'Checks', 'QC', and 'Options'. The main area is titled 'QC sample definition' and contains a table with columns for 'QC 1', 'QC 2', and 'QC 3'. The rows are 'QC Sample ID', 'Autosampler Loc', 'Count as Sample', and 'Subtract Reagent Blank'. The 'Count as Sample' and 'Subtract Reagent Blank' rows have checkboxes for each QC column. On the right side, there is a vertical navigation pane with buttons for 'QC Sample Definition', 'Concentrations and Limits', 'Schedule QCs', 'Actions: Calib. & Periodic', and 'Actions: End & Retry'.

	QC 1	QC 2	QC 3
QC Sample ID			
Autosampler Loc			
Count as Sample	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Subtract Reagent Blank	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

**Concentration and Limits:** Use this page to enter the concentration and the upper and lower concentration limits for the QC samples.

The screenshot shows the 'QC sample concentrations and limits' page. At the top, there are tabs for 'Spectrometer', 'Sampler', 'Calibration', 'Checks', 'QC', and 'Options'. The main area is titled 'QC sample concentrations and limits' and contains a dropdown for 'QC sample ID', radio buttons for 'Concentration units' (Calibration and Sample), and a 'Calculate limits...' button. Below this is a table with columns for 'Analyte', 'Units', 'Conc', 'Lower', and 'Upper'. The first row contains '1', 'Cu 324.75', and empty cells for the other columns. On the right side, there is a vertical navigation pane with buttons for 'QC Sample Definition', 'Concentrations and Limits', 'Schedule QCs', 'Actions: Calib. & Periodic', and 'Actions: End & Retry'.

Analyte	Units	Conc	Lower	Upper
1 Cu 324.75				

**Schedule QCs:** Use this page to select when each QC sample is to be analyzed. You can also set a schedule for periodically analyzing QC Samples using the Sample Information Editor. The schedule set in the Sample Information Editor takes precedence over the schedule set in the Method Editor.

Spectrometer | Sampler | Calibration | Checks | **QC** | Options

Schedule for QC analyses

QC Sample ID			
After Initial Calib			
After Recalibration			
Periodically			
Frequency			
At End			

Periodic timing of analyses

Frequency  Same for all QC's 1  Variable

Maximum time between QC's 30 minutes

Count  Samples  Replicates

Interrupt sample to analyze QC

QC Sample Definition

Concentrations and Limits

Schedule QCs

Actions: Calib. & Periodic

Actions: End & Retry

**Actions: Calib. & Periodic / Actions: End & Retry:** Use these pages to select the actions that you want the system to perform when the measured concentration of a QC sample is outside the acceptable limits. You also select the maximum number of times the system can reanalyze a group of standards or samples to prevent the system from going into an infinite loop.

Spectrometer | Sampler | Calibration | Checks | **QC** | Options

Failure actions for after-calibration QC's

QC Sample ID			
Times to retry QC			
When All Tries Fail			
Additional Message			

Failure actions for periodic QC's

QC Sample ID			
Times to retry QC			
When All Tries Fail			
Additional Message			

QC Sample Definition

Concentrations and Limits

Schedule QCs

Actions: Calib. & Periodic

Actions: End & Retry

Spectrometer | Sampler | Calibration | Checks | **QC** | Options

Failure actions for at-end QC's

QC Sample ID			
Times to retry QC			
When All Tries Fail			
Additional Message			

Maximum retries after QC failure

After a group of standards or unknowns has been reanalyzed 1 times, then Continue

QC Sample Definition

Concentrations and Limits

Schedule QCs

Actions: Calib. & Periodic

Actions: End & Retry

## Options

You use the entries on the Options page to set up your Results Display and Printed Log. You also set some options for information to be stored with a Results Data Set for an analysis.

The screenshot shows the 'Options' dialog box with the following settings:

- Include in results and printed log:**
  - Headers:**
    - Analytical header
    - Method header
      - Short
      - Expanded
    - Sample header
      - Short
      - Expanded
    - Start each sample on a new page
  - Summary items:**
    - Analysis list
    - Matrix test reports
    - Calibration curves
    - Calibration summary
- Sample data items:**
  - Replicate Data
  - Means and Statistics
  - Transient Peak Plots
    - All
    - First
    - Last
  - Display over calibration message (110 %)
- Save with results:**
  - Transient Peak Profiles
- Remarks:** (Empty text area)

### ***Include in Results and Printed Log***

Select the type of information you wish to include in the Results Display and the Printed Log for your analysis. For detailed descriptions of the following headers, see Results Display window.

**Analytical Header:** Select this to include a header when a new analysis is begun. This header includes the analysis start time, technique, the sample information file name, the results data set name, the results library name, and other general information. Each time the current method is modified and another sample is analyzed, a new analytical header is displayed.

**Method Header:** Select this to include a header that contains the name of the method, the method description and the date the method was last saved. The expanded header includes information from the method on the calibration equation, peak processing, plasma viewing, and spectral corrections. You can select from a **Short** or **Expanded** method header.

**Sample Header:** Select this to include a header with sample information, including sample ID, sample weight, dilution, and sample prep volume. You can select from a **Short** or **Expanded** sample header.

You have the option to **Start each sample on a new page**.

### ***Sample Data Items***

Select the type of information you wish to include in the Results Display and the Printed Log for your analysis.

**Replicate Data:** Select this option to include data for each replicate.

**Means and Statistics:** Select this option to include the mean values of each set of replicates, the standard deviation, and the relative standard deviation.

**Transient Peak Plots:** Select this option to include graphs showing the shape of the transient peak signal. You can select from All, First, or Last.

**Display over calibration message:** Select this option to display an over calibration message when the sample concentration is greater than the entered percentage of the highest standard. When this option is checked the % spin box is enabled. In the % spin box enter a value between 100 and 999 %.

## ***Summary Items***

**Analysis List:** Select this option to include a summary of the operations that were performed on all of the samples.

**Matrix Test Reports:** Select this option to include information about matrix check samples (duplicates, recovery samples and spikes) analyzed.

**Calibration Summary (Auto Analysis only):** Select this option to include a calibration summary in the Results Display window. If this is selected, the calibration summary is automatically included for automated analyses after the last standard is analyzed.

**Note:** *For manual analyses, you must select the Calibration Summary command in the Analysis menu.*

**Calibration Curves:** Select this option to include a graph of absorbance versus concentration showing the calibration standards and calculated curves.

## ***Save with Results***

**Transient Peak Profiles / Signal Profiles:** Select this option to save the raw absorbance versus time data for the atomic signal and background.

**Note:** *The raw data must be saved to reprocess the data after they have been collected.*

## ***Remarks***

Use this entry field to type any comments that you think may be useful to persons who may use this method.

# **Sample Information Editor**

## Sample Information Editor

The Sample Information Editor allows you to enter all the information from the sample. This information is recorded in the database after sample data has been collected.

**We recommend that you use a sample information file to store information about the samples.** The system uses this file to label the data from your samples both on the printed log of the results and in the results data set. Information in this file is also often needed by the system to calculate final concentrations.

For the sample description and sample preparation parameters, you decide whether the information will be the same for all samples or will vary for particular samples:

- If the information you enter will be the same for all samples, you assign the parameter to the **Parameters common to all samples** table.
- If the information you enter will vary for individual samples, you assign the parameter to the **Parameters that vary by sample** table.

To display this window:

- On the **Analysis** tab, in the **Sample Information** group, click the **Sample Info** button.

**File format:** The sample information is written as a text file, a format that you can also create using other software such as a BASIC program, a spreadsheet program, or a database program. You can also create this file on a laboratory information management system and load it into your instrument control computer to perform analyses.

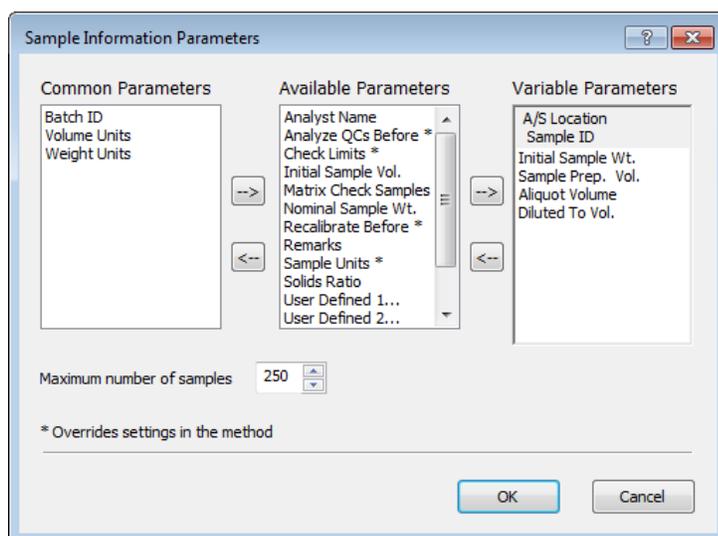
**Entering information:** Enter IDs only for samples and matrix check samples in the sample information file. Enter IDs for the blanks, standards, and QC samples in the Method Editor. If you enter IDs for blanks, standards, or QC samples in the Sample Information Editor, these solutions are analyzed as samples.

**Sample Information parameters:** The parameters in the Sample Information Editor fall into three categories:

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- **Sample Description parameters:** These parameters include the sample and batch names used to identify the sample, the autosampler location, and other optional information for describing the sample.
- **Sample Preparation parameters:** These parameters include information about the way in which the sample was prepared and the units in which the final sample concentrations will be reported.
- **Analysis Schedule parameters:** These parameters are used to schedule QC's, periodic recalibration, and matrix check samples. You can also select a Read Delay or Wash Time for a sample that differs from the method .

You can select the exact parameters that you need to describe your samples and add them to the Sample Information Editor. You select the sample description, preparation, and scheduling parameters from a list of available parameters.

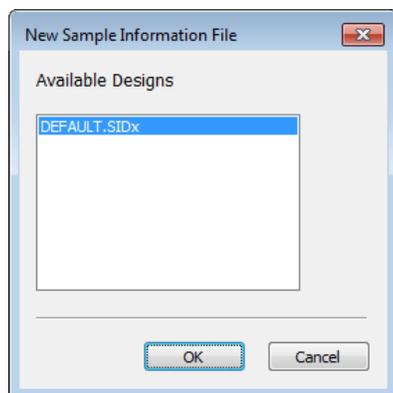


In addition, you can define your own parameters by selecting **User Defined** in the list of parameters.

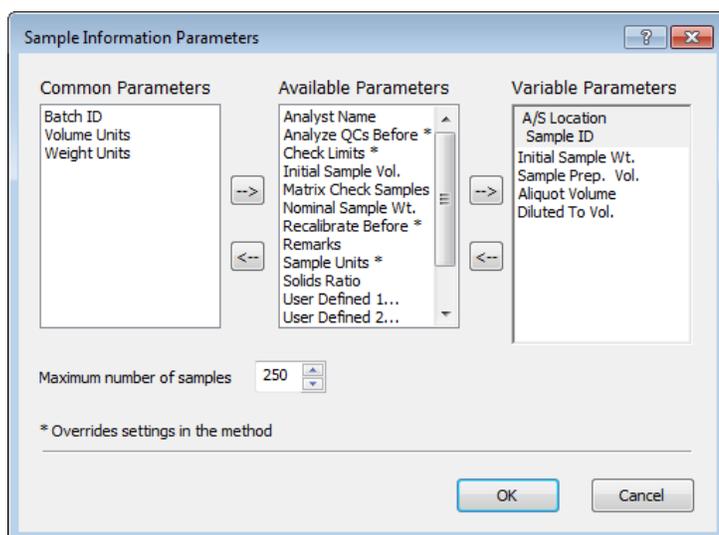
Once you have included all the parameters that you need, you can save this configuration as a sample information design. Select **Save As** from the **Save** drop-down in the **Sample Information** group to save as a .sidx file. By saving the design, you can reuse it later for similar sample information files.

## Creating a New Sample Information File

1. On the **Analysis** tab, in the **Sample Information** group, click **New**. The **New Sample Information File** dialog appears.



2. Select a design from the **Design List** and click on **OK**. This list includes a default design and any other designs that have been previously created and stored.
3. To create a name for the Sample Information file, click the **Save** drop-down, then click **Save As**.
4. In the Save Sample Information file As dialog, type a name for the new sample information file, then click on **Save**.
5. You can customize the Sample Information Editor by selecting the parameters you need to describe your samples. With the Sample Information file open, on the Analysis tab, in the **Sample Information** group, click on **Parameter List**.



6. In the **Available Parameters** list, click on a parameter to select it. (To deselect the parameter, click again.) The parameters are shown in alphabetical order.

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7. Click on the arrow button that points to the list where you wish to move the selected parameter. Parameters marked with an asterisk (\*) override settings in the method. When done click OK to close the dialog.
  - If the entry for the parameter is common to all samples, move the parameter to the **Common Parameters** list.
  - If the entry for the parameter varies for each sample, move the parameter to the **Variable Parameters** list. For example, the analyst name might be the same for all samples, while the sample IDs would vary for each sample.
8. Enter the sample information into the Sample Information Editor. For example, autosampler locations, Sample ID, Initial Sample Weight, etc. Use the arrow keys to move between columns and rows.
9. If desired, annotate the file using the File Description field to provide further descriptive information. When you move the mouse cursor to this text area and click with the right mouse button, a pop-up menu of editing commands appears.
10. When done, click **Save** in the **Sample Information** group.

## ***Editing Sample Information Parameters***

You can edit the entry fields and add or delete rows in the **Parameters that Vary by Sample** table.

### **To clear information in the table:**

When you clear information, the content in an entry field is removed, not the entry field itself.

1. Click on the entry field that contains the information you want to remove — click the row number to highlight an entire row.
2. On the **Analysis** tab, in the **Edit** group, click on **Clear**.  
-- or --  
Click with the right mouse button. In the pop-up menu that appears, click **Clear**.  
-- or --  
Press the **Delete (Del)** key.

### **To insert rows in the table:**

When you insert rows, the new rows are inserted before the first row you select in the table.

1. Select a row in the table by clicking on a number in the Sample Number column of the table. The entry fields in the row become highlighted to indicate that the row is selected.
2. If you want to insert more than one row, you select the same number of rows in the table. For example, to insert three new rows, you would select three existing rows. To select additional rows, hold down the Shift key while clicking on additional row numbers.
3. On the **Analysis** tab, in the **Edit** group,, click on **Insert Rows**.  
-- or --  
Click with the right mouse button. In the pop-up menu that appears, click **Insert Row**.

### To delete rows in the table:

When you delete rows, the contents of the row and all the entry fields in the row are removed.

1. Select a row in the table by clicking on a number in the Sample Number column of the table. The entry fields in the row are highlighted to indicate that the row is selected.
2. To select additional rows, hold down the Shift key while clicking on additional row numbers.
3. On the **Analysis** tab, in the **Edit** group,, click on **Delete Rows**.  
-- or --  
Click the right mouse button. In the pop-up menu that appears click **Delete Rows**.

### Modifying a Stored Sample Information File:

1. On the **Analysis** tab, in the **Sample Information** group, click the **Sample Info** button.
2. Select the Sample Information file that you want to open, then click on **Open**.
3. You can customize the Sample Information Editor by selecting the parameters you need to describe your samples. See Customizing the Sample Information Editor.
4. Change the sample information as desired.
5. Change the information in the **File Description** field as desired, using the pop-up menu for editing commands.
6. Save the file:
  - To save the file with the same name, in the **Sample Information** group click on **Save**.
  - To save the file with a new name, in the **Sample Information** group click on the **Save** drop-down then select **Save As**. The Save As dialog appears. Type a name for the file, then click on **Save**.

**Note:** *If you modify a sample information file and then attempt to create a new one, a message appears asking if you wish to save the changes to the first sample information file. This also happens when you attempt to exit the Syngistix software.*

## Appending Samples to an Automated Analysis

You can modify and append samples to an automated analysis.

1. While the instrument is performing an automated analysis, in the Sample Information Editor modify the information in samples as desired, then click on the **Append to Analysis List** button.
2. When the Append to Analysis List dialog appears, type the range of samples that you want to append and click on **OK** to add the samples to the end of the run list in the Automated Analysis Control window.

**Note:** *You can drag the mouse cursor through a range of samples in the Sample Information Editor and, when you click on the **Append to Analysis List** button and the Append to Run List dialog appears, the range of the selected samples already appears in the dialog.*

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## ***Opening a Stored Sample Information File***

1. On the **Analysis** tab in the **Sample Information** group, click **Open**.  
The Open Sample Information dialog appears.
2. Select the Sample Information file that you want to open, then click on **Open**.

## ***Deleting, copying, or renaming Sample Information Files***

- Use the Windows Explorer. These files are stored in C:\Users\Public\PerkinElmer Syngistix\AA\Data\Sample Information.

## ***Printing a Sample Information File***

1. Click on the **Sample Information Editor** window to make it active.
2. From the **Application** button select **Print Preview** from **Print Active Window** item.
3. Click the **Print** button on the print preview dialog that appears.
4. In the Print dialog that appears, check that the correct printer is shown.
5. To select a different printer, click on the drop-down arrow in the **File Name** field and make a selection. To make other changes, such as paper size or graphic attributes, click on the **Properties** button.
6. Click **OK** to start printing.

## ***Sample Preparation: An Example***

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The following is an example of sample preparation:

1. An analyst weighs 1.54 grams of sample into a beaker. This is the Initial Sample Weight.
2. Next, hydrochloric acid is added to the sample and the solution is heated so that the sample is dissolved. After the solution is allowed to cool, the analyst quantitatively transfers it into a 250 mL flask and fills the flask to the 250 mL mark. This is the Sample Prep Volume.
3. A 10 mL aliquot of this solution (the Aliquot Volume) is pipetted into a 100 mL volumetric flask and diluted to the 100 mL mark. This is the Diluted to Volume.

To summarize, for the above example, you would enter the following values:

Initial Sample Weight	1.54 grams
Sample Prep Volume	250 mL
Aliquot Volume	10 mL
Diluted to Volume	100 mL

**Note:** *You can also record the Diluted to Volume as the ratio of the original sample volume to the final sample volume. In this example, 10 mL of sample is diluted to 100 mL, so the ratio would be 10:100 or 1:10. You can enter 1 for Aliquot Volume and 10 for Diluted to Volume.*

## ***Sample Information Editor Pop-Up Menus***

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The following pop-up menus contain several convenient commands as you work with the Sample Information Editor.

To display the pop-up menus:

- Click with the right mouse button in the **Sample Information Editor**.
- When you click with the right mouse button in the **Parameters that Vary by Sample** table, a pop-up menu containing editing commands for the table appears.
- When you click with the right mouse button anywhere on the background area in the window, the Sample Information Editor pop-up menu appears.

### ***Sample Information Editor pop-up menu***

**Parameter List...** Adds new parameters to the Sample Information Editor.

**New Sample Info File...** Selects a design and creates a name for the new sample information file.

**Open Sample Info** Opens a stored sample information file.

**Save Sample Info** Saves the contents of the Sample Information Editor using the same file name.

**Save Sample Info As...** Saves the contents of the Sample Information Editor using a new file name.

**Save As Text...** Saves the contents of the Sample Information Editor to a text file or comma-delimited ASCII file.

**Save Sample Info Design As...** Saves the configuration of the Sample Information Editor as a design file. You can use a design file to quickly customize the Sample Information Editor with the parameters you need to describe your samples.

**Print...** Prints the contents of the Sample Information Editor.

**Print Preview...** Displays the formatted sample information report in a preview window. Use the Zoom In and Zoom Out buttons to enlarge or reduce the report. Click on **Close** to return to the Sample Information Editor.

### ***Table editing pop-up menu***

**Clear** Removes the contents of the selected entry fields.

**Insert Row** Inserts a new row before the currently selected row.

**Delete Rows** Removes the selected rows in the table.

**Append Rows...** Adds a column of your choice to the table.

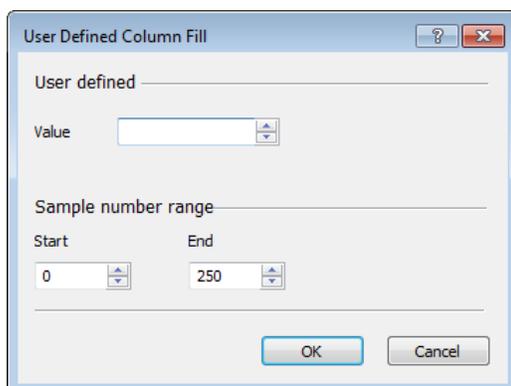
**Column Fill...** Displays the Column Fill dialog for the selected column. You use this dialog to automatically enter information for a range of samples.

**Entry Dialog...** Displays the Entry dialog for the selected entry field. You use this dialog to type information for a text entry field.

## ***Using Column Fill Dialogs***

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To automatically enter information for a range of consecutive samples, the Sample Information Editor contains Column Fill dialogs.



To display a Column Fill dialog:

- Double-click the column header;
- Or --
- Right-click the column header and select **Column Fill**;
- Or --
- Click an entry field, then in the Edit menu, click Column Fill.

### **To automatically enter information for a range of samples:**

1. Type the information in the entry field in the dialog. Enter values or text, as appropriate for the entry field.
2. In the **Start** box, select the sample number for the first sample in the group.
3. In the **End** box, select the sample number for the last sample in the group.
4. Click OK. The software enters the values in the Sample Information Editor.

### **To display a Column Fill dialog and pre-select a range of samples:**

You can pre-select the range of samples in the Sample Information Editor by selecting a range of entry fields in the column. When the dialog is displayed, this range will automatically be entered.

1. Click on the first row in the range of samples and drag the mouse cursor over the entry fields that you want to fill in the column. The rows are highlighted.
2. Right-click and select **Column Fill**.

## ***Analysis Schedule Parameters***

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**Recalibrate Before:** Select a recalibration, reslope, or autozero before the solution identified in this row is analyzed. Select None or leave the entry field blank if you do not want any of these options performed before this solution. To automatically enter the same information for a sequence of samples, double-click on the column header or right click and select Column Fill... and use the Recalibrate Before Column Fill dialog.

**Matrix Check Samples:** Use this parameter when analyzing a pair of matrix check samples. The first sample in the pair is the reference sample and the second sample is the matrix check sample. The first sample must be scheduled for analysis before the second sample. Double-click on the entry field for the second sample in the pair of matrix check samples. The Matrix Check Sample Entry dialog appears, in which you select options for the matrix check calculation and identify the two samples in the matrix check pair.

**Analyze QCs Before:** Use this parameter to analyze quality control samples before the selected samples. Type the numbers of the QC samples in the entry field. These numbers are found in the QC section of the method . Type individual QC numbers or a range of QC numbers. Use commas to separate the numbers and ranges. Example: 1, 3-5.

- To analyze QC samples at a specified frequency, double-click on the entry field. The Analyze QCs Before Column Fill dialog appears.

**Note:** *Periodic QC Scheduling in the sample information file will override Periodic QC Scheduling in the Method Editor.*

**Read Delay:** Use this parameter to use a Read Delay that differs from the read delay that is entered in the method. Enter the Read Delay in seconds. To automatically enter the same value for a sequence of samples, double-click on the column header and use the Column Fill dialog. May not be available for all techniques.

**Wash Time:** Use this parameter to use a Wash Time that differs from the Wash Time that is entered in the method. Enter the Wash Time in seconds. To automatically enter the same value for a sequence of samples, double-click on the column header and use the Column Fill dialog. Note that the Wash Frequency is selected in the method. You must select Between Samples for the Wash Frequency in order for a wash to occur. May not be available for all techniques.



# **Data Viewer**

## **Data Viewer Window**

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Use this window to view detailed information about your current sample and to track data from multiple quantitative analyses as your sample batches are processed. Scrolling results tables provide an Intensity view that displays the measured signal for each element examined by the instrument-with or without related RSD's; a Concentration view; an Unfactored Concentration view; and a QC (Quality Control) view.

The Report View window is made up of multiple tabs, each of which present the running analytic data from your samples in a different way:

- Intensities/Absorbances tab
- Conc. in Caib. Units tab
- Conc. in Sample Units tab
- QC tab

When you initially start a new software session, or after you click Clear Data, the Report View tabs are empty. They become populated as data is acquired, regardless of whether or not the window is open in your workspace. As you run samples, the tabs are updated in real time. The table-based tabs collect a scrolling list of sample results collected during quantitative analyses to a maximum of 1000 samples, after which the first samples scroll off the top of the list as new samples continue to be added at the bottom. Index numbering of the developing list goes up to a maximum count of 9,999 before rolling over to begin at 1 again.

To help you keep track of where you are in the data, your position in the scrolling list on any table is retained when you move between the Intensities/Absorbances, Conc. in Calib Units, and Conc. in Sample Units tabs, so that you can compare multiple types of data for a single sample without losing your place.

In the tables, sample data is displayed in alternating rows of white and gray to improve readability. Additional color cues employed in the tables include the use of a red font to indicate QC failures. Note that all tables take their base colors from your system colors; if you change from the default Windows system colors, you may change the table background colors.

### **Report View Common Controls**

The following controls are common to multiple tabs in the Report View window:

**Show RSDs:** Enable this check box to display the related RSD (Relative Standard Deviation) for each sample displayed in the report view tables. If you have chosen to display RSDs onscreen and you click Export..., the RSDs are exported to the worksheet corresponding to the tab where they are displayed. And whether displayed or not, RSD information is always exported to separate Intensity RSDs and Concentration RSDs sheets.

**Advanced...:** Click this button to open the Advanced Report View Display Options dialog box, and configure display preferences for the Intensities/Absorbances, Conc. in Calib Units, Conc. in Sample Units, and QC tabs.

**Export All...:** Click this button to export all current data from the Intensities/Absorbances, Conc. in Calib Units, Conc. in Sample Units, and QC tabs to Microsoft Excel. RSDs are always exported to a separate sheet in the Excel workbook. Additional information, including the relevant dataset name, method name, time and date of acquisition, reprocessing indicators, and QC status is also made available in the exported file to provide more clear and complete sample identification, even though it may not be present in the on-screen report views in the software.

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The default file format for the export function is .xlsx, but .xls is also generally available. However, due to limitations in Microsoft Excel, if you are exporting more than 256 columns of data, you can only export in .xlsx format.

You do not need to have Microsoft Excel installed on the same computer as your instrument software in order to perform a report view export. If Excel is not installed, the export file will still be saved with all applicable data, and with the Internal Standards graph drawn in .jpg form (rather than the usual editable Excel graph object). You can then transfer the file to another computer, or open the file with an Excel-compatible reader.

If you have a version of Microsoft Excel earlier than 2007 installed on your computer, you will be allowed to save to .xlsx format, but you will not be able to correctly open the resulting file in that version of Excel (the file will appear to contain garbage information). In this case, you can choose to instead save to .xls format, which will open in any version of Excel, or you can open the resulting .xlsx file in an Excel-compatible viewer or on another computer running Excel 2007.

**Clear Data:** Click this button to clear all current data from the report view tabs, except the Current Sample report. Note that you may wish to export your data before clearing in order to preserve it for future examination.

## ***Intensities/Absorbances Tab***

The Intensities/Absorbances tab displays the measured signal intensity for each element measured by the instrument. The column headings consist of the analytes as named in the related method along with the mass in amu. The relevant units are also displayed, again as defined in the method, below the analyte name in parentheses.

Select the **Show RSDs** check box to display the related Relative Standard Deviation values for each sample. You can also display additional columns to show the sample acquisition date and time, reprocessed data flags, and QC function status indicators — click **Advanced** to configure these options.

When the QC Status column is displayed, you can click on any **Failed** cell to go to the corresponding detailed data section of the Report View QC tab. Note that if a QC measure specifies that there be a valid calibration in the current workspace, and none exists, the QC Status column will appear blank, rather than showing **Passed** or **Failed**. The QC status will also be blank if QC checking is not enabled in the given method; or when it is enabled, but no QC limits have been specified.

	Sample Id	Cu 324.75 (Absorbance)
1	Calib Blank 1	0.0012
2	Calib Std 1	0.0499
3	Calib Std 2	0.1000
4	chk blk	0.0015
5	Calib Blank 1	0.0000
6	Calib Std 1	0.0511
7	Calib Std 2	0.1038
8	chk blk	0.0019
9	Calib Blank 1	0.0000
10	Calib Std 1	0.0499
11	Calib Std 2	0.1000
12	chk blk	0.0015
13	Calib Blank 1	0.0000
14	Calib Std 1	0.0511

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## ***Conc. in Calib. Units Tab***

The Conc. in Calib. Units tab displays the adjusted sample concentration for each element measured by the instrument. This tab consists of a tabular display with the sample name in the first column and masses in subsequent columns with the concentration units directly beneath. The column headings consist of the analytes as named in the related method along with the mass in amu. The relevant units are also displayed, again as defined in the method, below the analyte name in parentheses. Each row represents a single sample. For each internal standard, the IS percent recovery value is displayed, together with the related intensity RSD (if RSDs are displayed).

Select the **Show RSDs** check box to display the related Relative Standard Deviation values for each sample. You can also display additional columns to show the sample acquisition date and time, reprocessed data flags, and QC function status indicators — click Advanced to configure these options.

When the QC Status column is displayed, you can click on any **Failed** cell to go to the corresponding detailed data section of the Report View QC tab.

**Note:** *If a QC measure specifies that there be a valid calibration in the current workspace, and none exists, the QC Status column will appear blank, rather than showing **Passed** or **Failed**. The QC status will also be blank if QC checking is not enabled in the given method; or when it is enabled, but no QC limits have been specified.*

	Sample Id	Cu 324.75 (ug/L)
1	Calib Blank 1	0.000
2	Calib Std 1	10.000
3	Calib Std 2	20.000
4	chk blk	0.292
5	Calib Blank 1	0.000
6	Calib Std 1	10.000
7	Calib Std 2	20.000
8	chk blk	0.372
9	Calib Blank 1	0.000
10	Calib Std 1	10.000
11	Calib Std 2	20.000
12	chk blk	0.292
13	Calib Blank 1	0.000
14	Calib Std 1	10.000

## Conc. in Sample Units Tab

This tab is similar to the Concentrations view, but displays data measured *without* concentration or dilution factors. It consists of a tabular display with the sample name in the first column and masses in subsequent columns with the concentration units directly beneath. The column headings consist of the analytes as named in the related method along with the mass in amu. The relevant units are also displayed, again as defined in the method, below the analyte name in parentheses. Each row represents a single sample.

Select the Show RSDs check box to display the related Relative Standard Deviation values for each sample. You can also display additional columns to show the sample acquisition date and time, reprocessed data flags, and QC function status indicators — click **Advanced** to configure these options.

When the QC Status column is displayed, you can click on any **Failed** cell to go to the corresponding detailed data section of the Report View QC tab. Note that if a QC measure specifies that there be a valid calibration in the current workspace, and none exists, the QC Status column will appear blank, rather than showing **Passed** or **Failed**. The QC status will also be blank if QC checking is not enabled in the given method; or when it is enabled, but no QC limits have been specified.

	Sample Id	Cu 324.75 (ug/L)
1	Calib Blank 1	
2	Calib Std 1	
3	Calib Std 2	
4	chk blk	0.292
5	Calib Blank 1	
6	Calib Std 1	
7	Calib Std 2	
8	chk blk	0.372
9	Calib Blank 1	
10	Calib Std 1	
11	Calib Std 2	
12	chk blk	0.292
13	Calib Blank 1	
14	Calib Std 1	

## **QC Tab**

---

This tab displays relevant Quality Control data for samples run for which QC criteria has been defined in the selected method. The data displayed includes the basic sample information, such as the originating row index number and analyte sample information. When a sample falls outside of the specified QC criteria, the relevant data is displayed in red text. QC data is displayed for only as long as the corresponding sample entries appear on the Intensities/Absorbances, Concentrations, and Unfactored Concentrations tabs.

The data on the QC tab is organized into the following categories: *QC Standards*; *QC Spikes*; *QC Duplicates*; *QC Dilutions*; and *Samples, Blanks, and Calibration Standards*:

- For *QC Standards*, which are grouped by standard number, the original sample concentration is displayed, followed by the RSD and % recovery.
- *QC Spikes* display the % recovery of the spike. *QC Duplicate Spikes* are also listed here, showing the % difference. For all *QC Spikes* and *QC Duplicate Spikes* listed, this tab also displays the original row index of the parent sample.
- *QC Duplicates* and *QC Dilutions* display the % difference of the duplicate or dilution. For all *QC Duplicates* and *QC Dilutions* listed, this tab also displays the original row index of the parent sample.
- The *Samples, Blanks, and Calibration Standards* section displays the named information only where a sample fails the QC criteria specified — *Samples* display sample concentration, IS % recovery, RSD, and SD information; *Blanks* display measured intensity SD data; and *Calibration Standards* display net intensity RSD data.

The categories are each displayed in their own collapsible tree format — click the + and - signs beside each header to expand and view or collapse and hide the available data.

All QC types from the Method window QC tab are considered in this section. However, because the QC Calibration sub-tab deals with limits on the calibration as a whole (such as slope, intercept, and correlation coefficient limits) rather than on individual samples, no QC failure is flagged if an individual calibration standard goes outside specified limits, and no data, sample names or analyte headers appear in red if a calibration fails a QC check. When a calibration fails, the calibration information is displayed on the Intensities, Concentrations, and Unfactored Concentrations tabs as a *Calibration Curve*, and expanded upon on the QC tab with the addition of *Slope*, *Intercept*, and *Correlation Coefficient* values for each analyte. Also note that repeated samples and diluted samples as a result of QC failure actions are not added to this tab as QC Duplicates or QC Dilutions.

If a QC measure requires that there be a valid calibration in the current workspace, and none exists, the QC Status column will appear blank, rather than showing *Passed* or *Failed*, and the relevant cells on the QC tab will also appear blank, as no data could be properly calculated.

You can also access the data on this tab from any of the other tabular report views where a QC Status cell displays a Failed marker; simply click the Failed cell or the corresponding Sample ID to go to the relevant row on the QC tab. Note that QC failure messages are not displayed on this view — to view a failure message, you must look at the relevant individual Current Sample report.

You can display additional columns to show the acquisition date and time, and reprocessed data flags for relevant samples — click **Advanced** to configure this option.

## ***Advanced Display Options Dialog***

---

The **Advanced...** button displays a dialog to define report view display options. You can specify how the analytes are sorted in the tables; whether or not to display the acquisition date and time for each sample; whether or not to display reprocessed data and QC pass/fail indicators where relevant; and set the number of decimal places to display for Intensity, Concentration, RSD, SD, and % Recovery values.

To define display options:

1. Click **Advanced...**  
The **Advanced Report View Display Options** dialog box appears.
2. In the **Sort Analyte header by** drop-down list, select the type of sort order to use for analytes in the report view table headers.
3. If you have enabled QC (Quality Control) checking in one or more of your methods, and wish to display whether or not the QC measures have passed or failed on the Intensities, Concentrations, and Unfactored Concentrations tabs, enable the **Display Quality Control Status** check box . Whether displayed onscreen or not, QC information is always exported with the sample data.
4. If you want to display the Sample Acquisition Date and Time on the Intensities, Concentrations, and Unfactored Concentrations tabs, enable the **Display Sample Acquisition Date and Time** check box. Whether displayed onscreen or not, time and date information is always exported with the sample data.
5. In the **Intensity** field, select the number of decimal places to display for Intensity values. Valid values = 0-4
6. In the **Concentration** field: Select the number of decimal places to display for Concentration values. Valid values = 0-4
7. In the **RSDs** field: Select the number of decimal places to display for RSD (*Relative Standard Deviation*) values. Valid values = 0-4
8. In the **SDs** field: Select the number of decimal places to display for SD (*Standard Deviation*) values. Valid values = 0-4
9. In the **% Recoveries** field: Select the number of decimal places to display for Percent Recovery values in general, and for Percent Difference values on the QC tab. Valid values = 0-4
10. Click **OK** to save your changes.

## ***Data Export Functions***

---

You can export data from the Data Viewer to Excel. With the touch of a button, you can export the running data from the Intensities, Concentrations, Unfactored Concentrations, Internal Standards, and QC Report View tabs to a Microsoft Excel compatible file.

**Note:** *You do not need to have Microsoft Excel installed on the same computer as your instrument software in order to perform a report view export. If Excel is not installed, the export file will still be saved with all applicable data, and with the Internal Standards graph drawn in .jpg form. You can then transfer the file to another computer, or open the file with an Excel-compatible reader.*

At any point in your determinations, click the **Export All...** button to export all currently available report data from the Intensities, Concentrations, Unfactored Concentrations, Internal Standards, and QC Report View tabs to a Microsoft Excel compatible file. Each tab is given a separate worksheet in the resulting .xls or .xlsx file.

Additional information, including the relevant dataset name, method name, QC pass/fail, and time and date of acquisition, is also made available in the exported file to provide more clear and complete sample identification, even though it may not be present in the onscreen report views in the instrument software.

The default file format for the export function is .xlsx, but .xls is also generally available. However, due to limitations in Microsoft Excel, if you are exporting more than 256 columns of data, you can only export in .xlsx format.

**Note:** *If you have a version of Microsoft Excel earlier than 2007 installed on your computer, you will be allowed to save to .xlsx format, but you will not be able to correctly open the resulting file in that version of Excel (the file will appear to contain garbage information). In this case, you can choose to instead save to .xls format, which will open in any version of Excel, or you can open the resulting .xlsx file in an Excel-compatible viewer or on another computer running Excel 2007.*

**Tip:** *If you will be printing your exported reports to a black and white printer, append the mode you are using to each analyte name in your method so that this information is included in your print-outs (otherwise, mode is indicated by color only).*



# **Setup Windows**

## ***Setup Windows***

---

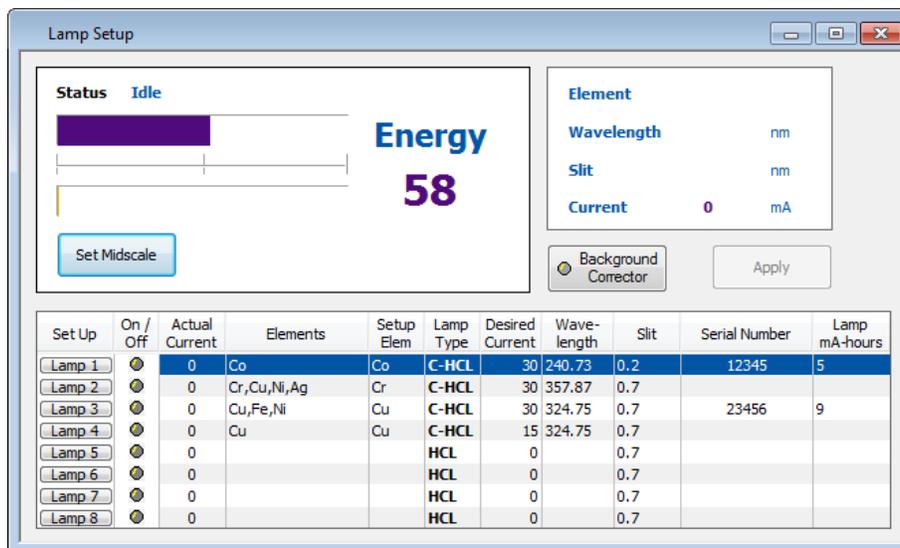
Use these windows to set up the analysis system before you start an analysis. For example to ignite the flame and adjust the position of the burner, or to align the furnace and the autosampler pipet tip. The status of the atomizer and is shown in these windows, for example the fuel flow rates, and the furnace or FIAS program status.

You can normally only use the controls in these windows when there is no analysis in progress.

**Fehler! Verwenden Sie die Registerkarte 'Start', um Heading 1 dem Text zuzuweisen, der hier angezeigt werden soll.. 129**

## Lamp Setup

You use this window to set up the lamps that you will use for the analysis. When you set up the lamps, set the same operating conditions that you intend to use when you perform the analysis.



**Status:** The status display shows information about the lamps and the relevant spectrometer settings. There are bar graphs and corresponding numerical energy values for the source lamp and the background correction lamp, if this lamp is switched on.

**Set Midscale:** Use this button to set the bar graph to mid-scale when you are setting up a lamp. The system does this automatically for a lamp when you click on **Set Up Lamp #**. When you click on this button, the system set the detector parameters to the optimum value for the active lamp.

**Apply:** Clicking on this button will set the instrument to the parameters that have been changed in the Lamp Setup window.

### Lamp Setup Table

**Set Up -- Lamp #** - When you have set the lamp parameters, click on **Lamp #** to set up the system with the lamp parameters. The system sets up the optical path, switches the lamp on, sets and peaks the wavelength, sets the slit, and performs an Automatic Gain Control (AGC).

**On/Off** - To switch the lamp on or off, click on this button. When the button is green, the lamp is switched on. This does not set up the system with the lamp parameters; use the **Setup Lamp#** button for this. The actual current reflects the current that the lamp has been set to.

**Actual Current** - It displays the actual current being applied to each lamp.

**Elements** - This is a list of the elements contained in the lamp. The system automatically enters the atomic symbols for elements in coded lamps. For uncoded lamps, type the atomic symbol for the element. For a multi-element lamp, separate the symbols by a comma. For example: Ca, Mg, Zn.

The system uses the list of elements to find the first lamp that contains the element selected in the active method. If two lamps contain the same element, the system uses the lamp installed in the location with the lowest number.

**Setup Element** - When a multi element lamp is used you can select one element from the drop down menu in this column.

**Lamp Type** - This shows the type of lamp installed. The system automatically fills in this entry for coded lamps on automatic wavelength instruments.

C - HCL -- Hollow cathode lamp (coded)

C - EDL -- Electrodeless discharge lamp (coded)

HCL -- Hollow cathode lamp (uncoded)

EDL -- Electrodeless discharge lamp (uncoded)

**Note:** *If you have uncoded lamps, select HCL or EDL. HCL or EDL may be selected by clicking on the drop down cell and selecting the arrow in the Lamp Type column.*

**Desired Current** - This is the operating current for the lamp. The system sets the recommended current. To change this, enter the desired current for the lamp. By clicking on Apply or the Lamp # button you will apply the value entered. For uncoded lamps, you must enter the atomic symbol in the **Element** entry-field before the system can set the current. You may change this value if necessary. When the lamp is nearing the end of its useful life, you may want to use a higher current; the maximum permitted current is shown on the label of the lamp.

**Wavelength** - This is the wavelength you use to setup the lamp. The system sets the recommended wavelength for the lamp. For uncoded lamps, you must enter the atomic symbol in the Element entry-field before the system can set the wavelength. To use a wavelength other than the one that is recommended, click on the drop down cell and selecting the arrow in the wavelength column and select from the wavelength list. You select the wavelength to use for the analyses in the method.

**Slit** - This is the slit width used to setup the lamp. The system sets the recommended slit width for the lamp. For uncoded lamps, you must enter the atomic symbol in the **Element** entry-field before the system can set the slit width. To use a slit width other than the one that is recommended, select a value from the list of options. You select the slit width to use for the analyses in the method.

**Serial Number** - This column displays a unique ID for each lamp. No serial number value is displayed for uncoded lamps.

**Lamp mA-Hours** - This column displays the number of milliamperes-hours (mA-hours) logged by each lamp (typically EDL and HCL lamps placed in PinAAcle analyzers. No lamp hours value is displayed for older lamps and uncoded lamps.

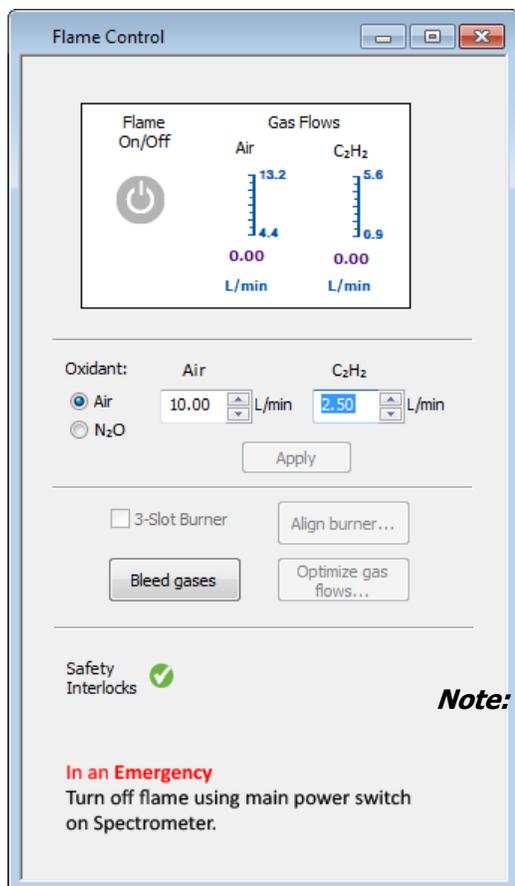
**Note:** *The Serial Number and Lamp mA-Hours columns displays information for all lamps, however for older coded lamps (older coded lamps can be identified by the serial number on the actual lamp; the serial numbers printed on the labels of these lamps start with 00000 and no hyphens are used), the lamp hours are not shown, instead the cell will be blank. For un-coded lamps the Serial Number and Lamp Hours cells are blank.*

## ***Background Correction for Flame Applications***

This switches the background correction lamp on or off. When the lamp is on, a bar graph and energy value for the background correction lamp appear in the status display.

## Flame Control

You use the Flame Control window to control the gas flows, bleed gases, align the burner and turn the flame on and off. You can only use these controls when there is no analysis in progress. The status of the gas flows are shown at the top of this window.



**Flow L/min (C<sub>2</sub>H<sub>2</sub>):** Enter a value for the flow rate of fuel (acetylene, C<sub>2</sub>H<sub>2</sub>). The flow meter shows the allowed range. Click on the **Apply** button to activate your change.

**Flow L/min (Oxidant - Air or N<sub>2</sub>O):** Enter a value for the flow rate of oxidant. The flow meter shows the allowed range. Click on the **Apply** button to activate your change.

**3-Slot Burner:** If you are using a 3-slot burner check this box. When 3-Slot Burner is checked, the system automatically switches over to gas flow ignition settings that will help prevent damage to the 3-slot burner. These flow settings result in a relatively richer flame, compared to the default condition for a standard single slot burner head. The default flow settings for a 3-Slot Burner are: 10 L/min for compressed air and 3 L/min for acetylene.

**Note:** *When a 3-slot burner is in use it is recommended that you avoid a very lean (clear blue) flame, because this type of flame can warp the burner slots. In situations where a blue flame is needed, damage to the slots can be prevented by continuously aspirating solvent. Never leave the flame unattended. If the burner top starts to glow,*

*either increase the fuel flow or restore the solvent aspiration. A few minutes after the ignition the flame tends to become lean and requires adjustment of the fuel flow. For best precision let the flame burn while aspirating solvent for at least 10 minutes before starting an analysis.*

**Safety Interlocks:** The Safety Interlocks box is used to indicate if problems exist which would prohibit you from igniting the flame. A green box with a check mark shows that the safety interlocks are satisfied and that you can ignite the flame. A red box with an X indicates a problem with the interlock/s. If there is a red box with an X, you must correct the interlock/s before you can ignite the flame. To find out which safety interlocks are not satisfied, double click on the red X; and a dialog box appears with information about the problem/s you must correct.

**Oxidant:** Select the correct oxidant for the type of flame that you require for your analyses, air or nitrous oxide. The system copies the selection you make here onto the Instrument page of the active method. Click on the Apply button to activate your change.

**Off / On:** Ignites or extinguishes the flame. In an emergency, depending upon the instrument you are using, either switch the spectrometer Off to extinguish the flame, or press the red emergency button on the spectrometer. The system will extinguish the flame safely.

**Bleed Gases:** Vents the burner gas lines to the atmosphere. Use this control after you have extinguished the flame and shut the valves of the gas supplies to the spectrometer at the cylinder or wall outlets.

**Align Burner:** Select this button to align the burner. Follow the step by step directions in the Align Burner Wizard.

**Note:** *Please note that the Align Burner feature is only available with the AAnalyst 700/800 and PinAAcle 900F and 900T.*

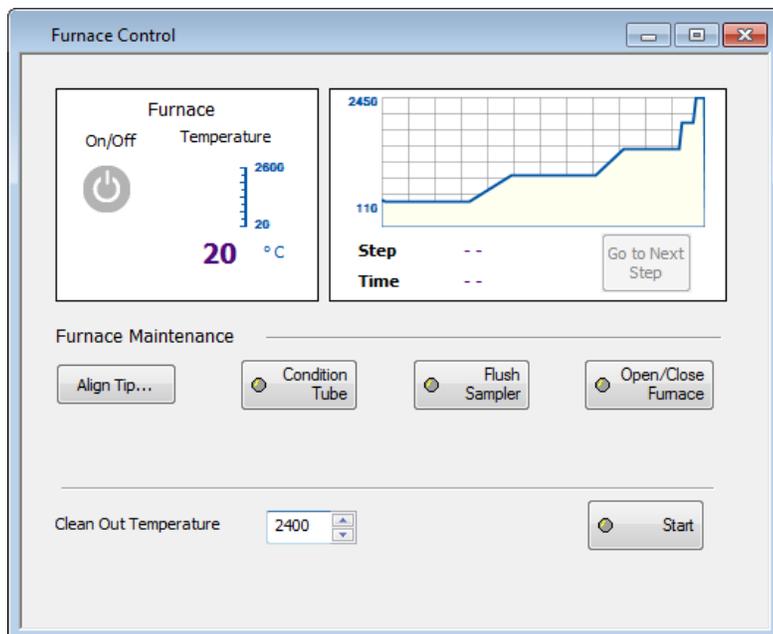
**Optimize Gas Flow:** Select this button to optimize the flame for maximum absorbance.

**Note:** *Please note that the Optimize Gas Flow feature is only available with the PinAAcle 900F and 900T.*

*For more information, see Gas Flow Optimization Wizard.*

## ***Furnace Control***

You use the **Furnace Control** window to control the furnace, condition the graphite tube and align the autosampler. You can only use these controls when there is no analysis in progress. The status of the furnace and the furnace program are shown at the top of this window.



**Furnace On/Off:** Starts or stops the furnace program defined in the active method.

**Go To Next Step:** This stops the current furnace program step and starts the next step in the furnace program. If the current step contains the read step or eliminates the time required for the BOC prior to the read step, this button will be disabled.

**Cleanout Temp.:** To heat the furnace to a selected temperature, enter the temperature, then click on **Start**. The system heats the furnace to the selected temperature. For temperatures above 2000 °C, the system maintains the temperature for 20 seconds, then switches the heating off.

**Start:** Starts or stops the furnace heating. The system heats the furnace to the temperature selected for **Cleanout Temp.**

**Open/Close:** Opens or closes the furnace by releasing or activating the pneumatic pressure that holds the furnace closed. If the furnace is open, before you can use the system, you must click on **Open / Close** to close the furnace.

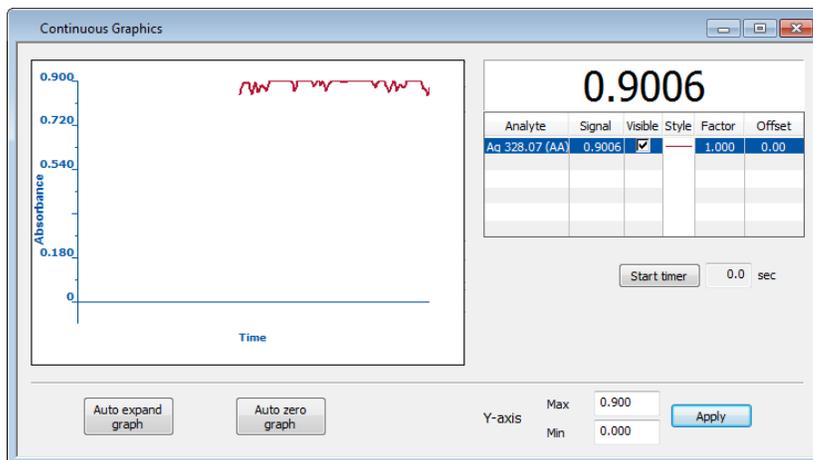
**Align Tip:** This displays the Align Autosampler Tip Wizard that you use to align the pipet tip. Follow the prompts in the wizard to align the autosampler tip.

**Condition Tube:** Starts or stops the special furnace program that heats the furnace to successively higher temperatures to condition the graphite tube.

**Flush Sampler:** Starts or stops a series of autosampler wash steps that flushes the furnace autosampler pipet. Do this when you refill the rinse bottle or change any of the rinsing system tubes.

## Continuous Graphics

This screen is divided into four sections. The display in the first section contains a continuous real-time plot. The second section has a numerical reading for the signal of the highlighted element. The element selected in the method is shown in the third section of this screen. The fourth section of this window has a list of the analyte chosen, the absorbance, whether it is visible, the line style shown on the graph and the factor.



**The Auto Expand Graph Button:** Click on this button to set the reading for the current signal to the top of the vertical axis of the graph.

**The Auto Zero Graph Button:** Click on this button to set the reading for the current signal to zero on the graph.

**Set Graph Maximum Button:** Enter a number between 0.05 and 2 in the field below this button. Click on this button to set the absorbance axis on the graph. This will allow you to customize the field to view the peak properly.

**Display Options:** Right click in this window to display the Continuous Graphics Options dialog.

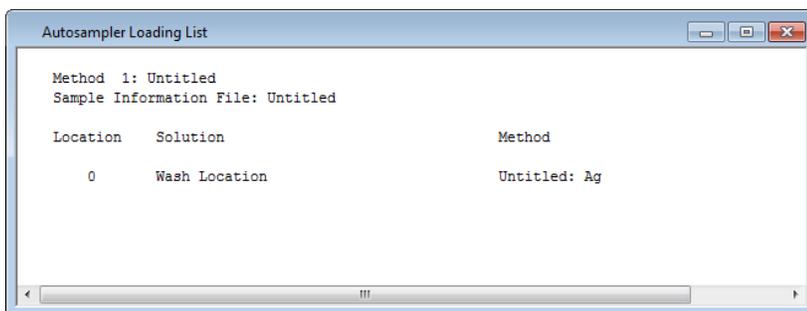
**Print:** From the **Application** button select **Print Preview** from the **Print Active Window** menu item.

**Note:** If you right mouse click in this window a pop-up screen will appear. This screen will allow you to select any of the above buttons.

## ***Autosampler Loading List***

---

Use this window to view and print the list of solutions you need to fill the autosampler tray. The information shown is taken from the active method and the current sample information file.



### ***Using this window***

1. Set up an automated or manual analysis by selecting a method and sample information file.
2. In the **Autosampler Loading List**, review the following information: the name of the method used, the sample information file used and the blanks, calibration standards and samples in the order that they are to be placed in the autosampler tray.
3. To print this window, from the **Application** button select **Print Preview** from the **Print Active Window** menu item.

**Note:** *This window will only update when opened.*

## Characteristic Mass

You use this dialog to calculate the characteristic mass, defined as the mass of analyte, in picograms, that will absorb 1% of the incident radiation ( 99% transmission). This is equivalent to a peak area of 0.0044 or a peak height of 0.0044, calculated as follows:

$$A = \log 1/( T ) = \log 1/(0.99) = 0.0044$$

The screenshot shows a dialog box titled "Characteristic Mass". It has several sections:

- Element:** Cu 324.8
- Mass of analyte atomized:**
  - Solution volume: 20 µL
  - Solution concentration: 0.000 µg/L
  - Mass of analyte: 0.00 ng
- Instrument readings:**
  - Test solution: 0.0000
  - Blank: 0.0000
  - Net: 0.0000
- Measured characteristic mass:** ---- pg/0.0044 A-s
- Comparison characteristic mass:** 17 pg/0.0044 A-s

At the bottom, there are "Print" and "Close" buttons.

### Mass of Analyte Atomized

**Solution Volume:** This is the volume of the test solution, in microliters, that was analyzed.

**Solution Concentration:** This is the concentration of the analyte in the test solution, in micrograms per liter.

**Mass of Analyte:** This is the mass of the analyte, in nanograms, that was atomized.

### Instrument Readings

These are the peak area or peak height readings for the test solution and the blank. The net reading is the difference between the test solution reading and the blank reading.

**Note:** *If more than one blank is analyzed, then the value displayed is the average of all the blanks.*

**Measured Characteristic Mass:** This shows the characteristic mass calculated from the values for Net Reading and Mass of Analyte. Normally, the measured value and the comparison value should agree within 20% if your instrument is properly set up and optimized.

**Note:** *Press the **Tab** key to get the calculated value.*

**Comparison Characteristic Mass:** This is a typical characteristic mass obtained for a simple reference solution, analyzed using the recommended analytical conditions.

**Print:** This button puts the measured characteristic mass in the results window so it can be printed with the results.

## ***Characteristic Concentration***

---

This window is used in the **flame technique** when a given concentration of an analyte produces a continuous absorbance. Characteristic concentration is defined as the standard concentration in mg/L that gives a signal of 0.0044 absorbance units.

Characteristic Concentration	
Element	Ag 328.07
Sample concentration	<input type="text"/> mg/L
Instrument reading	1.0000 abs
Measured characteristic concentration	0.000 mg/L
Comparison characteristic concentration	
Stainless steel nebulizer	0.054 mg/L
High sensitivity nebulizer	0.020 mg/L

**Solution Concentration:** The concentration of the analyte in the test solution, in the units shown. The test solution is a sensitivity-check solution containing a known amount of analyte.

**Instrument Readings:** The absorbance reading for the test solution, shown in the Results window.

**Measured Characteristic Concentration:** The characteristic concentration calculated from the values for Solution Concentration and Instrument Readings. Normally, the measured value and the comparison value should agree within 20% if your instrument is properly set up and optimized.

**Comparison Characteristic Concentration:** This is a typical characteristic concentration obtained for a simple reference solution, analyzed using the recommended analytical conditions. Comparison values are displayed for a Stainless Steel Nebulizer and a High Sensitivity Nebulizer.

**Print:** This button puts the measured characteristic concentration in the results window so it can be printed with the results.



# **Data Windows**

## ***Data Windows***

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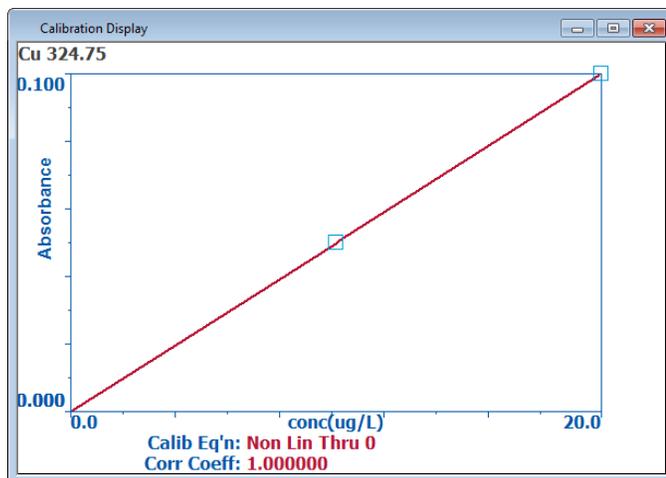
Syngistix contains a number of windows that you use to view the data as the instrument collects it, and afterwards, to view stored data and if necessary recalculate results.

- During an analysis you can select options to save the data in a data set and to print the data. You can also print any active window from the **Application Button** select **Print Preview** from the **Print Active Window** menu item
- To organize the data in the data sets after an analysis you use the Data Manager. You can start Data Manager from the Ribbon by clicking the **Utilities** tab and selecting **Data Manager**.

## ***Calibration Display***

---

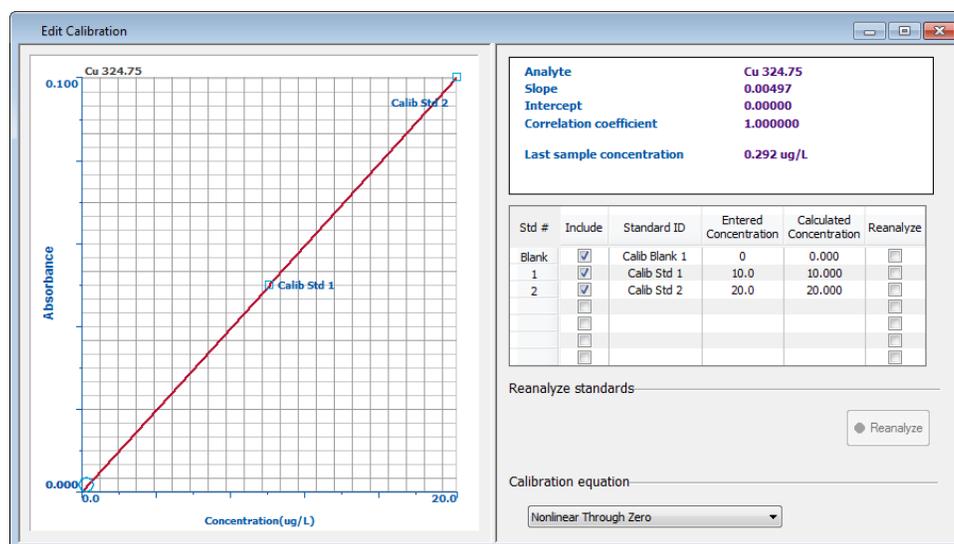
The Calibration Display shows the active calibration as it is being generated and when it is being used by the system. This window is just for viewing, you cannot make changes to the calibration curve from this screen. If this window is empty, there is no active calibration curve.



### ***Edit Calibration***

You use this window to:

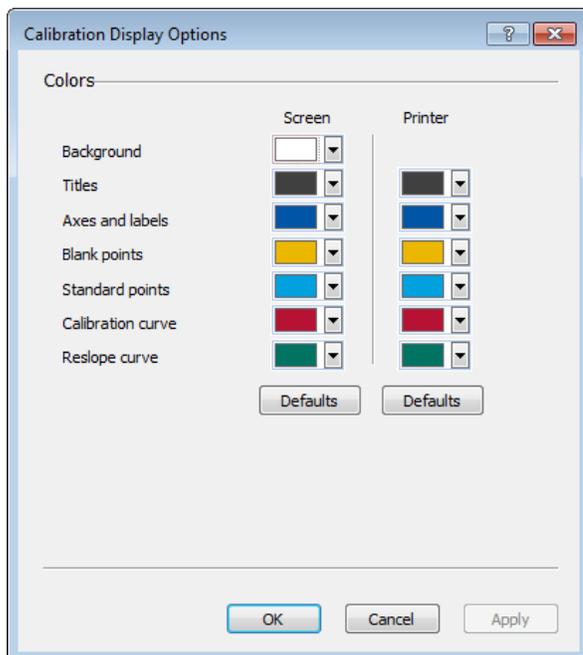
- Determine whether the standards lie on the curve and compare this graphic display of the calibration to the correlation coefficient.
- Check that you have selected the correct algorithm (nonlinear through zero, linear, calculated intercept, linear through zero, linear-bracketing, methods of additions-sample intercept, methods of addition-calculated intercept, methods of additions-calibrate) for the calibration.
- View the effect on the calibration after selection of different algorithms or other Method parameters.
- Print this window for your reports to present a graphical display of the calibration.



## Selecting Colors

To select the colors for both the on-screen and printed Calibration window, you use the Calibration Display Options dialog.

- To display this dialog, right-click anywhere inside of the Calibration Display window.



## Resizing

You can resize the window by placing the cursor on any side or corner of the window until the cursor changes to a double-headed arrow shape. Click and hold the left mouse button as you drag the mouse and change the window size.

**Fehler! Verwenden Sie die Registerkarte 'Start', um Heading 1 dem Text zuzuweisen, der hier angezeigt werden soll.. 143**

### ***Printing the Calibration Display***

To print the contents of the **Calibration** display at any time, click the **Application** button and click **Print Active Window**.

During an analysis the system will print data if you select Print log on the Automated Analysis Setup page or Manual Analysis window. To select the data that will appear on the printed log, use the Options page of the Method Editor.

### ***Calib Eq'n***

This is the calibration equation that is specified in the current method. (A list of calibration types is shown on the Calibration page of the Method Editor window.) After the calibration curve has been created, you can clear (delete) the calibration by clicking on **New Calibration** in the **Calibration** group on the **Results** tab.

### ***Corr. Coeff.***

The correlation coefficient indicates how well the data fit the generated calibration curve. A value of 1.0000 would indicate a perfect fit.

## Results

During an analysis this window shows the numerical results for the signal measurements and the calculated analyte concentrations. When the system finishes the analysis of each solution, the results are added to this window. When there is no analysis in progress this window may show the results from the most recent analysis.

To display this window:

- On the **Results** tab, **Results** group, click on **Results**.

The results window appears.

The screenshot shows a window titled 'Results' with the following content:

```

Results Data Set (original): 121912Cu
Results Library (original): C:\Users\Public\PerkinElmer\AA\Data\Results\Results.mdb
Results Data Set (reprocessed):
Results Library (reprocessed):

-----
Method Loaded
Method Name: Cu
Method Description: Cu
Method Last Saved: 12/13/2012 12:25:40 PM

-----
Sequence No.: 1
Sample ID: AutozeroRead
Analyst:
Logged In Analyst (Original) : Administrator
Autosampler Location:
Date Collected: 12/19/2012 2:35:36 PM
Data Type: Reprocessed on 8/20/2014 11:33:20 AM

-----
Replicate Data: AutozeroRead
Analyte: Cu 324.8
Repl SampleConc StndConc BlnkCorr Peak Peak Bkgn Bkgn Time Peak
# mg/L ug/L Signal Area Height Area Height
1 [0.00] 0.0001 0.0001 0.0004 -0.0003 0.0002 2:35:36 PM No
Auto-zero performed.

-----
Sequence No.: 2
Sample ID: ManualRead
Analyst:
Logged In Analyst (Original) : Administrator
Autosampler Location:
Date Collected: 12/19/2012 2:36:19 PM
Data Type: Reprocessed on 8/20/2014 11:33:20 AM

-----
Replicate Data: ManualRead
Analyte: Cu 324.8
Repl SampleConc StndConc BlnkCorr Peak Peak Bkgn Bkgn Time Peak
# mg/L ug/L Signal Area Height Area Height
1 -0.0002 -0.0001 0.0004 -0.0001 0.0003 2:36:20 PM No

-----
Sequence No.: 3
Sample ID: AutozeroRead
Analyst:
Logged In Analyst (Original) : Administrator
Autosampler Location:
Date Collected: 12/20/2012 9:36:46 AM
Data Type: Reprocessed on 8/20/2014 11:33:20 AM

-----
Replicate Data: AutozeroRead
Analyte: Cu 324.8
Repl SampleConc StndConc BlnkCorr Peak Peak Bkgn Bkgn Time Peak
# mg/L ug/L Signal Area Height Area Height

```

To print this window:

- During an analysis the system will print the data if you select **Print log** on the Automated Analysis page or Manual Analysis window. To print the contents of the Results window at any time go to the Application button drop-down and click **Print Active Window**.

## The Design of this Window

In the Method Editor Options page select the options that you would like to include in this results page.

**Method Header:** This header displays which method was used.

**Sample Header:** This displays descriptive information for each sample.

**Replicate Data:**

Data for Replicate 1

Data for Replicate 2

Individual data values under the relevant **Column headings**

**Means and Statistics:** This shows the mean concentration in sample units, the standard deviation (SD) and the relative standard deviation (%RSD) for each sample. The relative standard deviation is also referred to as the coefficient of variation.

## ***Data Reprocessing***

---

You use this window to reprocess sample data that is stored in a **Results** data set. There are several reasons why you might want to reprocess data:

- You chose peak height and wanted peak area.
- You entered 0.1 for a concentration of a standard and it is actually 1.0.
- You chose mg/mL but you need the results to print out in ppb or oz/ton.
- You chose a linear calibration equation instead of nonlinear.
- You ran just the samples and forgot to recall the calibration from another data set. Therefore, no concentrations are given and you need that information.
- You entered the wrong QC concentration or wrong QC limits the first time.

Reprocess cannot be accessed unless the Analysis Control Windows are closed (i.e. Manual or Automated Control Windows). In addition, you must save the transient peak to reprocess results.

### ***Using this Window***

**Note:** *You must have the method that was used to generate the data **open**.*

1. Next to **Data Set to Reprocess**, click on **Browse...** and select a results data set that contains the data you want to reprocess.

In the Data Reprocessing window, the results from the reprocessed data will be saved to the data set shown in the entry field. This field defaults to the data set from the most recent analysis. A check mark appears in the **Save Reprocessed Data** box, confirming that reprocessed data will be saved.

To change to a different data set, click on Browse... and in the **Select Results Data Set** dialog that appears, type a new data set name or select an existing one. A check mark appears in the **Save Results in Data Set** box, confirming that reprocessed data will be saved. If you do not want to store reprocessed data, click on the check box to clear it.

2. The Method should be open in the Method Editor so if you want to reprocess using different method parameters, that information can be used. Confirm that the method in use contains the correct settings for the results data set that is to be reprocessed.
3. In the table, review the information. The IDs in the selected results data set are listed along with the sample information that was used when the data was originally collected. To edit this information, type the new information into the fields as desired. To access a pop-up menu containing commands for editing the table, right click anywhere in the table. This pop-up menu applies to the selected rows or cells in the spreadsheet. To hide columns that do not contain data, select the **Hide Empty Columns** check box.

**Note:** *There is a column fill dialog available for each of the parameters in the table, except Sample Type and Original Method. To access a column fill dialog, double-click on the parameter's column header.*

To select items of interest for reprocessing, select the associated row numbers in the table.

To select a series of rows, click on the first row number of interest, hold down the Shift key, and click on the last row number of interest. You can also drag over the row numbers column using the mouse cursor. To select non-consecutive rows, hold down the Ctrl key and click on each row number.

**Tip:** *The order in which samples are selected is the order in which reprocessing occurs. As you select each row, the reprocessing sequence appears in the Sequence column.*

4. Click on **Reprocess**.

## **Data Reprocessing Window Settings**

This shows the status of the reprocessing operation.

**Reprocess:** Click on this button to begin reprocessing. Click again to interrupt reprocessing.

**Save Reprocessed Data:** This box is selected automatically (a check mark appears), indicating that the reprocessed data generated will be saved to the results data set shown in the entry field. To select a different results data set, click on Browse..., and in the Select Results Data Set dialog that appears, type a new data set name or select an existing one. Note that the peak data are not saved with the reprocessed results and do not change with reprocessing.

**Print Log:** Select this box to print a log of signals, analytical results, and other information about the analysis. The log includes an analytical header and, for each sample, a sample header and the data that are shown in the Results Display window as selected on the Options page of the Method. Look at all of the selections on the Method Editor Window Options page to get an overview of the selected analytical results that will appear in the printout.

**Hide Empty Columns:** Select this box to hide columns that do not contain data.

**Data Set to Reprocess:** Select the results data set that contains the data you want to reprocess. Click on Browse... and in the Results Data Set dialog that appears, select an existing data set name. The sample parameters from the results data set you selected are brought into the Data Reprocessing window. The column heads in bold indicate that this information from the original analysis cannot be modified.

**Note:** *For an example using Initial Sample Weight, Sample Prep Volume, Aliquot Volume, and Diluted to Volume see, Sample Preparation: An Example.*

## **Column Headers**

**Sequence:** This is the sequence in which samples will be reprocessed. This sequence appears as you select each row number.

**Sample ID:** This is the name you gave to each sample.

**Sample Type:** This is the solution type: blank, standard, sample, etc.

**Omit Replicates:** This is the entry for replicate numbers that you do not wish to reprocess for a sample.

**Matrix Check Samples:** This shows any samples that are designated as matrix checks.

**Date/Time:** This shows the date and time that each sample was analyzed.

**Initial Sample Wt.:** This is the sample mass prior to sample preparation.

**Initial Sample Vol.:** This is the quantity of sample volume before sample preparation.

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**Sample Units:** Use this column to change the sample units on a per sample basis before reprocessing data. The concentration will be calculated based on the new units.

**Weight Units:** This shows the units of the Initial Sample Quantity. These are either weight or volume units.

**Sample Prep. Volume:** After a solid sample has been dissolved or a liquid sample has been acidified (or otherwise treated), the resulting solution is prepared to a specific volume. This is the Sample Prep Volume.

**Aliquot Volume:** If an aliquot of the sample solution is taken and diluted to a final volume, record the aliquot volume for this entry and the final volume for the Diluted to Volume entry.

**Diluted to Volume:** This is the final volume of solution obtained by diluting an aliquot of the sample solution. You can also record the dilution as the ratio of the original sample volume to the final sample volume. For example, if 10 mL of sample is diluted to 200 mL, this ratio would be 10:200 or 1:20. Enter 20 for the Diluted to Volume entry and 1 for the Aliquot volume.

**Volume Units:** If the final sample concentrations are being reported in weight/weight units, you must enter the units for the Sample Volume.

**Solids Ratio:** This is the ratio of the wet and dry weights for the sample. This ratio is used to correct the sample concentration. For more information, see the Solids Ratio Column Fill dialog.

**Nominal Sample Weight:** This is the target weight when samples are weighed. This entry is required only if corrections are being made to weight/weight measurements to compensate for weight variations among samples. The Nominal Sample Weight is divided by the Initial Sample Weight to correct the final concentration value.

**Batch ID:** This is the name you give to this batch of samples.

**Original Method:** This shows the method you used in the analysis. This information cannot be modified.

**Remarks:** The remarks you entered in the Sample Information file before the initial analysis.

**Check Limits:** Check this box to enable sample limit checks as defined in the method. If you uncheck this parameter, then sample limit checks will not be performed for the particular sample.

## Reprint Data

---

You use this window to specify which results data you want to reprint. The Reprint function will allow you to create an exact copy of your original results data printout.

To display this window:

- On the **Results** tab, in the **Results** group, click on



### Using this window

**Note:** *If you plan on using the **Reprint Data** function, we recommend that you enable the **Spectral Data** option when collecting data. You enable **Spectral Data** by checking this option on the **Options** tab page of the **Method Editor**. If **Spectral Data** is not checked and you run an analysis, the samples will still be stored in a batch and will be available for reprinting, however, no data will be shown for those samples.*

1. Next to **Results Data Set Name**, click on the folder icon and select a results data set that contains the data you want to reprint.
2. Next to **Analysis Batch Date/Time**, click on the folder icon to select a batch that you want to reprint.

The **Select Analysis Batch** dialog appears and displays the batches that are available in the data set you selected. Batches are identified by the date and time they were initially created.

The rules for how batches are created are as follows:

- When you are performing **Manual Analyses**, a batch is created when you run the first solution after opening the Manual Analysis window. The batch will end when you close the Manual Analysis window. All samples that are run in between are stored as part of the same batch.
  - When you are performing **Automated Analyses** a new batch is created when you first select one of the analyze buttons (**Analyze All**, **Calibrate**, and **Analyze Samples**). The batch will end when you close the Automated Analysis Control window. If the analysis is paused and then continued, the continuation of the analysis will be part of the same batch.
  - When you are **Reprocessing Analyses** a new batch is created when you first open the Data Reprocessing window and click the **Reprocess** button. The batch will end when you close the Data Reprocessing window.
3. Click **Preview** to preview the selected data in the Results window, without printing.
  4. Click **Print** to print the selected data.

Output is sent to the Results window. It should be noted that no new data is stored to the Results database when you use the Reprint function.

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## ***Examine Transient Peaks***

With the furnace technique you can use this window to display the peaks for the elements that you have analyzed and saved in a data set. You can examine the peaks for the standards and samples that were analyzed in the method file.

The main function of the **Examine Transient Peaks** window is to display peaks that were saved to a **Data Set** so that you can:

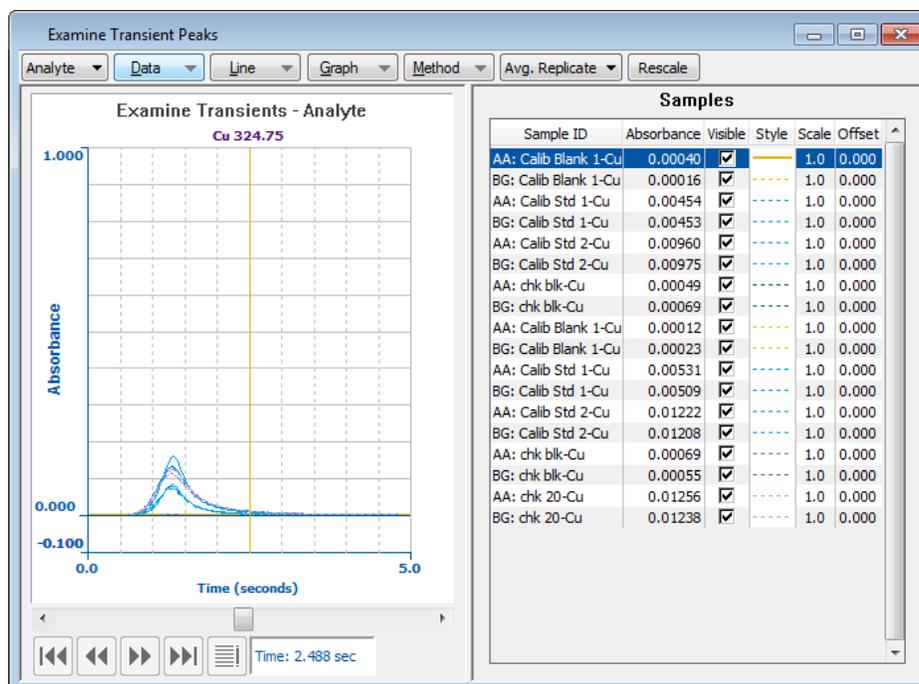
1. Modify Method parameters during method development.
2. Change the presentation of the peaks to aid in Method Development.
3. Set up peak displays for your printouts.
4. Troubleshoot possible hardware problems by evaluating standard peaks.

### ***Using this Window***

**Tip 1:** To ensure that you save the peaks data, make sure to check **Transient Peaks Profile** under **Save with Results** heading in the **Method Editor** window **Options** page.

**Tip 2:** Save the method, if you wish to retain the changes made to method parameters from the **Examine Transient Peaks** window.

**Tip 3:** Use the **Overlay Mode** to analyze peaks from multiple data sets.



The lists and menus along the top of this window are:

<b>Menu/Drop Down List</b>	<b>Description</b>
Analyte Mode	If you select Analyte mode you will be able to compare peaks from a single data set.
Overlay Mode	If you select Overlay mode you will be able to compare peaks from multiple data sets.

The **Analyte selection buttons** are only active in the analyte mode in this window. They are visible but grayed out when the Overlay mode is selected.

### ***Transient Peaks Display***

In the furnace technique, you can use this window to display the peak for the element selected in the active method or from another data set. You can examine the peaks for the standards and samples that were analyzed in the method file. You can also use this window to overlay peaks from another element.

## ***Using the Examine Transient Peaks Window***

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Before you begin using the Examine Transient Peaks window, open the method that was used to generate the peaks. If you are not sure which method was used, select **Import From Results Library...** in the file menu, then select the results data set. If you want to use a different method, it must contain some (but not all) of the elements that were originally used when the data was collected.

### ***Selecting peaks to display***

1. Open the Examine Transient Peaks window (in the Toolbar, click on the **Examine** button). Select **Analyte or Overlay** from the top-left drop-down list, if necessary. If you select **Analyte** mode you will be able to compare peaks from a single data set. If you select **Overlay** mode you will be able to compare peaks from multiple data sets.
2. In the Examine window, click on the Data menu, and click on **Select Data Set** in Analyte Mode or **Add Data Set Signals** in Overlay Mode.
3. Complete the Data Selection Wizard to select samples and analytes.

### ***What You See in the Examine Transients Peaks Window***

The window is split vertically with the graph (Analyte) on the left and the legend (Samples) on the right. The graph shows all peaks of a chosen analyte for all the samples. The legend shows you the AA and BG peaks which are graphed. It displays columns to indicate and set the hide visible, scaling and offset. Since there is an entry for each sample, it is easy to tell at a glance how these settings are adjusted relative to all of the samples. More importantly, all of the samples' absorbencies are listed together in one column. Also you can click on one sample and it is highlighted in the graph.

Along the **bottom of the graph** are buttons which are operable in the **Analyte Mode**. As shown in the illustration below the buttons from left to right are Select First Analyte, Select Previous Analyte, Select Next Analyte, Select Last Analyte, and Select Analyte. (You can also access these commands from the Data Menu of the Analyte Mode.)



At the **top of the graph** there is a drop-down list to select which replicate mode is displayed. There are four replicate modes: Average Replicate, First Replicate Last Replicate, and All Replicates.

### ***To allow more space for the legend or graph***

By default, the Auto Position Splitter Bar is checked in the Examine Transient Peaks Options Dialog. This causes the system to automatically position the splitter bar, which separates the graph from the legend, so that the legend is exactly wide enough to display the text it contains. You can easily allow more space for the graph or legend.

First uncheck the Auto Position Splitter Bar check box in the Examine Transient Peaks Options Dialog, and then position your mouse over "splitter bar" that separates the left and right panes. Your cursor changes to a double-headed arrow. Drag left or right to increase the size of a pane. (If your cursor does not change to a double-headed arrow, you must disable the "auto-position splitter" option in the Examine Display Options dialog.)

## ***Examine Transient Peaks Keyboard Shortcuts***

The following keyboard shortcuts exist only in the Analyte mode in the Transient Peaks window:

- f First Analyte
- < Previous Analyte
- > Next Analyte
- e Last Analyte
- g Go to Analyte

The rest of the cursor keys (up, down, page up, page down, home, end) always apply to the legend. For example, to advance to the next sample in the legend, press the down-arrow key. Provided that there is indeed another sample to advance to, that will become the active sample and be highlighted.

**More Keyboard Shortcuts** (only available in the Analyte mode)

- d add read delay point
- r add read end point
- m opens Update Method Parameters dialog

## ***Using the Examine Transient Peaks Data Menu Options***

---

Before you begin using the Examine Transient Peaks window, open the method that was used to generate the peaks. If you are not sure which method was used, in the **File** menu, select **Import from Results Library...**, then select the results data set. If you want to use a different method, it must contain some (but not necessarily all) of the elements that were originally used when the data was collected. To ensure that you save both the data and the method used to collect them, make sure to check the Transient Peaks profiles check box a from the Method Editor window Options page.

**Save the method**, if you wish to retain the changes made to Method parameters from the Examine Transient Peaks window.

The Examine Transient Peaks Data Menu Options in the Analyte Mode has the following drop-down menu:

Select Data Sets

Select Samples

Select Analytes

Export Transient Peaks

First Analyte

Previous Analyte

Next Analyte

Last Analyte

Go to Analyte

## ***Examine Transient Peaks Data Menu Options In Overlay Mode***

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Before you begin using the Examine Transient Peaks window, open the method that was used to generate the peaks. If you are not sure which method was used, in the File menu, select Import from Results Library..., then select the results data set. If you want to use a different method, it must contain some (but not necessarily all) of the elements that were originally used when the data was collected. To ensure that you save both the data and the method used to collect them, make sure to check the Transient Peaks profiles check box a from the Method Editor window Options page.

Save the method, if you wish to retain the changes made to Method parameters from the Examine Transient Peaks window.

The Examine Transient Peaks Data Menu Options in the Overlay Mode has the following drop-down menu:

- Add Data Set Signals
- Add Sample Signals
- Add Analyte Signals
- Clear Display

### ***Add Data Set Signals***

In the Overlay Mode of the Examine Transient Peaks Data Options select this option to add data from previously collected data. Follow the steps in the Data Selection Wizard to add these data set signals to the Examine Transient Peaks window for further analysis. The data are taken from the Results Data Set.

### ***Add Sample Signals***

In the Overlay Mode of the Examine Transient Peaks Data Options select this option to add sample signals from previously collected data. Follow the steps in the Data Selection Wizard to add these sample signals to the Examine Transient Peaks window for further analysis. The sample signals are taken from the Results Data Set.

### ***Add Analyte Signals***

In the Overlay Mode of the Examine Transient Peaks Data Options select this option to add sample signals from previously collected data. Follow the steps in the Data Selection Wizard to add these analyte signals to the Examine Transient Peaks window for further analysis. The analyte signals are taken from the Results Data Set.

### ***Clear Display***

Press this selection to completely clear the display.

### ***Analyte Mode***

Analyte mode allows you to compare peaks from a single dataset.

**If you have selected the Analyte Mode in the Examine Transients Peaks Window the following drop down menus options appear:**

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Data

Line

Graph

Method

Replicate

## ***Overlay Mode***

Overlay mode allows you will be able to compare peaks from previous analyses.

**If you have selected the Overlay Mode in the Examine Transients Peaks Window the following drop down menus options appear:**

**Note:** *The screen will change to a shade of blue to emphasize that you have switched to the Overlay Mode*

Data

Line

Graph

Replicate

## **Select Data Set**

---

To display data in the Examine Transient Peaks window, select **Data Set** from the Data menu.

Use the Data Selection Wizard to perform any of the following functions:

### **Select a results library from which to retrieve a data set**

- Click on the Browse button to select a path from the Results Path dialog. (The default pathname appears.)

### **Select peaks to display in the Examine Transient Peaks Window**

- Click on a data set name to select a data set from which you wish to display peaks. (You will specify the sample(s) and analyte (s) in subsequent dialogs.)

**Note:** *In Analyte Mode you can select only one data set per Examine Transient Peaks session. Overlay mode allows you to select from multiple data sets.*

### **Sort the data set list**

- Click on the appropriate option button to sort the Data Set list by Name or Date/Time.

### **Select samples and elements from a data set**

- After you choose a data set, click Next to display Step 2., the Select Samples page of the Data Selection Wizard.

## ***Select Samples***

---

Open the Data Selection Wizard by choosing **Select Samples** from the **Data** menu in the Examine Transients Peaks window. If this option is not available, choose **Select Data Set**. Use the Select Samples dialog to perform any of the following functions:

### ***Select every sample from the data set***

- Click on the **Select All** button and then click on **Next**. By default, all samples are initially selected (highlighted). To deselect the samples, click on any sample in the list.

### ***Select a specific sample from the data set***

- Click on a specific sample from the list.

**Note:** *If you wish to view the replicates for a sample follow these steps below:*

1. Select only one sample from this dialog
2. From the Replicates drop-down list, in the Examine Transient Peaks window select **First Replicate**, **Last Replicate**, **Average Replicate**, or **All Replicates**.

### ***Select a set of samples that are listed sequentially***

- Click on a sample, then press and hold the **Shift** key and click on another sample. All samples between these two will be selected (highlighted). Click on the **Finish** button.

### ***Select a set of samples that are NOT listed sequentially***

- Press and hold the **Ctrl** key while clicking on any samples you wish to highlight. Release the **Ctrl** key, confirm your selections, and then click on the **OK** button.

**Note:** *If you accidentally highlight a sample, simply unhighlight it by **Ctrl/clicking** on that sample again. (You can use this technique unhighlighting no matter how you originally chose to highlight an item).*

## **Select Analytes**

---

Open the Data Selection Wizard by choosing Select analytes from the Data menu in the Examine Transients Peaks window. If this option is not available, choose Select Data Set.

Use the Select Analytes dialog to perform any of the following functions:

### **Select every analyte in the data set**

- Click on the **Select All** button then click on **Finish**. (By default, all samples are initially highlighted.)

### **Select a specific analyte in the data set**

- Click on a specific analyte from the list.

### **Select a set of analytes that are listed sequentially**

- Click on a sample, then press and hold the **Shift** key and click on another sample. All samples between these two will be selected (highlighted). Click on the **Finish** button.

### **Select a set of analytes that are Not list sequentially**

- Press and hold the **Ctrl** key while clicking on any analysis you wish to highlight. Release the **Ctrl** key, confirm your selections, and click on the **OK** button.

**Note:** *If you accidentally highlight an analyte, simply unhighlight it by **Ctrl/clicking** on that analyte again. (You can use this technique unhighlighting no matter how you originally chose to highlight an item).*

## **Analyte Selection Buttons**

The analyte selection buttons are only operable in the Analyte Mode of the Examine Transient Peaks window.

### **First, Previous, Next, Last analyte in the list.**

- Use these buttons to change the currently displayed analyte to either the first, next previous or last analyte on the list.

### **Go to Analyte button.**

- Click this button to view a list of selected analytes. You can select any analyte from the list to display it.

## ***Exporting Transient Peaks***

---

In Analyte Mode open the Export Transient Peaks dialog by selecting **Export Transient Peaks** from the Data menu in the Examine Transient Peaks window. You must have a data set open to use this option.

You can export Transients Peaks data, which includes all the data points collected in the measurement range for each analyte to construct the peak that represents the absorbance values. Then you can view the exported data in a spreadsheet or database program of your choice and graph the data points, if desired.

Fill in the appropriate choices in the Export Transient Peaks dialog:

- **Format:** Choose the column format you wish to use for displaying the absorbance data for each sample. If all samples share the same time, select the option for **Single Time Column**, and the first column in the resulting spreadsheet will display the single time in the spreadsheet. If one or more of the samples have different times, select the option for **Time Column for Each Sample**, and the time column in the spreadsheet will be repeated for each sample.
- **Analytes:** Choose to export data for the analyte currently displayed in the Examine window, or choose all analytes.
- **Replicates:** Choose to include data from the first or last replicate, the average (mean) values, or all replicates.
- **Data Delimited by:** Choose the delimit character preferred by your spreadsheet or database program. Columns of data can be separated by commas, tabs, semicolons or the @.
- **File name:** Select a name for the export file. Choose the same name as the data set or create a different name.
- **Extension:** Choose the extension preferred by your spreadsheet or database program. The file extension can be .cvs, .prn, or .txt.
- **Directory:** Use the default Reports directory or browse to locate the directory where you want to save the exported file.

## ***Using the Examine Transient Peaks Line Menu Options***

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The Examine Transient Peaks **Line** Menu Options has the following drop-down menu:

- Select Scale & Offset
- Hide/Visible Active Sample
- Hide/Visible Column Fill
- Delete

### ***Using the Scale & Offset Option***

You can also display this dialog if you double-click anywhere in the Scale or Offset column of the legend.

**Note:** *If the dialog does not appear, you must first open a data set.*

**Tip 1:** *Select an Active peak BEFORE YOU SELECT THIS DIALOG.*

*To apply a Scale Factor and/or a Baseline Offset to a transient peaks, you must first select that peak by clicking on one of the sample names in the legend (i.e., the sample list in the right-hand side of the Examine Transient Peaks window). Notice that the transient peaks name will be highlighted and data points (which are indicated by small squares) appear on the associated peak to designate it as the active peak. (Data points will only appear if the data points option is selected from Select Graph Display Options Dialog.)*

**Tip 2:** *View the current status of an active peak by noting the right-hand side of the Examine Transient Peaks window. You can check the absorbance of the peak at the current cursor position, as well as the offset value and the scale factor that have been applied to the active Transient Peaks. (The values for the offset and scale will be zero and one respectively, when you first select an active peak).*

*For example, if you use this dialog to apply both an offset and scale factor, then you will see those values listed.*

*Use the Select Scale & Offset dialog to perform any of the following functions:*

**Apply the Scale and Offset to the current sample only or to all samples**

***Select a scale factor to apply to the sample(s)***

- **Type a value.** The appearance of the peak will be scaled larger or smaller based on the specified value. Click on the **Apply** or **OK** button to apply this factor to the scale for the active peak.

**Note 1:** *Check the box next to **Automatically determine full scale factors** and the software fills in the scale and offset factors that cause the sample(s) to appear to utilize the entire y-axis dynamic range. If the **All Samples** is selected, the factors for each sample will be optimized (separately.)*

**Note 2:** *A Scale factor only changes the appearance of the peak; the original data (stored in the data set) remains unchanged.*

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**Note 3:** *It is possible to detect a low level analyte by using scale factors, since an expansion factor is applied uniformly across the peak. A change in peak shape or a shift in time may indicate an interference problem.*

### **Select an offset to apply to the sample(s)**

- **Type a value** . Click on the Apply or OK button to move the baseline position of the peak up or down based on the specified value.

**Note 1:** *An Offset only changes the appearance of the y-axis of the peak and so the original data (stored in the data set) remains unchanged.*

**Note 2:** *When you have a group of peaks that are closely spaced (and sometimes overlaid on top of each other), you can apply an offset to move the active peak up or down (which does not change the scaling) so that you can make a direct comparison to the other peaks.*

Reset the Scale and Offset factors for the active sample or all samples.

With the appropriate option selected for Current Sample Only or All Samples, click on the Reset button. A scale factor of 1.0 and an offset of 0.0 will be displayed. Click Apply or OK to apply the factors.

### **Using the Hide/Visible Active Sample Line Option**

In the Line menu of the Examine Transient Peaks window, click on the **Hide/Visible Active Sample** option to perform the function listed below.

#### **Remove a peak from the display but retain the name in the samples list**

- Select the active peak and then click on Line menu and then click on the Hide option. The active peak is automatically removed from the display.

**Note 1:** *The peak name remains in the Samples list but the line showing its color is removed to indicate that this peak is "hidden."*

**Note 2:** *You can hide any number of peaks.*

#### **Re-display a previously hidden peak**

- Select a Hidden peak from the samples list (it will have a peak name but there will be no line color next to it) and then click on Line menu **Hide/Visible Active Sample** (or click the box in the Visible column of the legend). The active peak reappears in the display.

### **Using the Hide/Visible Column Fill Line Option**

In the Line menu of the Examine Transient Peaks window, click on the **Hide/Visible Column Fill** option to perform the function listed below. Also you can perform the same functions in the right side of the Examine Transient Peaks window, under the Hide/Visible Column Fill by checking or unchecking the box next to each sample for either the AA or BG peaks, independently.

### ***To remove or display all samples***

- Double-click on the word "visible" at the legend's visible column heading to open a column-fill dialog. There is a single checkbox in the dialog, label "visible". Checking checkbox and clicking the **OK** button will cause all samples to be visible. Unchecking that checkbox and clicking the **OK** button will cause all samples to hide (not be visible).

### ***Using the Delete Line Option***

From the Line menu in the Examine Transient Peaks window, click on the Delete option to perform the following function:

To Delete a peak from the display:

- Select the active peak and then in the Line menu, click on **Delete**. The active peak is removed from the current analyte's display (but not from the data set).

**Note 1:** *To redisplay a "deleted" peak you will need to reselect it: In the Data menu, click on **Select Samples** .*

**Note 2:** *You can delete any number of peaks*

## ***Using the Examine Transient Peaks Method Menu Options***

---

The Examine Transient Peaks Method Menu Options in the Overlay Mode has the following drop-down menu:

- Add Read Delay Point
- Add Read End Point
- Update Method
- Import Method From Results Library

### ***Add Read Delay Point***

The read delay is the time in seconds that the system waits before it starts to measure the signal. This option will allow you to manually set the read delay point which you can then save. Once it is saved this information will be modified in the method for future use.

The system receives a read command from the read delay you have manually entered, the system waits for the time set for the Read Delay, then measures the signal for the time set for the Read Time.

### ***Add Read End Point***

The read end point is the time in seconds that the system stops measuring the signal. This option will allow you to manually set this point which you can then save. Once it is saved this information will be modified in the method for future use.

The system receives a read end point command that you have manually entered. The system will stop measuring the signal when it reaches the read end point.

### ***Update Method***

To update method parameters, choose Update Method from the Method menu in the Examine Transient Peaks window.

To Update a Method

- Click on the **OK** button to modify the method according to the selections you have made in this dialog. However, the method changes will not be saved to disk. Make sure that the appropriate check boxes for Read Time or Read Delay are checked to reflect the changes you want. Click on **OK**.

### ***Import Method from Results Library***

Use this dialog when you need to open the method that was used to generate a data set. For example, if you need to reprocess data, you would open the method that was used to generate the data set before starting reprocessing.

To import a method:

1. Click on **Import from Results Library** or in the Examine Transient Peaks Window, click on Method and from the drop-down menu select Import Method from Results Library.
2. The Select Results Data Set dialog will appear if you started from the Analysis tab > Method group > Import Method. Select a results data set and click on OK.

**Note:** *If you started from the Examine Transient Peaks Window, the results data set that is currently in use in the Examine window is automatically selected and the Select Results Data Set dialog will not appear.*

3. When the Import from Results Library dialog appears, select the method you want to import. Click on OK.

The method is opened in the appropriate windows.

## ***Using the Examine Transient Peaks Graph Menu Options***

The Examine Transient Peaks Graph Menu Options has the following drop-down menu:

Define Y-axis  
Label Options  
Display Options  
Add Label

### ***Define Y-axis Options Dialog***

Open the Define Y-axis dialog by choosing Define Y-axis from the Graph menu in the Examine Transient Peaks window. If this option is not available, you must first open a data set.

**Note:** *Double-clicking on the graph area (the left-hand side) of the Examine Transient Peaks window, but to the left-hand side of the y-axis, is a convenient way to open the Define Y-axis Options dialog.*

Use this dialog to perform the following functions:

#### ***Change the y-axis options for ONLY the Current Analyte or All Analytes in the data set***

- Click on the appropriate option button at the top of the dialog.

#### ***Select the maximum value for the y-axis***

- To automatically scale the y-axis so the maximum Y value is at least 1, click on the Automatic (min 1) option button.
- To automatically scale the y-axis for the highest absorbance peak in the window, click on the Automatic option button.
- To enter a specific maximum value for the y-axis scale, click on the Manual option button and enter a value (that ranges from -10 to 100, inclusive).

#### ***Select the minimum value for the y-axis***

- To automatically scale the y-axis so that the zero point on the Y-axis must be shown, click on the Automatic with zero axis option button.
- To automatically scale the y-axis for the minimum intensity in the window, click on the Automatic option button.
- To enter a specific minimum value for the y-axis scale, click on the Manual option button and enter a value (that ranges from -10 to 100, inclusive).

### ***Select Label Options Dialog***

Open the Label Options dialog by choosing Label Options from the Graph menu in the Examine Transient Peaks window. If this option is not available, you must first open a data set.

Use this dialog to perform the following functions:

### ***Apply label options to the Current Analyte Only or All Analytes in the data set***

- Click on the appropriate option button at the top of the dialog.

#### ***Select the desired label options:***

Click on the appropriate option button for the desired graph title (i.e., to use the analyte name, to enter your own title, or no title at all.)

- Click on the appropriate option button to display x-axis and/or y-axis labels.

### ***Display Options Dialog***

The Examine Transient Peaks Display Options dialog has three tabs:

Settings  
Window  
Lines

Open the Examine Transient Peaks Display Options dialog by choosing Display Options from the Graph menu in the Examine Transient Peaks window.

You can also reach this dialog from the Options menu and select **Examine Transient Peaks** from the drop-down menu. If this option is not available, you must first open a data set. Also double clicking in the Analyte window, but to the right-hand side of the Y-axis of Examine Transient Peaks will also display this window.

#### ***Settings in Display Options***

This tab, in the Examine Transients Peaks Display Options window, allows you to select your display option choices for either all the analytes or just the current analyte .

You may also check off options to automatically set the:

- Autoposition Splitter Bar (Disabling this option lets you resize the Graph and Legend panes of the Examine window by positioning your mouse on the bar and dragging left or right.)
- Show the X and Y axis Grid divisions (When enabled, the number of x-axis grid divisions as indicated and the number of Y-Axis Grid Divisions can also be selected from 1 to 100.)
- Show Active Signal Points (When enabled, it shows the location of each data point for the selected peaks profile.)
- Show the Time Cursor.(When enabled, it display a time cursor on a graph. The cursor can be moved to a mark location where the absorbance will be display for each graph and to select locations for Read Delay and the Read End Points.)

Click on the **OK** button to apply your choices.

You can always return to the default settings by clicking on the **Set Defaults** button.

#### ***Window in Display Options***

This tab, in the Examine Transients Peaks Display Options window, allows you to select the colors for the screen and your printer for various parts of the Examine Transients Peaks window.

**Fehler! Verwenden Sie die Registerkarte 'Start', um Heading 1 dem Text zuzuweisen, der hier angezeigt werden soll.. 167**

**Note:** *You can choose Printer colors in this dialog and then print the graph display in the Examine Transient Peaks window as follows:*

- From the File menu, choose **Print Active Window**  
**Select the Examine Transient Peaks Options dialog to perform the following functions:**

**Select colors for the following items:**

- Axes and Label
- Graph Title
- Analyte Mode Background
- Overlay Mode Background
- Read Delay and Read End Marks
- Time Cursor
- Axis Grid Divisions
- Active Signal Points
- Peak Maximum Mark

Click on the **OK** button to apply your choices.

You can always return to the default settings by clicking on the **Set Defaults** button.

### ***Lines in Display Options***

This tab, in the Examine Transients Peaks Display Options window, allows you to select the colors styles and line widths for the lines which will appear on the screen and your printer. Clicking on the style column of the style section displays a drop-down menu of various line choices which you can select to display in the Examine Transient peaks window.

Click on the **OK** button to apply your choices.

You can always return to the default settings by clicking on the **Set Defaults** button.

### ***Add Label Dialog***

Open the Add Label dialog by choosing Add Label from the Graph menu in the Transient Peaks window. If this option is not available, you must first open a data set.

Use this dialog to add text labels to an active peak by following the steps below:

1. Select the active peak.
2. Click on the peak name.
3. Open the Add Label dialog.
4. Click on the Graph menu and then click on Add Label.  
Enter the desired title for the active peak.
5. Type a label name for the active peak and click on OK. The text appears in the window.
6. To move the text, position the mouse cursor where you want the text to appear. Hold down the Shift key and click on the desired position.
7. To label another peak on the window repeat steps 1 through 3.

***Automatically use the peak Sample ID as the label text:***

Click the Use Sample ID button to automatically enter the Sample ID as the label text.

***Label all samples with their Sample ID's as their label text:***

Check the Label all samples with their Sample ID's checkbox to enable this feature. If this checkbox is checked when the OK button is pressed, all of the samples for the current analyte will be assigned labels and each will be the Sample ID for the respective peak.

***Clear all labels:***

Check the Clear labels from all samples checkbox to enable this feature. If this checkbox is checked when the OK button is pressed, any existing labels will be removed from the display of the current analyte.

***Printing from the Examine Transient Peaks Window***

You can print the graph and legend displayed in this window as follows:

- From the **Applications** button click **Active Window** (or Active Window Preview).

## ***Selecting Replicates***

---

You can choose the replicates you wish to view in the Examine Transients Peak window. The Replicates list is next to the Graph menu. Click on the drop-down arrow to make a selection, as described below.

### ***View the Transient Peaks of the first replicate only***

- Click on **First Replicate** in the Replicate drop-down list.

**Note:** *You may wish to view a single replicate when you are optimizing instrument parameters for the maximum signal/noise which will be critical for detection limit measurements.*

### ***View the Transient Peaks of the last replicate only***

- Click on **Last Replicate** in the Replicate drop-down list.

### ***View the Transient Peaks of the average of all replicates***

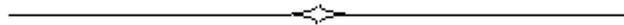
- Click on **Avg. Replicate** in the Replicate drop-down list.

**Note:** *During routine analysis you will most often just want to view an average of the replicates, which is the default setting. An exception to this may be if the Replicate Data from the Results Display window shows any significant discrepancies in replicate results.*

### ***View the Transient Peaks for all replicates***

- Click on **All Replicates** in the Replicate drop-down list.

**Note:** *All Replicates displays all of the replicates for a particular sample. This is different than the other modes, which display the first, the last, or the average of all replicates for all samples.*





## **Recommended Conditions**

## ***Recommended Conditions***

You use this window to show the recommended analytical conditions for the analyte (element) that you will determine. The pages that appear depend on the analytical technique that you have selected. Make sure that the accessories that you require are correctly installed and switched on. Refer to the user's guides for the instruments for installation instructions.

The analytical conditions shown can often be used to produce acceptable results for determining elements in samples with a simple matrix. For more complicated samples these conditions can be used as starting conditions for method development.

The following is an example dialog.

Recommended Conditions	
Data Remarks	
Element	Cu (Copper)
Setup data	
Wavelength	324.75 nm
Slit	0.7 nm
Rollover	0.70 abs
Temperatures	
Pyrolysis	1200 °C
Atomization	2000 °C
Atomization site	Pyro/Platform
Chemical modifier	0.005 mg Pd + 0.003 mg Mg(NO3)2
Performance checks	
Characteristic mass (typical)	17 pg/0.0044 A-s
Sensitivity check	25 ug/L for 0.15 A-s

The Pages of the Recommended Conditions Window:

- **Furnace Data** -- The recommended conditions for determining elements using the furnace technique.
- **Flame Data** -- The recommended conditions for the element when you use the flame or FIAS-flame technique.
- **FIAS-MHS Data** -- The recommended conditions for the element when you use the flow injection technique.
- **Remarks** -- Special conditions and other useful information for determining elements using the analytical technique that you have selected.

### ***Furnace Data***

This page shows the recommended analytical conditions for determinations using the graphite furnace technique. For determinations of individual elements in samples with simple matrixes, these conditions often produce acceptable results. For samples, you can use these as starting conditions for method development.

## ***Element***

- To display the conditions for a particular element, select the element from the drop-down list.

**Wavelength (nm):** This is the recommended wavelength for measuring the absorption of the element.

**Slit (nm):** The slit is normally used in the furnace technique.

**Rollover:** This is the absorbance at which you will begin to notice rollover of the Peak profile when using Zeeman background correction. Use this value to estimate the upper concentration limit for the calibration.

### **Temperature (°C):**

**Pyrolysis:** The recommended temperature for the pyrolysis step when you use the recommended modifier (see below). The optimum temperature depends on the sample matrix, the modifier and the combination of elements you are determining.

**Atomization:** The recommended temperature for the atomization step of the furnace program. The optimum temperature depends on the sample matrix, the modifier and the combination of elements you are determining.

**Atomization Site: Pyro/Platform** - Atomize the sample from the L'vov platform of a graphite tube. The platform and tube should have a coating of pyrolytic graphite.

**Atomization Site: Pyro/Wall** - Atomize the sample from the wall of a graphite tube. The platform and tube should have a coating of pyrolytic graphite.

**Chemical Modifier:** This is the recommended modifier for the selected element. The recommended amount of modifier is given as an absolute mass to add to each sample aliquot.

### **Performance Checks**

**Characteristic Mass : Typical:** This is the mass of analyte in picograms required to produce a peak height signal of 0.0044 or an integrated peak area signal of 0.0044. Use the method you have developed to analyze a reference solution of the element. The value you obtain for the characteristic mass should typically be within 20% of the value shown here.

**Sensitivity Check:** This shows the expected absorbance signal from a 20- $\mu$ L aliquot of a reference solution of the given concentration, analyzed using the recommended analytical conditions.

## **Flame Data**

You use this page to show the recommended analytical conditions for determinations using the flame technique using either the atomic absorption or the emission technique.

The analytical conditions shown can often be used to produce acceptable results for determining elements in samples with a simple matrix. For more complicated samples these conditions can be used as starting conditions for method development.

## ***Element***

Select the element from the drop-down list.

## ***Nebulizer***

Select the type of nebulizer in use. The information displayed in the Atomic Absorption table is updated to reflect the type of nebulizer you have selected

## ***Atomic Absorption***

**Wavelength (nm):** This is the recommended primary wavelength for measuring the absorption of the element. For some elements there are other wavelengths that you can use, for example to decrease the sensitivity .

**Slit Width (nm):** The slit width that provides the optimum sensitivity, the best signal-to-noise ratio and good linearity of the calibration curve at the recommended wavelength.

**Relative Noise:** The standard deviation for measurements with the flame on and using the recommended conditions compared to that for the primary wavelength and the associated recommended conditions. This value is therefore 1.0 for the primary wavelength. For other wavelengths, this value is a guide to the precision you can expect.

**Char. Conc. (mg/L):** An analysis of a simple reference solution containing this concentration of analyte, using the recommended conditions, will produce an absorbance of approximately 0.0044 ( 1% absorption).

**Sensitivity Check:** An analysis of a simple reference solution containing this concentration of analyte, using the recommended conditions, will produce an absorbance of approximately 0.200.

**Linear to (mg/L):** The approximate upper limit of the concentration for the linear part of the calibration curve. If you use a non-linear calibration equation and at least three calibration standards, you can normally create a useable calibration with an upper concentration limit of up to six times the value shown here.

**Oxidant:** The recommended oxidant, air or nitrous oxide, for analyses at the recommended wavelength.

**Oxidant Flow (L/Min):** The recommended flow rate of oxidant.

**Acetylene Flow (L/Min):** The recommended flow rate of acetylene.

## ***Flame Emission***

**Wavelength (nm):** This is the recommended wavelength for measuring the emission of the element.

**Slit (nm):** The slit width that provides the optimum sensitivity, the best signal-to-noise ratio and good linearity of the calibration curve at the recommended wavelength.

**Oxidant:** The recommended oxidant, air or nitrous oxide, for analyses at the recommended wavelength.

**Oxidant Flow (L/Min):** The recommended flow rate of oxidant.

**Acetylene Flow (L/Min):** The recommended flow rate of acetylene.

## ***FIAS-MHS Data***

You use this page to show the recommended analytical conditions for determinations using the FIAS-MHS technique.

The analytical conditions shown can often be used to produce acceptable results for determining elements in samples with a simple matrix. For more complicated samples these conditions can be used as starting conditions for method development.

### ***Element***

- Select the element from the drop-down list.

### ***Setup Data***

**Wavelength (nm):** This is the recommended wavelength for measuring the absorption of the element.

**Slit (nm):** For measurements at the recommended wavelength, this is the slit width that provides optimum analytical sensitivity with the best signal-to-noise ratio and good linearity of the calibration curve. This parameter is only relevant for instruments with variable slits.

**Cell Temp (°C):** This is the temperature of the quartz tube when using the electrically heated mantle for determinations.

**Note:** *This field does not appear if you are running a FIMS 100/400.*

**Pump #1 Speed:** This is the speed for the pump (#1) that fills the sample loop with sample.

**Pump #2 Speed:** This is the speed for the pump (#2) that controls the flow rate of the carrier solution, reductant and waste.

**Note:** *This field does not appear if you are running a FIMS 100.*

**Reductant:** This is the reducing reagent for the analysis. For example, 0.2% NaBH<sub>4</sub> is often used.

**Carrier Solution:** This is the solution that carries the sample solution through the system. For example, a 10% solution of HCl is often used.

**Carrier Gas Flow (mL/min):** This is the flow rate of the inert gas, normally argon, used to carry the gaseous hydride or mercury vapor to the quartz tube. The flow rate can have a significant influence on the sensitivity.

**Reaction Coil:** This is the length of the reaction coil where the carrier solution, containing the sample, mixes with the reducing reagent. Typically this tube is 110 mm long, with an inside diameter of 1.0 mm.

**Sample Volume (µL):** This is the volume of the sample loop on the flow-injection valve. The sample loops range in volume from 40 µL up to 1000 µL. To obtain larger volumes, you can combine two loops.

### ***Performance Checks***

**Characteristic Mass, Typical:** This is the mass of analyte in picograms required to produce a peak height signal of 0.0044 or an integrated peak area signal of 0.0044. Use the method you have developed to analyze a reference solution of the element. The value you obtain for the characteristic mass should typically be within 20% of the value shown here.

**Sensitivity Check:** This shows the expected absorbance signal, from the given volume of a reference solution of the given concentration, analyzed using the recommended analytical conditions.

## **Remarks**

This page shows any extra information that may be useful when determining the selected element using the selected atomization technique, for example, special precautions and alternative conditions.

- To display the remarks for an element, select the element from the drop-down list.
- To print the recommended conditions and remarks, click **Print**.

# *Glossary*

**Absorption:** A decrease in radiant energy when passing through matter, resulting in a corresponding increase in the energy of the absorbing system.

**addition calibrate:** See method of additions calibrate.

**Analyte:** The element whose concentration is determined in an analysis.

**analyte addition:** See methods of additions.

**analytical curve:** See calibration curve.

**Aspiration:** A high speed gas flow is directed across an open tube to draw solution into the nebulizer.

**atomization step:** The step in a program in which the analyte element is converted into an elemental state and can be quantitated.

**Atomizer:** The sample cell used to produce the ground state atoms necessary for atomic absorption to occur.

**Autozero:** A procedure that instructs the system to subtract the reading of the current sample (a blank or the average of several blanks) from subsequent measurements.

**background absorbance:** The absorption of radiation, at the analytical wavelength, that is not due to the analyte.

**Blank:** There are different types of blanks, for example: reagent blanks, sample blanks, and solvent blanks. They all contain one or more of the reagents used in sample or calibration solutions but do not intentionally contain the analytes.

**calibration curve:** The plot or the equation that describes the relationship between the concentration of an analyte and the variable that is measured to indicate the presence of the analyte. Once established, this relationship can be used to determine the analyte concentration in a sample.

**carrier gas:** The gas, usually argon, used to transport mercury vapor or hydride to the measurement cell when using the FIAS.

**char step:** Used to condition the sample before atomization by ashing or volatilizing the matrix. Also called the pyrolysis or thermal pretreatment step.

**characteristic concentration:** The amount of analyte in mg/L required to give a signal of 0.0044 A when performing Flame or FIAS-Flame analyses.

**characteristic mass:** The amount of analyte in picograms required to give a signal of 0.0044 A or A-s in Furnace or FIAS-MHS analyses.

**continuum background correction:** Background correction using a deuterium arc or tungsten halide lamp to allow subtraction of spurious absorption signals from the desired atomic absorption signal.

**correlation coefficient:** Indicates the quality of the fit between the calibration curve and the points it is fitting. A value of 1,000 indicates a perfect fit.

**detection limit:** The detection limit is defined as the concentration of the element which will produce a signal/noise ratio of 3. Thus, the detection limit considers both the signal amplitude and the baseline noise and is the lowest concentration which can be clearly differentiated from zero.

**Directory:** Contains one or more files and/or subdirectories, each of which contains one or more files and/or subdirectories and so on.

**dry step:** The step in a furnace program when the sample solution is gently dried and the solvent swept from the furnace tube.

**element file:** See method.

**Emission:** The creation of radiant energy in matter resulting in a corresponding decrease in the energy of the emitting system.

**external gas:** Argon or nitrogen protective gas around the outside of the graphite tube.

**FIAS:** Abbreviated for Flow Injection Analysis System.

**FIAS-Flame:** A technique that combines Flow Injection (FI) and Flame. The FIAS is used to introduced the sample into the flame.

**FIAS-MHS:** A technique that combines Flow Injection (FI) and the Mercury\Hydride System (MHS). The FIAS is used with MHS for analysis of mercury cold vapor and gaseous hydrides.

**graphite furnace:** A heated, semi-enclosed graphite device used to generate atomic absorption analyses.

**HGA:** An abbreviated for Heated Graphite Atomizer.

**hold time:** The time that a particular temperature is maintained in a furnace heating program.

**inert gas:** see carrier gas

**integrated absorbance:** see peak absorbance

**interference:** An enhancement or depression of the atomic absorbance signal of an analyte in a sample when compared with an aqueous standard of the same concentration.

**L'vov platform:** A small pyrolitic graphite plate that is inserted into a grooved graphite tube. Delays atomization of the sample until the internal atmosphere of the furnace tube reaches a stable temperature.

**Matrix:** The components in a sample mixture other than the element of interest.

**maximum power heating:** A term describing the result of entering a zero ramp time in a graphite furnace program. The furnace is heated as rapidly as possible until the programmed temperature is reached.

**Method:** Contains the operating parameters required to determine an element.

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**method of additions:** An analyte addition technique that allows you to compensate for matrix interferences by adding one or more standard spikes to the sample.

**method of additions calibrate:** A variation of method of additions, which can be used for a group of samples with the same matrix. Additions are used for the first sample only. The calibration curve that is established for the first sample is used in calculating the concentration of subsequent samples.

**MHS:** An abbreviation for Mercury Hydride System.

**Modifier:** A chemical or chemicals added to a sample in the furnace to modify its properties, for example, to increase the volatility of the matrix components or decrease the volatility of the element of interest.

**Parameters:** The values or selections that guide the software and hardware in performing determinations.

**peak absorbance:** See peak height.

**peak area:** The area under a peak, designated as A-s.

**peak height:** The highest absorbance signal of an absorbance peak profile.

**peak profile:** The absorbance versus time signal.

**pyrolysis step:** Used to condition the sample before atomization by ashing or volatilizing the matrix. Also called the thermal pretreatment or char step.

**pyrolytic coating:** A dense, layered graphite coating deposited onto a graphite tube or L'vov platform.

**QT-furnace:** Quartz tube furnace. The QT-furnace holds the quartz tube in position and heats it. You use the quartz tube in the FIAS-MHS technique.

**quartz tube:** An abbreviation for quartz tube atomizer (QTA). This is used in the hydride-generation AAS (HG AAS) technique and the cold vapor AAS (CV-AAS) technique to trap the gaseous hydrides or mercury vapor. In the HG-AAS technique, the analyte is then atomized by the QT-furnace that holds the quartz tube atomizer (QTA) in position and heats it.

**ramp time:** The controlled gradual rise in temperature between two steps in a furnace program.

**recommended conditions:** Analytical conditions defined for each element.

**Recovery:** The measured change in concentration divided by the concentration of a spike multiplied by 100.

**Sensitivity:** The slope of the analytical curve or calibration curve. It should not be used to mean characteristic mass or characteristic concentration.

**sequence number:** The number assigned to each sample when it is stored in a data set. This number is printed on the log during an analytical run. You will need to know this number to recall peak profiles to be replotted from data set.

**Spike:** Addition of a known quantity of an element to a sample, generally to test the recovery of the spike or analyte in a sample.

**standard deviation:** A statistical definition of the variation in a group of similar measurements.

**standard solution:** A solution that contains a known amount of analyte. It is used for calibration and reslope solutions, and it is added to sample solutions when the method of additions is being used and when recovery measurements are being made.

**stock standard solution:** A concentrated solution containing known amounts of one or more elements used to prepare a range of standards by dilution.

**thermal pretreatment step:** Used to condition the sample before atomization by ashing or volatilizing the matrix. Also called the pyrolysis or char step.

**THGA:** An abbreviation for Transversely Heated Graphite Atomizer. This is the type of furnace typically used with the longitudinal Zeeman ( ZL ) systems.

**Volatilization:** Passing from a solid or liquid state to a vapor.

**wall atomization:** Atomization in a furnace without a L'vov platform. The sample is actually deposited on the graphite tube wall.

**Workspace:** An arrangement of one or more windows on the screen. Workspaces can be saved on disk for later recall using the Save Workspace...command in the File menu.

**Zeeman:** A background correction system based on the splitting of an atomic spectral line in a magnetic field. The atomic signal is affected by the magnet whereas the background attenuation is not.

**ZL:** An abbreviation for Zeeman Longitudinal, a technique that uses the longitudinal Zeeman effect to compensate for background interferences.

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