CERTARA

Phoenix® Framework User's Guide

Applies to:

Phoenix WinNonlin® 8.3
Phoenix NLME™ 8.3
IVIVC Toolkit™ 8.3 for Phoenix
CDISC® Navigator 8.3
AutoPilot Toolkit™ 8.3 for Phoenix
Validation Suite™ 8.3

Legal Notice

Destination Control Statement

United States Government Rights

Certara, L.P.
100 Overlook Center, Suite 101, Princeton, NJ, 08540 USA
Telephone: +1.609.716.7900
www.certara.com

Contents

Phoenix Architecture

Phoenix is based on a modular framework, which results in a flexible and robust application platform for future expansion, promotes interchangeability between major and minor system components, and permits development of new, specialized tools through the use of the Phoenix API (**A**pplication **P**rogramming **I**nterface). Contact Certara Support for information on contracting with Certara to use the API.

This type of architecture is called a plug-in architecture because you can add and remove ***plug-ins*** (referred to in Phoenix as ***operational objects***) without affecting the core application. The Phoenix core application itself does not carry out any useful analytic tasks. It requires operational objects in order to perform any meaningful analysis. Each object provides a specific function. Descriptive statistics, noncompartmental analysis, and linear mixed effects modeling are all operational objects created for use with the Phoenix platform.

Phoenix allows you to work in an MDI (**M**ultiple **D**ocument **I**nterface) or an SDI (**S**ingle **D**ocument **I**nterface) environment. Workflows, operational objects, and datasets can be opened in their own window separate from the main Phoenix interface, or you can choose to work completely within the Phoenix user interface.

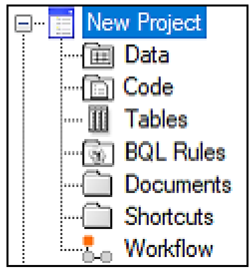
When using Phoenix, you will create projects that consist of one or more workflows of connected operational objects. For details on these concepts see:

Projects
Phoenix workflows
Workflow template
Operational objects

Projects

A Phoenix project is the workspace in which workflows, operational objects, and worksheets are combined to perform an analysis. Phoenix projects contain the following items:

– Data folder for worksheets and other datasets
– Code folder for PML, ASCII, and NONMEM code
– Tables folder for HTML formatted tables
– BQL Rules folder for BQL rules
– Documents folder for binary objects not placed in the other folders
– Shortcuts for pointers to input data files that were imported as shortcuts
– Workflow object that is used to group operational objects



Two of the benefits of Phoenix projects is that they allow analysis work to be easily organized and saved. You can save projects as Phoenix project files (*.phxproj) locally or save them to a database, such as Integral.

Phoenix projects are designed to be easily updated and shared, which allows for better data management. A project file contains all the datasets, such as study data, that were imported into a project so project files can be exchanged between users without also having to exchange external data sources. Sharing Phoenix projects has two main advantages:

- multiple users can review the steps and processes used in an analysis
- the amount of time needed to validate the results of an analysis is decreased.

Phoenix project files might be rejected by some email servers since they are password protected, in which case the user will need to adjust permissions to allow the `.phxproj` files.

Phoenix does not automatically save projects. Users must choose to save the project. Phoenix also prompts users to save projects when the application is closed. By default, Phoenix project files are saved in your `Documents` folder in `\Certara\Phoenix Projects`.

Note: Certain operations in Phoenix may occasionally generate “out of memory” errors. Merging in large datasets, generating plots with a large number of pages or lattices, running covariate shotgun on an NLME model, and saving multiple projects on the close of Phoenix are some examples of cases where a user’s computer may not have enough free memory to complete the operation. Many times the error only results in the offending object not displaying properly, while the remainder of output is unaffected.
To reduce the occurrence of memory errors while working with Phoenix: ensure that only the active Phoenix project is open; close any other applications that are open on the computer (email, web browsers, etc.); work with only relevant subsets of very large datasets so as not to carry around unused data in the workflow; create multiple plot or table objects to subset a large dataset. Of course, it is always a good working practice to save projects at regular intervals.

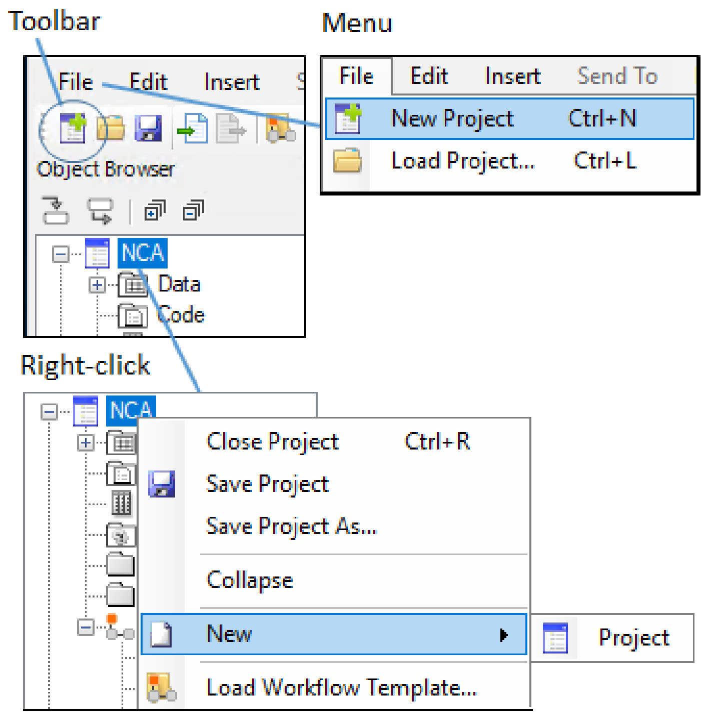
See also:

Creating or opening a project
Closing a project
Saving a project

For a brief, step-by-step example of using the Phoenix interface, see "Quick Tour of Phoenix".

Creating or opening a project

To create a project in Phoenix

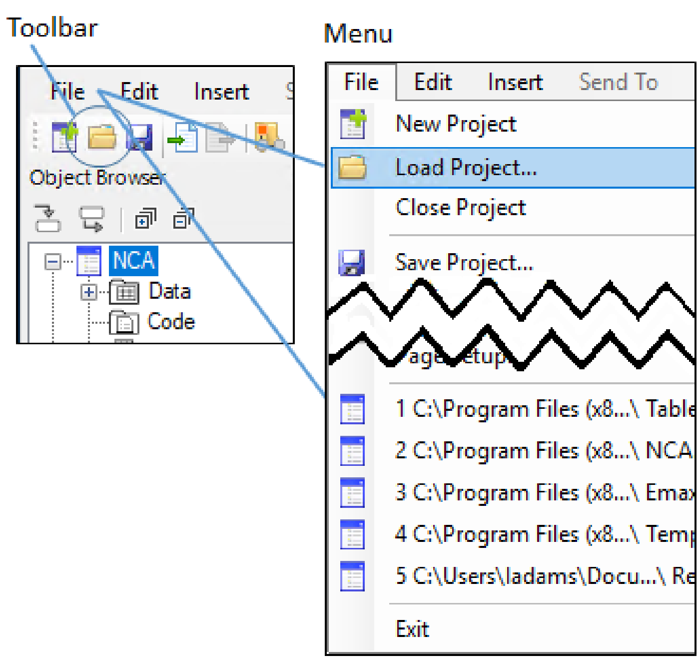


Click (**New Project** icon) in the toolbar.

Or select **File > New Project**.

Or right-click an object in the Object Browser and select **New > Project** in the menu.

To open a saved Phoenix project



Click (**Load Project** icon) in the toolbar.

Or select the project from the bottom of the **File** menu, if it was one of the last five projects opened in Phoenix.

Or select **File > Load Project**, choose the project file (`.phxproj`) and click **Open**.
(If the project file is in a different location, use the *Load Project* dialog to browse to the location.

Or outside of Phoenix, double-click a Phoenix project file (`.phxproj`).
By default, Phoenix project files are saved in your `Documents` folder in `\Certara\Phoenix Projects`.

Note: It is not recommended to open two conflicting projects since the re-serialization occasionally causes project corruption.

To restore a project from a backup file

Phoenix's auto-backup feature was implemented to aid in recovering from corrupt projects. When saving a project, a backup project file (with an extension of .phxbackup) is created in the same directory as the project. This provides a recent "checkpoint" from which most of the work can be recovered in the event that a project becomes corrupt. Note that there is only one backup file maintained for a project, i.e., subsequent save operations overwrite the project's backup file.

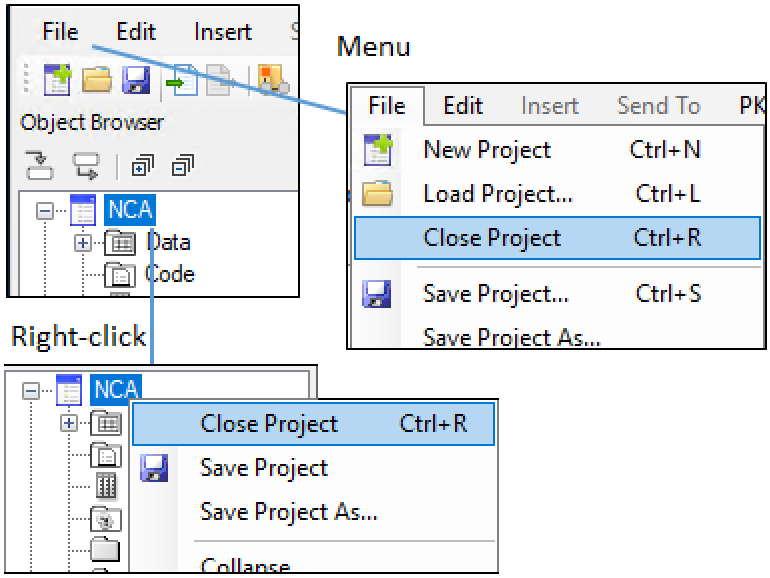
Right-click the **<project_name>.phxbackup** file in a file browser and select **Properties**.

On the General tab, change the extension from `.phxbackup` to `.phxproj` and the project_name (if the original project exists).and press **OK**.

Press **Yes** in the confirmation popup to rename the file.

The backup file is saved as a project file and can be opened in Phoenix.

Closing a project



Right-click the project in the Object Browser and select **Close Project**.

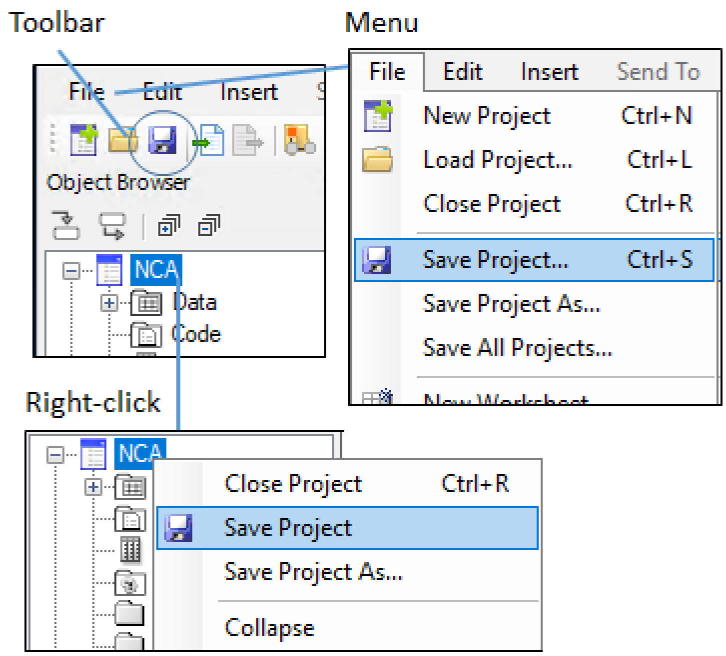
Or select **File > Close Project**.

Then, in the message dialog:

> Click **Yes** to confirm that changes to the project should be saved and use the *Save Project* dialog to specify a directory and file name for the saved project.
>
> Or click **No** to not save changes. A warning message is displayed stating that all project changes will be lost if the project is not saved. Click **Yes** to close the project or **No** to keep it open.

Note: Should a Named User Server license become disconnected while there are still unsaved projects open, you must ensure that a license is retrieved before attempting to close Phoenix. Otherwise, there will be no ability to save the project, and all changes will be lost.

Saving a project



To save a project

Click (**Save Project** icon) in the toolbar.

Or select **File > Save Project**.

Or type `CTRL+S`.

Or right-click a project in the Object Browser and select **Save Project**.

If a project has not been previously saved, Phoenix displays the *Save Project* dialog.

Specify the directory in the *Save Project* dialog.

Specify a file name in the **File name** field.

Click **Save** to save the project.

To save a project under a new name

Select **File > Save Project As**.

Or right-click a project in the Object Browser and select **Save Project As**.

Then, in the *Save Project* dialog, type a new file name in the **File name** field.

To save all open projects

Select **File > Save All Projects**.

If a project has not been previously saved, Phoenix displays the *Save Project* dialog. Type a new file name in the **File name** field.

Phoenix workflows

There are two types of workflows: ***project*** and ***operational***. The first type of workflow, the project workflow, refers to the series of steps needed to complete an analysis. This includes importing data, manipulating data, using model objects to analyze data, and saving or exporting the results. Project workflows contain the data, models, and other objects needed to complete an analysis, from data setup through reporting of results.

The second type are "Operational objects". The Workflow operational object is the root of all analysis work in Phoenix. It allows users to put together as many types of operational objects as needed to complete an analysis and, thereby, execute only a certain group of operational objects in a project. In a complex analysis that requires a large number of operational objects, Workflow objects provide a way of organizing various operational objects into larger, more complex functional units.

Workflow objects allow users to map data and code to operational objects in the workflow, and manage the flow of data between operational objects. Users can also access the Diagram tab through Workflow objects, which can be used to add operational objects, map data, and execute objects.

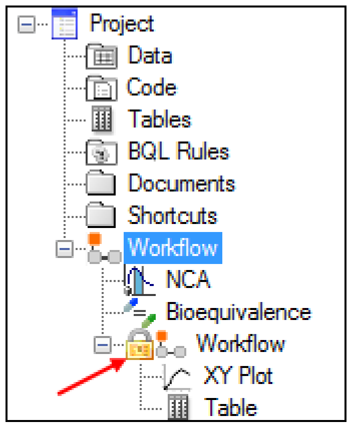


Figure 4-1. Root workflow with a locked sub-workflow

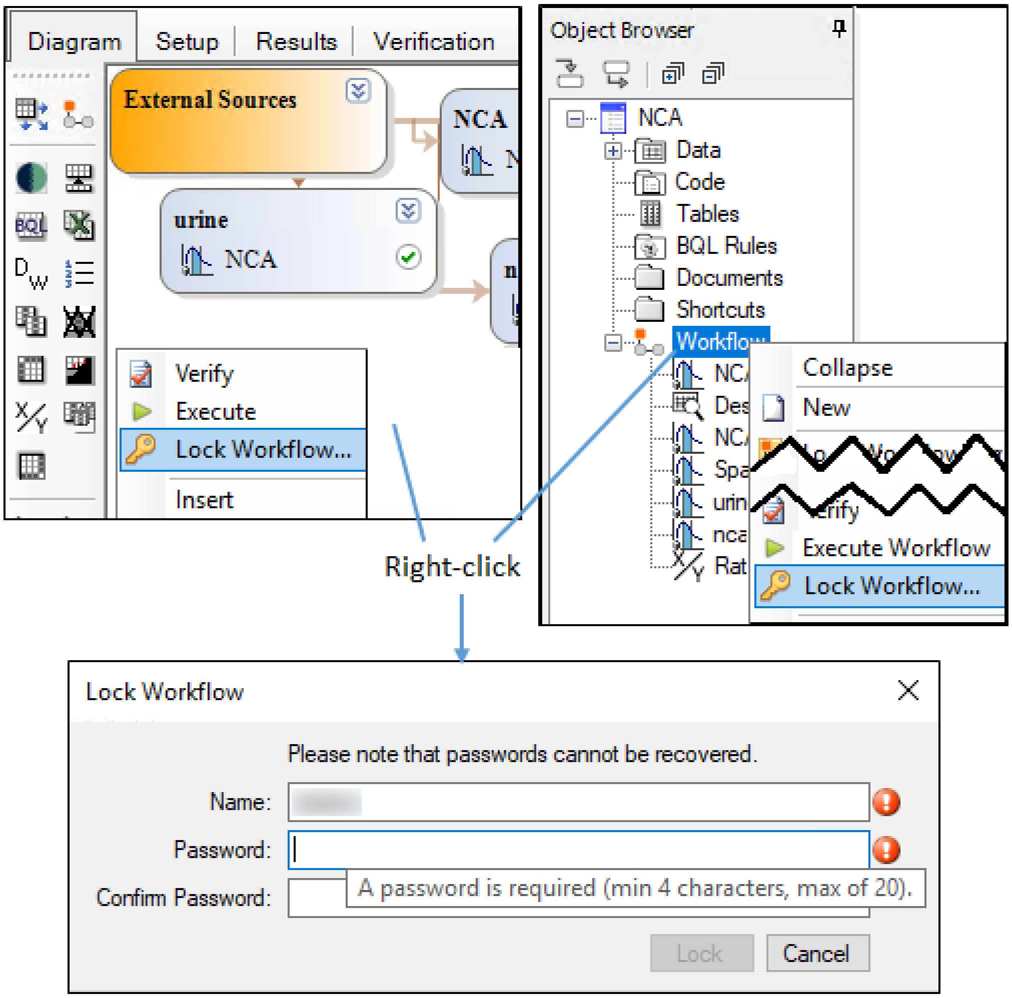
One or more Workflow objects can be inserted into a project like any other operational object. Multiple workflow objects can also be added to a project's root Workflow object, with each subsequent Workflow object containing its own group of operational objects.

A Workflow operational object does not, itself, perform any sort of analysis. It is only used to group the other operational objects, such as NCA, NLME, or Convolution, that do perform the analyses. Once a Workflow object is set up with all of the objects required to complete a desired set of analysis operations, it can be saved as a template for later use (see "Workflow template" for more information).

Locking and Unlocking a workflow

Locking a Workflow object protects it from modification, preserving the operational object settings and data flow between them.

To lock a workflow



Right-click the Workflow object or empty area in the Object Browser or Diagram and select **Lock Workflow**.

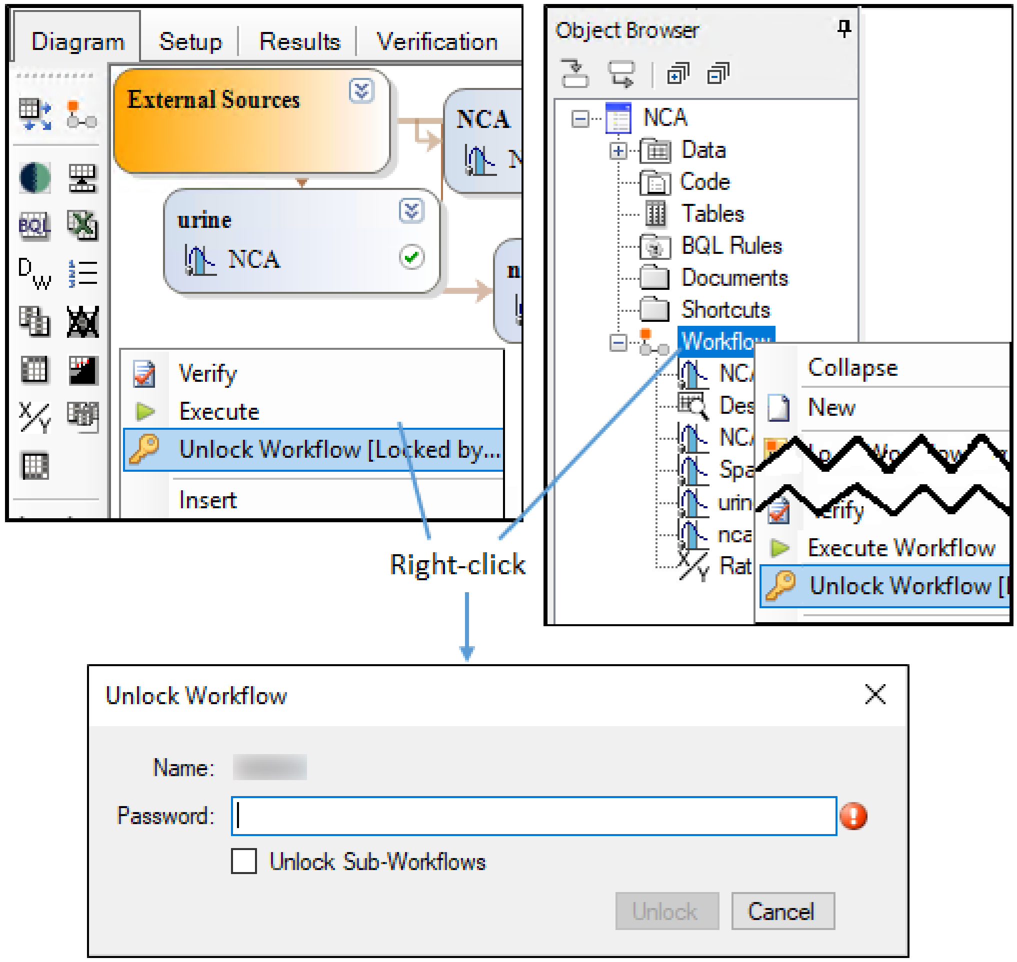
Then, in the *Lock Workflow* dialog, enter the password to be used to unlock the workflow (enter it a second time to confirm the password) and press **Lock**.

When a workflow is locked, a padlock  is added to the workflow icon.

All unlocked objects within the workflow (and any nested workflows) will be locked with the same username/password. If any nested workflow is already locked, a message is displayed asking for confirmation to continue.

Note: Phoenix does not track passwords used to lock workflows. Therefore, if a password is forgotten, the workflow will need to be recreated.

To unlock a workflow



Right-click a locked Workflow object or an empty area in the Object Browser or Diagram and select **Unlock Workflow**.

In the *Unlock Workflow* dialog, enter the password that was used to lock the workflow.

Use the **Unlock Sub-Workflows** checkbox to indicate if only the main workflow is to be unlocked (unchecked) or unlock all nested workflows as well (checked).

Press **Unlock**.

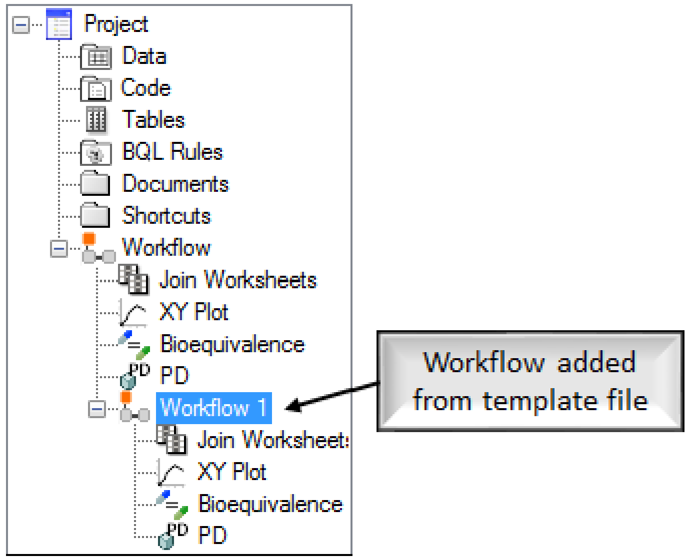
Note: Nested workflows within a locked workflow cannot be unlocked without first unlocking the outer workflow.

When a workflow is locked, it cannot be copied/pasted or saved as a template. However, an unlocked workflow that contains a nested, locked workflow can be copied/pasted or saved as a template (the password will still be required to unlock the nested workflow).

Locking a workflow also limits the functionality of operational objects within the workflow. The Setup, Verification, and Information tabs become unavailable, and the Options area becomes disabled. Adding or removing operational objects from locked workflows is not allowed. New input data mappings are not allowed either; to re-use locked workflows, use Data Links and the Data Wizard to map data to the workflow before locking.

Workflow template

A Workflow Template in Phoenix works like a template in Microsoft Word, it allows you to recreate the same steps over and over, and gives you a form or fields that can be used to automatically recreate a workflow to use with a new dataset.



Workflow Templates are `.phxtmplt` files that contain the specific configuration of each operational object in a workflow. Any pointers to results data are saved with the template (e.g., NCA Final Parameters worksheet), but not the original data input sources. (Note that older WinNonlin Template (`*.wnlt`) files can still be loaded into Phoenix, but are no longer created by Phoenix.)

Note: Workflow Template files do not contain any mappings or links to external data sources, which means templates do not have data mappings to external sources, or with any parameter settings in external scripts (e.g., scripts for connecting with third-party tools). This information must be remapped each time the template is used. The incorporation of Data Links in the workflow can streamline the process of connecting external data sources when a template is used.

By saving a workflow as a Workflow Template you can quickly reapply an analysis on new data. This allows a common analysis to be predefined for automated performance of repetitive analyses. Templates contain the specific configuration of each operational object in a workflow, but do not contain the original data input sources.

Tip: Default templates can be shared with others by having an administrator set up the template preferences file `default_templates.binconfig`, located in `C:\Users\<username>\AppData\Roaming\Certara\Phoenix\Configuration` to point to a common location where the shared templates will be stored. Notifications can then be sent by the administrator with the configuration file, template files, and instructions on where to store the files.

This section contains the following topics:

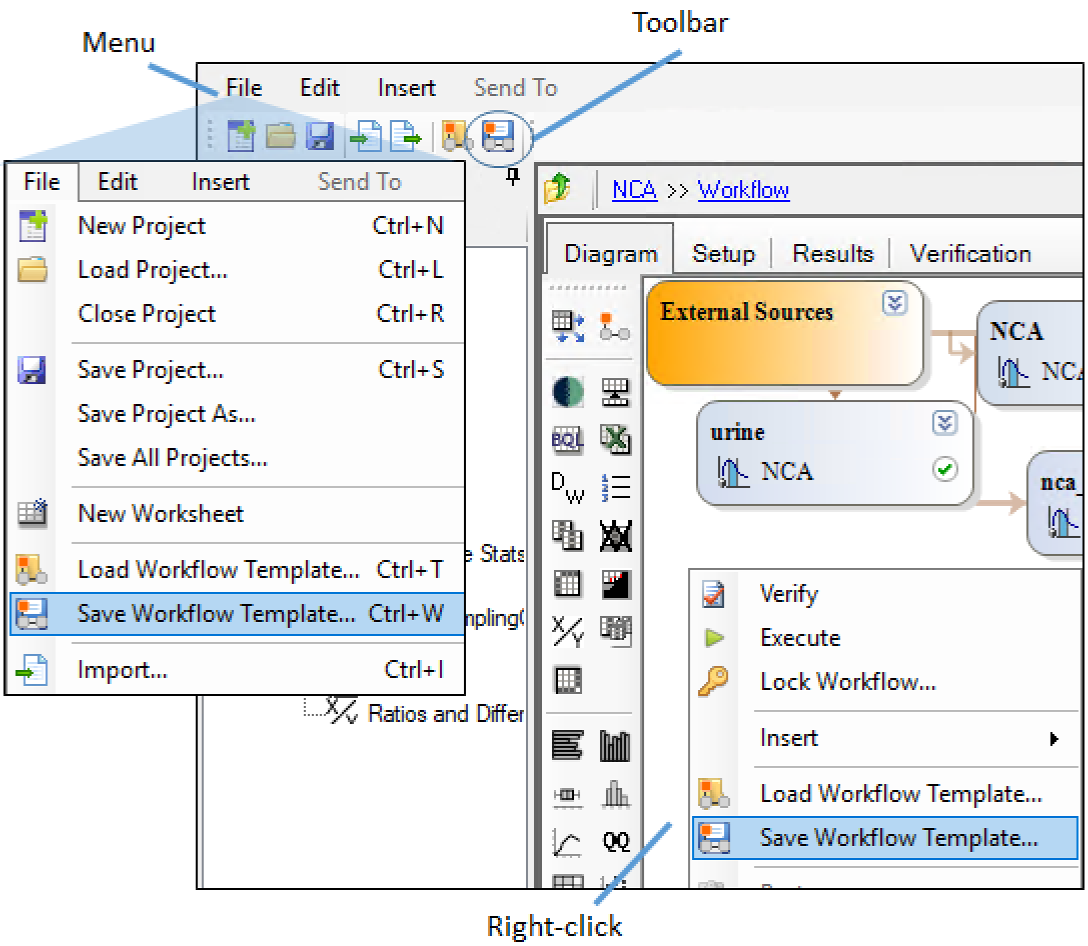
See also "Workflows and Templates example".

Saving and loading Workflow Templates

In situations where a particular workflow is commonly used, saving it as a Workflow Template allows you to simply load the template file rather than recreate the entire workflow every time.

The default location for saved Workflow Templates is set through the Project Settings page of the *Preferences* dialog (**Edit > Preferences**, select **General > Projects**).

To save a workflow template



Select the Workflow object in the Object Browser or in the Diagram.

Click  (**Save Workflow Template** icon) in the Phoenix toolbar.

Or select **File > Save Workflow Template** in the Phoenix menu.

Or right-click the Workflow object or empty area in the Object Browser and select **Save Workflow Template**.

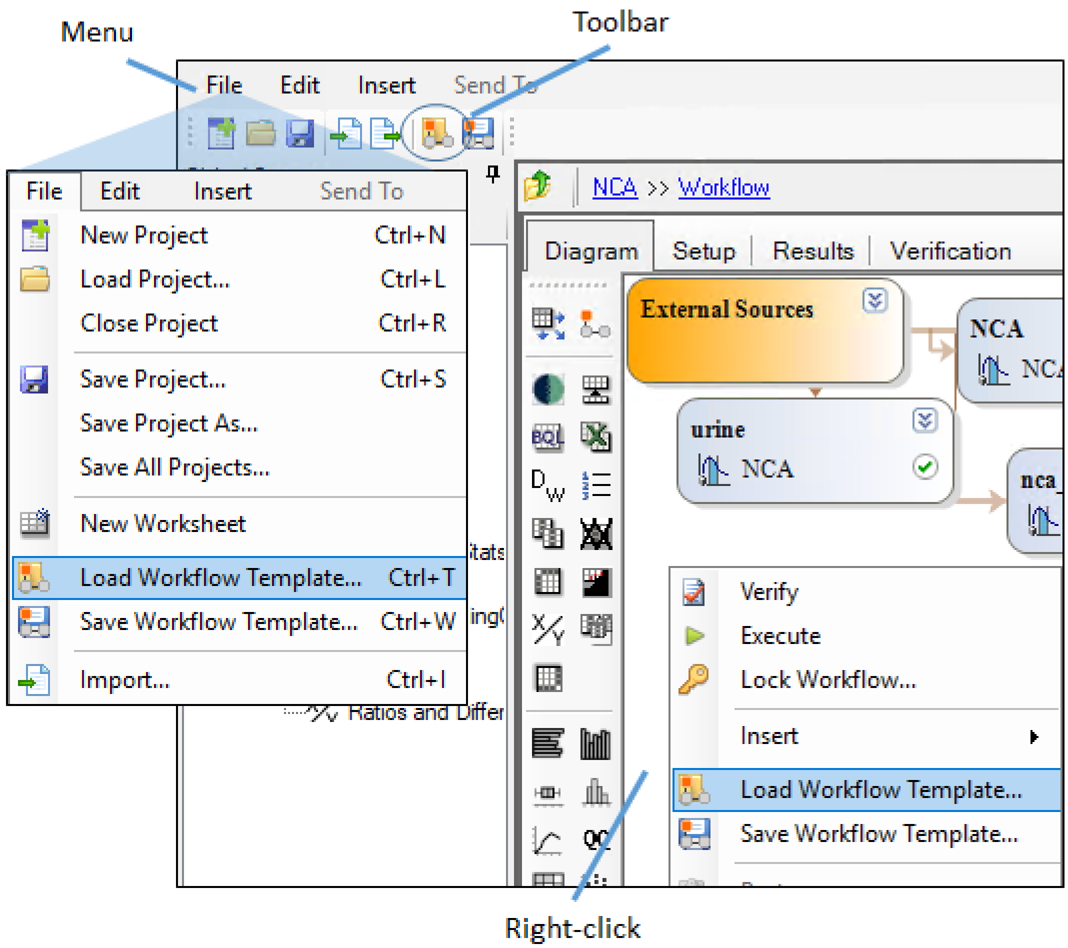
Or right-click an empty area in the Diagram and select **Save Workflow Template**.

In the *Save Workflow Templates* dialog, enter a name for the template file.

If you want to save the workflow's history with the template file, uncheck the **Clear History** checkbox.

Click **Save**.

To add a workflow template to the current workflow



Select a project or any Workflow object in the Object Browser or in the Diagram:

Click  (**Load Workflow Template** icon) in the Phoenix toolbar.

Or select **File > Load Workflow Template** in the Phoenix menu.

Or right-click the Workflow object or empty area in the Object Browser and select **Load Workflow Template**.

Or right-click an empty area in the Diagram and select **Load Workflow Template**.

In the *Load Workflow Templates* dialog, select the template.

If desired, enter a suffix to append to the names of the imported objects.

Click **Open**.

Note: Workflow templates do not load internal worksheets with sort variables, since sorts usually indicate profile-specific data. Use an external worksheet or Data Links to optimize re-use of templates.

Workflows and Templates example

The purpose of the example is to show Phoenix's ability to create and reuse workflows. This example shows users how to create a workflow to perform an analysis, save the workflow as a template, and use the template to complete the same analysis using different data.

This example assumes that a drug company wants to create a generic form of a popular drug. The company wants to test two formulations of a compound in order to decide which formulation is closest in bioequivalence to the name brand drug. In this example users will create a workflow to test the first formulation, save the workflow as a template, and reuse the template to test the second formulation.

Data for this study were created using Certara's Trial Simulator™.

The completed project (`Templates.phxproj`) is available for reference in …`\Examples\Data and Plots`.

Most Phoenix objects require the same basic steps for their use. However, there may be multiple paths to accomplishing a step (e.g., main menu, right-click menu, drag-and-drop, etc.). For simplicity, only one is listed here.

Any object added to a project can be viewed in its own window by selecting the object in the Object Browser and double-clicking it or pressing **ENTER**. All instructions for setting up and executing an object are the same whether the object is viewed in its own window or in Phoenix's viewing.

See also:

Phoenix workflows
Workflow template

Set up the workflow

A Workflow object is the part of the project that is used to contain and manage operational objects, similar to how the Data folder is used to contain and manage datasets.

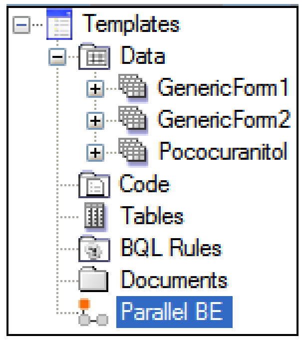
Workflows can be set up to perform complex operational procedures using operational objects. A Workflow can be saved as a template file, which allows users to create complex operational procedures once, and reuse and share them multiple times.

The advantage of a template is that it saves the configuration settings in each of the operational objects it contains. However, templates do not save mappings to external datasets. This means that a template can be created that can be easily reused with multiple datasets.

1. Create a project called `Template`.
2. Import the datasets.
   From …`\Examples\WinNonlin\Supporting files\`, import:
   `GenericForm1.xls`
   `GenericForm2.xls`
   `Pococuranitol.xls`
3. Select the **Has units row** option for each worksheet (except the History worksheets), using the **Right Arrow** button to advance to the next preview screen.
4. Once you get to the last screen, click **Finish**.

Note: Datasets in XLS (Microsoft Excel Workbook) format are added to the Data folder as workbooks.

5. Rename the workflow as `Parallel BE`.



Add Data Link objects

1. Drag the following worksheets from the Data folder to the display area: **Pococuranitol_data**, **Pococuranitol_dose**, **GenericForm1_data**, and **GenericForm1_dose**. This creates a Data Link object for each input dataset.
2. Execute the **Parallel BE** workflow object.

Later in the tutorial, you will switch the input datasets for two of the Data Link objects and then re-execute the workflow objects using the new datasets. Without the Data Link objects, you would have to redefine the input for each of the individual objects affected by the dataset change.

Add BQL objects

BQL is an acronym for Below Quantifiable Limit. BQL rules are used to exclude values in a dataset that are too low to be useful in an analysis. See "BQL" for information.

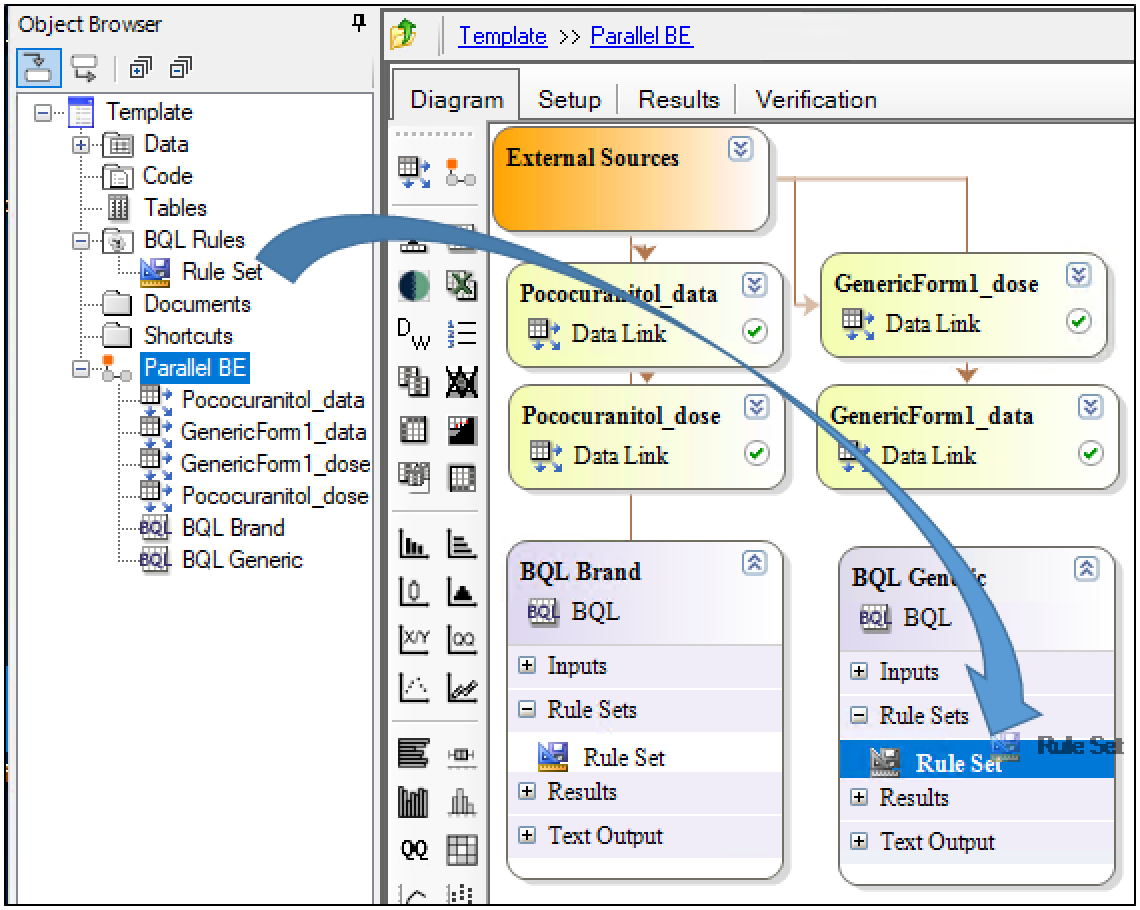
1. Right-click the **Parallel BE** workflow object, select **New > Data Management > BQL**.
2. Rename the BQL object as `BQL Brand`.
3. Insert a second BQL object named `BQL Generic`.

Create and map the BQL rule set

BQL rule sets are created and stored in the BQL Rules folder.

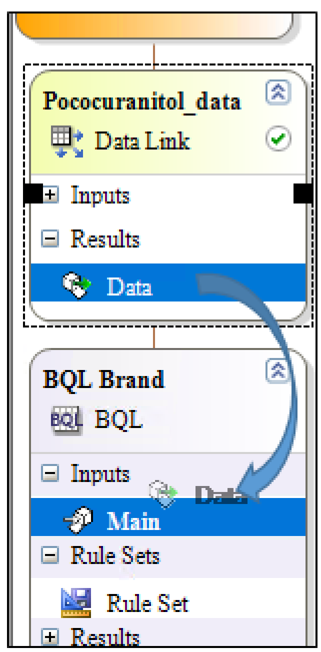
1. Right-click the **BQL Rules** folder, select **New > Rule Set**.
2. Type `ERR` under **Nonnumeric Code**.
3. Type `0` (zero) under **Unconditional Substitution**.
4. Check the **Use When < LLOQ** checkbox.
5. In the Properties tab, check the **Use Static LLOQ Value** checkbox.
6. Type `0.01` in the **LLOQ Value** field.
7. Select the **Parallel BE** workflow in the Object Browser.
8. In the Diagram, for both **BQL Brand** and **BQL Generic** objects:

   – Click the  button.
   – Click the (+) symbol to expand **Rule Sets**.
   – Drag the **Rule Set** from the BQL Rules folder to the BQL Rule Set input.



Setup BQL objects

1. In the Diagram, expand **Pococuranitol_data** and the **Results** section.
2. Drag **Data** to **BQL Brand > Inputs > Main**.



3. Expand **GenericForm1_data** and the **Results** section.
4. Drag **Data** to **BQL Generic > Inputs > Main**.
5. Select the **BQL Brand** object in the Object Browser.
6. Map the data types in the Main Mappings panel as follows:
   Subject to the **Sort** context.
   Time to the **Time** context.
   Concentration to the **Concentration** context.

   Leave all other data types mapped to **None**.
7. In the Properties tab, type `BrandConc_gt_0_01` as the **Output Column Name**.
8. Execute the object.
9. Select the **BQL Generic** object.
10. Map the data types as follows:
    Subject to the **Sort** context.
    Time to the **Time** context.
    Concentration to the **Concentration** context.

    Leave all other data types mapped to **None**.
11. Type `GenericConc_gt_0_01` as the **Output Column Name**.
12. Execute the object.

Set up two Descriptive Statistics objects

1. Go to the Results tab of the BQL Brand object.
2. Right-click the **Output** worksheet, select **Send To > Computation Tools > Descriptive Statistics**.

   A Descriptive Statistics object is inserted into the Parallel BE workflow. The columns in the Output worksheet are automatically mapped to the Descriptive Stat object's Main Mappings panel. See "Descriptive Statistics" for more information.)
3. Rename the Descriptive Statistics object `Descriptive Stats Brand`.
4. Map the data types as follows:
   Subject mapped to **None**.
   Time to the **Sort** context.
   BrandConc_gt_0_01 to the **Summary** context.
5. In the Options tab:
   – Check the **Confidence Intervals** checkbox.
   – Check the **Number of SD Statistics** checkbox.
   Do not change the default value.
6. Execute the object.
7. Go to the Results tab of the BQL Generic object.
8. Right-click the **Output** worksheet, select **Send To > Computation Tools > Descriptive Statistics**.
9. Rename the Descriptive Statistics object `Descriptive Stats Generic`.

10. Map the data types as follows:
    Subject mapped to **None**.
    Time to the **Sort** context.
    GenericConc_gt_0_01 to the **Summary** context.
11. In the Options tab:
    – Check the **Confidence Intervals** checkbox.
    – Check the **Number of SD Statistics** checkbox.
    Do not change the default value.
12. Execute the object.

Plot the concentration values over time

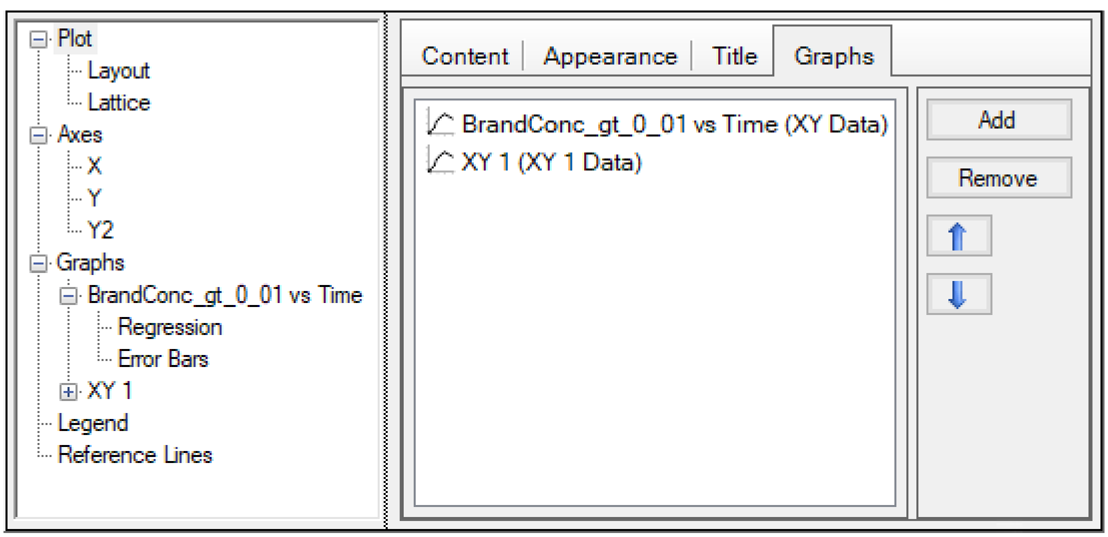
In this example, XY Plot objects will be used to graphically look at the data. Refer to “Plotting” for information on other plot objects.

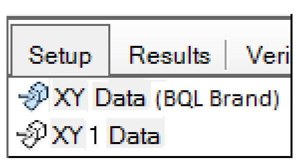
1. Go to the Results tab of the BQL Brand object.
2. Right-click the **Output** worksheet, select **Send To > Plotting > XY Plot**.
3. Rename the XY Plot object `XY Plot Brand vs Generic`.
4. Map the data types as follows:
   Subject to the **Group** context.
   Time to the **X** context.
   BrandConc_gt_0_01 to the **Y** context.

Add a second graph to the XY Plot object.

5. With **Plot** selected in the Options tab menu tree, click the Graphs tab.
6. Click **Add**.

   A second XY Plot input named XY 1 Data is added to the Setup list.





7. Map the Output worksheet from BQL Generic as input for the second graph:
   – Click the **XY 1 Data** object in the Setup panel.

   – In the XY 1 Data Mappings panel, click (**Select Source** icon).
   – In the dialog, select the BQL Generic **Output** worksheet and click **OK**.
8. Map the data types as follows:
   Subject to the **Group** context.
   Time to the **X** context.
   GenericConc_gt_0_01 to the **Y** context.
9. Execute the object.

Examine the output in the Results tab. The plot shows that the concentration values peak at different times for the two formulations.

Plot the mean concentration values over time

1. Go to the Results tab of the Descriptive Stats Brand object.
2. Right-click the **Statistics** worksheet and select **Send To > Plotting > XY Plot**.
3. Rename the XY Plot object `XY Plot Mean Brand vs Generic`.
4. Map the data types as follows:
   Time to the **X** context.
   Mean to the **Y** context.
   SD to the **Lower Error Bars** and **Upper Error Bars** contexts.

   Leave all other data types mapped to **None**.

Add a second graph to the XY Plot object.

5. With **Plot** selected in the Options tab menu tree, click the Graphs tab.
6. Click **Add**.
7. Click the **XY 1 Data** object in the Setup panel.
8. In the XY 1 Data Mappings panel, click the **Select Source** icon.
9. Select the Descriptive Stats Generic **Statistics** worksheet and click **OK**.
10. Map the data types as follows:
    Time to the **X** context.
    Mean to the **Y** context.
    SD to the **Lower Error Bars** and **Upper Error Bars** contexts.

    Leave all other data types mapped to **None**.
11. Execute the object.

The plot shows that the mean concentration values peak at very different times for the two formulations.

The plot does not place the points close to the axes, it is hard to differentiate between the overlaid plots, and the plot does not have a title. Use the Options tab to change the X and Y axes ranges, change the plot colors, and add a title.

12. In the Options tab, select **Plot** and go to the Title tab.
    – In the title field, type `Brand and Generic Mean Concentration`.

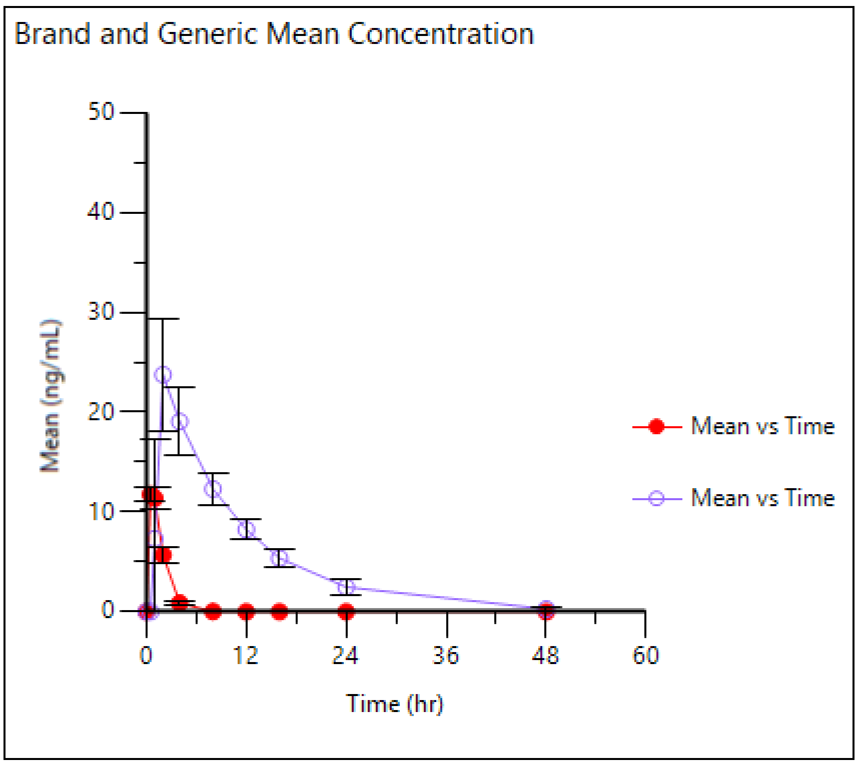
13. Select **Axes > X**.
– In the **Range** area, select the **Custom** option button.
– Leave the **Minimum** field set to `0`.
– In the **Maximum** field enter `60`.

14. Select **Axes > Y**.
– In the **Range** area, select the **Custom** option button.
– In the **Minimum** field, enter `0`.
– In the **Maximum** field enter `50`.

15. Select **Graphs > Mean vs Time** (the first one in the list).
– In the Appearance tab, select **Red** from the **Marker Color** menu.
– In the **Marker Border Color** menu, select **Red**.
– In the **Line Color** menu, select **Red**.

The Descriptive Statistics Brand plot is now highlighted in red.

The plot is automatically updated to reflect the new axes ranges, plot colors, and the title. Note that the XY Plot object did not have to be re-executed.



Set up two noncompartmental analysis objects

Refer to "NCA" for more information on the NCA object.

1. Go to the Results tab for the BQL Brand object.

2. Right-click the **Output** worksheet, select **Send To > NonCompartmental Analysis > NCA**.

3. Rename the NCA object `NCA Brand`.

4. Map the data types as follows:
Subject to the **Sort** context.
Time to the **Time** context.
BrandConc_gt_0_01 to the **Concentration** context.

In this example, one dose of 50 mg was administered at time zero. The Pococuranitol workbook has dosing data stored in the Pococuranitol_dose worksheet.

5. Select **Dosing** in the NCA Setup tab.
6. In the Mappings panel, click the **Select Source** icon.
7. Select the **Pococuranitol_dose** worksheet and click **OK**.
8. Map the data types as follows:
   Subject to the **Sort** context.
   Dose to the **Dose** context.
   Time_of_Dose to the **Time** context.
9. Execute the object.
10. Once the job finishes, go to the Results tab for the BQL Generic object.
11. Right-click the **Output** worksheet, select **Send To > NonCompartmental Analysis > NCA**.
12. Rename the NCA object `NCA Generic`.
13. Map the data types as follows:
    Subject to the **Sort** context.
    Time to the **Time** context.
    GenericConc_gt_0_01 to the **Concentration** context.

In this example, one dose of 50 mg was administered at time zero. The GenericForm1 workbook has dosing data store in the GenericForm1_dose worksheet.

14. Select **Dosing** in the Setup tab.
15. In the Mappings panel, click the **Select Source** icon.
16. Select the **GenericForm1_dose** worksheet and click **OK**.
17. Map the data types as follows:
    Subject to the **Sort** context.
    Dose to the **Dose** context.
    Time_of_Dose to the **Time** context.
18. Execute the object.

Create the formulation dataset for the bioequivalence model

Combine the Final Parameters Pivoted worksheets from both NCA objects and use the combined output in a bioequivalence model. The new column created by the Append Worksheets object will contain the formulation information for the bioequivalence model.

1. Go to the Results tab for the NCA Brand object.
2. Right-click the Final Parameters Pivoted worksheet, select **Send To > Data Management > Append Worksheets**.
3. Map **Subject**, **Cmax**, and **AUClast** to the **Source Column** context.
   Leave all other data types mapped to **None**.
4. Click the **Worksheet2** object in the Setup panel.
5. In the Worksheet 2 Mappings panel for the Append Worksheets object, click the **Select Source** icon.
6. Select NCA Generic **Final Parameters Pivoted** worksheet and click **OK**.

7. Map **Subject**, **Cmax**, and **AUClast** to the **Source Column** context.
   Leave all other data types mapped to **None**.
8. Execute the object.

Set up the first bioequivalence model

Refer to "Bioequivalence" for more information on the Bioequivalence object.

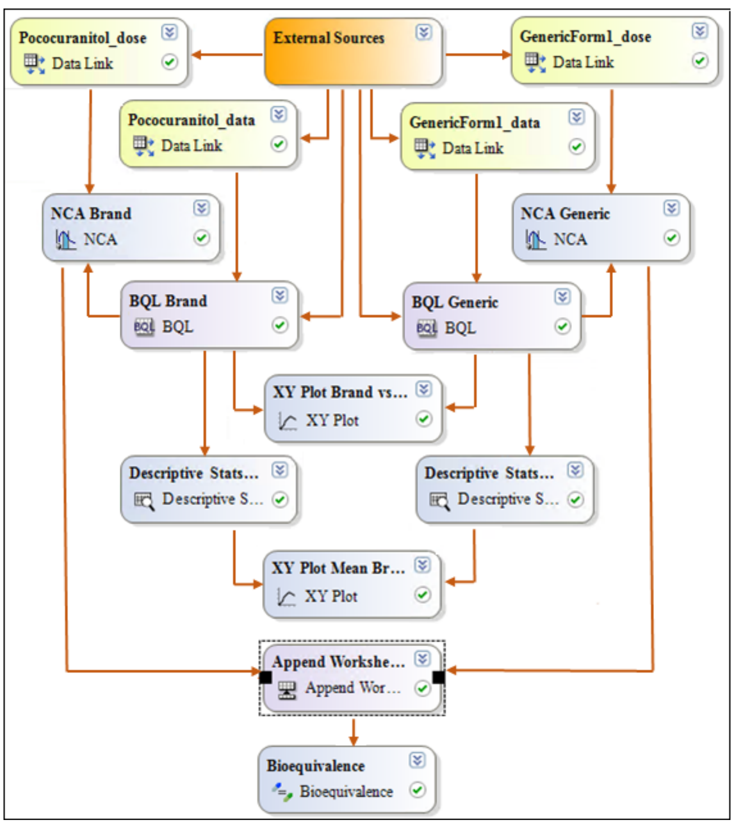
1. Right-click the Results worksheet for the Append Worksheets object, select **Send To > Computation Tools > Bioequivalence**.
2. Map the data types as follows:
   Source to the **Formulation** context.
   Subject mapped to **None**.
   Cmax to the **Dependent** context.
   AUClast to the **Dependent** context.
3. In the Model tab, select the **Parallel/Other** button.
   This option sets the model to a parallel bioequivalence model.

   Leave **Reference Formulation** set to **NCA Brand**.
4. Execute the object.

Examine the output in the Results tab.

Create and add a template

The Parallel BE workflow looks like this:



In Phoenix templates, any data mappings that are internal to the workflow are retained. For example, all expected output from the BQL objects, such as subject, time, and concentration, are retained in the NCA objects' Main Mappings panel. Mappings that are external to the template, such as the BQL rules and the datasets used with the BQL objects are not retained.

1. Select the **Parallel BE** workflow.
2. Click (**Save Workflow Template** icon) in the toolbar to save the workflow as a template.
3. In the dialog, enter the name as `Parallel BE`.
4. Click **Save**.

The workflow is saved as a Workflow template file in the location set in the *Preferences* dialog (by default `<default Project directory>/templates`) and named `Parallel BE.phxtmplt`.

5. Select **Template** in the Object Browser.
6. Click (**Load Workflow Template** icon) in the toolbar to load the template file.
7. In the dialog, select **Parallel BE.phxtmplt** and click **Open**.

The template is added to the project as a second workflow. The second workflow is nested below the first one and named Parallel BE 1.

Note: All references to workflows and operational objects in this section of the example refer to the Parallel BE 1 workflow and the operational objects it contains.

Set up the objects in the template workflow

1. Map the rule sets for both BQL Brand and BQL Generic objects.
   – In the **Parallel BE 1** workflow object, expand the objects, if necessary.
   – Drag **Rule Set** from the BQL Rules folder to the Rule Set input for both objects.
2. Drag the external data sources from the Data folder to the Data Link objects as follows:
   GenericForm2_data to Inputs > Data for the **GenericForm1_data** object.
   GenericForm2_dose to Inputs > Data for the **GenericForm1_dose** object.
   Pococuranitol_data to Inputs > Data for the **Pococuranitol_data** object.
   Pococuranitol_dose to Inputs > Data for the **Pococuranitol_dose** object.
3. Execute each object in the Parallel BE 1 workflow.
4. Select the **XY Plot Brand vs Generic** object, select Output in the Results tab.

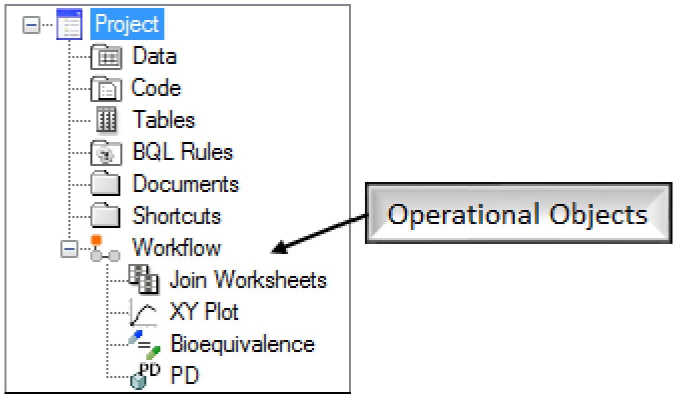
   The plot shows that the concentration values peak at very different times in the two different study groups. The second generic formulation lasts longer and has much higher concentration values than the brand name formulation.
5. Select the **XY Plot Mean Brand vs Generic** object, select Output in the Results tab.

   The plot shows that the mean concentration values peak at very different times in the two different study groups.
6. Examine the Bioequivalence output against the results from the first Bioequivalence object.
7. Right-click the project and select **Close Project**.

This concludes the Workflows and Templates example.

Operational objects

Phoenix analysis work is done using operational objects. An operational object contains a pointer to input data, a model, plot, or some other function, plus worksheet results, plot results, and text results. Examples of operational objects include data manipulation objects such as Column Transformation and Pivot Worksheet, models like Semicompartmental Modeling and PK Models, and plots like the XY Plot.



All operational objects can be inserted from the **Insert** menu, the Object toolbox, the **Send To** menu, and the workflow menu. They have user-defined settings and options that can be accessed in the Setup tab list and in the option tabs located beneath the Setup tab. Results in the form of worksheets, plots, and text, which are output from an executed operational object.

Operational objects use two types of data: external and internal.

An external data source for an operational object points to an imported dataset in the Data folder. The data is not contained in the object.

Internally generated data sources include worksheets created within Phoenix. These can be created either by users or by executing an operational object to get output results (e.g., the Final Parameters worksheet from a model can be sent as input to a Descriptive Statistics object for further analysis). These data are also not contained in the object.

This section contains information about the following topics:

Inserting operational objects
Using the Setup tab
Object settings
Renaming results
Using the Results tab

Inserting operational objects

Operational object menus in Phoenix are arranged by groups. There are several ways to insert an operational object, but the operational object menus are always grouped the same way.

Insert an operational object in ***one*** of the following ways.

- Select a project or workflow in the Object Browser and then select the **Insert >** <Mouse Click> (object group) **>** (operational object) menu item.
- Select a workflow in the Object Browser. On the left side of the Diagram tab that is displayed, click the object button in the Object Toolbox.
- Right-click a workflow in the Object Browser and then select **New >** <Mouse Click> (object group) **>** (operational object) from the menu.

- Right-click a data set in the Data folder or a results worksheet and then select **Send To >** <Mouse Click> (object group) **>** (operational object) from the menu.

The object is added to the project in the Object Browser and to the workflow Diagram tab. In addition, the inserted object is automatically opened in the right viewing panel. Each object's default view is the Setup tab, which contains all the steps necessary to set up an object.

Note: Any object added to a project can be viewed in its own window by selecting the object in the Object Browser and double-clicking it or pressing the **ENTER** key. All instructions for setting up and executing an object are the same whether the object is viewed in its own window or in Phoenix's viewing panel.

Plotting	**Computation Tools**
Bar Plot ( )	Bioequivalence ( )
Box Plot ( )	Convolution ( )
Column Plot ( )	Crossover ( )
Histogram Plot ( )	Deconvolution ( )
QQ Plot ( )	Descriptive Statistics ( )
Scatter Plot ( )	Linear Mixed Effects ( )
XY Plot ( )	Ratios and Differences ( )
X-Categorical XY Plot ( )	
NonCompartmental Analysis	**IVIVC**
NCA ( )	IVIVC ( )
NonParametric Superposition ( )	Levy Plot ( )
Semicompartmental Modeling ( )	Loo-Riegelman ( )
	Wagner-Nelson ( )

Modeling	Data Management
Maximum Likelihood Models ( ) Maximum Likelihood Model Comparer ( ) Least-Squares Regression Models interface Dissolution Model ( ) Indirect Response Model ( ) Linear Model ( ) Michaelis-Menten Model ( ) PD Model ( ) PK Model ( ) PKPD Model ( ) User ASCII Model ( )	Append Worksheets ( ) BQL ( ) CDISC Data Preparer ( ) Crossproduct Worksheets ( ) Data Wizard ( ) Enumerate Worksheets ( ) Join Worksheets ( ) Merge Worksheets ( ) Pivot Worksheet ( ) Rank Worksheet ( ) Split Worksheet ( ) Stacker ( )
Reporting	**External Software**
Reporter ( ) Table ( )	NONMEM Shell ( ) NONMEM Comparer ( ) PsN Shell ( ) R Shell ( ) SAS Shell ( ) SigmaPlot Shell ( )
System	
Data Link ( ) Workflow ( )	

Using the Setup tab

Every operational object has a Setup tab, which contains a list of items that must be specified before a model or other operational object can be executed. Each Setup tab has two common items: a panel used to map a dataset to an object's input and a toolbar. Some operational objects contain an additional tab used to sort the input columns or the output columns.

The following topics are discussed in this section:

Using the Setup tab toolbar

Each item in the Setup tab list contains a toolbar. The Setup tab toolbar allows users to select a data source, copy an internal worksheet to the Data folder, and view or delete the mapped data source.

Select source identifies an input data source for a Setup tab item.

Publish source copies an internal worksheet to the Data folder. (This button is only available for internal worksheets.) Displays the *Select Object* dialog. Select the Data folder or a worksheet in the Data folder in which to place the worksheet and click **Select**. Copying an internal worksheet to the Data folder converts the worksheet to an external source and automatically maps the column headers in the worksheet to the context associations.

Toggle source data panel displays the external source mapped to the Setup tab item. (This button is only available if a Setup tab list item has an external worksheet mapped to it.)

Remove source unmaps an external source worksheet from an operational object.

Load Object Settings displays the *Load Object Settings* dialog for selecting a saved settings file, in the default settings directory, to apply to the selected object.

Import Object Settings displays the *Import Object Settings* dialog for selecting a saved settings file, not in the default settings directory, to apply to the selected object.

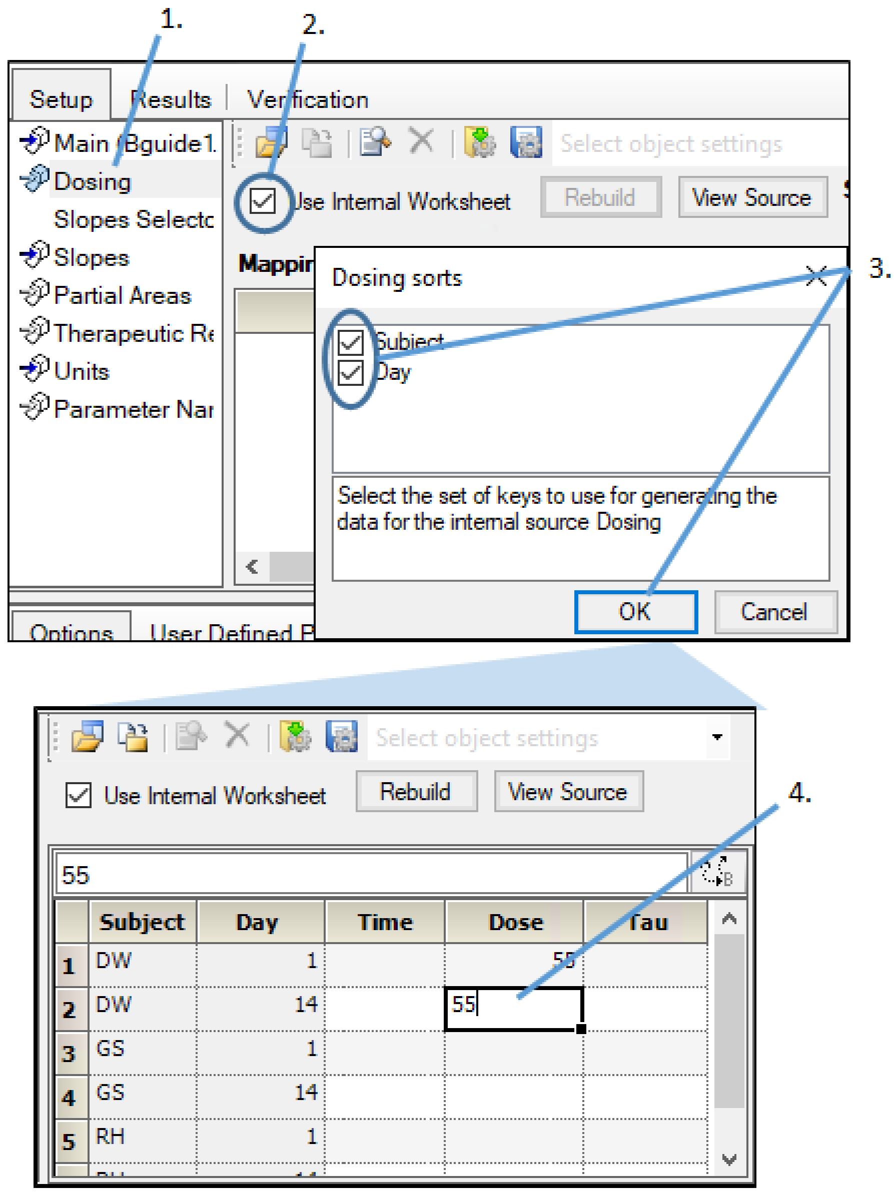
Save Object Settings displays the *Save Object Settings* dialog for saving the current object settings to a file for later use.

The pull-down menu lists all of the saved settings files that are located in the default settings directory and pertain to the selected object type. Selecting one from the menu displays a confirmation dialog for applying the settings. Click **Yes** to load the settings.

Entering data manually

Users do not have to use an external worksheet to provide input to operational objects. Internal worksheets can be used to enter the information necessary to set up an operational object.

Note: The primary data input for any operational object does not allow users to manually enter data.



1. Select an item in the Setup tab list other than the primary data input.
2. Select the **Use Internal Worksheet** checkbox.

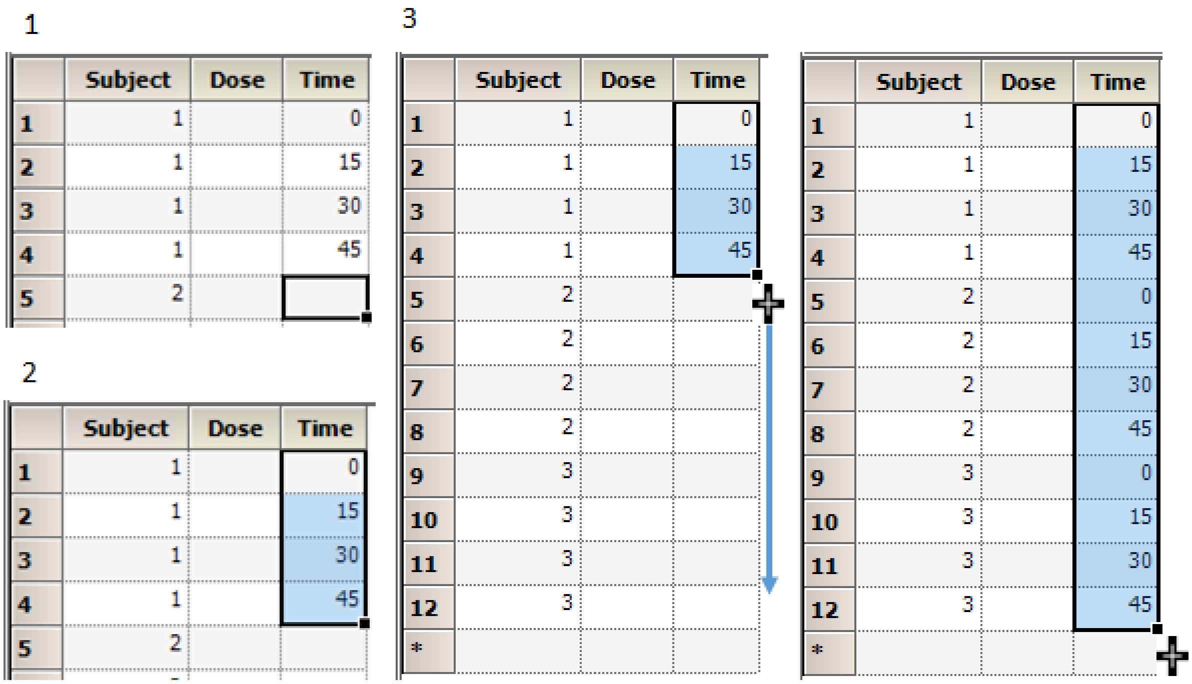
If the operational object uses sort keys, a dialog asks for the sort keys to use.

3. Check the boxes beside the sort keys to use and click **OK**.
4. Add the rows and columns of input data (refer to “Editing data values in worksheets”).

Note: The **Rebuild** button in the mappings panel can be used to rebuild the worksheet, incorporating any changes that affect the contents of the worksheet.

When entering data manually into cells, there are a couple of features that can help with copying and moving values: "drag and fill" feature and "drag" feature.

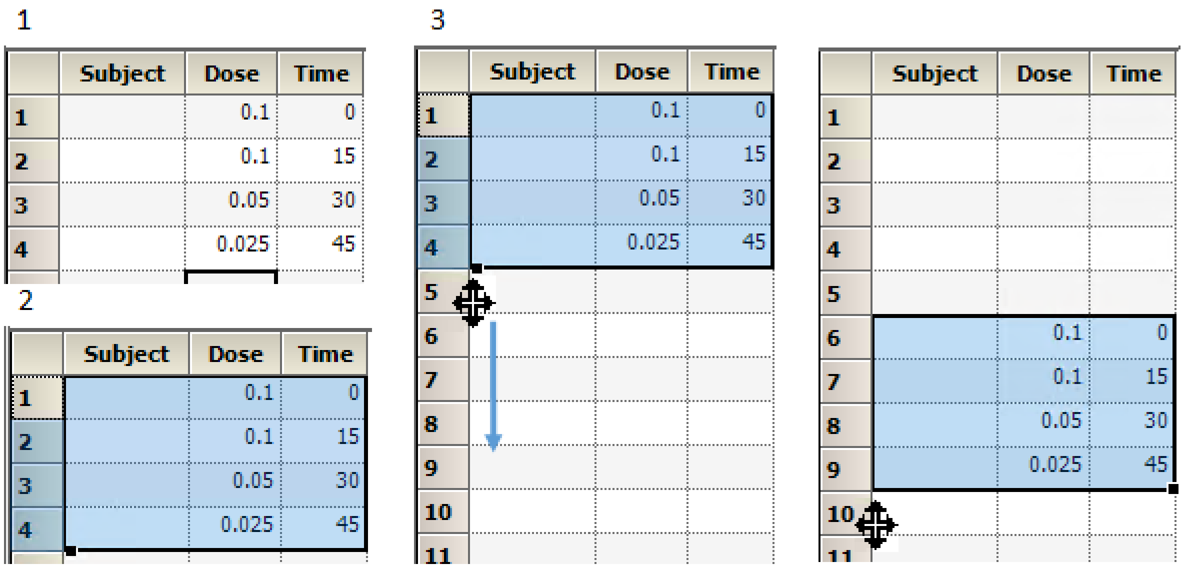
To use the drag and fill feature to propagate values



1. Enter the value(s) to propagate.
2. Use the pointer to highlight those cells.
3. Place the pointer over the black square on the lower right side of the selection.
   When the pointer changes shape, press the left mouse button and drag the selection down or across to fill the other cells.

In the image above, the same set of times when a dose is administered is being propagated to all subjects.

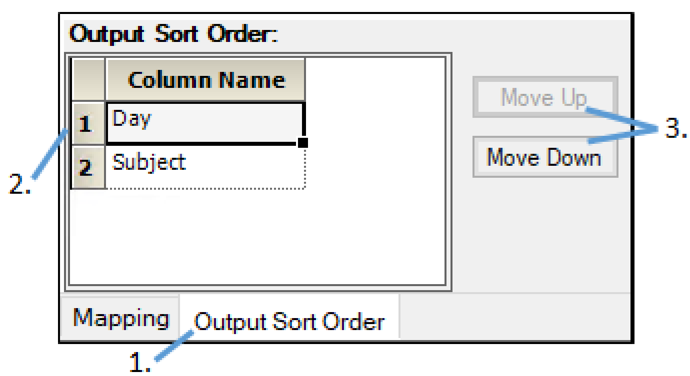
To use the drag feature to move values



1. Enter the value(s).
2. Use the pointer to highlight the entire row(s).
3. Place the pointer over the black square on the lower left side of the selection.
   When the pointer changes shape, press the left mouse button to drag the selected row of values to the destination row.

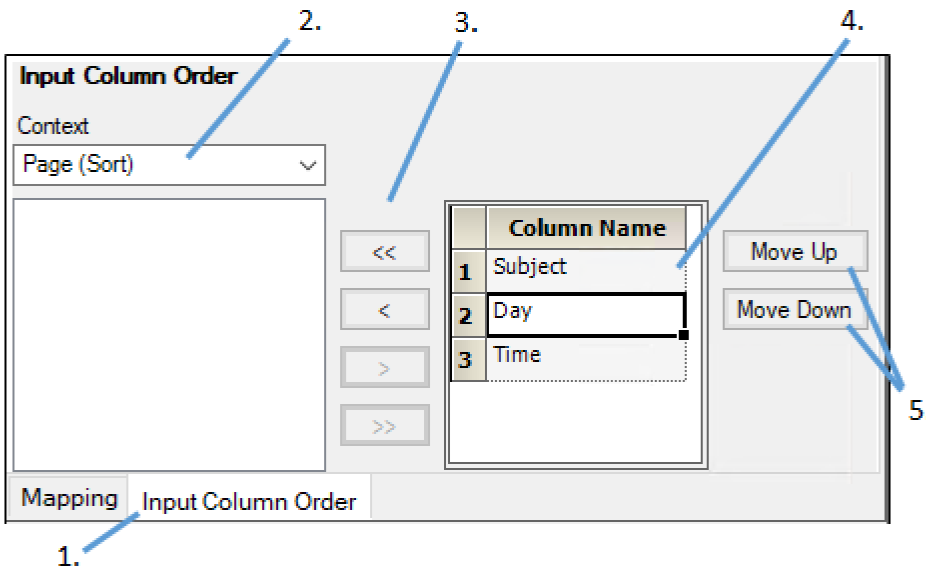
Output Sort Order and Input Column Order tabs

Most operational objects have an Output Sort Order tab used to arrange results worksheets based on the sort keys mapped in the primary data input. The Output Sort Order tab is located beside the Mapping tab.



1. Select the **Output Sort Order** tab.
   Data types mapped to the object's Sort context are listed.
2. Select a column name.
3. Click the **Move Up** or **Move Down** buttons to change the position of the columns.
   Results worksheets are sorted based on the selections made in the Output Sort Order tab.

Plotting operational objects have an Input Column Order tab for sorting the input columns used to create graphs. Users can select column headers mapped to different sorting contexts and specify how the points, bars, or lines are sorted in the output.



1. Select the **Input Column Order** tab.
2. From the **Context** menu select the context to which the sort keys are mapped.
   Plot objects have multiple sorting contexts, so the menu options are different for each plot object.

   The data types mapped to the selected context are listed below the **Context** menu.
3. Select a sort key in the list, then use the **>** and **<** buttons to move it between lists.
   Use the **>>** and **<<** buttons to move all sort keys between the lists.
4. Select a column name.
5. Click the **Move Up** or **Move Down** buttons to change the position of the columns.

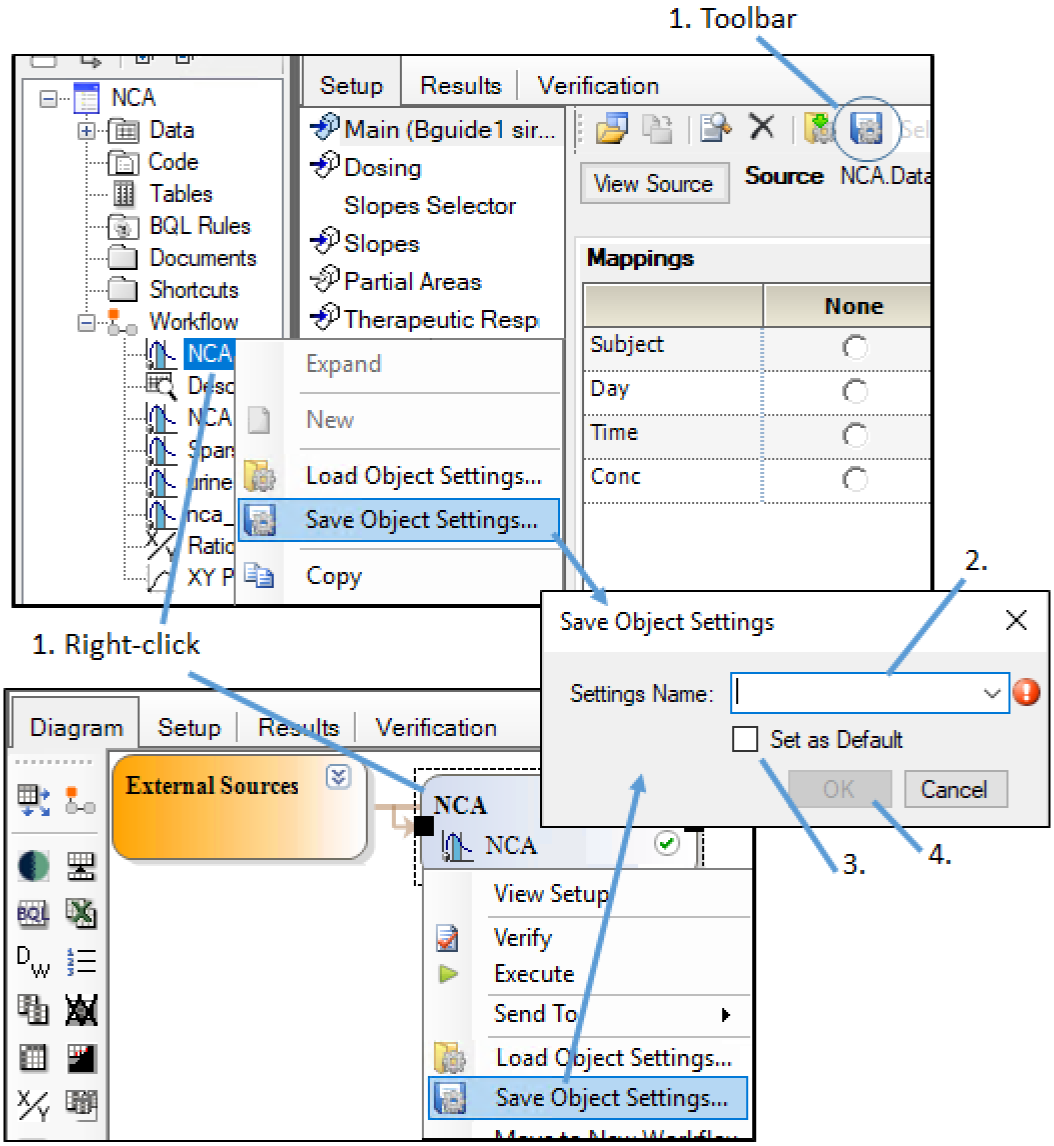
Object settings

An Object Settings file contains all of the settings used with an operational object and has a `.phx-setting` extension. The Object Settings file can be used to expedite future analysis of operational objects that are created to perform complex or specific functions. The file contains the specific configuration of an operational object, but does not contain the original data input sources. The configuration in the file can be loaded into an operational object of the same type or it can be specified as the default configuration for that object type, so that the settings in the file are loaded when each new operational object of that type is added to a workflow.

Note: Unlike other objects, the Data Wizard can contain many steps. Saving and loading object settings for Data Wizard objects includes settings for all steps, but input mappings for the first step only.

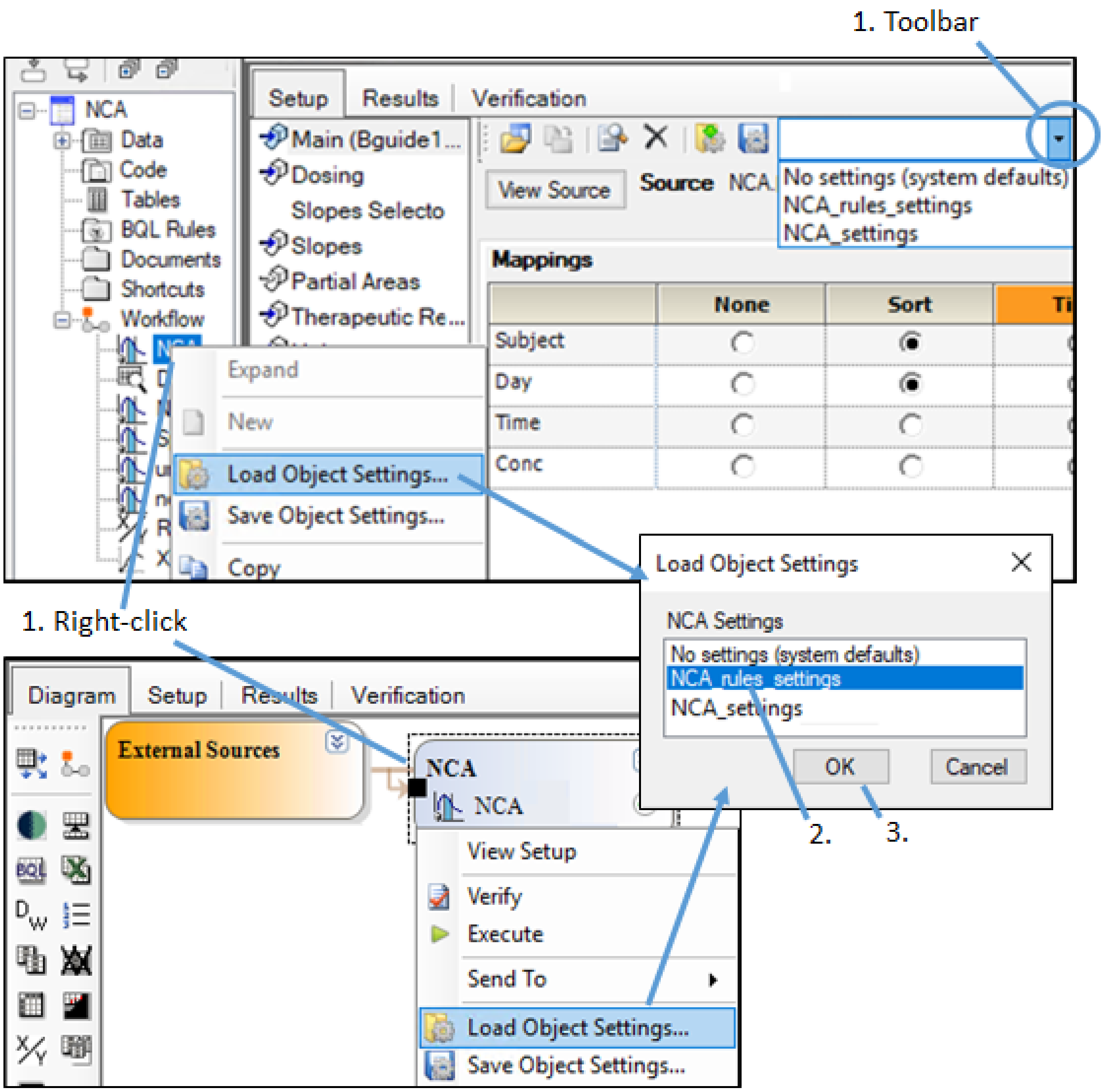
To save object settings

Once an object has the desired settings it can be saved to an Object Settings file. Settings files are saved to `C:\Users\<username>\Documents\Certara\Phoenix Object Settings`. See “To set object settings preferences for operational objects” for additional information.



1. With the object selected in the Object Browser, click  (**Save Object Settings** icon) in the Setup tab toolbar. Or right-click the object in the Object Browser or Diagram and select **Save Object Settings**.
2. In the dialog, enter a name for the file.
3. Check the **Set as Default** checkbox to use this settings file as the default settings when an object of the same type is inserted in Phoenix.
4. Click **OK**.

To load object settings to an existing object



1. With the object selected, choose the settings file from the pull-down list in the Setup panel toolbar. Or right-click the object in the Object Browser or Diagram and select **Load Object Settings**.

Note: Selecting the **No settings (system defaults)** option ignores any user-specified settings and uses the Phoenix default settings.

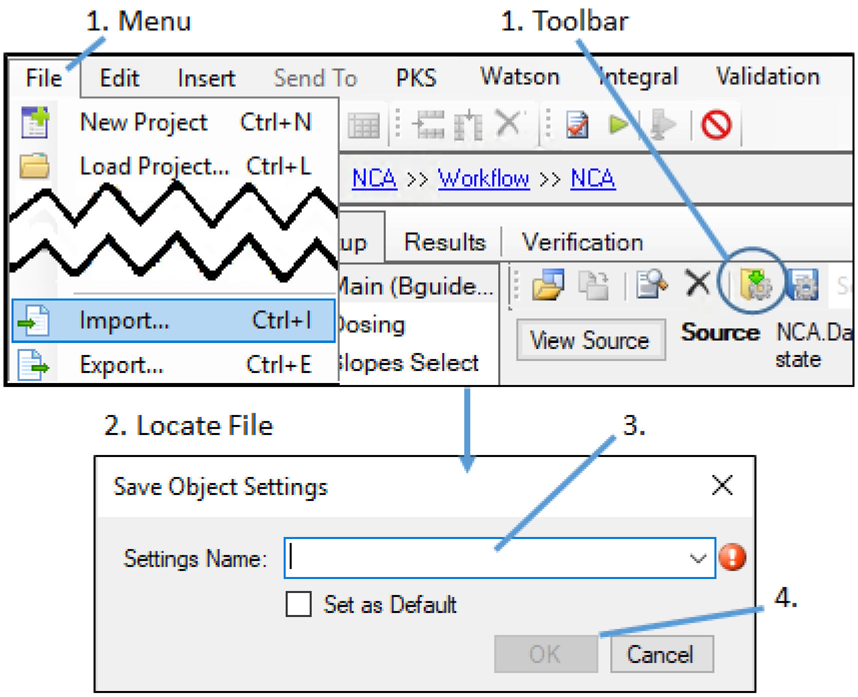
2. In the dialog, select the settings file from the list available for the same operational object type.
3. Click **OK**.

A note about internal and external worksheet handling

If an internal worksheet has one or more Sorts, then this indicates that the worksheet is data-specific and would not be applicable to other data, so it is not saved with the object settings. If there is no Sort in an internal worksheet (e.g., the same dosing or partial area was applied to all Sorts), then that internal worksheet is saved with the object settings and will be applied when those object settings are loaded. Thus, worksheets that do not allow for Sorts (e.g., NCA Parameter Names, NCA Units, and BQL Rules) will always be saved and loaded with object settings.

External mapped worksheets have priority over internal worksheets. If an external worksheet is mapped as an auxiliary worksheet in an object (e.g., NCA Dosing worksheet) and the object settings that are loaded have an internal worksheet saved with them, the external worksheet and mappings will override.

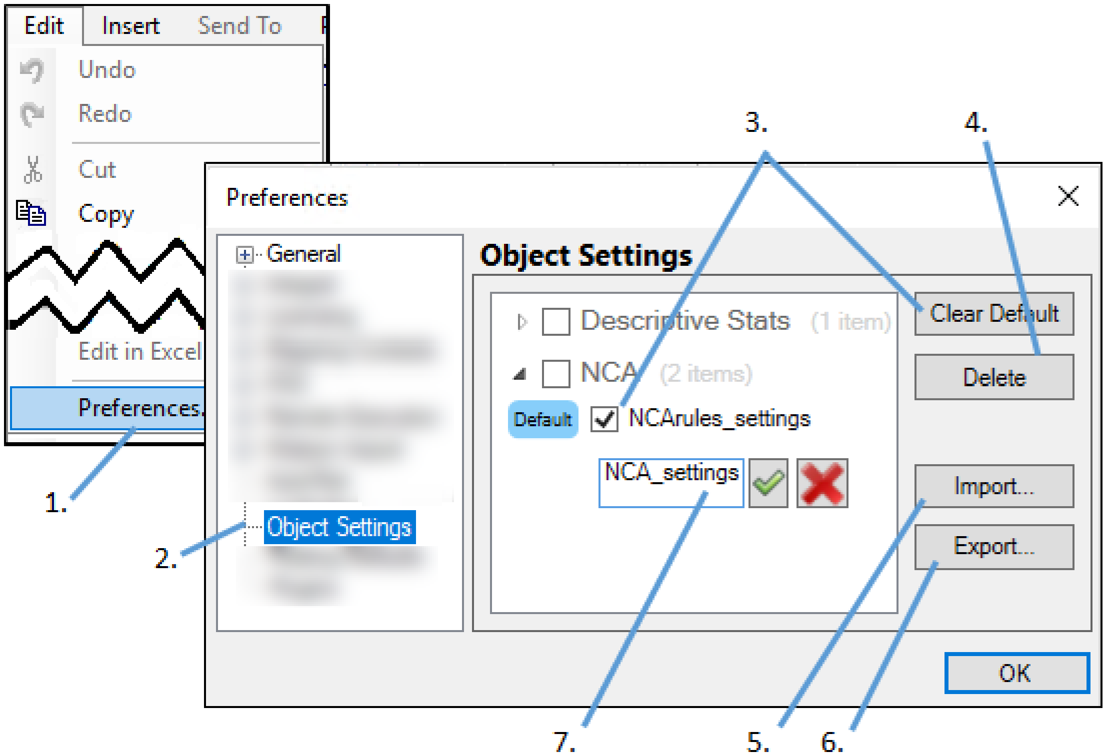
To apply an imported object settings file



1. Click  (**Import Object Settings** icon) in the Setup toolbar or select **File > Import**.
2. In the file browser, navigate to and select the desired object settings file.
   (The settings file must be for the same object type.)
3. In the dialog, enter a name for the settings file for use in Phoenix.

The settings are automatically loaded from the selected file and the settings file is managed by Phoenix.

To set object settings preferences for operational objects



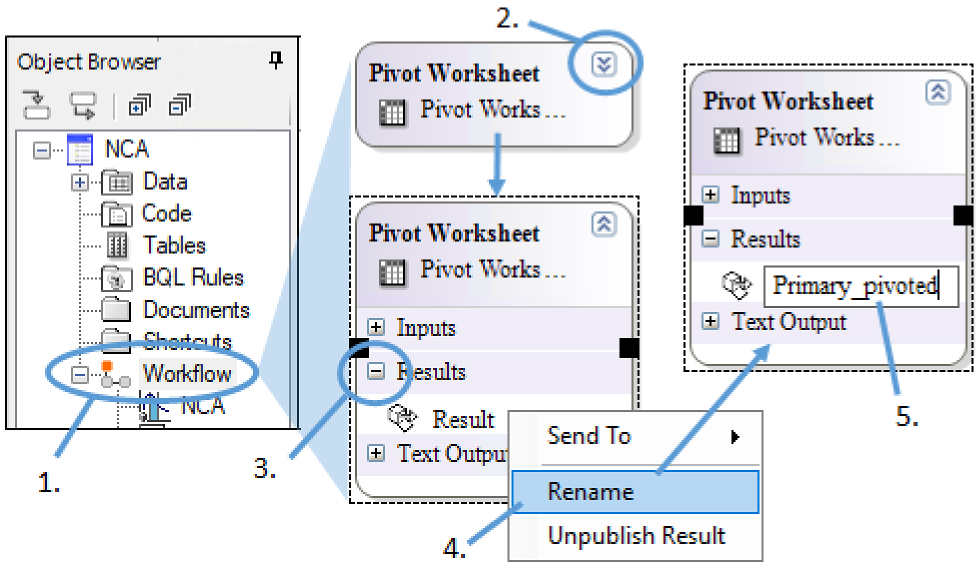
1. Select **Edit > Preferences**.
2. In the dialog, select **Object Settings**.
3. To ***specify the default settings*** for an operational object, select the object settings file to use as the default and click the **Set Default** button.

   If only the default setting for an object is selected, the **Set Default** button will change to **Clear Default**. Clicking the **Clear Default** button returns to a state where none of the user-specified settings are applied by default and the Phoenix default settings will be used for any new objects.
4. To ***delete*** object settings file(s) from the file system, select the file(s) and click **Delete**.
5. To ***import*** object settings file(s) that have been exported into the Settings directory, click **Import** or from the object's Setup panel, click the **Import** icon in the toolbar (see "To load object settings to an existing object" for more information).
6. To ***export*** object settings file(s), select the file(s) and click **Export**. In the dialog, select the directory to which the files are to be exported and click **OK**.

   Exported settings files can be shared with other users.
7. To ***rename*** object settings file(s), double-click the settings name and type the new name.

Renaming results

Prior to the execution of an object, the name of the results worksheets, plots, and text files can be changed through the Diagram tab.



1. Select the Workflow object to display the Diagram tab.
2. Click  to expand the desired object.
3. Click the (+) sign next to **Results**, **Text Output**, or **Plots** to expand the list of output items.
4. Right-click the item, and select **Rename**.
5. The name of the output item becomes editable and you can type in a new name.

Using the Results tab

The results of any operational object are located in the Results tab. There are four types of output created by operational objects:

Worksheets
Plots
Text files
Tables

Each type of output has its own set of options.

The Results tab also contains a toolbar that allows users to group, save, and print the results.

Do not group lists the output alphabetically.
Group by type lists the output in grouped by type.
Group by executable lists the output grouped by operational object. Group by executable is only available in the workflow object’s Results tab.
Expand all results shows all results items in the list.
Collapse all results collapses results so only the group headings are visible.
Copy to Documents copies the selected item to the Data, Tables, or Documents folder.

Export exports and saves the selected item.
Print sends the selected object to the printer.

An out-of-date result is shaded pink in the Object Browser. If the result is open in a separate window (by double-clicking the item in the Object Browser), the title bar will show "(Out of Date)" after the title. A result is considered out-of-date if some part of the operational object or its source data changes once the object is executed.

Worksheets

Result worksheets cannot be edited unless they are exported or copied to the Data folder. They are shaded gray to denote that they cannot be edited.

To use a results worksheet as input

Right-click a worksheet in the Results tab and select **Send To > (Object group) > (Operational object)**.

The operational object is added to the workflow and the result worksheet is mapped to it as the primary input data source. This is much simpler than exporting the worksheet or copying the worksheet to the Data folder.

To copy a result worksheet to the Data folder

Select the worksheet and click (**Copy to Data Folder** icon) or right-click the worksheet and select **Copy to Data Folder**.

Note: When a Data Wizard result worksheet is copied to the Data folder, the History tab will also contain all of the history records from the source worksheet that was mapped into the Data Wizard.

To save a worksheet

Select the worksheet and click (**Export** icon) or right-click the worksheet and select **Export**.

In the dialog, select an export location and a file format and click **Save**.

To print a worksheet

Select the worksheet and click (**Print Results** icon) or right-click the worksheet and select **Print**.

In the dialog, click **OK** to print the worksheet.

Plots

Result plots can be edited like any other plot object. Editing a plot does not mark an object as out-of-date, because Phoenix automatically updates the object as the plot is edited.

To copy a plot to the Windows clipboard

Right-click the plot and select the image format to use when copying the plot to the clipboard: **Copy high resolution image (vector)** or **Copy image (bitmap)**.

To save a single plot to a file

Right-click the plot image and select **Export**.

In the dialog, select a location and a file type, then enter a name for the file.

In the **Image Settings** part of the dialog, make any changes to the size of the image and click **Save**.

To export all plot images associated with a result plot

Select the result plot in the Results tab and click the **Export** icon.

In the dialog, select an export location and a file format, then click **Save**.

In the next dialog, make any changes to the size of the image and click **OK**.

If there are multiple tabs of plots for the selected plot result, all of the plots in all of the tabs are exported as the selected file type. For example, if there are five tabs of plots in the results and the selected filetype is JPEG, five separate JPEG files are saved and named sequentially.

To print a plot

Select the plot and click the **Print Results** icon.

In the dialog, click **Print** to print the plot.

Text files

Result text files typically contain object settings and a plain text version of the worksheet output.

Note: Right-clicking a text file and using the **Send To** menu creates a new object, but does not map the text file to the object.

To copy a result text file to the Documents folder

Select the text file and click the **Copy** icon.

Or right-click the text file and select **Copy to Documents**.

To save a text file

Select the text file and click the **Export** icon.

Or right-click the text file and select **Export**.

Then, in the dialog, select an export location and a file format and click **Save**.

Note: For rtf file format, if the exported file contents do not appear to line up properly, change the font to Courier New 9pt.

To print a text file

Select the text file and click the **Print Results** icon.

Or right-click the text file and select **Print**.

Then, in the dialog, click **OK** to print the text file.

Tables

Note: Right-clicking a table and using the **Send To** menu creates a new object, but does not map the table to the object.

To copy a result table to the Tables folder

Select the table and click the **Copy** icon.

Or right-click the table and select **Copy to Tables folder**.

To save a table

Select the table and click the **Export** icon.

Or right-click the table and select **Export**.

Then, in the dialog, select an export location and click **Save**.

To print a table

Select the table and click the **Print Results** icon.

Or right-click the table and select **Print**.

Then, in the dialog, edit the page setup and click **OK**.

In the next dialog, click **OK** to print the table.

Quick Tour of Phoenix

Using a number of the sample files provided with the Phoenix software, this tutorial introduces the steps to complete the following common tasks:

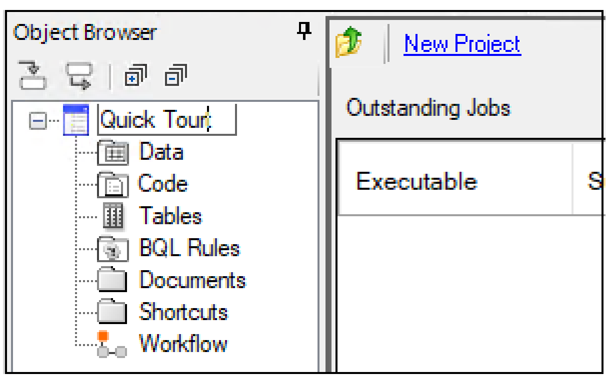
- Start Phoenix and create a new project
- Import a dataset
- Create a plot
- Create a table
- Execute noncompartmental analysis
- Perform pharmacokinetic modeling
- Execute a bioequivalence model

Most Phoenix objects require the same basic steps for their use. However, there may be multiple paths to accomplishing a step (e.g., main menu, right-click menu, drag-and-drop, etc.). For simplicity, only one is listed here.

Note: Any object added to a project can be viewed in its own window by selecting the object in the Object Browser and double-clicking it or pressing **ENTER**. All instructions for setting up and executing an object are the same whether the object is viewed in its own window or in Phoenix's viewing.

Start Phoenix and create a new project

1. Double-click the Phoenix icon ( ) on your desktop to start Phoenix.
2. Select **File > New Project** to create a new project.
   A new project is created in the Object Browser and is in edit mode for you to name.
3. Name the new project by typing `Quick Tour`.



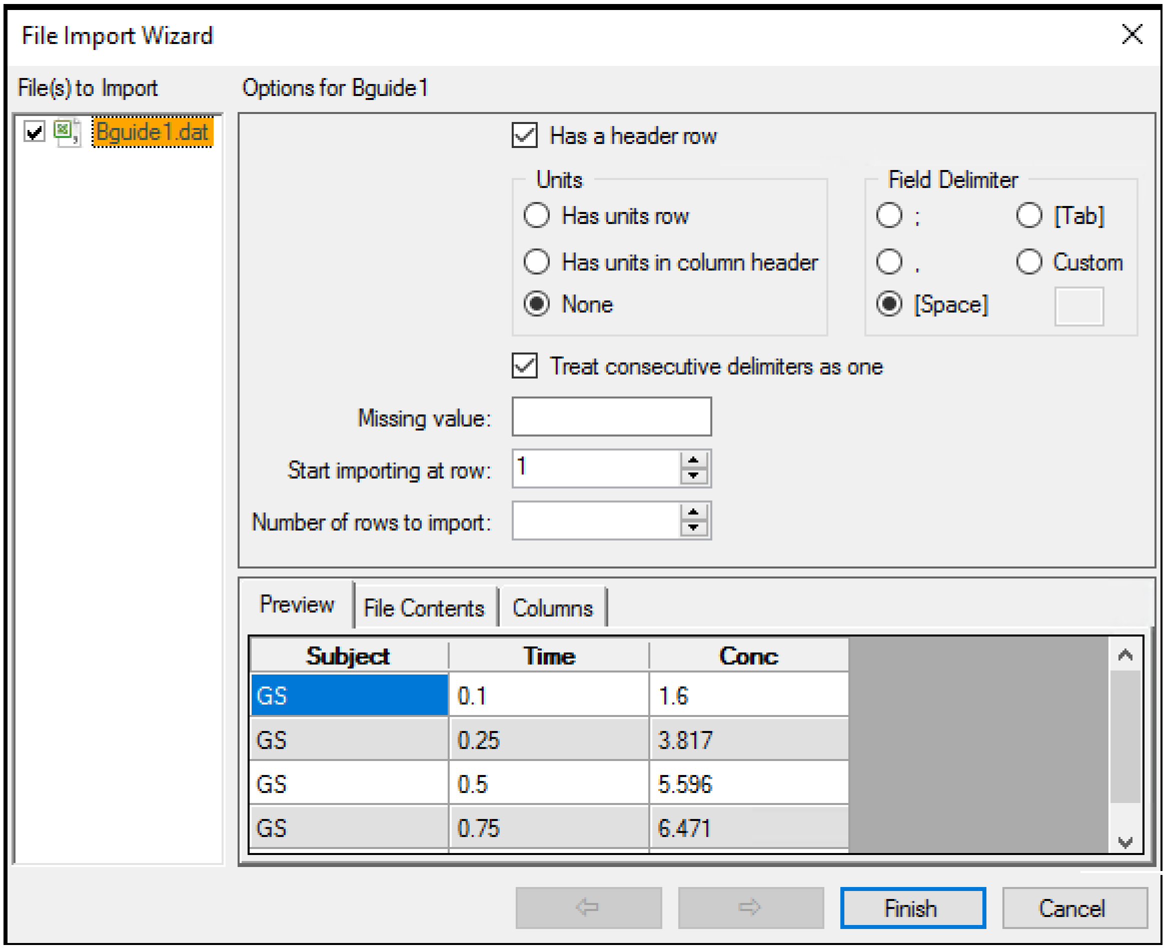
The left panel's default view is the Object Browser, which contains the project, and the other folders and objects that are contained in the project. The right viewing panel's default view is blank, unless one of the project folders or the workflow is selected.

Import a dataset

The dataset `Bguide1.dat` will be used to test key Phoenix functions.

1. Select **File > Import** or click (**Import File** icon).

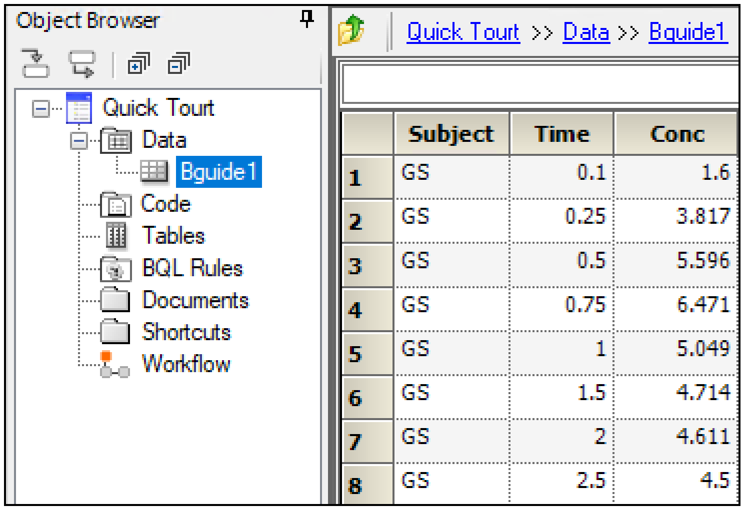
2. Navigate to <Phoenix_install_dir>\application\Examples\WinNonlin\Supporting files.
3. Select the file **Bguide1.dat** and click **Open**.
   The *File Import Wizard* is used to assign options for how the data are imported and presented.



No changes need to be made to the default options for this dataset.

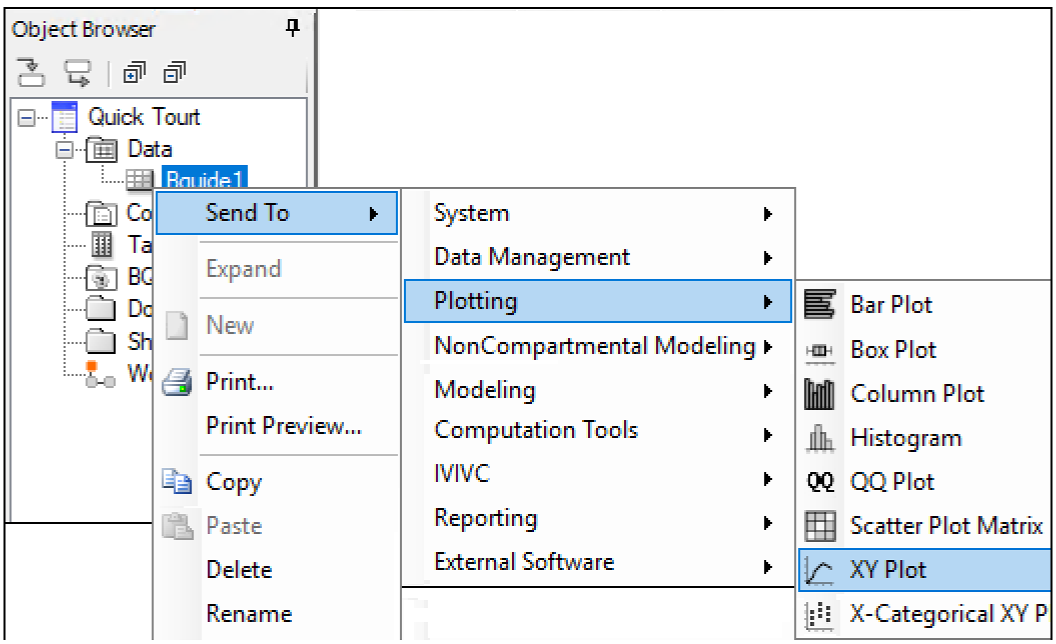
4. Click **Finish**.

The dataset is added to the project Data folder and the worksheet is displayed in the right viewing panel.



Create a plot

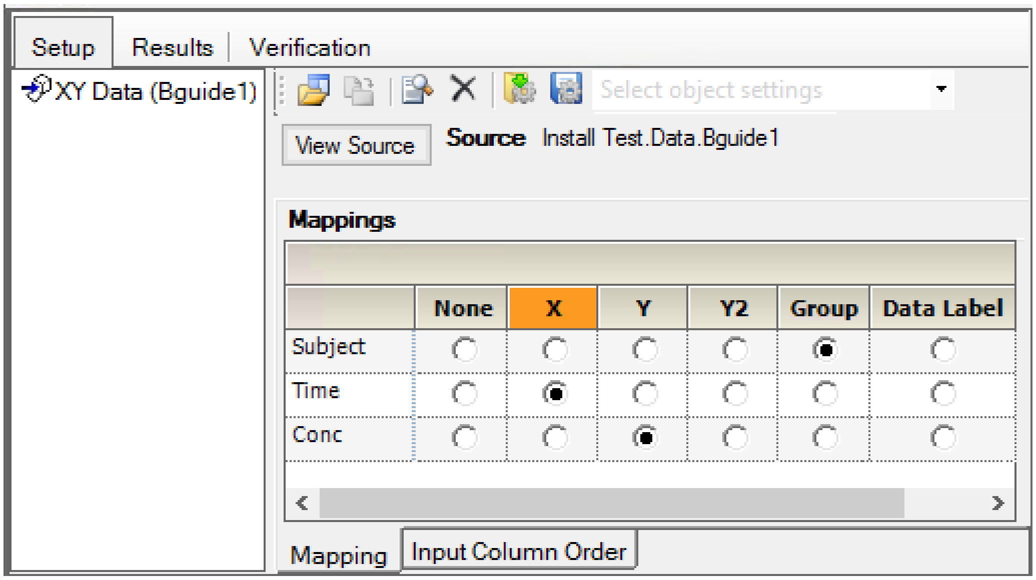
1. Right-click **Bguide1** in the Data folder and select **Send To > Plotting > XY Plot** from the menu.



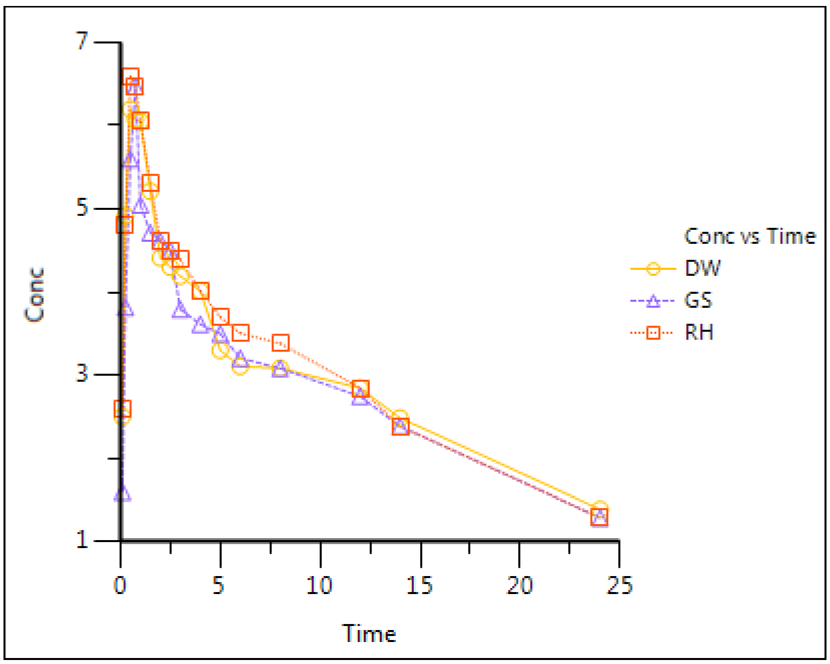
An XY Plot object can also be added to a Workflow by selecting the Workflow object in the Object Browser and then selecting **Insert > Plotting > XY Plot**. Or by right-clicking the Workflow object, selecting **New > Plotting > XY Plot**, and then using the pointer to drag the **Bguide1** worksheet from the Data folder to the XY Data Mappings panel.

The default view of an object is the Setup tab, which contains all the steps necessary to set up an object.

2. Use the option buttons in the XY Data Mappings panel to map the data types to the contexts as follows:
   Map **Subject** to the **Group** context.
   Map **Time** to the **X** context.
   Map **Conc** to the **Y** context.



3. Click (**Execute** icon) to execute the workflow.

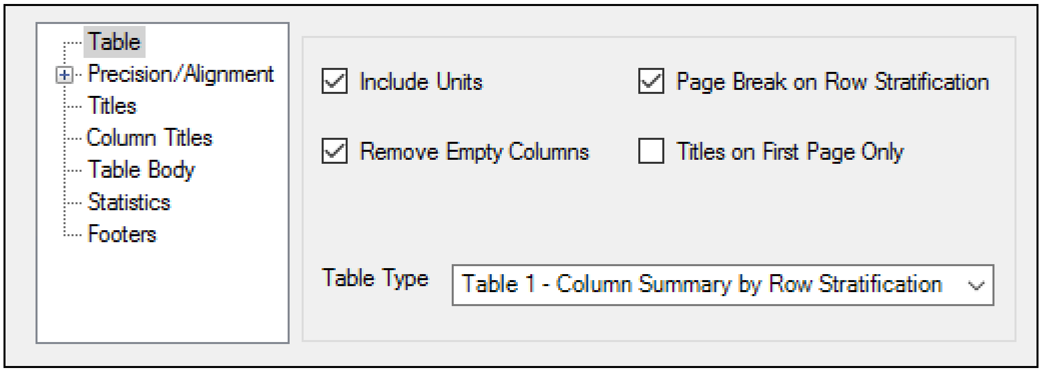


Now use the Bguide1 dataset to test the Table object and its summary statistics function.

Create a table

1. Right-click **Bguide1** in the Data folder and select **Send To > Reporting > Table**.
2. In the Main Mappings panel, map the data types as follows:
   Map **Subject** to the **Stratification Row** context.
   Leave **Time** mapped to **None**.
   Map **Conc** to the **Data** context.
3. In the Options tab below the Setup tab, select **Table 1 - Column Summary by Row Stratification** as the **Table Type** to use.

4. Check the **Page Break on Row Stratification** box.



5. Select the **Statistics** tab, which is also located below the Setup tab.
6. Click **Select All** to select all output statistics.
7. Execute the object.

The results are presented as three HTML tables in the Results tab. Compare the table for the DW subject in the Results tab to the table pictured below.

Subject		Conc
DW	N	16
	NMiss	0
	NObs	16
	Mean	4.004
	SD	1.432
	SE	0.358
	Variance	2.051
	CV%	35.8
	Min	1.39
	Median	4.10
	Max	6.20
	Range	4.81
	Mean Log	1.3179
	SD Log	0.4039
	Geometric Mean	3.736
	Geometric SD	1.498
	Geometric CV%	42.10
	CI 95% Lower	0.95
	CI 95% Upper	7.06
	CI 95% Lower Mean	3.24
	CI 95% Upper Mean	4.77
	CI 95% Lower Var	1.12
	CI 95% Upper Var	4.91
	CI GEO 95% Lower	1.58
	CI GEO 95% Upper	8.84

CI 95% Lower GEO Mean	3.01
CI 95% Upper GEO Mean	4.63
Lower 1SD	2.572
Upper 1SD	5.436
GEO Lower 1SD	2.494
GEO Upper 1SD	5.595
1%	1.39
2.5%	1.39
5%	1.39
10%	2.15
25%	2.90
50%	4.10
75%	5.14
90%	6.11
95%	6.20
97.5%	6.20
99%	6.20
IQR	2.24
Sum	64.06
Harmonic Mean	3.434
Skewness	0.0595
Skewness Pop	0.0537
Kurtosis	-0.8084
Kurtosis Pop	-0.9299
Pseudo SD	1.7578
KS PValue	0.96

Execute noncompartmental analysis

1. Select **File > Load Project**.
2. In the dialog, navigate to `<Phoenix_install_dir>\application\Examples\WinNonlin`.
3. Select **Multiple_Profiles.phxproj** and click **Open**.

This project contains:
– A dataset worksheet (profiles)
– A worksheet of dosing information (Dosing published from NCA)
– An XY Plot object
– An NCA model object
– A Descriptive Statistics object
– A Data Wizard object
– An X-Categorical XY Plot object

4. Expand the workflow node.
5. Select the **NCA** model object in the Object Browser.
6. Select items in the Setup tab list to explore the data mappings and option settings.
7. Execute the object.

Text output

The **Core output** contains the model settings and the same data as the worksheets, but presented in plain ASCII text. If there were errors in the model they would be listed here. Below is part of a Core output text file.

```
…
Model: Plasma Data, Extravascular Administration
Number of nonmissing observations:   12
Dose time:       0.00
Dose amount:      100.00
Calculation method: Linear Trapezoidal with Linear Interpolation
Weighting for lambda_z calculations: Uniform weighting
Lambda_z method: Find best fit for lambda_z, Log regression
Compute Concentrations at: 75

Summary Table
-------------
 Time   Conc.   Pred. Residual    AUC         AUMC      Weight
 min    ng/ml   ng/ml  ng/ml   min*ng/ml  min*min*ng/ml
-------------------------------------------------------------
  0.0000 0.0000                   0.0000      0.0000
  5.000  340.3                     850.8        4254.
  10.00  1914.                     6487.    5.636e+04
  15.00  2069.                 1.644e+04    1.818e+05   1.000
  20.00  1471.                 2.529e+04    3.329e+05   1.000
  30.00  788.8                 3.659e+04    5.983e+05   1.000
  45.00* 496.4  460.9   35.54  4.623e+04    9.434e+05   1.000
  60.00* 372.8  357.2   15.63  5.275e+04    1.279e+06   1.000
  90.00* 204.3  214.6 -10.33   6.141e+04    1.890e+06   1.000
  120.0* 124.1  128.9 -4.852   6.633e+04    2.389e+06   1.000
  180.0* 39.25  46.52 -7.266   7.123e+04    3.048e+06   1.000
  240.0* 19.32  16.79  2.531   7.299e+04    3.389e+06   1.000
```

The **Settings** file lists all the settings used to specify the noncompartmental analysis. Below is part of a Settings text file.

```
…
  Sort: Subject, Form
  Time: Time [min]
  Concentration: Conc [ng/mL]
  Carry:
Dosing: (Internal)
Slopes: (Internal)
Partial Areas: (Internal)
Therapeutic Response: <None>
```

```
Units: (Internal)
Parameter Names: <None>
…
Plasma Model
Title=Processing Multiple Profiles with Model 200
Linear Trapezoidal Linear Interpolation
Sparse=False
Weighting=Uniform Weighting; 0
Dose Type=Extravascular
Dose Unit=ng
Dose Normalization=None
Compute Concentrations at: 75
```

Output data

The NCA object creates several results worksheets including: Dosing Used, Exclusions, Final Parameters, Final Parameters Pivoted, Partial Areas, Plot Titles, Slopes Settings, and Summary Table. Selections from the Final Parameters and Summary Table worksheets are shown below.

	Subject	Form	Parameter	Units	Estimate
1	1	Capsule	N_Samples		12
2	1	Capsule	Dose	ng	100
3	1	Capsule	Rsq		0.99267305
4	1	Capsule	Rsq_adjusted		0.99084131
5	1	Capsule	Corr_XY		-0.99632979
6	1	Capsule	No_points_lambda_z		6
7	1	Capsule	Lambda_z	1/min	0.016987622
8	1	Capsule	Lambda_z_intercept		6.8975665
9	1	Capsule	Lambda_z_lower	min	45
10	1	Capsule	Lambda_z_upper	min	240
11	1	Capsule	HL_Lambda_z	min	40.803072
12	1	Capsule	Span		4.7790519
13	1	Capsule	Tlag	min	0
14	1	Capsule	Tmax	min	15

Figure 8-1. Part of the Final Parameters worksheet

	Sub	Form	Time (min)	lam	Conc (ng/mL)	Predicted (ng/mL)	Residual (ng/mL)	AUC (min*ng/mL)	AUMC (min*min*ng/mL)	Weighting
1	1	Capsule	0		0			0	0	0
2	1	Capsule	5		340.3167			850.79175	4253.9588	0
3	1	Capsule	10		1914			6486.5835	56357.918	0
4	1	Capsule	15		2069.167			16444.501	181801.68	0
5	1	Capsule	20		1470.917			25294.711	332941.29	0
6	1	Capsule	30		788.75			36593.046	598345.49	0
7	1	Capsule	45	*	496.4167	460.87344	35.543259	46231.796	943354.88	1
8	1	Capsule	60	*	372.8333	357.20475	15.628553	52751.171	1278670.5	1
9	1	Capsule	90	*	204.25	214.57954	-10.329536	61407.421	1889958	1
10	1	Capsule	120	*	124.05	128.90192	-4.8519188	66331.921	2388985.5	1
11	1	Capsule	180	*	39.25	46.515912	-7.2659123	71230.921	3047515.5	1
12	1	Capsule	240	*	19.31667	16.785864	2.5308059	72987.921	3398545.5	1
13	1	Tablet	0		0			0	0	0

Figure 8-2. Part of the Summary Table worksheet

A total of 12 pages of plots are generated; one for each of two formulations, for each of the six subjects. The first two charts for subject one are shown below.

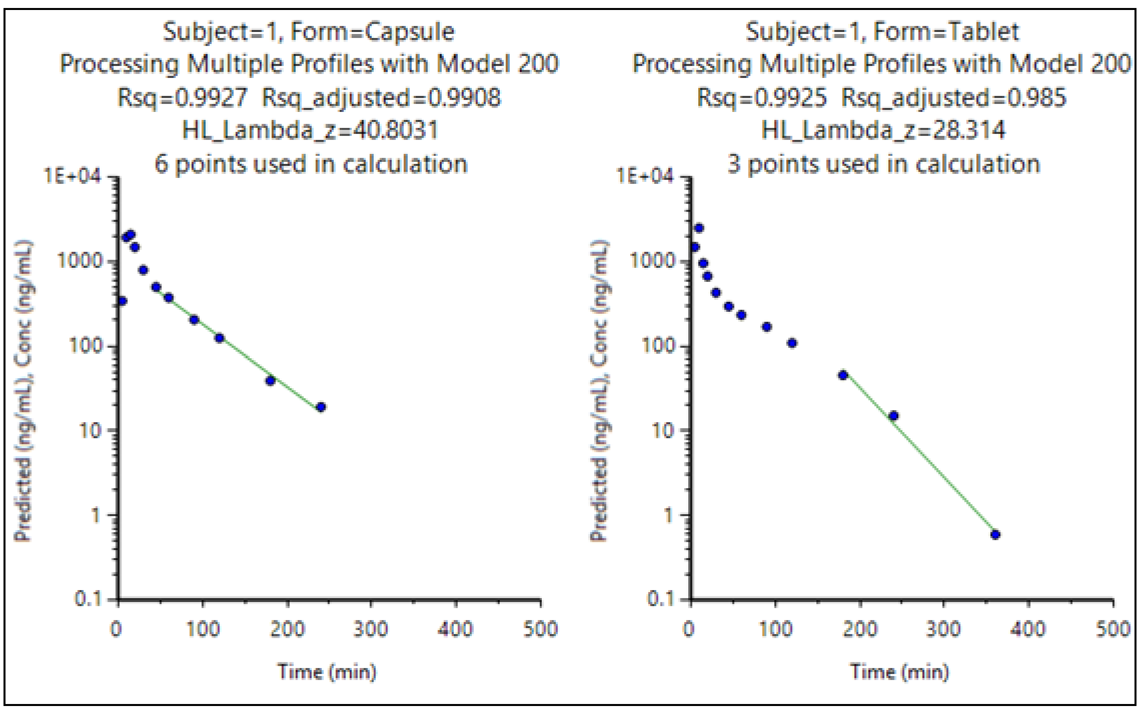


Figure 8-3. Plots for subject one, capsule and tablet formulation

Perform pharmacokinetic modeling

1. Select **File > Load Project**.
2. In the dialog, navigate to <Phoenix_install_dir>\application\Examples\WinNonlin.

3. Select **PK_Model.phxproj** and click **Open**.

   This project contains:
   – A dataset worksheet (study1)
   – An XY Plot object
   – A PK model object

4. Expand the workflow node.
5. Select the **PK** object in the Object Browser.
6. Select items in the Setup tab list to explore the model’s data mappings and option settings.

   The imported PK Model object uses PK Model 3, which is a one-compartment model with 1st order absorption.

7. Execute the object.

Worksheet results

The PK Model object’s output worksheets partially include Condition Numbers, Diagnostics, Dosing Used, Final Parameters, Initial Estimates, Secondary Parameters, and Summary Table. The Final Parameters, Secondary Parameters, and Summary Table worksheets are shown below.

	Sub	Param	Units	Estimate	StdError	CV%	UnivarCI_	UnivarCI_U	PlanarCI_L	PlanarCI_
1	1	V_F	mL	301.28617	5.4850738	1.8205528	289.3352	313.23713	283.22832	319.34401
2	1	K01	1/hr	2.1586326	0.090628388	4.1984166	1.96117	2.3560951	1.8602676	2.4569975
3	1	K10	1/hr	0.21483403	0.007340839	3.4169816	0.1988397	0.23082837	0.19066667	0.2390014

Figure 8-4. Final Parameters worksheet

	Subject	Parameter	Units	Estimate	StdError	CV%
1	1	AUC	hr*ng/mL	30.899234	0.63214664	2.0458327
2	1	K01_HL	hr	0.32110476	0.013467848	4.1942224
3	1	K10_HL	hr	3.226431	0.11013642	3.413568
4	1	CL_F	mL/hr	64.726523	1.3255206	2.0478785
5	1	Tmax	hr	1.1870389	0.026332083	2.2182999
6	1	Cmax	ng/mL	5.1439722	0.046900364	0.91175384

Figure 8-5. Secondary Parameters worksheet

	Sub	Time_ob (hr)	Conc_ob (ng/mL)	Time (hr)	Conc (ng/mL)	Predicted (ng/mL)	Residual (ng/mL)	We	SE_Yhat	Standard_Re
1	1	0.1	1.29	0.1	1.29	1.2745998	0.015400175	1	0.033025914	0.15795305
2	1	0.25	2.81	0.25	2.81	2.6889731	0.12102695	1	0.055940643	1.4005554
3	1	0.5	4.16	0.5	4.16	4.1158923	0.044107747	1	0.058589906	0.52112365
4	1	0.75	4.6	0.75	4.6	4.8144531	-0.21445309	1	0.049693255	-2.3788162
5	1	1	5.13	1	5.13	5.0953875	0.034612464	1	0.045856544	0.37556116
6	1	1.5	5.03	1.5	5.03	5.051743	-0.021742964	1	0.050117469	-0.24181407
7	1	2	4.78	2	4.78	4.6987536	0.081246401	1	0.050279037	0.90448852
8	1	2.5	4.39	2.5	4.39	4.2750813	0.11491872	1	0.045791316	1.2464824
9	1	3	3.68	3	3.68	3.8583222	-0.17832217	1	0.041419535	-1.8922238
10	1	4	3.2	4	3.2	3.1202607	0.079739284	1	0.040325291	0.84190556
11	1	5	2.55	5	2.55	2.5179435	0.03205647	1	0.044871579	0.34601201
12	1	6	2.03	6	2.03	2.0312675	-0.001267533	1	0.048709632	-0.013977098
13	1	8	1.28	8	1.28	1.3218078	-0.041807823	1	0.049677892	-0.46370881
14	1	12	0.552	12	0.552	0.5597105	-0.007710497	1	0.037020818	-0.080273645
15	1	14	0.321	14	0.321	0.36421764	-0.043217644	1	0.029360941	-0.43802838

Figure 8-6. Summary Table worksheet

Text output

The **Core output** text results include all model settings and iterations, including the output from the worksheets. Any model errors would be listed here. Below is part of the Core output text file.

```
…
Listing of input commands
 MODEL 3
 NVAR 3
 NPOI 1000
 XNUM 2
 YNUM 3
 NCON 3
 CONS 1,2,0
 METH 2'Gauss-Newton (Levenberg and Hartley)
 ITER 50
 INIT 0.25,1.81,0.23
 MISS '.'
 DATA 'WINNLIN.DAT'
 BEGIN
```

The **Settings** file lists all the settings used to specify the noncompartmental analysis. Below is part of the Settings text file.

```
…
Main: PK Model.Data.study1
  Sort: Subject
  Time: Time [hr]
  Concentration: Conc [ng/mL]
  Carry:
Dosing: (Internal)
Initial Estimates: (Internal)
Units: (Internal)
***** Other Parameters *****
…
```

```
PK 3-[PK]
Gauss-Newton (Levenberg and Hartley)
Convergence criteria of 0.0001 used during minimization process
50 maximum iterations allowed during minimization process
```

Plots

The plot results include Observed Y and Predicted Y vs X, Partial Derivatives Plot, Predicted Y vs Observed Y, Predicted Y vs X, Residual Y vs Predicted Y, and Residual Y vs X. Some plot results are shown below.

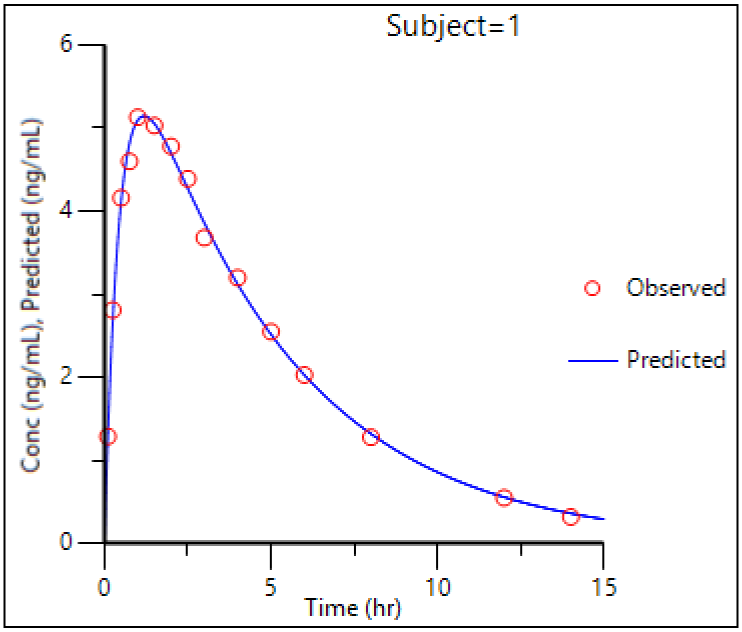


Figure 8-7. Observed Y and Predicted Y vs X

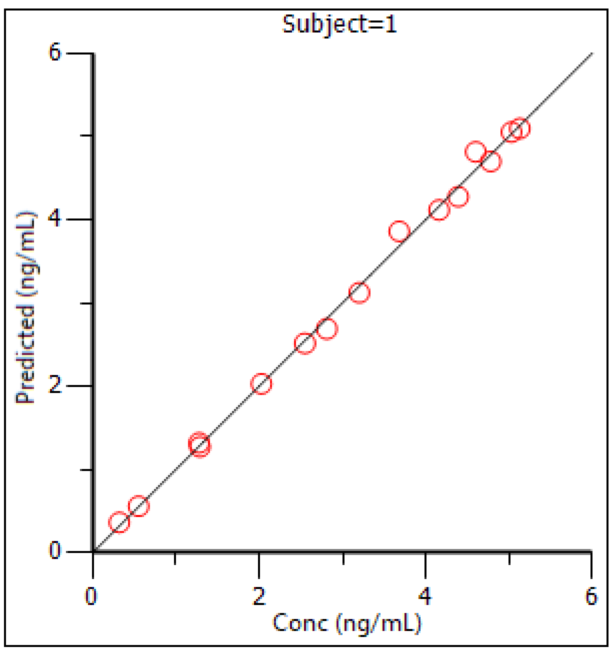


Figure 8-8. Predicted Y vs Observed Y

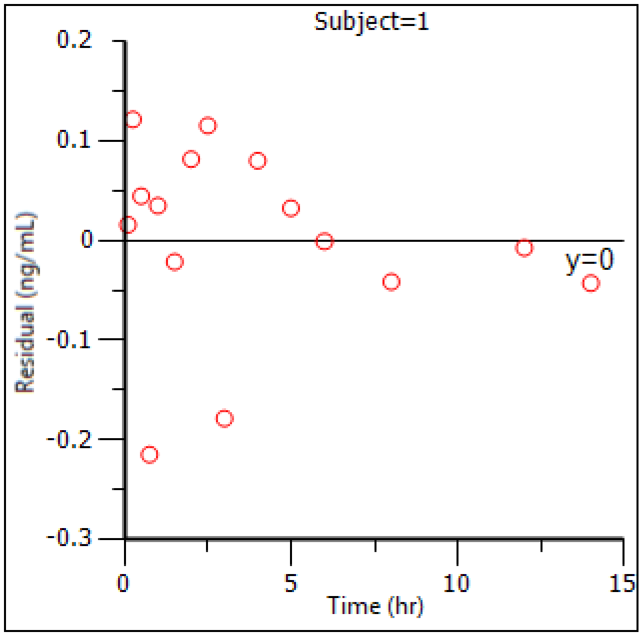
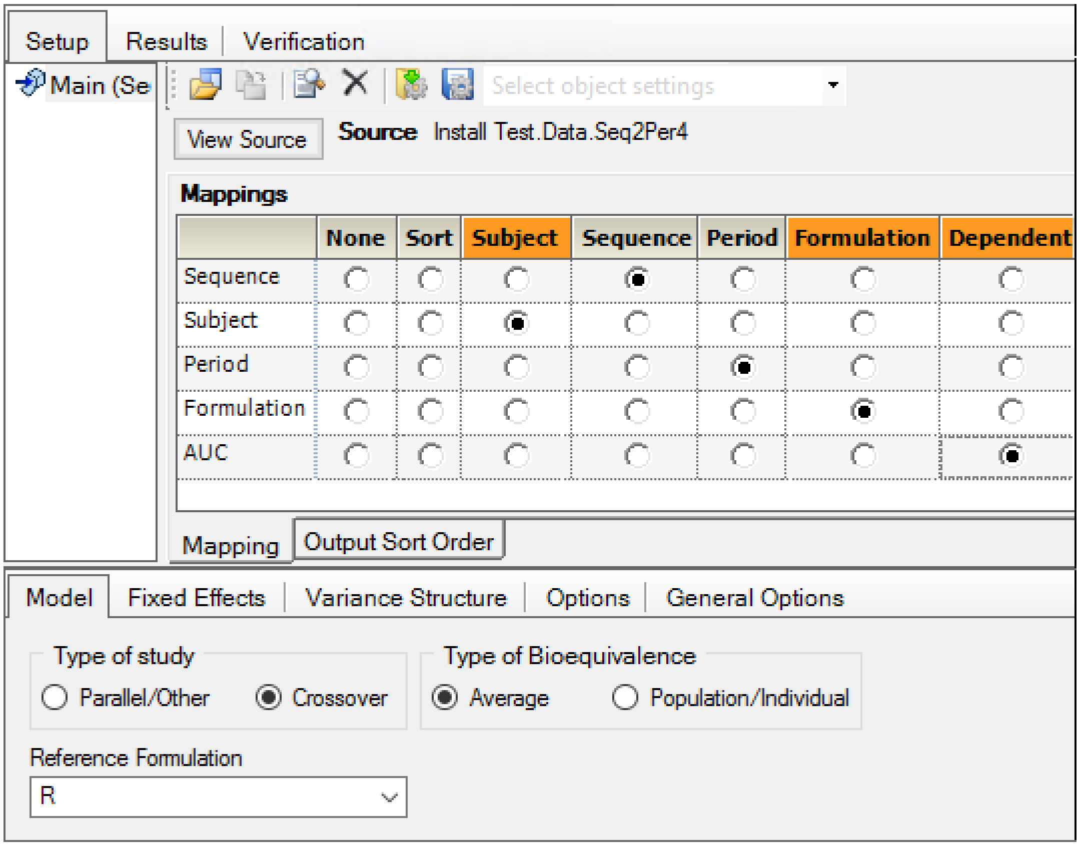


Figure 8-9. Residual Y vs X

Execute a bioequivalence model

1. Select the **Quick Tour** project in the Object Browser.
2. Select **File > Import**.
3. In the dialog, navigate to `<Phoenix_install_dir>\application\Examples\WinNonlin\Supporting files`.
4. Select the file `Seq2Per4.csv` and click **Open**.
   In the *File Import Wizard* dialog, click **Finish**. The dataset is added to the project Data folder.
5. Right-click the **Seq2Per4** worksheet in the Data folder and select **Send To > Computation Tools > Bioequivalence**.
   The **Bioequivalence** object is added to the workflow in the Object Browser and the following data types are automatically mapped to contexts.
   – **Sequence** to the **Sequence** context
   – **Subject** to the **Subject** context
   – **Period** to the **Period** context
   – **Formulation** to the **Formulation** context
6. In the Main Mappings panel, map **AUC** to the **Dependent** context.
7. In the Model tab (located below the Setup tab), ensure the following:
   – **Crossover** is selected as the **Type** of study
   – **Average** is selected as the **Type of Bioequivalence**
   – **R** is selected as the **Reference Formulation**



8. Select the **Fixed Effects** tab, which is located below the Setup tab.
9. **Ln(x)** is automatically selected in the **Dependent Variables Transformation** menu. Do not change this setting.
10. Execute the object.

Output data

The bioequivalence model worksheet output partially includes Average Bioequivalence, Diagnostics, Final Fixed Parameters, Final and Initial Variance Parameters, Least Squares Means, and Sequential Tests. The Diagnostics, Final Variance Parameters, and Sequential Tests worksheets are shown below.

	Depend	Units	FormVar	FormR	RefLSM	RefLSM_S	RefGeoL	Test	TestLSM	TestLSM_
1	Ln(AUC)		Formulation	R	5.5537097	0.10472836	258.1936	T	5.7481984	0.1196125

TestGeoLSM	Difference	Diff_SE	Diff_DF	Ratio_%Ref_	CI_80_Lower	CI_80_Upper
313.62513	0.19448871	0.09348619	24.829354	121.46898	107.40168	137.37878

CI_90_Lower	CI_90_Upper	CI_95_Lower	CI_95_Upper	t1_TOST	t2_TOST	Prob_80_00
103.53701	142.50665	100.1885	147.26953	4.4673151	-0.30651416	7.514E-05

Prob_125_00	MaxProb	TotalProb	Power_TOST	AHpval	Power_80_20	Prob_Eq_Var
0.38088443	0.38088443	0.38095957	0.08554966	0.38080929	0.7482755	

Figure 8-10. Average Bioequivalence worksheet

	Dependent	Units	Diagnostic	Value
1	Ln(AUC)		Total Observatio	48
2	Ln(AUC)		Observations Us	48
3	Ln(AUC)		Obs. Missing Mo	0
4	Ln(AUC)		Residual SS	0
5	Ln(AUC)		Residual df	0
6	Ln(AUC)		Convergence	Achieved
7	Ln(AUC)		REML log(likelih	-19.238555
8	Ln(AUC)		-2 * REML log(li	38.477111
9	Ln(AUC)		Akaike's Inform	60.477111
10	Ln(AUC)		Schwarz's Bayes	79.591476
11	Ln(AUC)		Hessian eigenva	855.2051
12	Ln(AUC)		Hessian eigenva	715.32814
13	Ln(AUC)		Hessian eigenva	158.63358
14	Ln(AUC)		Hessian eigenva	63.03212
15	Ln(AUC)		Hessian eigenva	21.604278

Figure 8-11. Diagnostics worksheet

	Dependent	Units	Parameter	Estimate
1	Ln(AUC)		lambda(1,1)_11	0.27893988
2	Ln(AUC)		lambda(1,2)_11	0.35567907
3	Ln(AUC)		lambda(2,2)_11	-1.97E-13
4	Ln(AUC)		Var(Period*For	0.10761781
5	Ln(AUC)		Var(Period*For	0.09035641

Figure 8-12. Final Variance Parameters worksheet

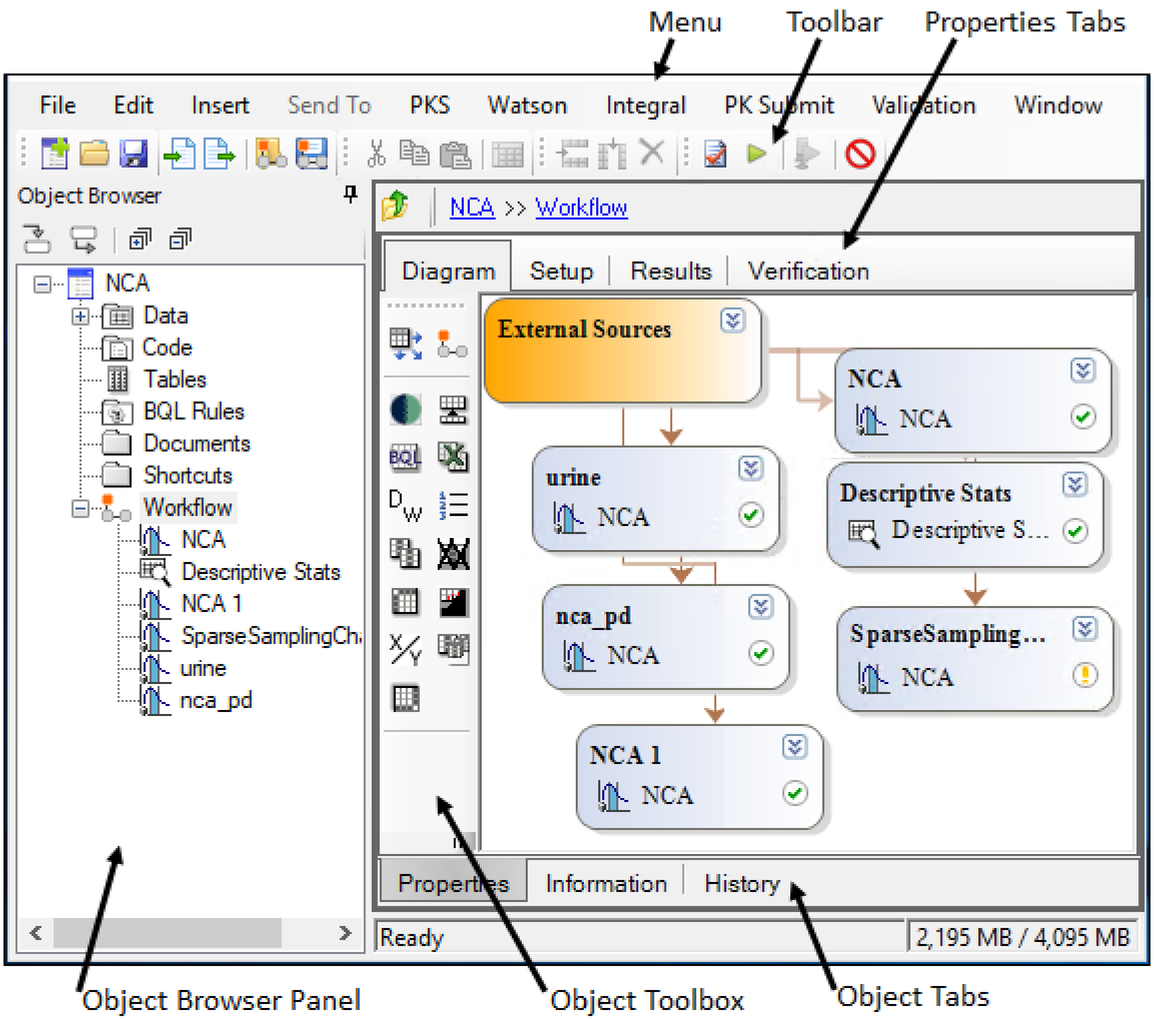
	Dependent	Units	Hypothesis	Numer_DF	Denom_DF	F_stat	P_value
1	Ln(AUC)		int	1	10.008139	3055.0348	8.9E-14
2	Ln(AUC)		Sequence	1	10.008139	0.095274924	0.7639047
3	Ln(AUC)		Formulation	1	24.829354	4.328066	0.047965077
4	Ln(AUC)		Period	3	28.392036	2.1673487	0.11384356

Figure 8-13. Sequential Tests worksheet

This concludes the Quick Tour of Phoenix.

The Phoenix User Interface

The Phoenix interface lets users control and organize multiple projects, workflows, operational objects, and data sources. The following image highlights the major components of the interface.



Additional information is available for the following:

- Main menu options
- Toolbar buttons
- Object Browser panel
- Diagram tab
- Setup and Results tabs
- Verification tab
- Information tab
- History tab and Settings file
- Phoenix log viewer
- Phoenix hotkeys

For a brief walk-through of the Phoenix user interface, try the "Quick Tour of Phoenix".

Note: The Phoenix interface is best rendered when there is no display scaling. If you are unable to select some buttons or tabs, or if parts of the interface overlap, try changing the scaling of text, applications, and other items to 100% (right-click on the Desktop and choose **Display**). A computer restart may be required to apply changes.
To set the scaling only for the Phoenix application on a high DPI display, browse to the Phoenix installation folder (by default, `C:\Program Files (x86)\Certara\Phoenix\application`), right-click on `Phoenix.exe`, select **Properties** menu item, and choose the **Compatibility** tab. For Windows 7, select [**x**] on **Disable display scaling on high DPI settings** option. For Windows 8 or Windows 10, select [**x**] on **Override high DPI scaling behavior. Scaling performed by:** option, and then select **Application** or **System (Enhanced)** in the drop-down menu. Then restart your computer to apply the changes.

Main menu options

The Phoenix main menu allows users to create and save projects, import datasets, export operational objects and worksheets, and connect to databases.

Note: All menu options are not always active and, therefore, are unavailable. Some options are only available when a user selects a certain part of the interface, such as a cell in a worksheet. For example, the **Insert** menu is only available when a project, workflow, or operational object is selected. The **Send To** menu is only available when a worksheet is selected.

File: Create, load, save, and close projects, create worksheets, load and save templates, import and export data, and print results.

Edit: Undo and redo worksheet edits, cut, copy, paste, find, and sort data, insert and delete rows and columns, freeze panes, locate a cell by column/row number, edit worksheet in Excel, and access the *Preferences* dialog.

Insert: Add operational objects to a workflow. This menu is only available when a project, a workflow object, or an operational object is selected.

Send To: Send worksheets to an operational object. The **Send To** menu is only available when a worksheet is selected.

Integral: Connect to Certara Integral, create and edit studies.

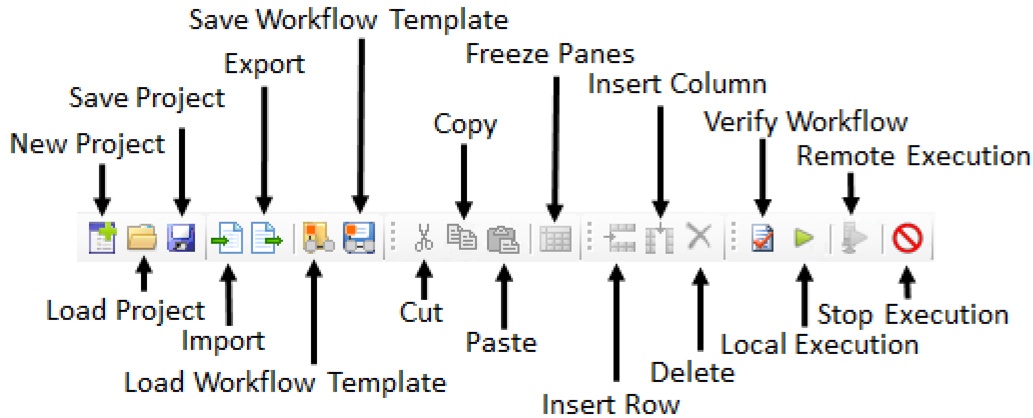
Watson: Import data from Watson LIMS into a Phoenix project as either a study Workbook or as a study in Integral.

Validation: Execute validation test packages, display results, and generate validation reports.

Window: View job status, display/undisplay the Object Browser, arrange open windows.

Help: Access the Phoenix Assistance Library, information about support, training, and the installed version of Phoenix, as well as view log files.

Toolbar buttons



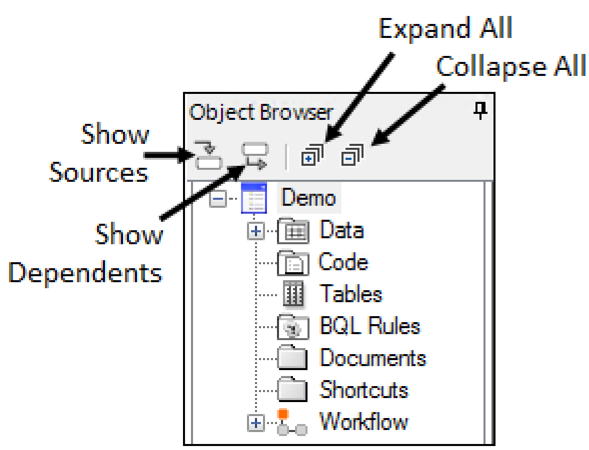
Load Workflow Template and **Save Workflow Template** are only available when a workflow is selected.

Cut, **Copy**, **Paste**, **Freeze Panes**, **Insert Row**, **Insert Column**, and **Delete** are only available when a cell in a worksheet is selected.

Verify Workflow, **Execute**, **Remote Execute**, and **Stop Execution** are only available when a work-flow or operational object is selected.

Object Browser panel

The Object Browser displays all the operational objects inserted into a project or a workflow.



The Object Browser contains the following items:

Project: All the operational objects inserted into a project. Also contains the Data and Library fold-ers.

Data folder: Imported datasets and user-created worksheets and workbooks.

Code folder: Imported PML, legacy ASCII model code, NONMEM scripts, SAS scripts, and any imported text or rich text format (*.rtf) files.

Tables folder: Imported or internally created output tables.

BQL Rules folder: Rules for importing datasets with uselessly low concentration data.

Documents folder: Any binary objects that do not belong in the other folders.

Shortcuts folder: Pointers to input data files that have been imported as shortcuts.

Workflow object: Any object that allows users to group operational object and nest workflows within a project.

Operational object: Any object that receives input, performs an operation, and produces results. An example is the NCA (noncompartmental analysis) object.

Select a folder object to display a list of the contents in the main panel area.

The objects in the tree can be re-ordered. Click and drag the item to the new location. The cursor will change to a blue arrow when it is possible to move the item to that location. Moving items to a different workflow will require re-execution; however re-ordering within a workflow will not require re-execution. Items cannot be moved after a workflow, as it is not possible to determine if the user intends to place it at the end of the workflow or after it. Consequently, move the workflow instead.

The Object Browser toolbar contains icons for the following:

Show Sources shows which data is mapped to an operational object.

Show Dependents shows all objects which depend on the selected object for data input.

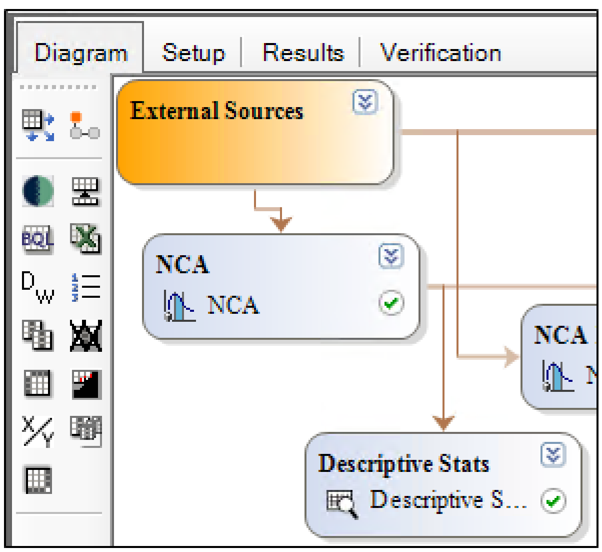
Expand all expands all of the nodes in the Object Browser.

Collapse all collapses all of the nodes in the Object Browser.

See Using the Object Browser for more information.

Diagram tab

Part of the Properties tab, the Diagram tab is only available when a Workflow object is selected in the Object Browser. Use the Diagram tab to visualize the flow of data between objects in your workflow.



Right-clicking in an open area of the diagram display area presents a menu with the following options:

Verify Workflow: Check if an executable object can be run.

Execute: Execute an object or workflow locally, depending on which is selected in the Object Browser.

Lock/Unlock Workflow: Enter the username and password to lock/unlock the workflow. (Note that passwords must be recorded by users as they are not maintained by Phoenix. If a password is lost, the workflow will need to be recreated.)

Insert: Add an object to the workflow.

Load Workflow Template: Adds a new workflow to the project along with the operational objects and settings that were saved within the Workflow Template.

Save Workflow Template: Save a workflow as a Workflow Template, in order to reapply an analysis on new data.

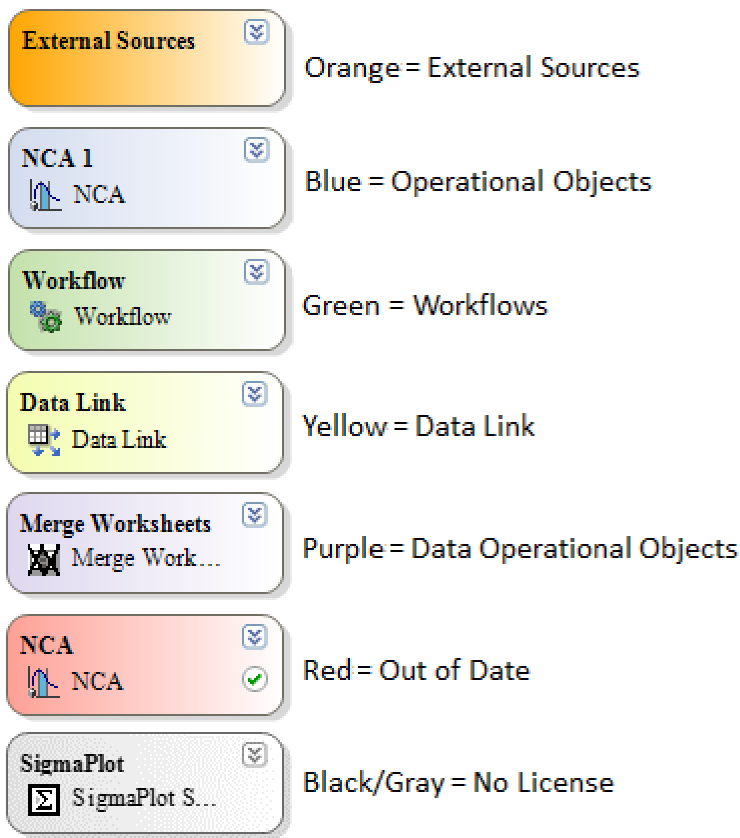
Paste: Add the object from the clipboard to the diagram.

Connect External Sources to Data Links: Create a data link object for every worksheet coming into the workflow.

Disconnect External Data Links: Remove data link objects from the workflow.

Copy Diagram to Clipboard: Place a copy of the diagram on the clipboard.

The Diagram tab contains the operational objects in a workflow, color-coded as shown in the following image.

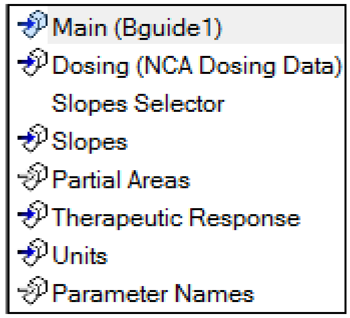


The Object Toolbox allows users to insert objects into a project by clicking the buttons in Object Toolbox. The objects in the Object Toolbox are grouped in the same way as they are in the **Insert** menu.

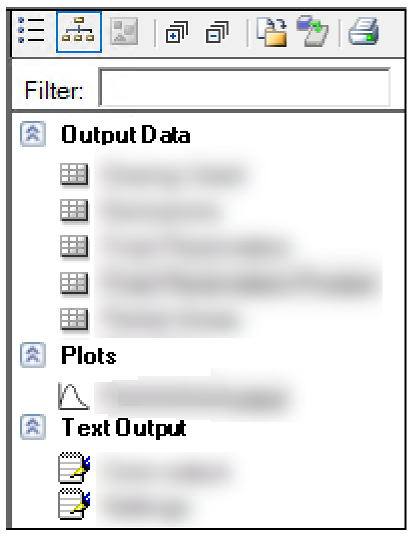
Setup and Results tabs

The Setup and Results tabs are sub-tabs of the Properties tab.

The Setup tab is the default view of any newly inserted operational object. This tab contains a list of the panels and options tabs that are used to set up the object. Through the Setup tab, users can map datasets and other worksheets to an object.



The Results tab displays the results of an executed object grouped by type. Result types are text, worksheets, and graphs.



The toolbar contains icons that perform the following functions:

Do not group lists results in alphabetical order.
Group by type organizes the results in three groups: tables, plots, and text output.
Group by executable groups the results of each executable together.
Expand all results expands all of the groups to make all results visible in the list (use when results are grouped).
Collapse all results displays only the groupings, hiding the list of individual results.
Copy to Data Folder copies results to the Data folder.
Export exports the results.
Print prints the results.

The Results tab of all Phoenix objects allows filtering. The filtering is not case sensitive and when a filtering string is entered, only results containing that string within their name are displayed in the Results tab. The filter persists until the object is closed or the filter is changed.

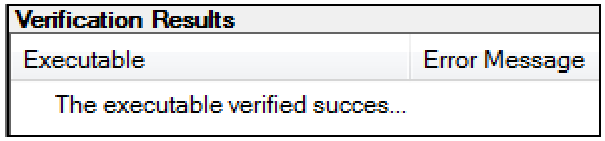
The list of results can also be simplified by collapsing/expanding the groups (i.e., results types) using the chevrons next to the group name. 

A plot can be viewed and modified in its own window by selecting it in the Results list and double-clicking it or pressing **ENTER**.

Re-execute the object by clicking  (**Re-execute Plot** icon) in the toolbar of that separate window.

Verification tab

Part of the Properties tab, the Verification sub-tab displays operational object status and execution error messages.



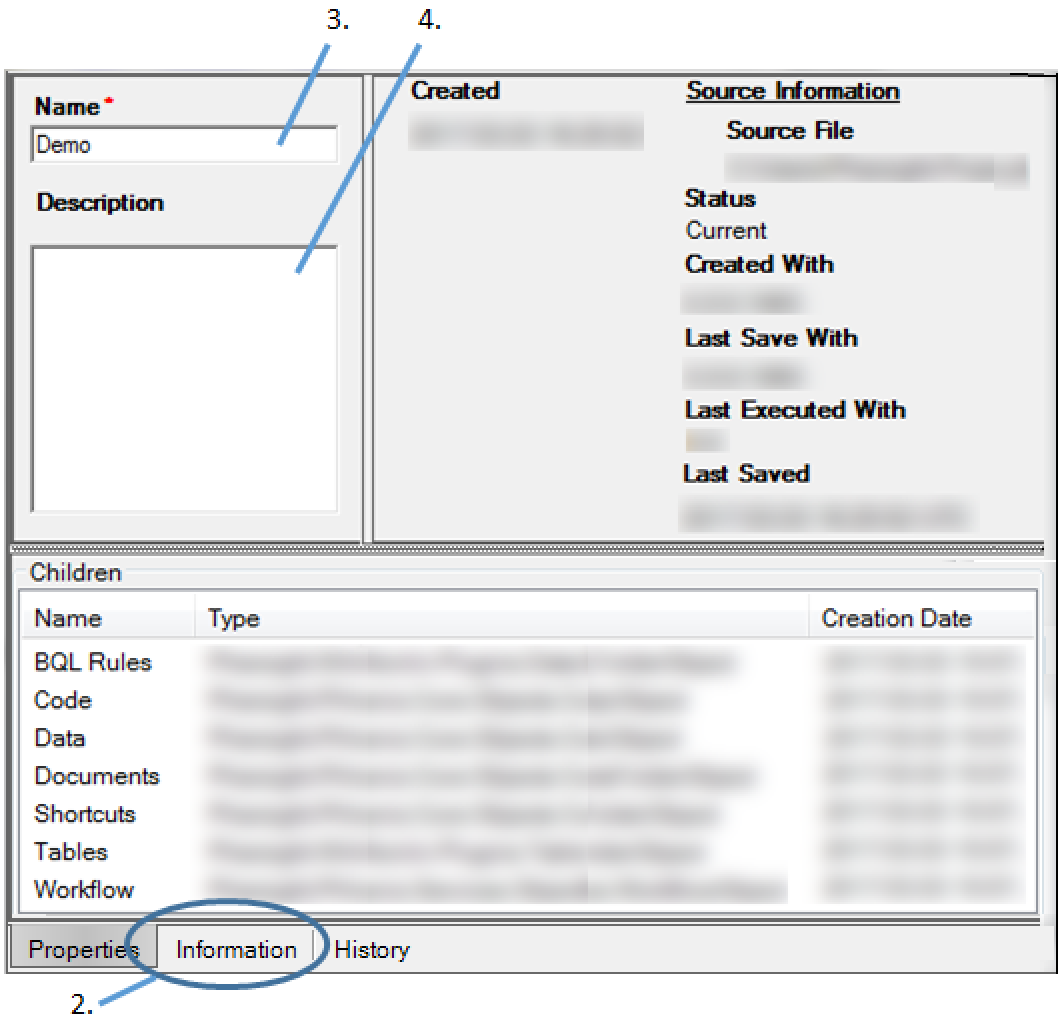
 (**Verify** icon) in the main menu verifies that the selected operational object can be executed.

Phoenix displays a popup indicating the success or failure of verification. The **Verification** tab will also indicate the verification results. If there is a failure, options in the operational object that need to be specified or any other problems will be listed in the **Error Message** column.

Information tab

The **Information** tab displays information about a selected object. Depending on the object selected, the following information may be available: the name, date created, status, Phoenix version used to create the object, Phoenix version used when last saved, the last date executed, and the last date saved. When a project is selected, the tab also includes the full path of the source file.

All Information tabs have two editable fields: the Name and the Description fields.



1. Select any item in the Object Browser.
2. Select the Information tab at the bottom of the right viewing panel.
3. To edit the item's name, type a new name in the **Name** field.
4. Add a description of the item in the **Description** text box.

The bottom portion of the tab lists any children of the selected item. The object type and creation time of each child is also listed. Children can be deleted from this list by selecting them and using either the **Delete** key or the right-click menu **Delete** option. If any of the selected children cannot be deleted, then pressing the **Delete** key will do nothing and the right-click menu **Delete** option will be disabled. Deleting a child from this list also removes them from the Object Browser.

History tab and Settings file

Phoenix provides two methods to track data analyses and manipulation. Operational objects, except for plot objects, create a text file called Settings that lists the options selected at the time of an object's last execution. The Settings files are located in the Results tab.

Every item in the Object Browser also has a history worksheet that tracks changes made to that item. The history worksheet for each item is located on the History tab. Information recorded for each action includes a timestamp, the user who performed the action, the name of the action, and a description. Although the automatically recorded information cannot be edited, notes can be added using the **Annotation** field (double-click in the cell or click in the cell and press the **F2** key).

Timestamp	User	Object Name	Event	Description	Annotation
[illegible]	[illegible]	Descriptive Stats	Object Created	Object Created	
[illegible]	[illegible]	Descriptive Stats	Executed	Phoenix Build 8.1.0.3436 Include Percentiles = False Confidence Interval = 95 Number of SD = 1	

The automatic history worksheet entries cannot be edited.

The events that the history worksheet records change depending on the item. The list below shows the events recorded in the History tab for each item.

Projects: creation, name change

Data folder: creation

Workbooks: creation, name change, copy and paste

Worksheets: creation, name change, column and row creation and deletion, cell value changes, copy and paste, column data type changes, and column unit changes, skipped worksheets on import, opening (including path and filename), fill-down event (including source and destination cell ranges). Worksheets that are copied from an operational object's results contain all the history information from that object.

Code folder: creation

Code files: creation, name change, copy and paste

Tables folder: creation

HTML tables: creation, name change, copy and paste

BQL Rules folder: creation

BQL rules: creation, name change, copy and paste

Documents folder: creation

Document files: Varies based on the type of object imported.

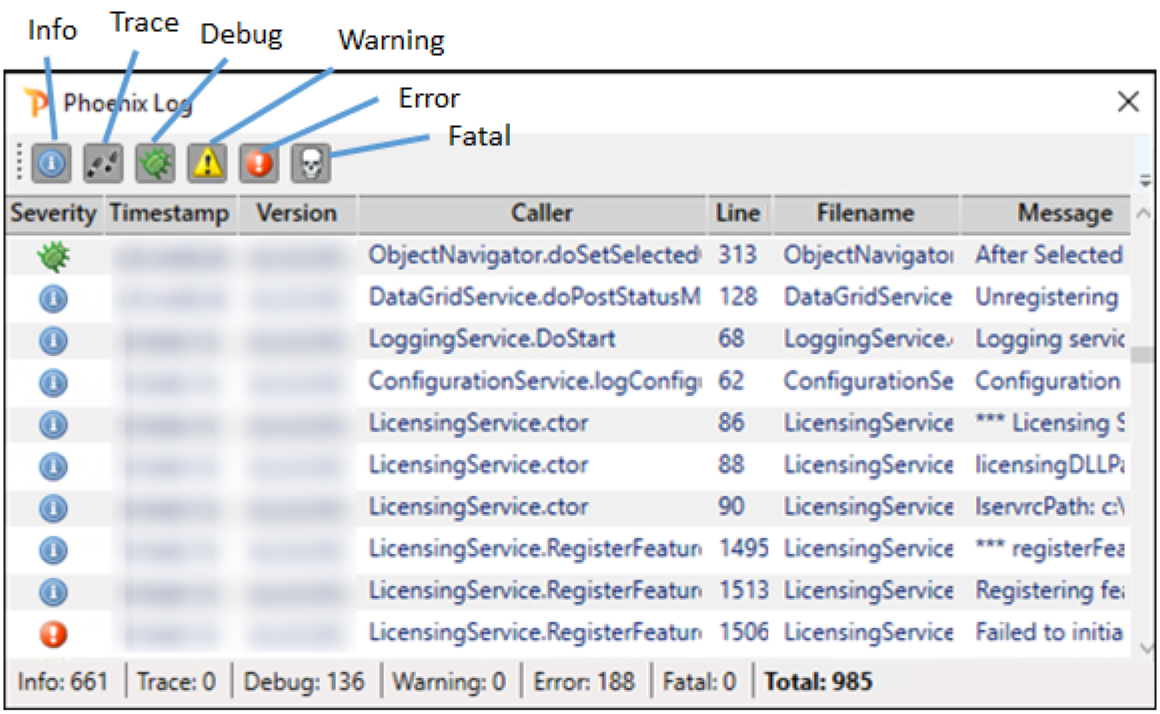
Workflow object: creation, execution, name change, copy and paste, copy from template

Operational object: creation, execution, name change, copy and paste, copy from template

The date-time values recorded in the History tab are Coordinated Universal Time and are displayed with the "UTC" designation to indicate the time zone. This standard time is implemented in the History tab to prevent confusion if Phoenix projects are shared across time zones. There is no option in Phoenix for the user to change the time zone used for recording times in the History worksheet. Settings, NCA, and modeling core text outputs will use the local time and timezone designation of the machine where Phoenix is installed; these do not conflict with the times in the History tab since the time zone being utilized is clearly indicated in each case.

Phoenix log viewer

Phoenix creates several log files that are primarily useful for network administrators and customer support. These files are accessed using the **Help > View Log** menu item. Use the buttons above the list to show/hide log entries of different severity. By default, entries for all levels of severity are displayed. The total number of entries for the different severity levels are reported at the bottom of the window.



Phoenix hotkeys

F1: Help
F2: Rename an object
F3: Find next
F7: Execute
F8: Validate
F9: Edit in Excel
Shift+F7: Execute all objects in workflow
Ctrl+N: New project
Ctrl+R: Close project
Ctrl+L: Open project
Ctrl+S: Save project
Ctrl+W: Save workflow template
Ctrl+P: Print
Ctrl+I: Import
Ctrl+E: Export
Ctrl+F: Find
Ctrl+H: Replace
Ctrl+J: View jobs
Ctrl+O: Orphan model

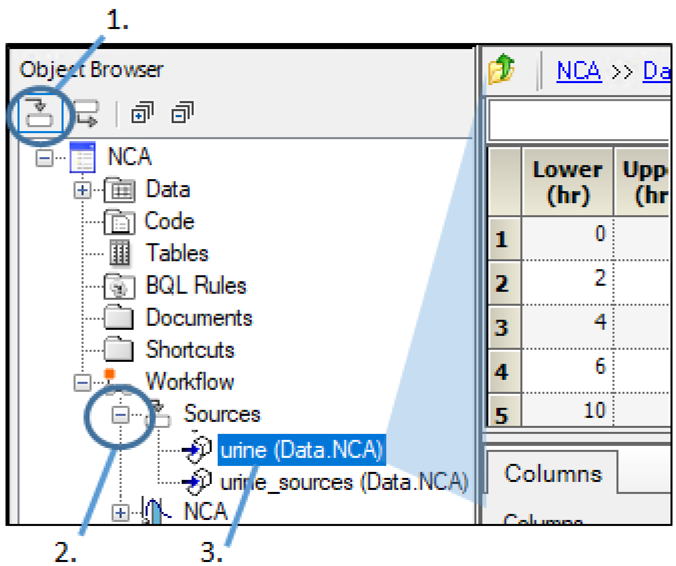
How To Do Common Tasks

The following is a list of several basic tasks that are required by a large number of the Phoenix modules. Becoming familiar with these tasks will help reduce the time spent setting up projects.

Using the Object Browser

The following topics are discussed in this section:

Showing sources

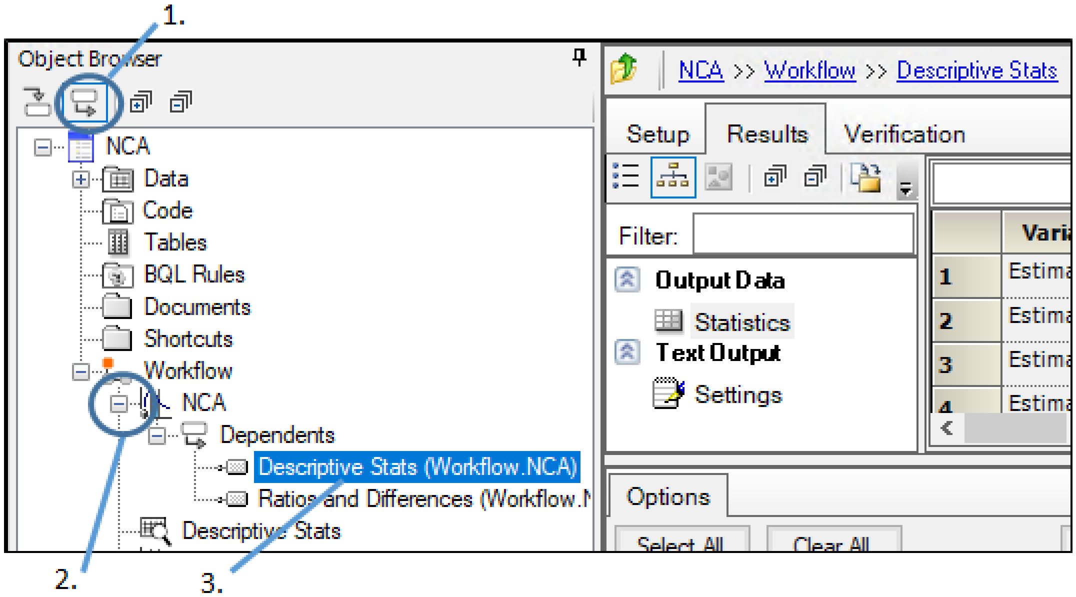


1. Click (**Show Sources** icon) to display the source worksheets for each workflow and operational object.
2. Click the (+) sign next to Sources to view the source worksheets for an object.
   Source worksheets include imported datasets and user-created datasets.
3. Select a worksheet to view it in the right viewing panel.
   The worksheet is displayed in the Grid tab, with the Columns tab below.

Right-click an item in the Sources list and select **Find Object in Browser** to automatically go to that item in the Object Browser.

Source worksheets can be edited like any other worksheet. If a worksheet or part of a worksheet is shaded gray, it cannot be edited. Be aware that editing a source worksheet that is used by an executed operational object marks the object, its results, and the workflow as out-of-date. Also, if multiple operational objects use the same worksheet, then changing the worksheet affects all of those objects, not just the selected one.

Showing dependents



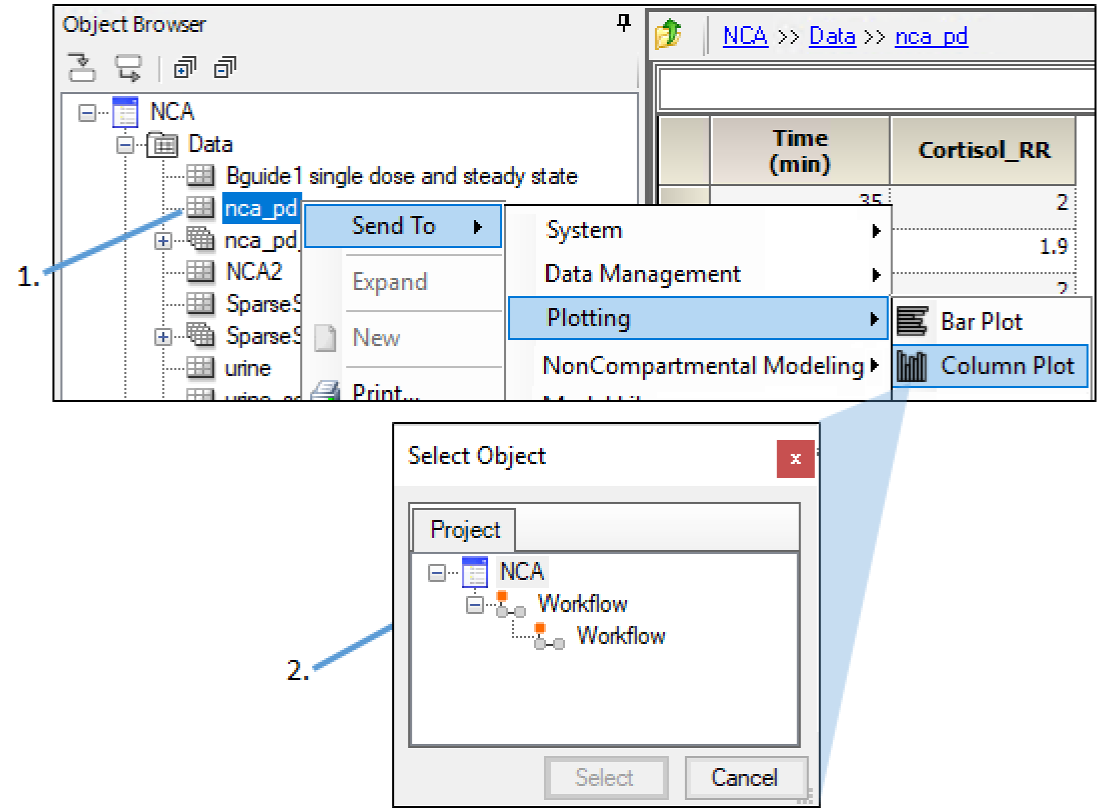
1. Click  (**Show Dependents** icon) to display dependent objects for each worksheet in the Data folder.
2. Click the (+) sign next to Dependents to view the dependent object list.
3. Select an object in the dependent object list to display it in the right viewing panel. Selecting a workflow object displays the Diagram tab for that workflow.

Right-click an item in the Dependents list and select **Find Object in Browser** to automatically go to that item in the Object Browser.

Note: Only dependents of final output are shown, dependents of intermediate or secondary results are not listed.

Send To menu

The **Send To** menu is used to insert an operational object, automatically mapping the selected dataset to it.



1. Right-click a dataset in the Data folder, select **Send To >** <object group> **>** <object>.
   For example, right-click a worksheet and select **Send To > Plotting > Column Plot**.
2. If there are multiple workflow objects, select the one in which to add the new object.
   The object is added to the workflow, with the dataset is automatically mapped to its main input.

The **Send To** menu is accessible from any dataset in the Data folder and from any results worksheet.

Items other than datasets can be sent to operational objects. Code and scripts in the Code folder can be sent to the User ASCII Model, NONMEM Shell, SAS Shell and SigmaPlot Shell operational objects. The Maximum Likelihood models, however, does not allow users to send a code file to be mapped to the object, because the Maximum Likelihood Models object always defaults to the built-in model, and not the text model.

BQL rules in the BQL Rules folder can be sent to a BQL object by right-clicking a rule set and selecting **Send To > Data Management > BQL**.

Copying/Pasting Data folder items

Right-click a worksheet, workbook, or subfolder in the Data folder and select **Copy**.
Or select the item and type **Ctrl+C**.

Right-click the Data folder or a Data subfolder and select **Paste**.
Or select the folder and type **Ctrl+V**.

A duplicate of the worksheet, workbook or subfolder and its contents will be added to the folder or subfolder with “Copy of” prepended to the name.

Copying/Pasting a workflow object

Right-click a Workflow in the Object Browser and select **Copy**.
Or select the Workflow and type **Ctrl+C**.

Right-click the target Workflow and select **Paste**.
Or select the target Workflow and type **Ctrl+V**.

A duplicate of the object will be added at the bottom of the list of workflow objects with “Copy of” prepended to the name.

When pasting an object using **Ctrl+V**, Phoenix identifies an appropriate parent for the copied object. For instance, if a Workflow object is copied and then an executable (not a Workflow) is selected, typing **Ctrl+V** will paste a copy of the Workflow object into the parent executable’s Workflow. If another location is selected, such as the Data folder, a copy of the Workflow object will be pasted in the root Workflow. (Similarly, copying a worksheet and trying to paste it into an executable with **Ctrl+V** will paste the worksheet into the Data folder.)

Caution: When copying and pasting objects, auto-mapping can take place. For example, a parameter worksheet with a Lower or Upper column can be unexpectedly mapped when pasting in an NLME model. It is a good idea to check mappings after pasting a copied object.

Moving a workflow object

Click and drag the object from one Workflow to another Workflow

Deleting items

Right-click an item in the Object Browser and select **Delete**.
Or select an item in the Object Browser and press the **Delete** key.

Click **Yes** in the confirmation dialog.

Since only one item can be selected at a time in the Object Browser, only one item can be deleted at a time. If there are multiple items that need to be deleted, use the Information tab. See “Information tab”.

Exporting a workflow

Phoenix can export all of the objects within a Workflow with one click. This option, called **Dependencies**, is intended to share work with users that might not have Phoenix. It provides a `.xml` summary that displays information about the Phoenix objects in the Workflow and the results. To use this functionality:

- Right-click a Workflow object and select **Dependencies**.
- In the dialog, navigate to an empty folder.
  All of the Workflow output will be exported to this location.
  (Plot results containing more than 100 chart tabs will only output the first 100 tabs.)
- Enter a file name and select **Save**.
  Exporting all objects in a Workflow may take a while, depending on the number of objects.
- In the next dialog, select **Yes** to open a browser window and view a summary.
  All objects are listed, including links to all results for each object.
  Select **No** to return to the main Phoenix window.

Note: Exporting a Workflow in this manner is not a substitute for saving Phoenix projects as `.phxproj` files. Files exported via the **Dependencies** option cannot be imported back into Phoenix as a Workflow.

Comparing or refreshing a dataset

Datasets in ASCII format, meaning those with `.csv` and `.dat` extensions, can be compared to the original dataset and updated from the original file.

To compare imported and original dataset

Right-click an ASCII dataset in the Data folder and select **Check State**.

Phoenix compares the imported version with the original version and tells the user if the datasets match.

To refresh a dataset

Right-click an ASCII dataset in the Data folder and select **Refresh from Source**.

The dataset is synchronized with the original dataset.

Importing Data

When a data is imported into Phoenix, whatever changes are made to those data only affects the data that is imported into Phoenix. The actual file that contains the data is not affected.

This means that any changes made to datasets imported into Phoenix are not reflected in the dataset that is saved on a hard drive or other storage media. Users can make as many changes as they want to a dataset in Phoenix without changing the original dataset.

What types of data does Phoenix use?

Imported datasets such as worksheets and workbooks.
User-created worksheets and workbooks.
Worksheets that are the results of operational objects.

How is data used in Phoenix?

The Data folder contains all the imported or created datasets that are used in a project.
All datasets used in a workflow are contained internally within Phoenix.
Changes made to imported datasets do not change the original dataset.
Data must be mapped to an operational object before it can be used.

This section contains information on:

Importing files
Importing datasets

Note: Computer accuracy for numeric data is limited to about 14 significant digits. This can cause two unique numbers with more than 14 significant digits to be treated as the same number. If the number represents an identifier, set the column type to text to preserve the full ID. The situation for actual numerical data needs to be handled carefully. As an example, using the NCA Slopes Selector when the time data has more than 14 significant digits, and two points differ at the 14th digit (e.g., 240.333333333333 and 240.333333333334), one point appears selected for the time range but it is not used in the Slopes Selector. Furthermore, the point representing a number, such as 240.333333333333, is selectable in the Slopes Selector and can show as the End Time for a user-specified range, but will not be used in the slope calculation, causing Lambda_Z_Lower and Lambda_Z_Upper in the output to be off by 1e-14. One workaround is to click on Slopes and paste the full number. Another possibility is, prior to NCA, to round the time data so it has 14 significant digits or fewer (use a custom transformation in the Data Wizard with a formula such as round(time,10) or roundsig(time,14)).

Importing files

To import files

Click  (**Import File** icon) in the Phoenix toolbar.

Or select the **File > Import** menu option.
Or press **CTRL+I**.
Or right-click the Data Folder in the Object Browser and select **Import**.

Navigate to and select the file(s) to import in the dialog.

To import files as shortcuts

Select **File > Custom Import > File Shortcut**.

To import all files within a folder

Select **File > Custom Import > Import Folder**. All files and sub-folders within the selected folder will be imported into the Documents folder, with the directory structure maintained.

Supported file types

Phoenix can import several file types beyond what are officially supported and displays different import options depending on the file type selected. Some files have no import options. Supported files types are listed below.

ASCII Data (*.csv;*.dat): Displays the *File Import Wizard* dialog.

BQL Rule Set (*.phxruleset): Adds new BQL rule set to the BQL Rules folder.

Enhanced Meta File (*.emf): Imported in the Documents folder.

Excel 97–2003 Workbook (*.xls): Displays the *File Import Wizard*.

Excel Workbook (*.xlsx): Displays the *File Import Wizard*.

Image File (*.bmp,*.gif,*.jpeg,*.jpg,*.png): Imported in the Documents folder.

Phoenix Projects (*.phxproj): Can only be loaded using the import function if a project is already open in Phoenix. No import options.

SAS Transport Files (*.xpt): Imported into the Data folder. (Phoenix supports SAS Transport Format (XPORT) Version 5.)

Text (*.bat,*.ctl,*.mdl,*.mod,*.r,*.sas,*.ssc,*.tdl,*.txt,*.vbs): Imported into the Code folder.

Windows Meta File (*.wmf): Imported into the Documents folder.

Extensionless files are placed in the Code folder. Files imported as shortcuts are placed in the Shortcuts folder.

Note: The following legacy file formats are no longer supported: .lib, .pwo, .pmo, .pto, .pco, .bql, .tdf, .xml, .lml, .cmd, .ivc, .map, .wsp, .pws. Files of these types can still be imported into a project using Pheonix32.exe and then save the project. The saved project is then ready for use in either 32- or 64-bit Phoenix.

Importing datasets

Phoenix can import datasets in several different file formats. During the import process, a copy of the data is created. The original dataset file, no matter where it is located, is not altered by Phoenix in any way.

The maximum worksheet size Phoenix can import depends on the amount of RAM in the computer running Phoenix.

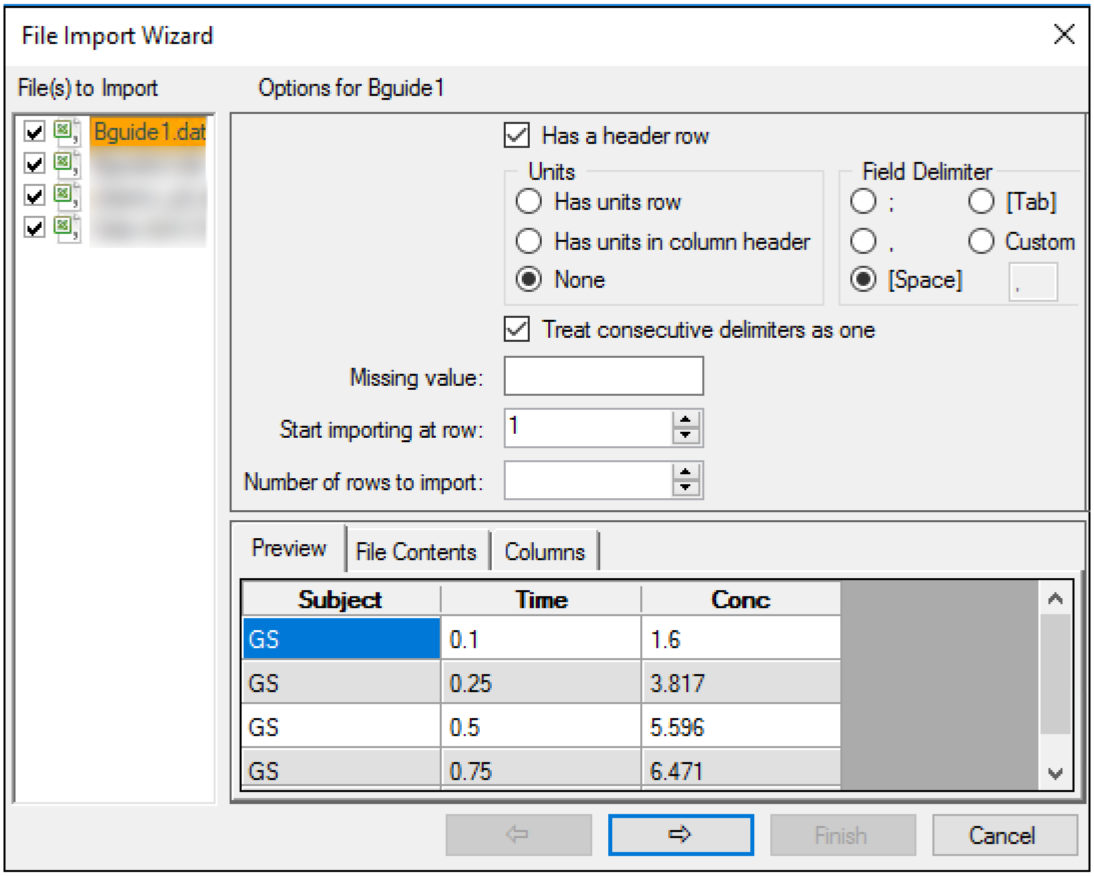
The following topics are discussed in this section:

Using the File Import Wizard dialog
Custom imports
See "ODBC" and "Watson Import Object" for data importing options.

Note: When subject IDs with many digits are imported (e.g., 100010901), they are changed upon import to G8 format by default (e.g., 1.0001090E-08), even if they are imported as text. Using the G9 format preserves the subject ID digits. See “To specify a Microsoft .NET format string” for more information on numeric formats.

Using the File Import Wizard dialog

The *File Import Wizard* dialog contains several options that allow users to determine how a dataset is imported into Phoenix. The *File Import Wizard* dialog is used to import .csv, .dat. .xls, or .xlsx files.



File(s) to Import: Lists the file or files that are being imported. Select a file in the list to view the options for that file.(Clear the checkbox to not import a particular item.)

Has header row: Check this box to indicate that a worksheet contains column headers.

Has units row: Check this box to indicate that a worksheet contains unit information for the column headers.

Has units in column header: Check this box to indicate that at least one of the columns in the worksheet has units included in the header. If checked, any characters that are after an underscore (_), within brackets ({}), or within square brackets ([]) in the source file will be considered as units for the column.

Treat consecutive delimiters as one: Check this box to have Phoenix treat two spaces, for example, as one space.

Field delimiter: Select the option buttons to indicate how the fields in a dataset are separated: by semi-colon, comma, space, tab, or a custom delimiter.

Missing value: If the dataset has a specific entry for instances where the value is missing, type that entry in this field. Any cells that match that entry will be left blank when they are imported. For example, a dataset may contain the word “None” in cells where a value is not available. Typing `None` in the **Missing value** field will import cells that contain the word “None” as a blank cell.

Start at row: Type the row number where importing is to start. The default value is 1.

Number of Rows to Import: Type the total number of rows in the dataset that are to be imported.

Worksheet Preview tab: Displays a preview of the data being imported based on the currently selected options. (Only the first 20 rows of a worksheet are previewed.)

File Contents tab: Displays the raw file contents. (Only the first 20 rows of a worksheet are shown in this tab.)

Column Options tab: Provides options to specify the data type of a column (**Numeric** or **Text**) and indicate any columns of data to ignore during the import (check the boxes in the **Ignore** column).

Click **Finish** to import the file and display it in the viewing panel. Click **Cancel** to cancel the file import.

Note: Numeric columns can switch to text if there is any non-numeric data in a cell. So, if there is an extra row in an input dataset containing text, it will cause entire columns to be treated as text. if this happens, change the column type to numeric.

Custom imports

Phoenix file imports are controlled by the file extension. Phoenix uses the file extension to determine where to place the file and its components, if any. The **Custom Import** menu allows users to force a file to be imported as a binary, ASCII, or text file, without regard to the file extension.

The **Custom Import** menu is useful for importing file types that are recognized by Phoenix, but do not contain data that is usable by Phoenix. For example, a user might want to attach an Excel table to a project. By selecting **File > Custom Import > Binary File** the Excel file is placed in the Documents folder, and not in the Data folder.

Additionally, the **Custom Import** menu allows users to import data for use with any of the third party objects (e.g., R, SAS, PsN, etc.) as a shortcut.

- To import a binary file, select **File > Custom Import > Binary File**.
  Files are placed it in a Documents sub-folder named after the imported file's extension. For example, an imported `.jpg` file is placed in `Documents/jpg`. These files cannot be viewed or used in Phoenix. The Binary File custom import is best used to keep files in a project that are associated with a project, but are not used directly in a project.
- To import an ASCII file, select **File > Custom Import > ASCII Data**.
  Files are placed in the Data folder.
- To import a text file, select **File > Custom Import > Plain Text**.
  Files are placed in the Code folder.
- To import a shortcut object, select **File > Custom Import > File Shortcut**.
  A shortcut object containing meta information about the selected file is added to the Shortcuts folder.

Data Mapping

Data mapping is the process of associating a dataset with an operational object so that objects can use the data in an analysis or other function. Data mapping in Phoenix is as simple as dragging a dataset from the Data folder to an object's input, or using the *Select Object* dialog to select a dataset.

There are multiple types of data mapping in Phoenix:

- Mapping a dataset to an operational object: Datasets can be mapped to the different panels in an object's Setup list, or they can be mapped to an object's inputs in the Diagram tab.
- Mapping results to an operational object
- Mapping context associations: Context mapping is the process of linking a specific column in a dataset to a specific context in an operational object, such as Time or Concentration.

Phoenix can complete context mappings if a column header in a worksheet matches the context name in an operational object. The Global Contexts and Context Association panels in the *Preferences* dialog can be used to automatically associate columns in a dataset with contexts in an operational object. For example, Phoenix can be set to map a concentration column named conc to an operational object's concentration context.

Mapping a dataset to an operational object

Every operational object includes a data input panel in the Setup tab that is used to identify how input variables are used in an operational object.

Most primary data input panels contain two tabs: the Mapping tab (where dataset columns are mapped to an object's inputs) and a sort order tab (allows users to sort dataset columns). The Table, NONMEM, PsN, R, SAS, and SigmaPlot objects only have a Mappings panel.

Users can map a dataset or other worksheet to almost any item in the Setup tab list using the instructions listed below. Note that the R and SAS Shell objects must have a script mapped to them before their inputs are defined. The PsN Shell object must have at least one model mapped to it before the input can be defined.

To map a dataset using the data mappings panel

In the data mappings panel, click (**Show Sources** icon).

In the dialog, click the (+) sign next to the Data folder.

Select a dataset and click **Select**.

Or use the pointer to drag a dataset from the Data folder to the Mappings panel.

To map a dataset using the Diagram tab

Select the Workflow object in the Object Browser.

In the Diagram tab, click to expand the object box.

Click the (+) sign next to Inputs.

Drag the dataset from the Data folder to the primary data input.

The line between the External Sources box and the object box represents the data mapping.

To map a dataset using the "Send To" menu option

Select the object in the Object Browser to return to the Setup tab.

Right-click an imported worksheet and select **Send To >** <object group> **>** <operational object>.

The **Send To** command inserts the new object into the Workflow with the right-clicked worksheet already mapped as the input source.

Mapping results to an operational object

The results worksheet of any operational object can also be mapped to another operational object.

To map results from the Setup tab

Click  (**Select Source** icon) in the operational object's Setup tab.

In the dialog, click the (+) signs to expand the menu tree.

Select the results worksheet and click **Select**.

To map results from the worksheet

Right-click a results worksheet and select **Send To >** <object group> **>** <operational object>.

Mapping context associations

Context associations are inputs to an operational object. Contexts that must have data mapped to them so the object can perform its function are shaded orange. Most items in an operational object's Setup list have a Mappings panel that allows users to match columns in a dataset to inputs in an operational object.

Column headers in the dataset are displayed on the left side and context associations for the operational object are displayed across the top.

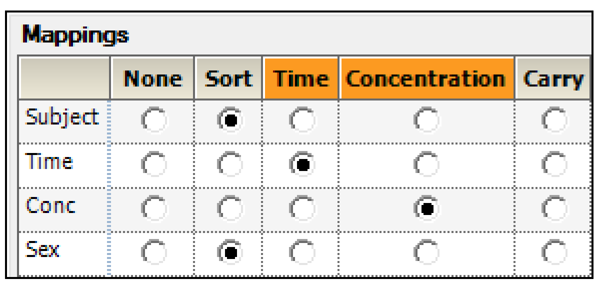


Figure 13-1. Context associations for NCA model 200

Select the option button to connect the input dataset column containing the data (row) to the corresponding context (column).

Repeat for each item in the Setup tab list that requires mapping data to inputs.

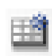
Working with Worksheets

This section includes information on the following topics:

There are also a number of operational objects designed specifically for modifying worksheets. See "Worksheet-Related Objects".

Creating a worksheet or workbook

To create a worksheet

Select **File > New Worksheet**  (**New Worksheet** icon).

Or right-click the Data folder and select **New > Worksheet**.

A new worksheet is added to the Data folder.

To rename the worksheet

Select the worksheet and press the **F2** key.
Or single-clicking the worksheet name a second time.
Or right-clicking the worksheet and selecting **Rename**.

Type a name for the new worksheet.

To create a workbook

Right-click the Data folder and select **New > Workbook**.

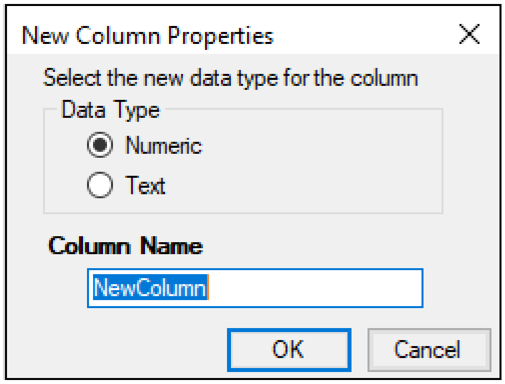
Click the (+) sign next to the workbook to view the worksheets it contains.

To add more worksheets to a workbook, right-click a workbook and select **New > Worksheet**.

Adding columns to a worksheet

With the worksheet displayed, click **Add** under the Columns box in the Columns tab.
Or right-click in the worksheet itself and select **Insert Column** from the menu.

In the dialog, select the **Numeric** or **Text** option buttons to set the data type for the new column.



Type a name for the new column in the **Column Name** field and click **OK**.

After a column is added to the Columns box its properties can still be edited.

Numeric versus text

Numeric-type columns are considered by Phoenix to contain only numeric values, and the application treats the values in a numeric column as numeric data. A numeric column contains only numeric values or substitution values such as those applied by BQL rules.

Text-type columns in Phoenix can contain mixed numeric and text values. Some important considerations regarding Text-type columns include:

Any beginning and trailing spaces in text columns are trimmed in Phoenix worksheets.

Preceding "0"s will be lost in the case of numeric subject identifiers that start with "0"s.

Columns with numbers as purely text will sort differently than numeric columns.

Very large integers will lose precision due to rounding of significant digits when they exceed precision capacity (approximately 14 digits);

Limitations on column names

Limitations on column names are necessary in Phoenix because certain characters can cause operational objects to either work incorrectly or not recognize a column in a worksheet.

Use only alphanumeric characters and underscores.

No spaces. Spaces are converted to underscores.

Start with a letter. Column names that start with a number have an underscore added to the beginning of the column name.

Any invalid characters are automatically converted to an underscore. For example, if a user types the column name `1 Conc%`, Phoenix automatically converts it to _1_Conc_.

Editing an existing column

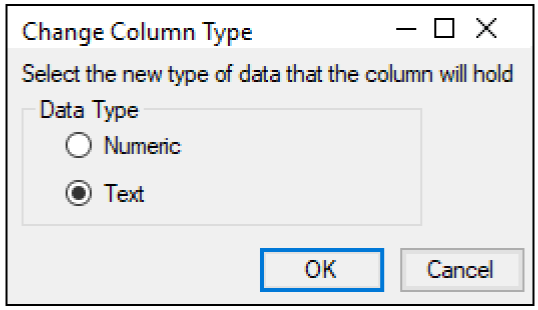
To ***change*** the column header, click the name in the Columns box to make it editable and type the new name.

To ***remove*** a column, select a column header in the Columns box and click **Remove** below the Columns box.
Or right-click the cell or column header in the worksheet itself and select **Delete** from the menu. In the confirmation dialog, click the **Selected Column(s)** option button and click **OK**.

Note that columns cannot be deleted from a worksheet that is mapped to an operational object.

To ***change the order*** of the columns, select a column in the Columns box and click the **Up Arrow** and **Down Arrow** buttons beside the Column box to move the column up and down.

To ***change a column's data type***, click **Change** beside **Data Type** to display the *Change Column Type* dialog and select the type.



Caution: Changing a column from text to numeric deletes any non-numeric values in the column.

To ***add units*** to a column header, type the unit in the **Unit** field or click **Units Builder** to open the *Units Builder* dialog. See "Using the Units Builder".

Adding and deleting rows in a worksheet

Right-click in the worksheet and select **Insert Row** from the menu.

If a cell is selected, the row is inserted above the selected cell. If multiple rows are selected, the same number of rows will be inserted above the first selected row.

To ***delete*** a row, right-click a cell in the row and select **Delete** from the menu. In the dialog, select the **Selected Row(s)** option button and click **OK**.

To ***move*** rows, select the contiguous rows, move the cursor over the lower right corner of the selected block of rows and, when the cursor changes to a four-arrow sign, drag the block of rows to the new location.

Note: A row-paste operation will only appear in the history when the data to be copied is selected by highlighting the individual cells and pasted by selecting the destination row number. If the data is copied by selecting a row number or pasted by selecting the destination cells, the history entry will not be created.

Moving cell values in a worksheet

Use the pointer to select a horizontal or vertical range of cells in a worksheet.

Select **Cut**, **Copy**, **Paste** from the right-click menu, **Edit** menu, or in the toolbar.

Cut moves the values in the cells to the clipboard.

Copy copies the values in the cells to the clipboard.

Paste pastes the values in the clipboard into cells, starting with the currently selected cell.

Or move the cursor over the lower right corner of the selected block of cells and, when the cursor changes to a four-arrow sign, drag the block of cells to the new location.

Editing data values in worksheets

Click in a cell and edit the content directly in the cell or in the field above the worksheet.

If you want the same value in multiple adjacent cells, enter that value in the first cell and then drag the lower right corner of the selection box until the block of desired cells is selected. When you release the mouse button all of the selected cells will have the entered value.

Note: If you are unexpectedly unable to edit a cell value, try double-clicking in the cell or selecting the cell and then using the field above the worksheet to enter the data.

Replacing a cell value with a new value

Select **Edit > Replace**.

In the **Find** field, type the text or number to be replaced.

In the **Replace With** field, type the text or number to replace the search value entered in the **Find** field.

Check the **Replace All** box to replace all instances of the value in the **Find** field. Unchecking the **Replace All** box only replaces the first instance of the search value.

Undoing and redoing actions

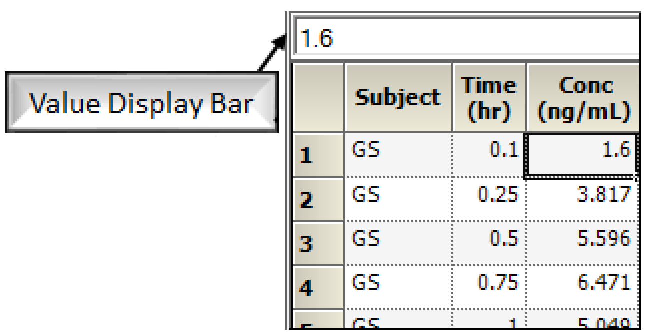
Select **Edit > Undo** to undo the last worksheet action.

Select **Edit > Redo** to redo the last worksheet action.

Note: The **Undo** and **Redo** functions have no effect on any part of Phoenix other than worksheets.

Changing the display format of numerical values

The numeric display format is only used to control how data is displayed. All operational objects use the raw data that is displayed in the Value Display bar, i.e., full precision is used in all calculations regardless of the display format.



Phoenix uses Microsoft .NET format strings to display numerical values in a worksheet.

To specify a Microsoft .NET format string

Select the **Custom** option button in the Columns tab.

Enter a format string in the field. The following lists some examples. The default is `G8`.

General format (e.g., G, G4, G8): Enter `G` in the **Custom** field to display the values in the cells in fixed-point or scientific notation, depending on the length of the number and the specified precision. Users can change the precision specifier after G to any whole number from one to 99. Any numerical value longer than the specified precision value is displayed in scientific notation. If no precision value is specified, then every number in the column is displayed without regard to significant digits or decimal places.

Exponential (e.g., E, E4, E8): Enter `E` in the **Custom** field to display the values in the cells in scientific notation. Users can change the precision specifier after E to any whole number from one to 99. If no precision value is specified, then six decimal places are used to display every number in the column.

Fixed (e.g., F, F4, F8): Enter `F` in the **Custom** field to display the values in the cells in real numbers. The F format determines how many decimal places are displayed. Users can change the precision specifier after F to any whole number from one to 99. If no precision value is specified, then two decimal places are used to display every number in the column.

To specify the number of decimal places

Users can set the number of required and optional decimal places to make sure that all values in a cell are represented and not altered. The number of required and optional decimal places needed to do this depends on the values in the column cells.

Select the **Numeric** option button.

In the **Required Decimals** box, select or type the number of required decimal places.

In the **Optional Decimals** box, select or type the number of optional decimal places.

Check the **Use Thousands Separator** box to place a comma between every third integer.

If a cell contains less than the specified number of required decimals, then zeros are appended to the end of the value. For optional decimals, no zeroes are appended. On the other hand, if a cell contains more decimal values than the number specified, then the values are truncated. The actual value is not changed in the cell, only the displayed value is changed.

Date and time formats

The time column in a worksheet is typically in numeric format. Phoenix also allows users to create worksheets that contain the date and time values in text format.

MM/dd/yyyy (8/22/2006)
dddd, dd MMMM yyyy (Tuesday, 22 August 2006)
dddd, dd MMMM yyyy HH:mm (Tuesday, 22 August 2006 06:30)
dddd, dd MMMM yyyy hh:mm tt (Tuesday, 22 August 2006 06:30 AM)
dddd, dd MMMM yyyy H:mm (Tuesday, 22 August 2006 6:30)
dddd, dd MMMM yyyy h:mm tt (Tuesday, 22 August 2006 6:30 AM)
dddd, dd MMMM yyyy HH:mm:ss (Tuesday, 22 August 2006 06:30:07)
MM/dd/yyyy HH:mm (8/22/2006 6:30)
MM/dd/yyyy hh:mm tt (8/22/2006 6:30)
MM/dd/yyyy H:mm (8/22/2006 6:30)
MM/dd/yyyy h:mm tt (8/22/2006 6:30)
MM/dd/yyyy h:mm tt (8/22/2006 6:30)
MM/dd/yyyy h:mm tt (8/22/2006 6:30)
MM/dd/yyyy HH:mm:ss (8/22/2006 6:30)
MMMM dd (22-Aug)
yyyy'-'MM'-'dd'T'HH':'mm':'ss.fffffffK (2006-08-22T06:30:07.7199222-04:00)
ddd, dd MMM yyyy HH':'mm':'ss 'GMT' (Tue, 22 Aug 2006 06:30:07 GMT)

yyyy'-'MM'-'dd'T'HH':'mm':'ss (2006-08-22T06:30:07)
HH:mm (6:30)
hh:mm tt (6:30 AM)
H:mm (6:30)
h:mm tt (6:30 AM)
HH:mm:ss (6:30:07)
yyyy'-'MM'-'dd HH':'mm':'ss'Z' (2006-08-22 06:30:07Z)
dddd, dd MMMM yyyy HH:mm:ss (Tuesday, 22 August 2006 06:30:07)
yyyy MMMM (2006 August)

Finding a cell value in a worksheet

To find a cell by column and row

With a worksheet displayed, select **Edit > Go To**.

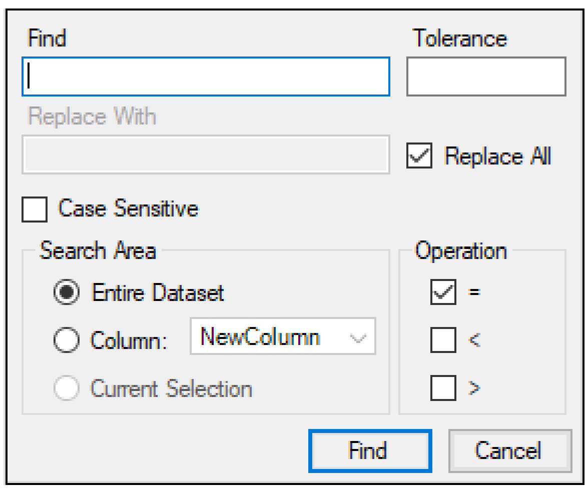
In the dialog, use the **Column** menu to select the column in which the cell is located.

In the **Row Number** field, type the row number in which the cell is located.

Click **OK** to select the corresponding cell and scroll to that location in the worksheet.

To find a cell by its value

Select **Edit > Find**.



In the dialog, type the number or text to search for in the **Find** field.

For numerical values, use the **Tolerance** field to enter a tolerance value. Numeric values that are +/- the tolerance of the search value are considered to match the search value.

For text or text and numbers, check the **Case Sensitive** checkbox to search for text that matches the capitalization of the search value.

In the **Search Area**, select the **Entire Dataset**, **Column**, or **Current Selection** option button to define the search range.

If the **Column** option button is selected, use the menu to select which column is searched.

In the **Operation** area, select one of the operator checkboxes to find values equal to, less than, greater than the search value. Multiple checkboxes can be selected to create additional operators.

= (equal to the search value)

< (less than the search value)

<= (less than or equal to the search value)

> (greater than the search value)

>= (greater than or equal to the search value)

<> (not equal to the search value)

Sorting a worksheet

Worksheet columns can be sorted in ascending or descending order, and the sorted column position can be further ordered in the *Sort Worksheet* dialog.

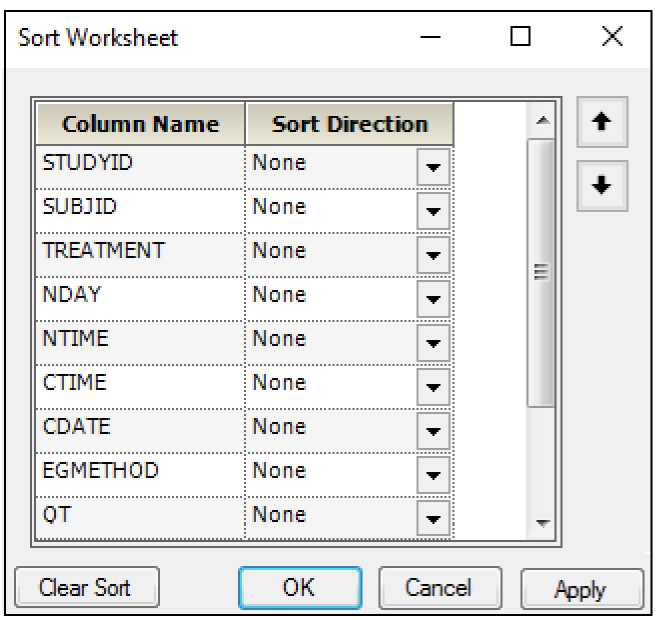
Any worksheet, including imported datasets and the results of an analysis can be sorted. Sorting a worksheet has two different effects, depending on the type of worksheet that is sorted.

- Sorting a source worksheet, creates a permanent change in the way the worksheet is ordered. It affects all operational objects that use that worksheet so they are marked as out-of-date.
- Sorting a results worksheet only changes the order in which the data is displayed. If users want to make permanent changes to the way a results worksheet is sorted, then that worksheet can be copied to the Data folder or mapped to a Column Transformation object.

To sort a worksheet

Click the **Sort Worksheet** (**Sort Worksheet** icon) button that is located above every worksheet.

Or select **Edit > Sort Worksheet**.



In the dialog, click the **Sort Direction** arrow next to a column name to select a sort direction. Sort direction options include **Ascending** (increasing) or **Descending** (decreasing). Changing the sort direction changes the column order in the dialog, but ***does not*** change the sort order in the worksheet.

Select a sorted column in the dialog and move it up or down in the list by clicking the **Up** and **Down** arrow buttons.

When finished, click **OK** to apply the changes and close the dialog, or click **Apply** to apply the changes and leave the dialog open.

Click **Clear Sort** to clear all specified sort orders.

Note: If a column has no specified sort direction, then the column order cannot be changed in this dialog. However, the column order can still be changed in the Columns tab.

Using Edit in Excel

If Microsoft Excel is installed, users can edit worksheets and HTML tables in Excel and re-import the edited worksheet or table into Phoenix. Excel can be used to enter formulas into worksheets or change the formatting of HTML tables.

The following topics are discussed in this section:

Note: Copying and pasting from Phoenix to Excel might not retain the same number of digits or trailing zeros, since the tools could have different column formats. An alternative method is to send the data to a Table object and create a table with the specified number of decimals or significant figures for each table column. Then right-click the Table and select **Copy to Tables folder**. Select the copied table in the Tables folder and right-click to select **Edit in Excel**, which will open the data in Excel with preserved formatting.

Editing a worksheet with Microsoft Excel

If a worksheet has no dependents, which means it is not mapped or connected to an operational object, and it is located in the Data folder, then it can be edited in Excel. In order to edit a Phoenix object's result worksheet in Excel, it first must be copied to the Data folder by right-clicking the worksheet and selecting **Copy to Data Folder**.

In the Object Browser, select a worksheet in the Data folder.

Select **Edit > Edit in Excel**.
Or right-click the worksheet and select **Edit in Excel**.

A dialog is displayed warning that all editing done in Excel is logged as a single, generic audit entry.

Click **OK** to open the worksheet in Excel.

Edit the worksheet using the Excel tools.

Note: While a worksheet is being edited in Excel, it cannot be mapped to any operational object.

When finished editing, save the worksheet in Excel using **File > Save** and close Excel.
Be sure to save the worksheet before closing Excel, or all changes will be lost.

Caution: Because of the way Phoenix handles its interactions with Excel, users cannot use the **Save As** option in Excel to save the worksheet with a different name or to a different location. The **Save** option must be used. If the worksheet name or file location is changed, the Excel edits cannot be imported into Phoenix.

In the dialog, click **Yes** to apply the changes.
An entry is written in the worksheet's History tab noting that it was edited in Excel.

In the next dialog, click **Yes** to save formulas in the worksheet.
The worksheet is ***no longer editable*** in Phoenix, but it can be edited in Excel and the worksheet can still be used with operational objects.
If formulas are not saved, only the formula results are saved, and the worksheet can be edited in Phoenix. However, the formulas will not be available the next time the worksheet is edited in Excel.

In addition to editing the data in a worksheet, users can edit the units associated with each column. If a worksheet has a units row, edit the units in that row. If a worksheet does not have a units row, entering units adds the units to a row in the worksheet, but not the column headers.

When the worksheet is open in Excel, it is stored in a temp directory located at `C:\Users\<user name>\AppData\Local\Temp\Phoenix`. The temp directory's name starts with `PhxExcel_`, followed by a unique identifier.

Note: For worksheets edited in Excel, with formulas saved, if the **Refresh from Source** option in the edited right-click menu is used, the worksheet is empty. To get the data back, use the **Edit in Excel** option again, make a change to the dataset and then save the changes back to Phoenix, the worksheet will be restored.

Editing an HTML table in Microsoft Excel

The Table object in Phoenix creates tables in HTML format. To edit a table in Excel, it first must be copied to the Table folder by right-clicking the table output and selecting **Copy to Tables Folder**.

In the Object Browser, select a worksheet in the Table folder.

Select **Edit > Edit in Excel**.
Or right-click the worksheet and select **Edit in Excel**.

When finished editing in Excel, select **File > Save As** and change the filename.
Excel cannot publish to the same file that is being edited.

In the **Save as type** menu, make sure that **Web Page (*.htm;*.html)** is selected.

Click **Publish**.

In the next dialog, click **Publish**.

Close Excel without saving.

When asked to apply the changes to the table, click **Yes**.
An entry is written in the table's History tab noting that it was edited in Excel.

In the next dialog, select the renamed HTML file and click **Open**.
The HTML file's name is the same one entered in Excel.

The HTML table in the Tables folder now contains the edits made in Excel.

When the table is open in Excel, it is stored as a temp file which, by default, is located in `C:\Users\<username>\AppData\Local\Temp\Phoenix`.

Rules for editing worksheets and HTML tables in Excel:

- Only worksheets and HTML tables in the can be edited in Excel.
- Worksheet format edits (fonts, shading, etc.) are not saved when saving back to Phoenix.

- HTML table format edits are saved when saving back to Phoenix and the user chooses to apply the changes.
- Only formatting available in standard Phoenix tables are supported. For non-standard tables, the HTML is passed to Excel as is.
- Multiple worksheets and HTML tables can be edited at once.
- If a text value is added to a Numeric-type column, then the column is changed to a Text-type when the changes are applied in Phoenix.
- The edited worksheet and table will match any changes that Excel automatically makes to those files.
- Formulas cannot be edited in Phoenix. If a worksheet contains formulas and the formulas are saved when the worksheet is imported back into Phoenix, then the worksheet can no longer be edited in Phoenix.
- Worksheets that cannot be edited in Phoenix are shaded gray.
- Detailed edits made in Excel are not recorded in the worksheet's or table's history tab. The History tab only records a single edit entry named "Object Edited in Excel."

Using the Units Builder

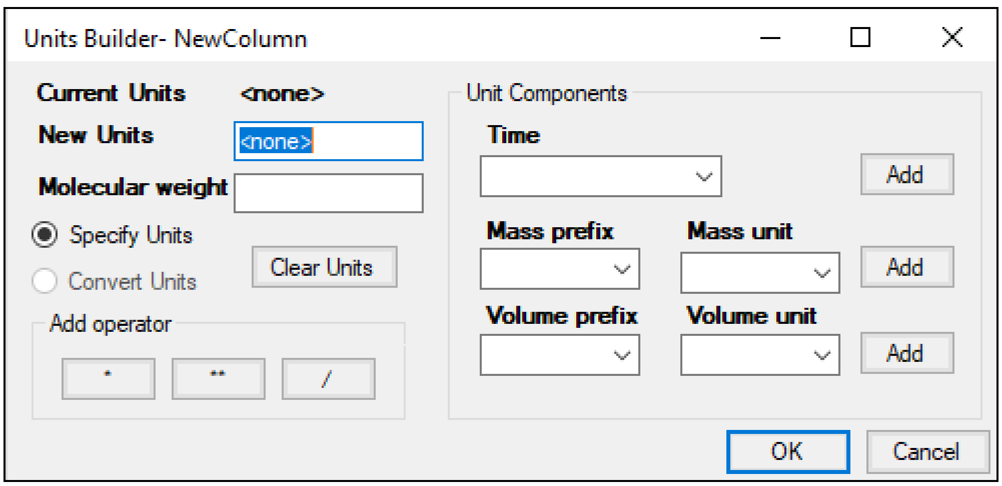
This section includes information on the following topics:

Adding new units
Converting existing units
Changing units without conversion
Removing units
Converting between grams (g) and moles (mol)
Valid units and prefixes in Phoenix

Phoenix recognizes certain units as valid, which means Phoenix can convert those units and their associated values. Invalid units can still be added but cannot be converted. Invalid units are placed inside curly brackets. For example, {mmHg} is an invalid unit and that is denoted by the curly brackets. When unsure of the unit abbreviations recognized by Phoenix, use the *Units Builder* dialog.

Note: Avoid using spaces in the units, as they are considered invalid characters, even though the *Units Builder* does not flag them with curly braces.

With a worksheet displayed, click **Units Builder** in the Columns tab.



Note: Conversions involving “deca” should be avoided as they will generate incorrect results due to a defect in a third party product.

Invalid, or nonstandard units are carried throughout any operation, such as descriptive statistics, but not used in any calculations. For a list of valid units and prefixes, see “Valid units and prefixes in Phoenix”.

Adding new units

In the *Units Builder* dialog, type the units in the **New Units** field and click **OK**.
Or

In the **Time** menu, select a time unit and click **Add** to add the unit to the **New Units** field.

In the **Mass prefix** menu, select a mass prefix.

In the **Mass unit** menu, select a mass unit.

Click **Add** to add the mass unit to the **New Units** field.

In the **Volume prefix** menu, select a volume prefix.

In the **Volume unit** menu, select a volume unit.

Click **Add** to add the volume unit to the **New Units** field.

To add an operator to a unit, click one of the operator buttons.
[*] (multiplication) [**] (square) [/] (division)

Click **OK** to add the unit to the column header.

Invalid units are displayed in red text in the **New Units** field. If an invalid unit is specified, Phoenix displays a warning message asking if you wish to continue. Clicking **Yes** adds the unit.

When importing a dataset with units, be sure the **Has units row** checkbox is checked in the *Import* dialog to display the units in the column headers. Otherwise, the units are displayed in the first row, since units are stored in a row in a worksheet.

When exporting a dataset with units, be sure the **Output units** checkbox is checked in the *Export* dialog. Otherwise, the units are not saved in the exported dataset.

Converting existing units

If a unit can be converted, the **Convert Units** option button is automatically selected. (Invalid units cannot be converted, and must be cleared before new units can be added.)

Type the new unit in the **New Units** field and click **OK**.

The new unit is added to the column header and the values in the selected column are automatically converted.

Note: Units cannot be converted using the **Unit Components** menus. Selecting a unit from these menus only appends the selected unit to the existing unit. It does not convert them.

If Phoenix cannot convert a unit and its values, a warning message is displayed if you would like to set the unit anyway. Clicking **Yes** sets the unit.

Changing units without conversion

In the *Units Builder* dialog, select the **Specify Units** option button.
(The **Convert Units** option button is selected by default if a column already has units.)

In the **New Units** field, type the new unit.
Or use the **Unit Components** menus and the operator buttons to enter the unit.

Click **OK**.

The unit is changed without converting the values in the column.

Removing units

Note: Only use the **Clear Units** button if want to change the unit label without changing the numbers, as clearing the units makes Phoenix "forget" the original unit.

In the *Units Builder* dialog, click **Clear Units** and then click **OK**.

The unit is removed from the column header.

Converting between grams (g) and moles (mol)

Select the column that contains units in grams (g) or moles (mol).

Click **Units Builder**.

In the *Units Builder* dialog, type `mol` in the **New Units** field if the values are in grams or `(mass prefix)g` if the values are in moles (mol).

In the **Molecular weight** field, type the molecular weight and click **OK**.

The new unit is added to the column header and all values in the selected column are automatically converted.

Valid units and prefixes in Phoenix

Valid units and prefixes for ***time*** include: hour [h], hour [hr], day [day], minute [min], second [sec], second [s], millisecond [ms], microsecond [us], nanosecond [ns], week [week], month [month], year [year]

Valid units and prefixes for ***mass*** include: gram [g], mol [mol], pound [lb], IU [IU], femto [f], pico [p], nano [n], micro [u], milli [m], centi [c], deci [d], deca [dk], kilo [k]

Valid units and prefixes for ***volume*** include: liter [L], femto [f], pico [p], nano [n], micro [u], milli [m], centi [c], deci [d], deca [dk], kilo [k]

Printing

The results of any executed operational object can be printed. Phoenix can also print worksheets, text files of any format, `.rtf` files, `.map` files, `.lib` files, `.mdl` files, and HTML tables.

Note: The only items in the Documents folder that can be printed are text files. Any other files imported into the Documents folder, including types that Phoenix can print, are not printable if they are in the Documents folder.

Printing object results

Select the Results tab of any executed operational object.

Select any text or plot object in the Results tab.

Click  (**Print Results** icon).

In the *Print* dialog, select a printer, the number of pages and copies to print, and click **OK**.

Printing items in the Object Browser

Not all objects in the Object Browser can be printed. For example, workbooks and most objects in the Documents folder cannot be printed.

If an item cannot be printed, the **Print** and **Print Preview** options in the **File** menu are disabled.

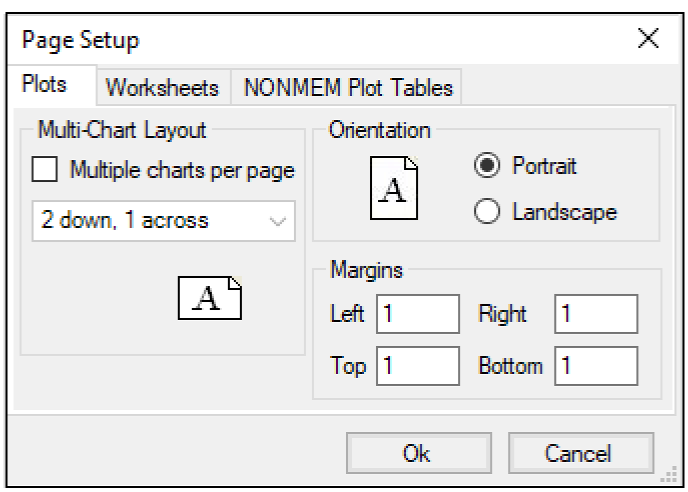
To set up a page for printing

Select **File > Page Setup**.

The *Page Setup* dialog has several tabs containing setup options for headers, footers, page orientation, margins and other options that are relevant for a particular type of object.

To set up plot printing

Select the **Plots** tab.



To specify how multiple charts are to appear on a printed page, check the **Multiple charts per page** box and choose a predefined layout from the pull-down menu.

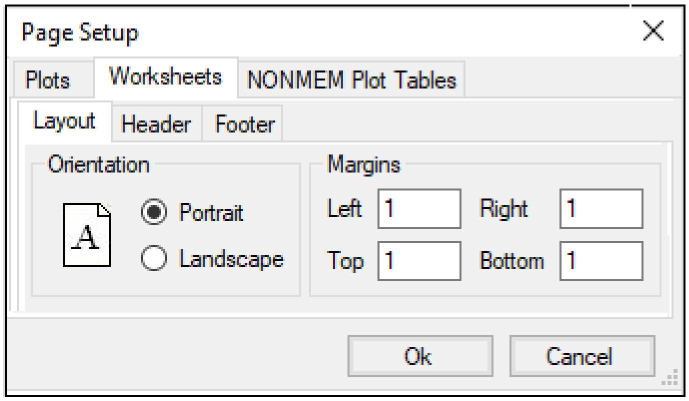
Specify the orientation of the charts on the page as either **Portrait** or **Landscape**.

Enter the size of each page margin (in inches).

To set up worksheet printing

Select the **Worksheets** tab.

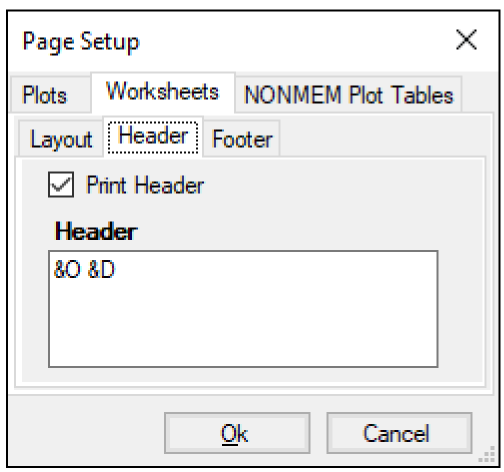
Select the **Layout** sub-tab.



Specify the orientation of the data on the page as **Portrait** or **Landscape**.

Enter the size of each page margin (in inches).

Select the **Header** sub-tab.



In the **Header** field, enter codes for information to include in the header in the order they should appear.

Codes supported for formatting headers and footers include:

&D (Date)
&N (Total number of pages)
&P (Current page number)
&T (Time)
&O (Object name)

The options on the Footer tab can be set in the same manner as described for the Header tab.

Note: The options on the DME Plot Tables tab and the NONMEM Plot Tables tab are identical to those in the Worksheets Layout tab.

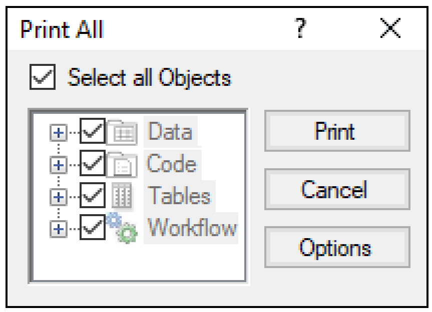
To print single objects

Select an object in the Data, Code, Tables, or Documents folders.

Select **File > Print**.
Or type `CTRL+P`.

To print multiple objects

Select **File > Print All**.



In the dialog, click **Print** to print all printable items in the Object Browser
This includes the results of any executed operational object, any internal worksheets created by operational objects, and any imported and user-created files.

Or

Uncheck the **Select all Objects** box and check/uncheck the boxes beside each item to include or exclude it in the print job and then click **Print**.

Click **Options** in the dialog.

Check the **Multiple charts per page** box to print multiple charts per page.

Click the chart layout menu to select how many charts to print down and across each page.

Click **OK**.

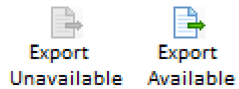
Exporting

Objects that Phoenix can export using **File > Export** or the **Export** icon include workflows, operational objects, workbooks, worksheets, text objects, BQL rules, plots, and HTML tables.

A separate Word Export tool allows users to export worksheets, HTML tables, plots, and text objects to Microsoft Word. See Exporting to Microsoft Word.

Exporting an object

With an object selected for export, choose **File > Export** or click the **Export** icon.
If an object cannot be exported the **Export** button is unavailable.



In the dialog, use the **Save in** menu to select a directory.

Type a file name in the **File name** field or accept the default.

Use the **Save as type** menu to select the file format for the exported file.

For more details, see:

Workbooks and worksheets
HTML tables
BQL rule sets
Text objects
Plots

Workbooks and worksheets

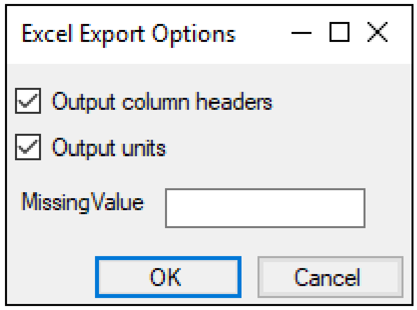
Workbooks in the Data folder are only exported as Excel files (`.xls` or `.xlsx`). Worksheets in the Data folder and in the Results tab can be exported as the following file types:

Excel 97-2003 Workbook (*.xls)
Excel Workbook (*.xlsx)
SAS Transport Format (XPORT) Version 5 (*.xpt)
Text (Comma delimited) (*.csv)
Text (Space delimited (*.dat)
Text (Tab delimited) (*.txt)

Caution: To export output in the **Results** tab, click the Export icon in the Results tab toolbar. Otherwise, the selected operational object is exported, and not the results.

To set options for Excel export

Exporting a worksheet or workbook as an Excel file displays the *Excel Export Options* dialog.



Check the **Output column headers** box to save the column headers in the Excel file.

Check the **Output units** box to save column units in the Excel file.

Type a value in the **MissingValue** field to have that value inserted in any blank cells in the worksheet.

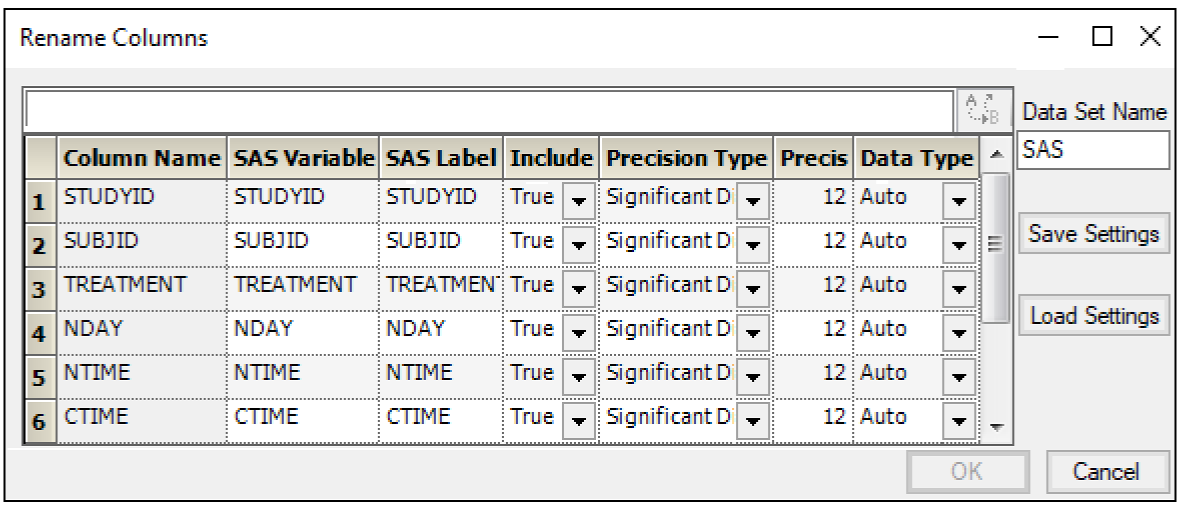
Click **OK** to save the worksheet or workbook as an Excel file or click **Cancel** to cancel the export.

Worksheets saved as an Excel file have their history worksheet saved with them.

Caution: Only the Excel export format supports saving the history worksheet with the dataset.

To set up for SAS export

Exporting a worksheet as a SAS Transport File displays the *Rename Columns* dialog.



Enter information in the table that is appropriate for the data being exported:

Column Name: The column name in Phoenix; it cannot be changed.

SAS Variable: Enter the name of the SAS variable or use the default (limited to eight characters).

SAS Label: Enter the SAS column label header or use the default name (limited to 40 characters).

Include: Set to **True** to include or **False** to exclude the column.

Precision Type: Set the precision type to either **Significant Digits** or **Decimal Places**.

Precision: Enter the number of significant digits or decimal places or use the default value.

Data Type: Select the data type as **Numeric** or **Text**, or leave it set to **Auto** to export the column as it is in Phoenix.

Data Set Name: Enter a name for the data set.
This name is internal to SAS and independent of the actual file name.

To ***save*** the SAS export settings in the Documents folder, click **Save Settings**.
The settings are saved as a text file and named after the dataset name.

To ***load*** the SAS export settings from the Documents folder, click **Load Settings**.
In the dialog, select an SAS export settings file in the Documents folder and click **Select**.

Click **OK** to save the worksheet as an SAS Transport File.

To set up a text export

Exporting a worksheet as a text (comma, space, or tab delimited) file displays the *Data Export Options* dialog.

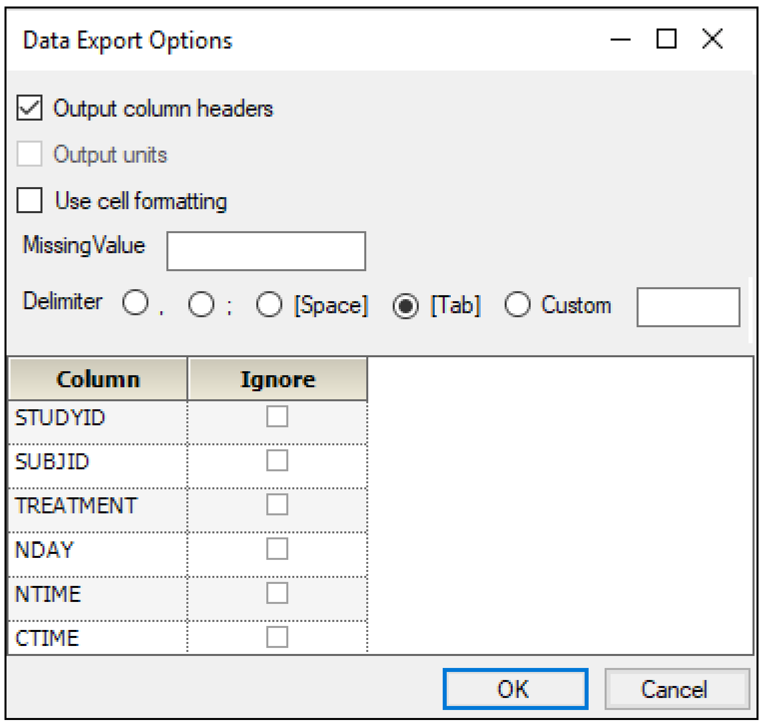


Figure 17-1. Data Export Options dialog for a .csv, .dat, or .txt data file

Check the **Output column headers** box to include column headers in the worksheet.

Check the **Output units** box to include column units in the worksheet.

Check the **Use cell formatting** box to preserve custom cell formatting in the worksheet.

Type the value in the **MissingValue** field that is to be inserted in any blank cells in the worksheet.

Select one of the **Delimiter** option buttons to choose how to separate values in the worksheet.

By default, `.csv` files use a comma to separate values, `.dat` files use a space to separate values, and `.txt` files use a tab to separate values.

Check the **Ignore** box beside a column name to exclude that column in the output file.

Click **OK** to save the worksheet as a `.csv`, `.dat`, or `.txt` file.

HTML tables

Select an HTML table in the Tables folder.

Export the selected table.

The table is exported as an HTML file.

BQL rule sets

Select a rule set in the BQL folder.

Export the rule set.

The rule set is exported as a `.phxruleset` file.

Text objects

Text objects in the Code folder, the Documents folder, and in the Results tab are exported as the following file types:

RTF File (*.rtf)
Text File (*.txt)

Caution: To export output in the Results tab, click the Export icon in the Results tab toolbar. Otherwise, the selected operational object is exported, and not the results.

Plots

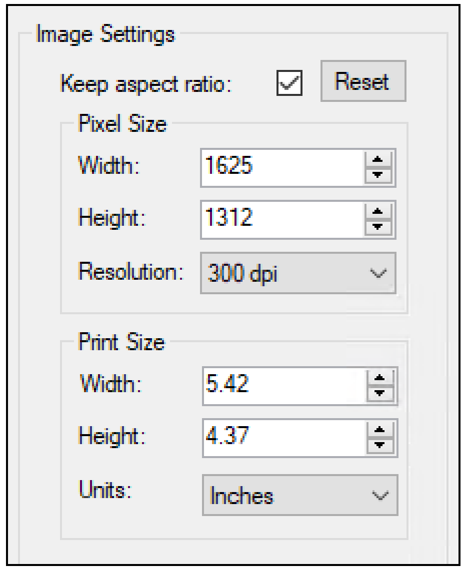
Plots in the Results tab are exported as the following file types:

Bitmap (*.bmp)
Enhanced Meta File (*.emf)
GIF (*.gif)
JPEG (*.jpg)
PNG (*.png)
Tiff (*

Caution: To export output in the Results tab, click the Export icon in the Results tab toolbar. Otherwise, the selected operational object is exported, and not the results.

To set up image export

Exporting a plot as an image file displays the *Export* dialog with the following additional options.



Check the **Keep aspect ratio** box to keep the original ratio of width to height as adjustments are made.

Click **Reset** to return the settings to the original values.

Adjustments to the image can be made based on pixels or print.

For pixel adjustments, use the **Resolution** pull-down to specify the dpi setting.

For print adjustments, select the units to use from the **Units** pull-down.

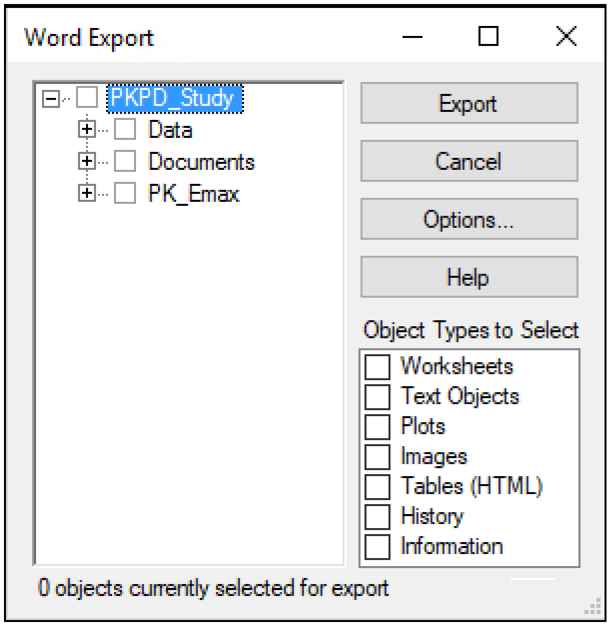
Make the desired changes to the **Width** and/or **Height** values.

Exporting to Microsoft Word

The Word Export tool allows users to export items, such as external and internal source worksheets, code files, images, results worksheets, results text, plots, Information tab text, and History worksheets, to a Word file.

To set up an export to a Word file

Select **File > Word Export**.



In the dialog, click the (+) signs next to Data, Code, or Workflow to expand each list.

Check the checkbox beside the project name to select all exportable items.
Or check the checkbox next to individual items to include them in the Word document.

Click **Export** to export the selected items to a Word document.

Click **Options** to display the *Word Export Options* dialog.

In the Document tab:

Choose the page orientation by selecting the **Portrait** or **Landscape** option button.

Check the **Add source line to object** box (the default) to include a source line stating the project, workflow, and object used to create each exported item.

In the Charts tab:

Check the **Multiple charts per page** box to export more than one plot per page.

In the **Down** and **Across** menus, select the number of rows of plots (**Down**) and columns of plots (**Across**) to display per page.

Check the **Add page break** box to add a blank page between each plot or grouping of multiple plots.

Check the **Include both linear and log charts** box to export linear and logarithmic Y-axes versions of plots.

Check the **Start chart numbers at** box to numerically label the charts. For example, Figure 1, Figure 2, etc. In the field, type the first number to use when labeling exported plots. The default is one.

In the Chart Format area, select the **Export chart as metafile** or **Export chart as bitmap** option button to choose the chart output format.

In the Workbooks tab:

Check the **Start table numbers at** box to numerically label the worksheets. For example, Table 1, Table 2, etc. In the field type the first number to use when labeling exported worksheets. The default is one. This option is ignored when exporting HTML tables created in Phoenix.

Check the **Heading rows repeat** box to have the worksheet column headers repeat on every new page.

Click **Finished** when all options are specified.

Click the checkbox of a particular type of object in the **Object Types to Select** list to select/deselect all objects of the specified type.

Click **Export** to export all selected items. The Word document is displayed when the export is finished.

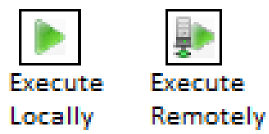
Executing Objects and Workflows

Individual objects in a workflow can be executed as well as an entire workflow. In many cases, the execution can be done locally or remotely. (See “RPS” for details on setting up Phoenix to use RPS for executing remotely.)

Note: Depending on the types of objects that make up the Workflow, executing the Workflow may sometimes fail if one object tries to start before another object, whose results are needed as input, finishes. In such cases, try executing the objects separately.

To execute an object

Select that object in the Object Browser and click the **Execute** icon or the **Execute Remotely** icon in the toolbar.



Or right-click an object in the Object Browser or in the Diagram and select **Execute** from the right-click menu.

Or with the object selected, right-click an empty space in the Object Browser or in the Diagram and select **Execute** from the right-click menu.

To execute an entire workflow

Select the workflow in the Object Browser or in the Diagram and click the **Execute** icon or the **Execute Remotely** icon in the toolbar.

Or right-click a workflow item in the Object Browser or in the Diagram and select **Execute** from the right-click menu.

Or with the workflow selected, right-click an empty space in the Object Browser or in the Diagram and select **Execute** from the right-click menu.

BQL

Data analysis, tabulation, plotting, and summarization are problematic when the data contain concentrations that fall below the lower limit of quantification (LLOQ) of the assay. The LLOQ is the concentration whose lower bound (of variability in the assay) includes zero. An analyte may be detectable below this concentration even though it is not quantifiable.The BQL object allows users to define rule sets to filter out unusable data in a dataset using a BQL (Below Quantifiable Limit) rule set.

Standard laboratory procedures can require that such data be reported as a character string rather than a numerical value. Representing such a concentration as zero is not always appropriate, as doing so can introduce a statistical bias or misrepresentation in some analyses. Different substitution rules are required depending on the intended use of the data, and substitution rules vary between companies and departments. As a result, it may be necessary to perform a custom transformation of the BQL column in your dataset. Refer to the “Data Wizard” section, specifically the “Example custom functions” has several example functions used for BQL columns.

The BQL object is used to create useful datasets by substituting different non-numerical codes for concentration levels too low to be used in an analysis.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Data Management > BQL**.
Or Main menu: **Insert > Data Management > BQL**.
Or right-click menu for a worksheet: **Send To > Data Management > BQL**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

This section contains information about the following:

User interface description
General BQL rules
BQL output

User interface description

Main Mappings panel
Rule Set panel

Main Mappings panel

Use the Main Mappings panel to identify how input variables are used in a BQL object. Required input is highlighted orange in the interface.

None: Data types mapped to this context are not included in any analysis or output.
Sort: Categorical variable(s) identifying individual data profiles, such as subject ID and treatment in a crossover study. A separate computation is done for each unique combination of sort variable values.
Time: Nominal time or actual time (time that a study dose or observation actually happened) collection points in a study.
Concentration: Drug concentration values in the blood.
Status Code: (Optional) Column containing the non-numeric status codes associated with each

datum in the Concentration column; determines transformation of the concentration values.
LLOQ: (Optional) Column containing the lower limit of quantification (LLOQ) associated with each measurement in the concentration variable.
Carry Along: Variables that are not required for the current analysis, but are copied and included in the output dataset.

Rule Set panel

The Rule Set panel allows users to map a BQL rule set to the BQL object, or define their own BQL rules using the internal BQL Rule Set worksheet. See “General BQL rules” for more information on BQL rules.

There are two ways to create a BQL rule set: create a rule set in Rule Set panel in the BQL object or in the BQL Rules folder.

Use the Rule Set panel

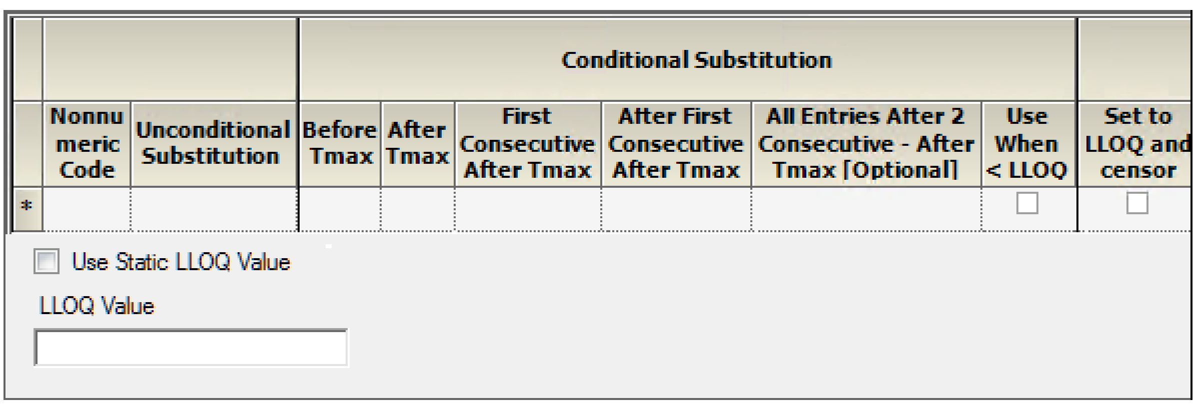
Select the **Rule Set** panel in the Setup tab.
Check the **Use internal BQL Rule Set** box.
Users can now define their own rule set as an internal worksheet in the Rule Set panel.

Use the BQL Rules folder

Select the **BQL Rules** folder in the Object Browser.
Right-click **BQL Rules** and select **New > Rule Set**. (Adds a new rule set to the BQL Rules folder.)
Rename the rule set or leave the default name.

Define a rule set

Note: The steps and interface used to define a BQL rule set are the same whether the BQL Rules folder or the Rule Set panel is used.



Enter the following information to define the rules:

Nonnumeric Code: Status code to be transformed.

Unconditional Substitution: If the transformation is the same regardless of whether the status code occurs before or after Tmax, or is repeated, this is the value to which the status code is transformed. An unconditional substitution is the same as a REPLACE ALL function within the column mapped to Concentration.

For ***conditional substitutions***, where the transformation depends on the status code's position relative to Tmax and whether or not the code is repeated in consecutive observations, then leave the cell in the **Unconditional Substitution** column blank and enter values in the subsequent four columns.

Conditional substitutions are based on being able to identify a Tmax (time when the maximum concentration is observed within a profile) and its corresponding concentration (Cmax). The first four parts of a conditional substitution need to be defined, but the fifth substitution is optional and not applied if left empty. The tool always sorts by the variable mapped to **Time** before applying the rule to the column mapped to **Concentration**:

Before Tmax: Value for any status code that occurs before Tmax.

After Tmax: Value to use for any status code that occurs after Tmax and ***is not*** followed, ***nor*** preceded, by the same status code (i.e., the value is isolated).

First of consecutive after Tmax: Value for any status code that occurs after Tmax and ***is*** followed, but ***not*** preceded, by the same status code (i.e., this value is assigned to the first of those contiguous observations).

After First of Consecutive after Tmax: Value for any status code that occurs after Tmax and ***is*** preceded by the same status code (i.e., this value is assigned to all status codes except the first of those contiguous observations).

All Entries After 2 Consecutive after Tmax [Optional]: Value for any status code that occurs after Tmax and is preceded by two identical observations (i.e., the value assigned to all trailing observations (status codes or values) except the first and second of those contiguous observations). This substitution is optional and should be left blank if one does not wish to apply it.

Any entry that is not equal to the non-numeric code breaks the consecutive assessment including blank and missing values. These should be removed prior to applying conditional substitutions if the consecutive rule should ignore them.

Tmax is considered the maximum value in the column concentration within unique combinations of sort variables (typically subject). If there is more than one Tmax within a profile, the first Tmax is used for the conditional substitution. Note that the tool automatically sorts by the sort variables and then by the column mapped to TIME.

Conditional substitution rules are only applied if there is at least one numerical value in the column mapped to concentration. For example, if all the values within a profile are equal the non-numeric code (e.g. BQL) then the resulting column will present blank data for the profile. However, if there is an unconditional substitution beforehand then the results will present the original values in the column mapped to concentration (e.g., BQL).

Use When < LLOQ: Check to indicate that, when numeric values less than the LLOQ are encountered, those values are transformed as though they contained the status code.

This checkbox can be used with conditional and unconditional substitutions, but an LLOQ needs to be defined either by entering a static value in the rule or by mapping a column with these values to the LLOQ column.

Only one non-numeric code can be assigned to **Use When < LLOQ**. When selected, the tool will compare concentrations values to the LLOQ for each row, and if the value is less than the LLOQ then it treats it as if it has been recorded as the non-numeric code and thus, the same rules as the non-numeric code will be applied to that number. For example, if the unconditional substitution is that BQL non-numeric code should be set to zero, the LLOQ is static to 0.5 and the **Use When <**

LLOQ is checked, any concentration equal to BQL and any concentration less than 0.5 will be set to zero.

If a profile has concentration values but all of those are < LLOQ a conditional substitution will consider the first value in the concentration column to be *tmax* and the substitution will take place based on this assessment. In other words, the first concentration will be set to substitution for first consecutive and the following concentrations will be set to the value for the after first consecutive.

Set to LLOQ and censor: Check to set the resulting concentration cell to the LLOQ value (the static value or the value from the LLOQ mapped column). A column named CObsBQL is created in the output.

This substitution is mutually exclusive from the other existing substitutions (conditional and unconditional) therefore only one type of substitution can be used for each rule. If the option to **Set to LLOQ and censor** is selected for a nonnumeric code it sets that resulting concentration cell to the LLOQ value (the static value or the value from the LLOQ mapped column) and creates an additional column: CObsBQL.

The cell that is modified by the censoring substitution (i.e. set to LLOQ value) gets a corresponding value of one for CObsBQL, if no substitution took place then a value of zero is assigned to CObsBQL. The values assigned to the censored column CObsBQL are either zero or one. If the option of **Use When < LLOQ** is checked in conjunction with the censoring substitution then any numeric value less than LLOQ is set to the LLOQ value and the censoring flag is set to one.

This option is designed to integrate with Maximum Likelihood models. A resulting worksheet of a BQL object with a censored column **CObsBQL** can be used as the input for a Maximum Likelihood model with the option **BQL?**. If **BQL?** is selected, a column can be mapped to the **CObsBQL** context in the Main Mappings panel. This column can contain two categories of values: non-zero (censored) or zero (non-censored). If a concentration value is marked as censored (**CObsBQL**<>0), it means that the true value of the observation is unknown but it is not greater than the observed value (e.g., LLOQ) and then the cumulative distribution function for the normally distributed error is used to calculate the likelihood. If a concentration value is flagged as non-censored, then the probability density function is used to calculate the likelihood.

Note: Maximum Likelihood models with censored data (**BQL?** option) use the log of the probabilities between 0 and the censored number in the log likelihoods. If the censoring numbers are very small, the loglikelihood might overflow, resulting in a Fortran error. This seems to be more often the case when using multiplicative error models. If the error occurs, try increasing the BQL value if possible or change error types.

Check the **Use Static LLOQ Value** box to set a fixed LLOQ value.

In the **LLOQ Value** field, type the LLOQ value.

Note: When a static LLOQ value is specified the static value is always used, even if a dataset column is mapped to the LLOQ context in the BQL object.

Additional status codes can be entered under **Non-numeric Code**. Each new status code that is entered creates a new row in the rule set. To ***remove a row***, left-click the row number to select the entire row and press the **Delete** key.

Syntax for the rules: The status rules are not case-sensitive. The values entered can include numbers, operators, and the variable LLOQ, if an LLOQ value or data column is assigned.

General BQL rules

- A rule in a rule set can only do a conditional substitution or an unconditional substitution, not both.
- If a rule set has rules for the same exact non-numeric value, then the last rule is applied.
- A rule set can list several non-numeric codes with different substitution rules. These rules are considered independent of each other. For example, if the rule set states to substitute concentrations equal to < LLOQ and set them to BQL, and then another rule within the same rule set indicates to take all BQL values and set them to zero, concentrations of < LLOQ are shown as BQL and not zero, regardless of the order of the rules.
- The BQL object provides the option to map a column with the LLOQ values or to enter a static LLOQ value within the rule set. If both options are used the static option takes precedence over the mapped LLOQ column.
- A numeric value is allowed to be entered as a non-numeric code. The tool will search for the exact value with the exact precision before a substitution takes place. The search will take place in the column mapped to Concentration unless the Status Code option is selected. In that case the search will take place in the column mapped to the Status Code instead.
- A rule that resides within the folder BQL Rules can be used in a BQL object or several BQL objects. An internal rule resides within a given BQL object and cannot be used by another object. If the rules are the same there is no difference in the results if an external or internal rule is used.

Common substitution rules

- Substitutions are either unconditional or conditional.
- The nonnumeric code column must contain non-numeric values.
- Only one column can apply rules for the below LLOQ concentration.

Some common substitution rules for BQL samples are presented in the table below.

		Conditional Substitution				
Nonnumeric Code	**Unconditional Substitution**	**Before Tmax**	**After Tmax**	**First Consecutive**	**After First Consecutive**	**Use rule for:**
BQL		0	Missing	LLOQ/2	Missing	PK analysis
BQL	0					Summary statistics
BQL	*BQL				"	Listing individual data
BQL	LLOQ/2					Plotting individual data on log-scale
BQL	0					Plotting individual data on linear scale

The substitution rules are typically defined in standard operating procedures or method sheets for a given company or department. The rules can become more complex when a user wishes to make a distinction between concentrations that are below the quantification limit (BQL) and below the detection limit (BDL). In general, a substitution rule is defined by the list of possible non-numeric representations for concentration and the values to be substituted for each. One possible substitution rule for PK analyses is presented below:

Nonnumeric Code	Unconditional Substitution	Before Tmax	After Tmax	First Consecutive	After First Consecutive
BQL		0	Missing	LLOQ/2	Missing
NS	Missing				
ISV	Missing				
NA	Missing				
...	...				

The BQL object transforms observation values from non-numeric status codes to number values for use in analyses and plots. It can also convert unusable concentration values to non-numeric status codes. The BQL object creates a new worksheet based on an existing one, by copying over selected columns.

It transforms values in the input worksheet as specified by user-defined rules. Numeric concentration data and the non-numeric concentration status codes can be in the same or different columns in the dataset.

The BQL object also stores information about the lower limit of quantification (LLOQ) for one or more sampling assays. Users can specify an LLOQ and the new column header into which it is placed, or identify an existing column containing the LLOQ for each observed concentration. The LLOQ, if any, can be used to define how status codes are transformed.

BQL output

The BQL object generates one worksheet and one text file.

Output: The worksheet with the updated concentration column.
Settings: The input worksheet used and the options selected.

CDISC Data Preparer

The CDISC Data Preparer object produces analysis ready datasets (SAMPLE and DOSE) in Phoenix, using CDISC formatted dataset inputs of either SDTM (Study Data Tabulation Model) or SEND (Standard for Exchange of Nonclinical Data).

- CDISC SDTM is a unified way of transmitting information in drug studies with precise column names and a common file format. CDISC Data Preparer produces output in the STDM format that is compliant with the standards in the *SDTM Implementation Guide 3.1.1*.
- CDISC SEND is an implementation of SDTM for nonclinical studies and specifies a consistent format for presenting and exchanging nonclinical data. The CDISC Data Preparer produces output in the SEND format that is compliant with the standards in the *SEND Implementation Guide 3.0*.

For further information, please visit the Clinical Data Interchange Standards Consortium Web site at www.cdisc.org.

CDISC input datasets must have the following domains in order for the CDISC Data Preparer object to generate a PK dataset:

DM: Demographic information; one row per subject
PC: PK concentrations data, one record per concentration per analyte
EX: Exposure, one record per constant dosing interval per subject

The input dataset can also include Finding domains such as:

EG: ECG tests
LB: Laboratory tests
PE: Physical examinations
QS: Questionnaire
SC: Subject characteristics
VS: Vital signs
MB: Microbiology specimens
PP: Pharmacokinetics parameters

Findings domains can contain time-dependent data, but the times do not necessarily match the times of the samples or treatments. The CDISC Data Preparer object uses processing rules to locate data corresponding to the time of data collection.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Data Management > CDISC Data Preparer**.
Main menu: **Insert > Data Management > CDISC Data Preparer**.
Right-click menu for a worksheet: **Send To > Data Management > CDISC Data Preparer**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Additional information is available for the following topics:

User interface description
Results

See also “CDISC Data Preparer Example”.

User interface description

Note: Required Mappings are highlighted in orange.

Demographics panel

Add data that is to be included in the output. The Demographics panel contains an internal worksheet that can be used to manually enter concentration data, or a concentration worksheet can be mapped to it.

None: Data types mapped to this context are not included in any analysis or output.
Subject Identifier: The unique identifier of the subjects in a dataset.
Demographic: Data to include in the output datasets.

Exposure panel

Specify how the exposure columns are treated when producing the Dose result dataset. The panel can also be used to identify the columns to use in joining the sample domain and the columns to include in the Sample dataset.

Dose context definitions:

None: Data types mapped to this context are not included in any analysis or output.
Pivot: Identifiers of the unique dose tests.
Dose: Actual dose amount.
Unit: Unit of the actual dose amount.
Carry to Dose Dataset: Data to include in the Dose result dataset.

Sample context definitions:

None: No action should be taken for the exposure field related to the Sample dataset.
Join: Set of columns to use to join the PK Findings domain. Typically, the EXSTDTC field (Start Date/Time of Treatment) from the EX domain is referenced in the PC domain PCRFTDTC field (Date/Time of Reference Point), and this field alone can be configured as the Join column; however, a combination of fields can be used to join the EX and PC domains.
Carry to Sample Dataset: Data to include in the Sample result dataset. It is often necessary to carry some fields from the EX domain to the Sample result dataset so that sort keys can be specified between the Dose and Sample datasets during analysis.

PK Findings panel

Specify the data from PK Findings tests.

None: Data types mapped to this context are not included in any analysis or output.
Test Identifier: Identifiers for unique PK Findings test. The unique tests are displayed in the PK Findings properties tab.

Row: Data to include, and that represent the unique set of rows. All unique combinations of Row and Join columns determine the number of sample rows in the result dataset.
Carry: Data to carry over unchanged in the output worksheets.

Each column selected as a Join column in the EX domain will appear as a column mapping context for the PC domain. This allows the user to specify what column in the PC domain corresponds to what column in the EX domain. In most cases, the EXSTDTC (Start Date/Time of Treatment) context will be mapped to the PCRFTDTC (Date/Time of Reference Point) field in the PC domain.

PCELTM column requirement

Although PCTPT (Planned Time Point Name), PCTPTNUM (Planned Time Point Number), and PCELTM (Planned Elapsed Time from Time Point Ref) tabulate the same information, they each have a different format and only PCELTM has a defined standard format. Therefore, PCELTM is the variable that CDISC Data Preparer uses to calculate Relative Nominal Times for the Sample result dataset. If your datasets usually have PCTPT or PCTPTNUM instead of PCELTM, you will need to create a PCELTM column from the other column. If PCELTM is not in the dataset, or not carried along, or not in the proper format, CDISC Data Preparer generates a warning.

The PCELTM column values need to be in hours and have units of “hr” specified in the header. The column type must be text.

To create the PCELTM column from a PCTPTNUM or PCTPT column:

1. Use the Data Wizard object’s **Transformation** action to copy the contents of the column to a new PCELTM column. You can use the arithmetic formula “x-n” and set “n” to 0.
2. Create a **Properties** step to specify the column units as “hr” and, if the data is from a PCTPTNUM column, set the column’s data type to **Text**.
3. If the data is from a PCTPT column, create a **Filter** step involving multiple filters to replace “PREDOSE” with “0”, “15MIN” with “0.25”, “30MIN” with “0.5”, “45MIN” with “0.75”, “1H” with “1”, etc.

Other Findings panel

Specify additional tests to include in the data preparation.

None: Columns mapped to this context are not used to identify the tests performed.
Pivot: The fields identified as **Pivot** fields are used to identify the tests to be included in the Sample results. For example, in the VS domain, the tests might be identified by the combination of the VSTEST (Vital Signs Test Name) and the VSPOS (Vital Signs Position of Subject) fields.

Options tab

Add or remove the Other Findings items listed in the Setup.

Add Other Findings: Add another Other Findings item (displays as **Other Findings1**) in the Setup panel list.
Remove Other: Remove an Other Findings item from the Setup panel list. This button only removes Other Findings item that were added using the **Add Other Findings** button.

Exposure tab

The Exposure tab allows users to view the list of unique exposure data combinations based on the Exposure context mappings.

Exposure Specification

	EXTRT	EXDOSFRM	EXDOSFRQ	EXROUTE
1	Sydneyol	TABLET	ONCE	ORAL
*				

EXTRT = Name of Actual Treatment, EXDOSFRM = Dose Form, EXDOSFRQ = Dose Frequency per Interval, EXROUTE = Route of Administration

The image above shows a study where, based on the Exposure context mappings, only one exposure specification was identified.

PK Findings tab

The PK Findings tab allows users to view the unique tests that were identified using the PK Findings context mappings and select the ones to include.

Tests(PC)

	PCTESTCD	PCSCAT	PCSPEC	Usage	Layout	Result Column
1	SYDN	NON-COMPARTMENTAL	PLASMA	Include	Stacked	All
2	SYDN	NON-COMPARTMENTAL	URINE	Include	Stacked	All
3	SYDN_OH	NON-COMPARTMENTAL	PLASMA	Include	Stacked	All
4	SYDN_OH	NON-COMPARTMENTAL	URINE	Include	Stacked	All
5	VOLUME	NON-COMPARTMENTAL	URINE	Include	Stacked	All

PCTESTCD = Pharmacokinetic Test Short Name, PCSCAT = Test Subcategory, PCSPEC = Specimen Material Type

Usage: whether to **Include** or **Exclude** the test in (from) the output.
Layout: control the display of the test data. See the "Layout Columns" section below for more information. Choices are:
– Stacked: create a PCORRES (Result or Finding in Original Units) and PCSTRESN (Numeric Result/Finding in Standard Units) result column for each unique unit found in the source dataset for the stacked test,
– Pivoted: for each pivoted test a set of result columns is added in the output.
Result Column: the result column to include for each test (select **All** to include all of the results columns). Result columns are those that match the CDISC specification for results columns in original, numeric, or text format.

Layout Columns

The table below shows the sets of columns that will be included in the output depending on the settings for **Layout** and **Result Column**.

For example, it would be common to stack urine concentration results for different analytes and pivot the urine volume such that the volume and concentration are shown on the same row.

Tests(PC)

	PCTESTCD	Usage	Layout	Result Column
1	SYDN	Include	Stacked	All
2	SYDN_OH	Include	Stacked	All
3	VOLUME	Include	Pivoted	All

With the set up shown above, note that the SYDN and SYND_OH concentration results are stacked, and the VOLUME data are pivoted to align with the concentrations.

	PCTESTCD	PCORRES (ng/mL)	PCORRESU	PCSTRESC	PCSTRESN_ (ng/mL)	PCSTRESU	VOLUME_PCOR (mL)	VOLUME_ PCSTRES	VOLUME_PCST (mL)
55	SYDN	LOQ	ng/mL	0	0	ng/mL	250	250	250
56	SYDN_OH	0.64	ng/mL	0.64	0.64	ng/mL	250	250	250
57	SYDN	LOQ	ng/mL	0	0	ng/mL	250	250	250
58	SYDN_OH	0.64	ng/mL	0.64	0.64	ng/mL	250	250	250
59	SYDN	3.95	ng/mL	3.95	3.95	ng/mL	1350	1350	1350
60	SYDN_OH	0.87	ng/mL	0.87	0.87	ng/mL	1350	1350	1350
61	SYDN	0	ng/mL	0	0	ng/mL	2835	2835	2835
62	SYDN_OH	0.99	ng/mL	0.99	0.99	ng/mL	2835	2835	2835

PCTESTCD = Pharmacokinetic Test Short Name, PCORRES = Result or Finding in Original Units, PCSTRESC = Character Result/Finding in Std Format, PCSTRESN = Numeric Result/ Finding in Standard Units, PCSTRESU (Standard Units)

Other Findings tab

Select data from multiple other findings domains that were identified using the Other Findings context mappings to include in the Sample output. Data is extracted from these datasets by finding the tests corresponding to subjects and occurring within a specified time-window relative to the concentration sample collection time.

Fixed and Dynamic Covs(Other Findings)

	SEX	Usage	Selection Rule	Tolerance Interval (hr)	Result Column
1	F	Include	Fixed Pick First		All
2	M	Include	Fixed Pick First		All
3	U	Include	Fixed Pick First		All

Usage: whether to **Include** or **Exclude** the covariate value in (from) the output.
Selection Rule: rule to use to extract data from the dataset. Choices are:

– **Dynamically Pick Closest**: Pick test value closest to the PC sample collection time*
– **Dynamically Pick Next**: Pick test value that occurred after the sample collection time*
– **Dynamically Pick Previous**: Pick test value that occurred prior to the sample collection time*
– **Fixed Baseline**: Use the first value marked as a baseline value
– **Fixed Pick First**: Pick first value for the test, based on the collection time
– **Fixed Pick Last**: Pick last value for the test, based on the collection time
– **Fixed Pick Mean**: Calculate the Mean of all numeric test results, regardless of time collected
– **Fixed Pick Median**: Calculate the Median of all numeric test results, regardless of time collected.

Tolerance Interval: The allowed tolerance in the covariate value.
Result: The result column to include for each covariate (select **All** to include all of the results columns).

*Value must be within **Tolerance Interval**, if specified, or no value is returned.

Results

Dose: Worksheet containing:

- USUBJID
- Selected **Demographics**, **Pivot**, **Dose**, **Dose Unit**, **Carry to Dose Dataset**, and **Join** columns
- Calculated Relative_Actual_Time and Relative_Nominal_Time

Sample: Worksheet containing:

- USUBJID (Unique Subject Identifier)
- Columns marked as **Include** in the PK Findings tab
- Columns selected for joining to the EX domain
- Result column and result unit column for each pivoted test (column name is the concatenation of the Test Identifier and the Result column name)
- LLOQ value for each pivoted test
- PCSEQ (Sequence Number) value for each pivoted test in the PK Findings domain
- Result column for PCORRES (Result or Finding in Original Units) and PCSTRESN (Numeric Result/Finding in Standard Units) for each unique unit found in the source dataset for stacked tests
- Result columns for attributes associated with the stacked values: PCORRESU (Original Units), PCSTRESU (Standard Units), PCLLOQ (Lower Limit of Quantitation), and PCSEQ for stacked results
- Columns from the EX domain marked as **Include in Sample Dataset**
- Demographics marked as **Demographic** in the DM domain
- Calculated time values for Relative_Actual_Time, Relative_Actual_End_Time, and Relative_Nominal_Time

If a single unit is found for all occurrences in a column, it is displayed in the column header.

Log: Text file containing a list of step performed during processing.

Settings: Text file containing the mapping selections and test selections made by the user and applied when processing the data.

CDISC Data Preparer Example

This example demonstrates the general steps to prepare a CDISC dataset so that it can be used within Phoenix. The CDISC Data Preparer object produces analysis-ready datasets (SAMPLE and DOSE worksheets) in Phoenix, using CDISC formatted datasets as input. This example will also walk through submitting the output of the CDISC Data Preparer as input to an NCA object, which will be successfully executed.

There are steps common to many Phoenix objects (e.g., inserting an object, importing and mapping data to an object, and executing an object) and can be completed in multiple ways (e.g., main menu selection, right-click menu selection, drag and drop operation, etc.). For simplicity, only one mechanism is listed. Please refer to the Phoenix Functions chapter of the *Phoenix Framework User's Guide* to familiarize yourself with the basic operations used in Phoenix and any alternative mechanisms available.

The sections in this example include:

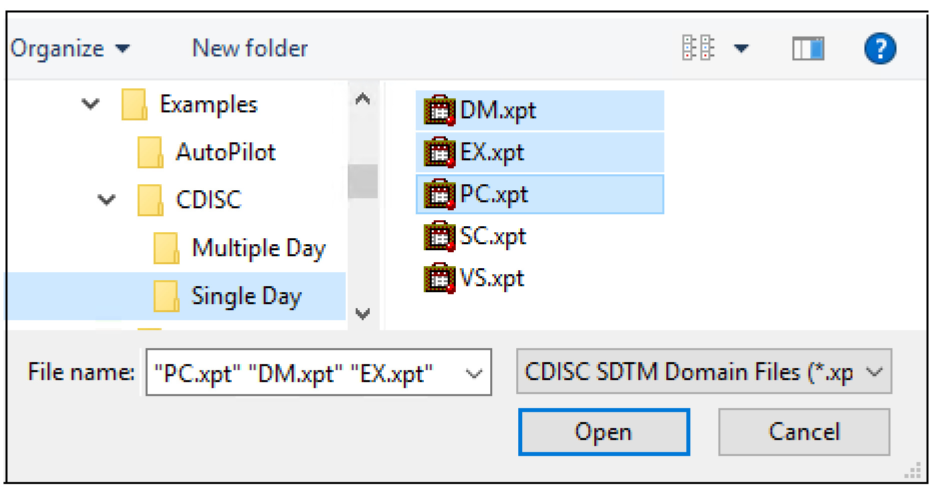
Setting up the project and data
Setting up the CDISC Data Preparer object
Exploring the results
Mapping the results to an NCA model

Setting up the project and data

1. Create a new project named `CDISC Prep Example`.

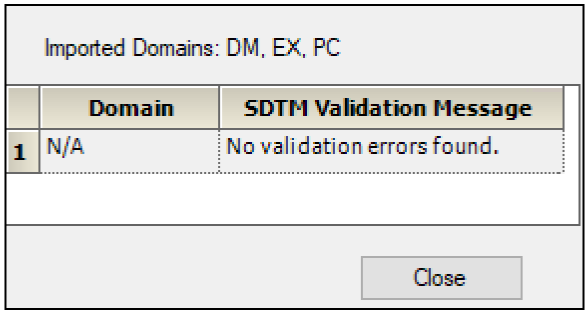
   The CDISC Data Preparer object is dependent on CDISC Navigator. The CDISC Navigator converts CDISC files, in SAS transport file format (.xpt), into Phoenix worksheets and verifies that the data conforms to the standards for the specified domain. Elapsed times are also converted from ISO format to numeric times in hours.

2. Select **File > CDISC > SDTM > Import**.
3. Import the **DM.xpt**, **EX.xpt**, and **PC.xpt** files from …`\Examples\CDISC\Single Day`.



4. Click **Open**.

   The *CDISC SDTM Import* dialog is displayed listing any problems that were encountered during the import and data validation processes.



Imported Domains: DM, EX, PC

	Domain	SDTM Validation Message
1	N/A	No validation errors found.

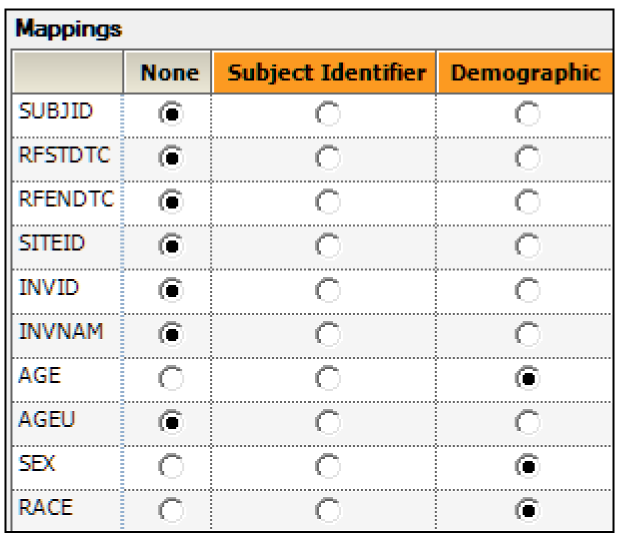
Close

For this example, there were no errors.

5. Click **Close**.

Setting up the CDISC Data Preparer object

1. Select **Workflow** in the Object Browser and then select **Insert > Data Management > CDISC Data Preparer**.
2. Drag the **DM** worksheet from the Data folder to the Demographics Mappings panel to map it as the input source.
   The columns are automatically mapped to the appropriate contexts:
   – USUBJID to the **Subject Identifier** context.
   – AGE, **SEX**, and **RACE** to the **Demographic** context.These are the columns to include in the output datasets.



Mappings

	None	Subject Identifier	Demographic
SUBJID	◉	○	○
RFSTDTC	◉	○	○
RFENDTC	◉	○	○
SITEID	◉	○	○
INVID	◉	○	○
INVNAM	◉	○	○
AGE	○	○	◉
AGEU	◉	○	○
SEX	○	○	◉
RACE	○	○	◉

3. Select **Exposure** in the Setup panel list
4. Drag the **EX** worksheet from the Data folder to the Exposure Mappings panel.

   There are two mapping section in the Exposure Mappings. The first section specifies how exposure columns are treated when producing the Dose result dataset. The second section specifies which data columns from the Exposure domain are used to join to the Sample domain and which exposure columns to include in the Sample result dataset.

   The columns are automatically mapped to the appropriate contexts:

   - **EXTRT** (Name of Actual Treatment),
     EXDOSFRM (Dose Form),

EXDOSFRQ (Dosing Frequency per Interval),
EXROUTE (Route of Administration)
to the **Pivot** context.
These columns identify unique dose tests as defined in the Exposure tab.

Exposure Specification

	EXTRT	EXDOSFRM	EXDOSFRQ	EXROUTE
1	Sydneyol	TABLET	Q24H	ORAL
*				

- **EXDOSE** to the **Dose** context. This column contains the actual dose amount.
- **EXDOSU** to the **Unit** context. This column contains the actual unit of the dose amount.
- **EXSTDY** (Study Day of Start of Treatment),
  EXENDY (Study Day of End of Treatment),
  EXTPT (Planned Time Point Name),
  EXTPTREF (Time Point Reference)
  to the **Carry to Dose Dataset** context.
- **EXSTDTC** (Start Date/Time of Treatment) to the **Join** context. This column will be used to match up data in the PK Findings domain.
- **EXTRT**, **EXDOSFRM**, **EXDOSFRQ**, **EXROUTE**, **EXSTDY**, **EXENDY**, **EXTPT**, **EXTPTREF** to the **Carry to Sample Dataset** context.
  This context enables sort keys to be specified between the dose and sample datasets during analysis.

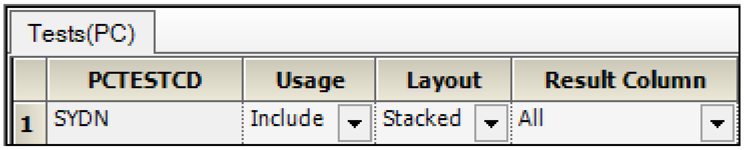
Mappings

						Sample		
	None	Pivot	Dose	Unit	Carry to Dose Dataset	None	Join_sample	Carry to Sample
EXTRT	○	●	○	○	○	○	○	●
EXDOSE	○	○	●	○	○	●	○	○
EXDOSU	○	○	○	●	○	●	○	○
EXDOSFRM	○	●	○	○	○	○	○	●
EXDOSFRQ	○	●	○	○	○	○	○	●
EXROUTE	○	●	○	○	○	○	○	●
EPOCH	●	○	○	○	○	●	○	○
EXSTDTC	●	○	○	○	○	○	●	○
EXENDTC	●	○	○	○	○	●	○	○
EXSTDY	○	○	○	○	●	○	○	●
EXENDY	○	○	○	○	●	○	○	●
EXTPT	○	○	○	○	●	○	○	●
EXTPTREF	○	○	○	○	●	○	○	●

5. Select **PK Findings** in the Setup panel list
6. Drag the **PC** worksheet from the Data folder to the PK Findings Mappings panel.

   Most of the columns are automatically mapped to the appropriate contexts.

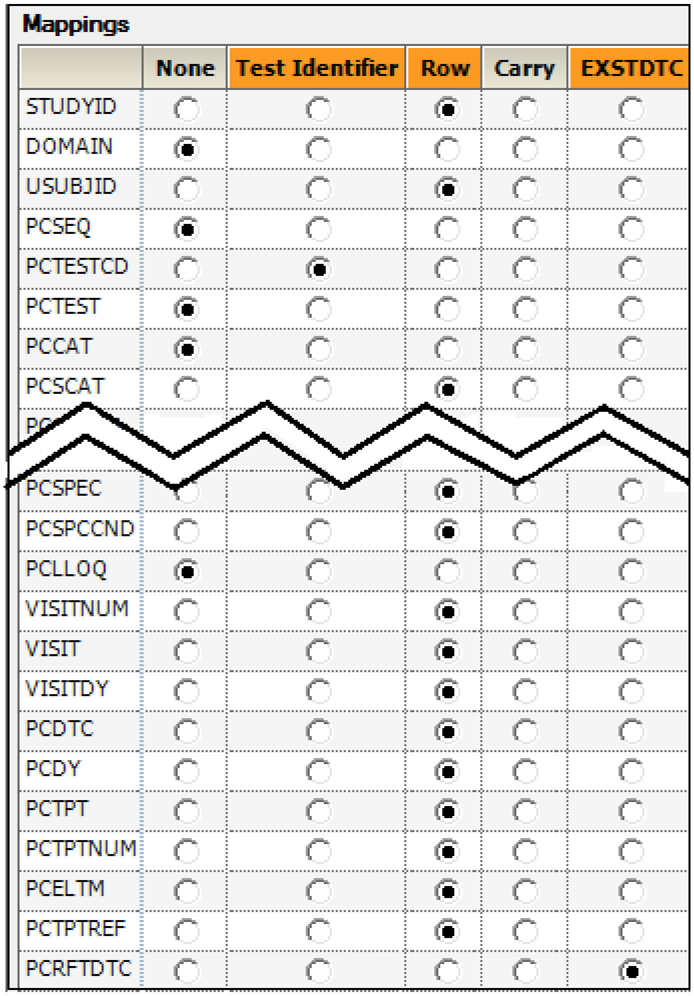
PCTESTCD (Pharmacokinetic Test Short Name) to the **Test Identifier** context.
These columns are used to identify unique PK Findings tests. The unique tests are displayed in the PK Findings (Tests (PC)) tab in the properties.



STUDYID (Study Identifier),
USUBJID (Unique Subject Identifier),
PCSCAT (Test Subcategory),
PCSPEC (Specimen Material Type),
PCSPCCND (Specimen Condition),
VISITNUM (Visit Number),
VISIT (Visit Name),
VISITDY (Planned Study Day of Visit),
PCDTC (Date/Time of Specimen Collection),
PCDY (Actual Study Day of Specimen Collection),
PCTPT (Planned Time Point Name),
PCTPTNUM (Planned Time Point Number),
PCELTM (Planned Elapsed Time from Time Point Ref),
PCTPTREF (Time Point Reference)
to the **Row** context.
These are columns to include and represent the unique set of rows. All unique combinations of the Row and Join columns determine the number of sample rows in the result dataset.

Each column selected as a Join column in the EX domain will appear as a column mapping context for the PC domain. This allows specification of the columns in the PC domain that correspond to columns in the EX domain.

PCRFTDTC to the **EXSTDTC** context.



Select PK Findings Tests

The PK Findings Tests(PC) tab on the Properties panel is used to select the tests to include, the layout, and the result columns to include in the result sample dataset.

In this example, the dataset only involves one test.

Do not change the default settings for the SYDN PK Findings test, which are.

> **Usage** set to **Include** to include the test in the output.
> **Layout** set to **Stacked** to have the results presented in a stacked format.
> **Result Column** set to **All** to have all results columns included in the output that match the CDISC specification for results columns in original, numeric, or text format.

Continue to the next section.

Exploring the results

Click (**Execute** icon) to execute the object.

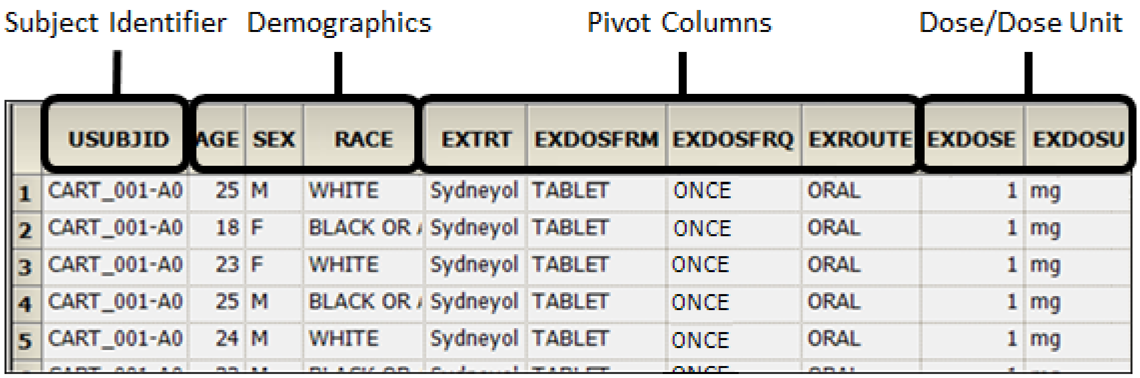
The Results are displayed on the Results tab. The CDISC Data Preparer object produces a Dose and Sample worksheet in the Output Data folder. A Log and Settings file are also produced. A Warnings and Errors file is generated if issues are encountered during execution.

Dose

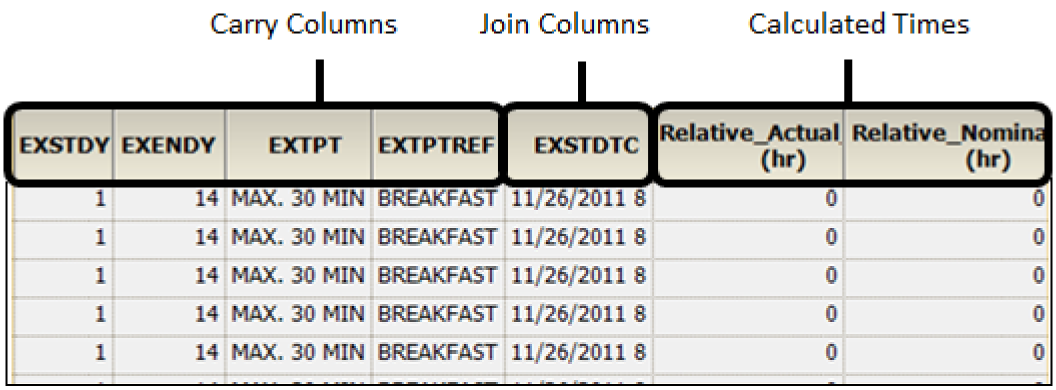
The Dose results worksheet contains the following columns in the order listed:

Subject identifier columns
Selected demographic columns
Selected pivot columns
Selected dose and dose unit columns
Selected **Carry to Dose Dataset** columns
Selected join columns
Calculated relative actual time and relative nominal time columns

The following images show a portion of the Dose worksheet generated as part of this example.



	USUBJID	AGE	SEX	RACE	EXTRT	EXDOSFRM	EXDOSFRQ	EXROUTE	EXDOSE	EXDOSU
1	CART_001-A0	25	M	WHITE	Sydneyol	TABLET	ONCE	ORAL	1	mg
2	CART_001-A0	18	F	BLACK OR /	Sydneyol	TABLET	ONCE	ORAL	1	mg
3	CART_001-A0	23	F	WHITE	Sydneyol	TABLET	ONCE	ORAL	1	mg
4	CART_001-A0	25	M	BLACK OR /	Sydneyol	TABLET	ONCE	ORAL	1	mg
5	CART_001-A0	24	M	WHITE	Sydneyol	TABLET	ONCE	ORAL	1	mg



EXSTDY	EXENDY	EXTPT	EXTPTREF	EXSTDTC	Relative_Actual (hr)	Relative_Nomina (hr)
1	14	MAX. 30 MIN	BREAKFAST	11/26/2011 8	0	0
1	14	MAX. 30 MIN	BREAKFAST	11/26/2011 8	0	0
1	14	MAX. 30 MIN	BREAKFAST	11/26/2011 8	0	0
1	14	MAX. 30 MIN	BREAKFAST	11/26/2011 8	0	0
1	14	MAX. 30 MIN	BREAKFAST	11/26/2011 8	0	0

Sample

The Sample results worksheet contains the following columns in the order listed:

Subject identifier columns
Columns selected as **Row** in the PK Findings context mapping
Selected join columns
Selected test identifier columns
Selected demographics
Selected **Carry to Sample Dataset** columns
PCORRES and PCRSTRESN columns for each unique unit in the source dataset for stacked tests
Result column and result unit column for each pivoted test
LLOQ column for each pivoted test
If any results are stacked, PCORRESU, PCRSTRESU, and PCLLOQ columns containing the attributes associated with the stacked values
Calculated relative actual time, relative actual end time, and relative nominal time columns

The following images show a portion of the Sample worksheet generated as part of this example.

Subject Identifier / Row Columns

	STUDYID	USUBJID	PCSCAT	PCSPEC	PCSPCCND	VISITNUM	VISIT	VISITDY	PCDTC	PCDY	PCTPT
1	CART_001	CART_001-A0	NON-COM	PLASMA		1	DAY 1	1	2011.12.2	1	PREDOSE
2	CART_001	CART_001-A0	NON-COM	PLASMA		1	DAY 1	1	2011.12.2	1	15MIN
3	CART_001	CART_001-A0	NON-COM	PLASMA		1	DAY 1	1	2011.12.2	1	30MIN
4	CART_001	CART_001-A0	NON-COM	PLASMA		1	DAY 1	1	2011.12.2	1	45MIN
5	CART_001	CART_001-A0	NON-COM	PLASMA		1	DAY 1	1	2011.12.2	1	1H30MIN

Row Columns / Join / Test Identifier / Demographics

PCTPTNUM	PCELTM (hr)	PCTPTREF	PCRFTDTC	PCTESTCD	AGE ({YEARS})	SEX	RACE
0	-0.083333333	Day 1 Dose	2011.12.26 07:4	SYDN	25	M	WHITE
0.25	0.25	Day 1 Dose	2011.12.26 07:4	SYDN	25	M	WHITE
0.5	0.5	Day 1 Dose	2011.12.26 07:4	SYDN	25	M	WHITE
0.75	0.75	Day 1 Dose	2011.12.26 07:4	SYDN	25	M	WHITE
1.5	1.5	Day 1 Dose	2011.12.26 07:4	SYDN	25	M	WHITE

Carry Columns

EXTRT	EXDOSFRM	EXDOSFRQ	EXROUTE	EXSTDY	EXENDY	EXTPT	EXTPTREF
Sydneyol	TABLET	ONCE	ORAL	1	1	MAX. 30 MIN BE	BREAKFAST
Sydneyol	TABLET	ONCE	ORAL	1	1	MAX. 30 MIN BE	BREAKFAST
Sydneyol	TABLET	ONCE	ORAL	1	1	MAX. 30 MIN BE	BREAKFAST
Sydneyol	TABLET	ONCE	ORAL	1	1	MAX. 30 MIN BE	BREAKFAST
Sydneyol	TABLET	ONCE	ORAL	1	1	MAX. 30 MIN BE	BREAKFAST

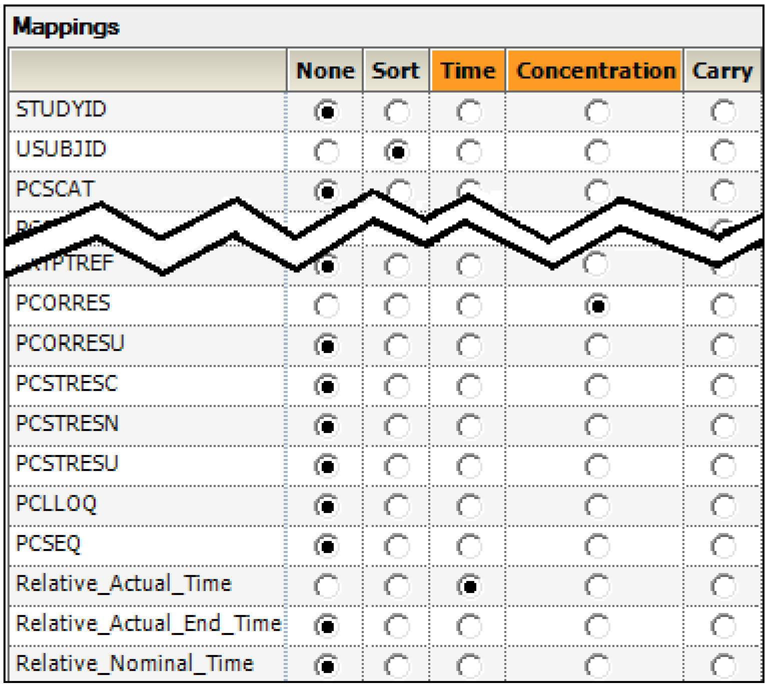
Stacked Test Columns / Calculated Times

PCORRES (mg/L)	PCORRESU	PCSTRESC	PCSTRESN (mg/L)	PCSTRESU	PCLLOQ	PCSEQ	Relative_ Actual_Tin (hr)	Relative_ Actual_En (hr)	Relative_ Nominal_Ti (hr)
BQL	mg/L	0	0	mg/L	0.5	1	-0.75		-0.083333333
LOQ	mg/L	0	0	mg/L	0.5	2	0.6		0.25
6.92	mg/L	6.92	6.92	mg/L	0.5	3	0.9		0.5
5.34	mg/L	5.34	5.34	mg/L	0.5	4	1.1		0.75
4.01	mg/L	4.01	4.01	mg/L	0.5	6	2		1.5

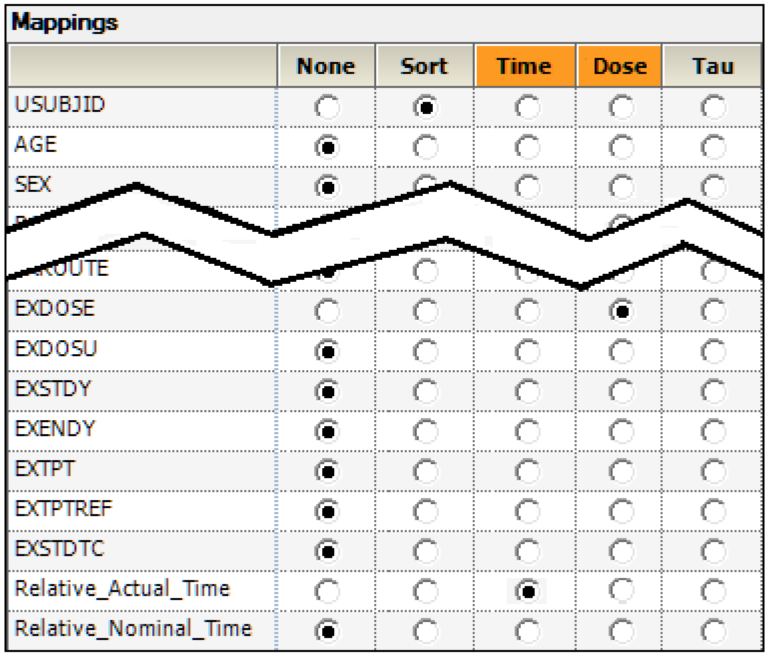
Mapping the results to an NCA model

1. Select **Workflow** in the Object Browser and then select **Insert > NonCompartmental Analysis > NCA**.
2. Map the CDISC Data Preparer Sample worksheet to the Main input of the NCA object.

   – In the NCA Mappings panel click  (**Select Source** icon).
   – Select the **Sample** worksheet under **CDISC Data Preparer** and click **OK**.
3. Use the option buttons in the NCA Mappings panel to map the following:
   – Map **USUBJID** to the **Sort** context.
   – Map **Relative_Actual_Time** to the **Time** context.
   – Map **PCORRES** to the **Concentration** context.

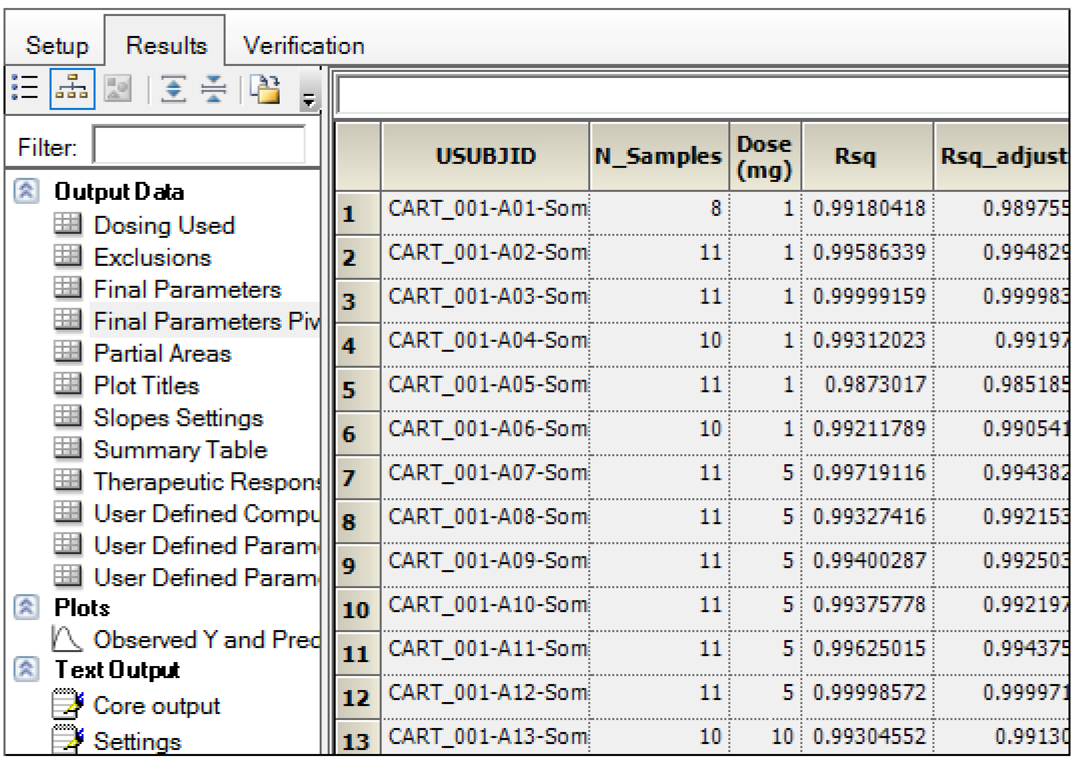


4. Map the CDISC Data Preparer Dose worksheet to the Dosing input of the NCA object.
   – Select **Dosing** in the Setup list.
   – In the Dosing Mappings panel click the **Select Source** icon.
   – Select the **Dose** worksheet under **CDISC Data Preparer** and click **OK**.
5. Use the option buttons in the NCA Mappings panel to map the following:
   – Map **USUBJID** to the **Sort** context.
   – Map **Relative_Actual_Time** to the **Time** context.
   – Map **EXDOSE** (Dose per Administration) to the **Dose** context.



6. Execute the object.

The results are displayed on the Results tab. The NCA object will produce worksheets and plots in the Output Data folder. It also produces a Core Output and Settings file. If any issues are encountered during execution, a Warnings and Errors file will be generated.



This example has shown how to use the CDISC Data Preparer object to convert CDISC data into a format that can be used by Phoenix. The object was set up and executed. The results of the CDISC Data Preparer were then mapped to another Phoenix object, NCA, as input. The execution of that NCA object was successfully completed without error.

CDISC Navigator

CDISC Navigator supports the importing and exporting of CDISC data in either the SDTM (Study Data Tabulation Model) or the SEND (Standard for Exchange of Nonclinical Data) format.

- CDISC SDTM is a unified way of transmitting information in drug studies with precise column names and a common file format. The CDISC STDM implementation in CDISC Navigator is compliant with the standards in the *SDTM Implementation Guide 3.1.1*.
- CDISC SEND is an implementation of SDTM for nonclinical studies and specifies a consistent format for presenting and exchanging nonclinical data. The CDISC SEND implementation in CDISC Navigator is compliant with the standards in the *SEND Implementation Guide 3.0*.

For further information, please visit the Clinical Data Interchange Standards Consortium Web site at www.cdisc.org.

A typical workflow using CDISC Navigator tools begins by obtaining the SEND files from the labs, then using CDISC Preparer to generate the data and format needed for the NCA analysis. The NCA analysis will generate the necessary PK parameters and SEND columns, which in turn can be exported to a PP SEND file.

CDISC domains supported by CDISC Navigator include:

DM (Demographics): Essential standard variables that describe each subject in a clinical study.
SC (Subject Characteristics): Subject-related data not collected in other domains.
EX (Exposure): A subject's exposure to protocol-specified study treatment.
PC (PK Concentration): Concentrations of drugs/metabolites in fluids or tissues as a function of time.
PP (PK Parameters): Pharmacokinetic parameters derived from pharmacokinetic concentration-time (PC) data.

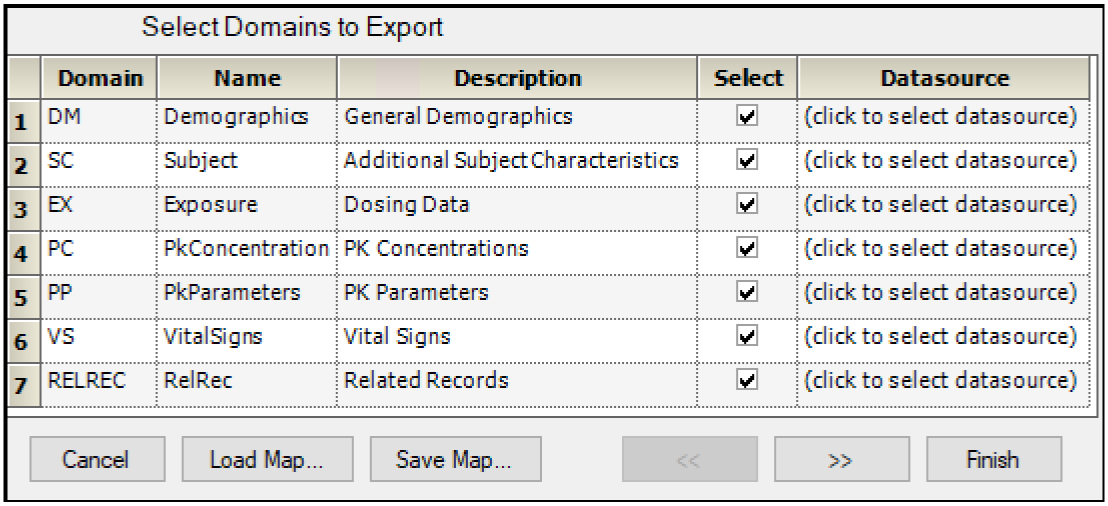
CDISC datasets are saved as SAS Transport Format (XPORT) Version 5 files (`.xpt`). Datasets exported from CDISC Navigator are automatically saved as SAS transport files.

This section contains the following topics:

CDISC Export

Note: The images in this section show the SDTM Export Wizard. The options are identical to those in the SEND Export Wizard.

Select **File > CDISC > SDTM > Export** for SDTM formatted datasets.
Or select **File > CDISC > SEND > Export** for SEND formatted datasets.



Clear the **Select** checkbox beside a domain to exclude it from the export.

To specify a file outside of Phoenix as the source

Click in the **Datasource** cell beside the domain.

Select **File System** and click **OK**.

In the file browser, locate and select the `.xpt` file and click **Select**.

Click **Finish** to export the data.

Upon export, the original `.xpt` file from the file system is overwritten. Because of this, there is no need to do any mapping for the domain.

To specify a Phoenix object as the source

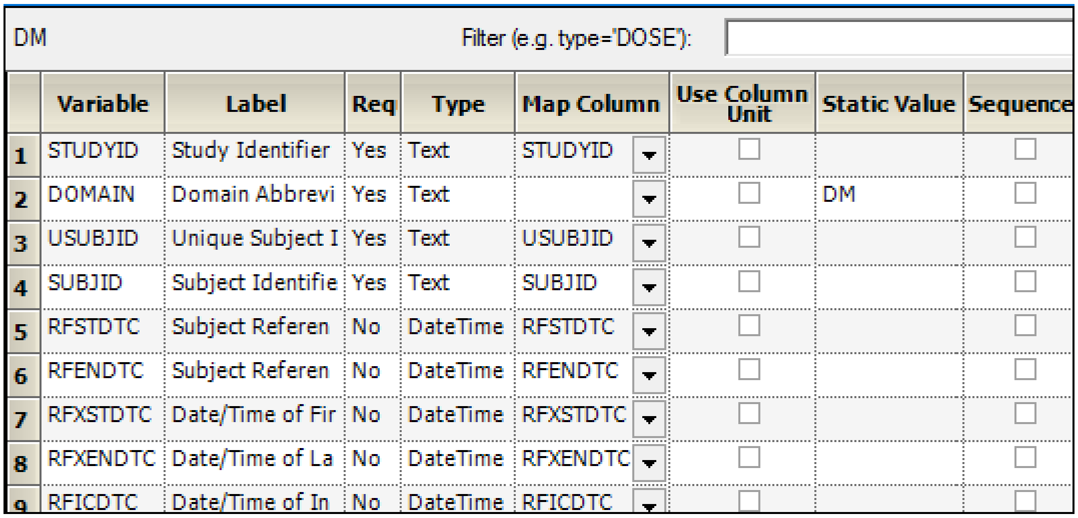
Select **Phoenix Project** and click **OK**.

Select a worksheet in the *Select Object* dialog and click **Select**.

Each domain has its own set of study variables that must be mapped. Users can map columns in a dataset to domain variables.

If a map file exists of the selected domains and data sources, click **Load Map** to load the file. Otherwise, click **>>** to proceed with the mapping.

The Variable column contains the CDISC variable names. The column headers in the data source are not required to match the variable names.


DM Filter (e.g. type='DOSE'):

	Variable	Label	Req	Type	Map Column	Use Column Unit	Static Value	Sequence
1	STUDYID	Study Identifier	Yes	Text	STUDYID			
2	DOMAIN	Domain Abbrevi	Yes	Text			DM	
3	USUBJID	Unique Subject I	Yes	Text	USUBJID			
4	SUBJID	Subject Identifie	Yes	Text	SUBJID			
5	RFSTDTC	Subject Referen	No	DateTime	RFSTDTC			
6	RFENDTC	Subject Referen	No	DateTime	RFENDTC			
7	RFXSTDTC	Date/Time of Fir	No	DateTime	RFXSTDTC			
8	RFXENDTC	Date/Time of La	No	DateTime	RFXENDTC			
9	RFICDTC	Date/Time of In	No	DateTime	RFICDTC			

Note: When exporting a PP domain, an additional checkbox is shown above the table, **Include REL-REC**. Turn on to include related records. See “Exporting related records” for more information.

In the **Filter** field, type a column name followed by a condition to filter the input for the current domain.

For example, if a user retrieves data from Certara Integral that contains dosing and sample data, entering `Type='Dose'` in the Filter field only exports the dosing data. Note that the Filter field is case sensitive.

Use the **Map Column** menus to select a column in the data source to map to each CDISC variable.

Select the **Use Column Unit** checkbox to remove the units from a column header and place them in their own column during export.

In the **Static Value** field, enter a static value for a CDISC variable.
Note that the Map Column selection supersedes any static value.

Select the **Sequence** checkbox if a column contains the order of the output, or the treatment sequence in a crossover study.

Click **>>** to continue mapping for each selected domain.

Optionally save the mappings for future use once the mapping is complete by clicking **Save Map** to save the mappings to an XML file.

Every selection in the export wizard, including domains, static values, etc., is saved in the map file.

To export the data, click **Finish** and, in the *Browse for Folder* dialog, select an export directory.

The exported data is placed in a directory with date and time stamps included in the name. A message is displayed telling users when the export is complete. If a required field is missing, the export continues, but an alert is presented to the user.

Exporting related records

Exporting related records provides a link between parameter calculations and the data in the original data source that went into the calculation.This is accomplished by creating a RELREC worksheet in the output that stores the connection information.

There are some limitations/considerations when exporting related records:

The original dataset must have a PCSEQ (Sequence Number) column.

The datasource for the PP domain must be an NCA result.

Some of the Final Parameters are calculated based on the points from which the regression line was fitted. For these parameters, the RELREC information should only contain the PC data that was used for Lambda Z calculations.

The `CdiscRelRecLZParams.xml` configuration file (located in `<Phoenix_install_dir>\application\Plugins\CDISC`) lists these Lambda Z-based parameters. Parameters specified in this file will have records in the RELREC table that link to a RELID defined as the profile number plus the suffix "LZ".

Assume that CDISC DM, EX, and PC domains are imported into Phoenix using the CDISC Data Preparer object.

1. Using the imported CDISC data as input, set up and execute an NCA object.
2. Map PCSEQ as a **Carry** column so that it appears in the Summary Table. The PCSEQ column enables referencing to the original sequence number in the source data.

   The Summary Table and Final Parameters table can be used to determine which entries from original PC dataset were used to calculate the profiles in the NCA analysis.
3. In the Final Parameters table (stacked), identify the sort key for the parameter of interest.
4. Go back to the Summary Table and find that sort key. Each associated sequence number that went into this calculation is listed as a separate row with the same sort key.
5. To export the Final Parameter Results back to CDISC, select **File > CDISC > SDTM > Export**.
6. Click in the Datasource cell for one of the domains to export.

   The user is able to pick datasources for the domains being exported that are either located in the file system or are part of the Phoenix project. For exporting related records, the datasource for the PC domain must be the original dataset.

Note: Selecting the dataset that was imported into the Phoenix project instead of the original dataset is not recommended. During import, modifications to the data have occurred (e.g., different date and time formations, relative time calculations, etc.) and the purpose of exporting related records is to be able to track the data that went into a calculation back to the original CDISC dataset.

7. Select **File System**, click **OK**.
8. Locate and select the original dataset.
9. Repeat for each of the domains to export.
10. For the PP domain, click in the Datasource cell.
    The PP domain datasource must be the Final Parameters worksheet from the NCA analysis.
11. Select **Phoenix Project**, click **OK**.
12. Locate and select the Final Parameters worksheet for the NCA analysis.

13. When finished mapping the domains to data sources, click the **>>** button at the bottom of the dialog.
14. For each domain being exported, make adjustments as needed to the column mappings in the corresponding page and click the **>>** button.
15. For the PP domain, turn on the **Include RELREC** checkbox above the table to create the RELREC.xpt file of related records.

PP ☑ Include RELREC Filter (e.g. type='DOSE'):

	Variable	Label	Req	Type	Map Column	Use Column Unit	Static Value	Sequence
1	STUDYID	Study Identifier	Yes	Text	STUDYID	☐		☐
2	DOMAIN	Domain Abbrevi	Yes	Text		☐	DM	☐
3	USUBJID	Unique Subject I	Yes	Text	USUBJID	☐		☐

16. Continue through the Export Wizard and click **Finish**.
17. Select the folder in which to export the domains.

The image below shows a portion of an exported RELREC.xpt file. For the rows where IDVAR=PCSEQ, each sequence has an identifier listed in the IDVARVAL column. The RELID column lists the NCA profile identifier. Thus, PCSEQs 11, 13, 17, 19, 23, 25, 30, and 32 all were included in calculating profile P1.

	STUDYID	USUBJID	RDOMAIN	IDVAR	IDVARVAL	RELTYPE	RELID
1	CART_001	CART_001-A0	PC	PCSEQ	11	ONE	P1
2	CART_001	CART_001-A0	PC	PCSEQ	13	ONE	P1
3	CART_001	CART_001-A0	PC	PCSEQ	17	ONE	P1
4	CART_001	CART_001-A0	PC	PCSEQ	19	ONE	P1
5	CART_001	CART_001-A0	PC	PCSEQ	23	ONE	P1
6	CART_001	CART_001-A0	PC	PCSEQ	25	ONE	P1
7	CART_001	CART_001-A0	PC	PCSEQ	30	ONE	P1
8	CART_001	CART_001-A0	PC	PCSEQ	32	ONE	P1
9	CART_001	CART_001-A0	PC	PCSEQ	79	ONE	P2
10	CART_001	CART_001-A0	PC	PCSEQ	87	ONE	P2

Looking further down in the RELREC.xpt file, where IDVAR=PPSEQ, each row reflects a different parameter. Each sequence number (IDVARVAL) can be tracked back to a parameter that was calculated.

	STUDYID	USUBJID	RDOMAIN	IDVAR	IDVARVAL	RELTYPE	RELID
208	CART_001	CART_001-A1	PC	PCSEQ	1356	ONE	P18
209	CART_001	CART_001-A1	PC	PCSEQ	1358	ONE	P18
210	CART_001	CART_001-A0	PP	PPSEQ	1	ONE	P1
211	CART_001	CART_001-A0	PP	PPSEQ	2	ONE	P1
212	CART_001	CART_001-A0	PP	PPSEQ	3	ONE	P1
213	CART_001	CART_001-A0	PP	PPSEQ	4	ONE	P1

CDISC Import

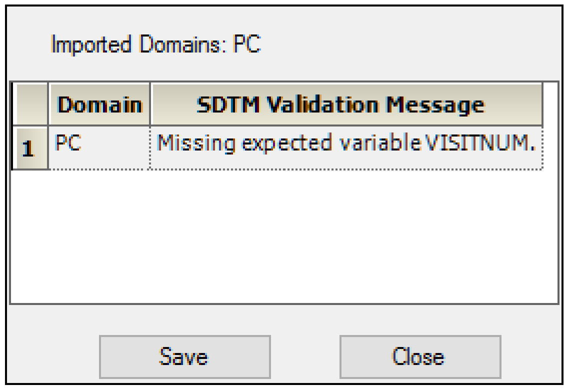
Select **File > CDISC > SDTM > Import** for SDTM formatted datasets.
Or select **File > CDISC > SEND > Import** for SEND formatted datasets.

In the *Open* dialog, choose the file format from the pull-down menu next to the **File name** field (`.xpt` domain file or `define.xml` file).

The `define.xml` file specifies all of the domains that are part of the CDISC dataset. Selecting this file will result in all of the specified domains being imported.

Locate and select the CDISC domain file(s) or `define.xml` file and click **Open**.

A message is displayed that lists any validation errors encountered during import. Users are alerted if a required field is missing but the import is not stopped.



Click **Save** to save the error messages to a file for later review or **Close** to close the dialog.

The imported dataset is added to the Data folder in the Object Browser.

CDISC time formats

Below are some important notes regarding the time formats used in CDISC.

All the date, time, and collection time fields are in ISO 8601 format as defined by the CDISC standards.

The format of CDISC data after import may differ depending upon the default local/regional ISO format for the environment in which Phoenix is running. The mm/dd/yyyy ISO date format may not be the default and may not even be an option in some regions.

CDISC Navigator selects the highest time unit when importing datasets.

When relative time values are exported, CDISC Navigator creates the 8601 format based on the values in the relative time column.

Data Link

Data Link is an operational object that allows adding/removing/renaming of required columns so the user can use datasets with different column names, without having to do a specific column rename. This facilitates reuse of workflows by standardizing the column names of input.

What happens if data links are not used? If a workflow template is saved without using data links, when it is applied to another workflow, all of the links from the external sources will be missing. The more complex the workflow, the harder it is to establish new links to replace those that were lost. If data links are included in the template being applied, simply connect the source data to the data links themselves. Each data link distributes the data to where it is needed in the workflow.

To add a Data Link object to a workflow

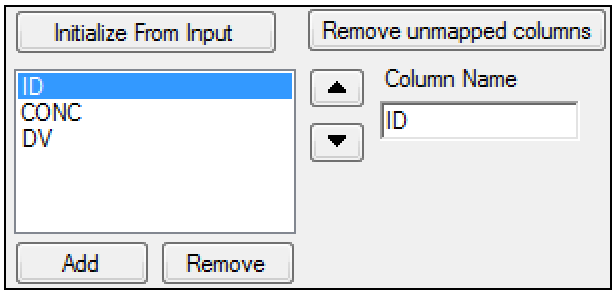
Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > System > Data Link**.
Or Main menu: **Insert > System > Data Link**.
Or right-click menu for a worksheet: **Send To > System > Data Link**.

Map an input dataset to Data in the Setup tab list.

To modify the required columns and their names

When creating a Data Link, by default all the columns in the original dataset are shown as a requirement. The user must map a column to each of the listed columns. If a new dataset does not have one of the columns listed in the Data Link, the user must remove that column from the Data Link or add the data to the dataset and map it before the Data Link can be executed.



In the Options tab of a Data Link object, click **Initialize From Input** to list only columns in the input dataset. Any columns that have been added by the user are removed from the list.

To ***add*** a column, click **Add** and the enter the name in the **Column Name** field.,

To ***remove*** a column(s), select the column name(s) from the list and click **Remove**.

To ***rename*** a column, select the column name from the list and enter a new name in the **Column Name** field.

Use the up and down arrows to ***reorder*** the columns.

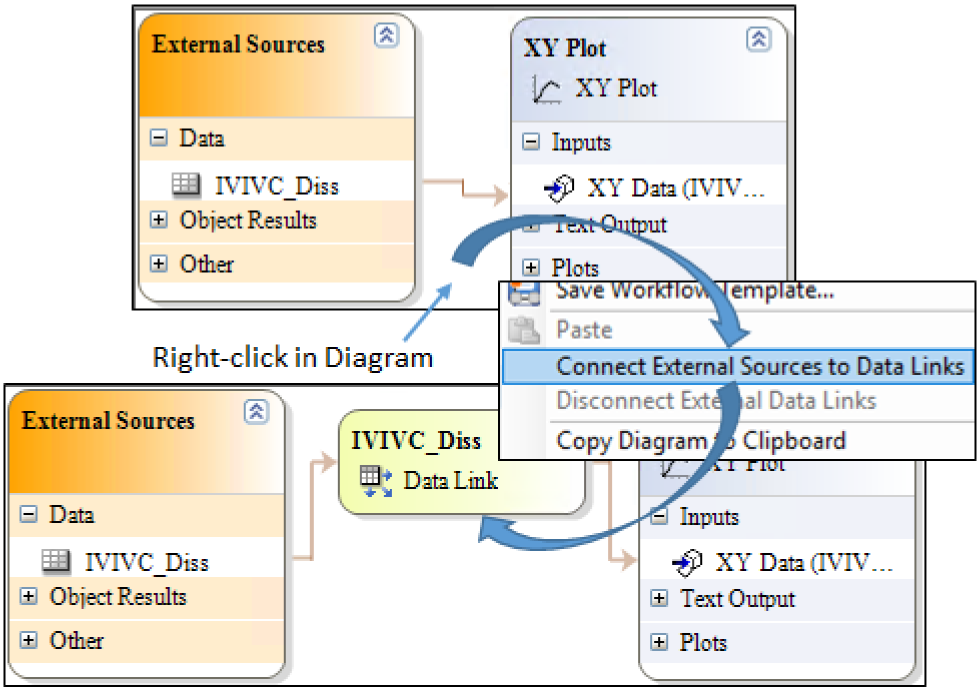
Click **Remove unmapped columns** to ***delete*** all columns that are not mapped to the input data.

To connect and disconnect external sources to data links

Before saving a workflow template, the **Connect External Source to Data Links** feature should be used. This feature allows you to create a data link object for every worksheet coming into the workflow. It is a way of making place holders in the workflow so someone using the template can see where external data are needed. Therefore, it is recommended that you first finalize your workflow, then connect the external sources using data links and then save the workflow as a template.

In a Diagram window that has external sources mapped directly to operational objects, right-click and select **Connect External Source to Data Links**.

- If there is an existing Data Link object and all columns in the input match the columns in the object, then the connections will be redirected through the Data Link object.
- If, on the other hand, columns in an existing Data Link do not match all the columns of the input, then the existing Data Link will not be used. Phoenix will create a new Data Link object to match all of the columns exactly.



To disconnect external sources from a Data Link object, right-click in the Diagram and select **Disconnect External Data Links**. The External Sources and operational objects will be directly connected.

Use of the **Connect External Source Data Links** feature is demonstrated in the "Workflows and Templates example".

Data Wizard

The Data Wizard is designed to facilitate repeated data operations on the same dataset. It also allows changes in the sequence of the operations. It replaces the following standalone tools: Column Properties, Filter Worksheet, and Column Transformation. (If a project created in an earlier version of Phoenix has those options, these objects are loaded and visible.) The Data Wizard provides the property computing, filtering, and transformation operations as well as generating an easy summary worksheet to keep the workflow organized.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Data Management > Data Wizard**.
Or Main menu: **Insert > Data Management > Data Wizard**.
Or right-click menu for a worksheet: **Send To > Data Management > Data Wizard**.

The manipulation of data is defined in the Data Wizard as Steps. When the Data Wizard object is added, **Step 1** is automatically listed in the Summary list of the Setup tab and is ready to be defined. From the **Action** menu in the Options tab, select **Properties**, **Filter** or **Transformation** and press **Add** to define the step.

Once that selection is made, the action is appended to the Step name in the Summary list and other controls on the Options tab are enabled appropriately.

A series of steps can easily be created (specifying column properties via **Properties**, filtering the data using **Filter**, and then doing a data transformation using **Transformation**). Each step in the Data Wizard identifies its action in the Summary. Delete steps, rearrange steps, insert new steps, and specify when to execute steps in a sequence using the buttons in the Options tab.

The first step in the Data Wizard allows the user to map the dataset, whether it is for filtering, transformation, or modifying column properties. After the dataset has been mapped in that first step, all subsequent steps use that source dataset in combination with the steps created in the Data Wizard.

The **Retain Intermediate Results** checkbox preserves all results for each step set up in the Data Wizard. It will add significantly to the amount of output (and requires more memory). This options is only recommended when the intermediate output is truly necessary.

This section contains information about the following:

Properties operation
Transformation operation
Filter operation
Results

See also "Ratios and baseline adjustments example".

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Properties operation

The **Properties** operation in the Data Wizard allows users to set column header names, units, and data types (text or numeric) for worksheets.

The interface consists of three main parts:

Main Mappings panel
Options tab
Defaults tab

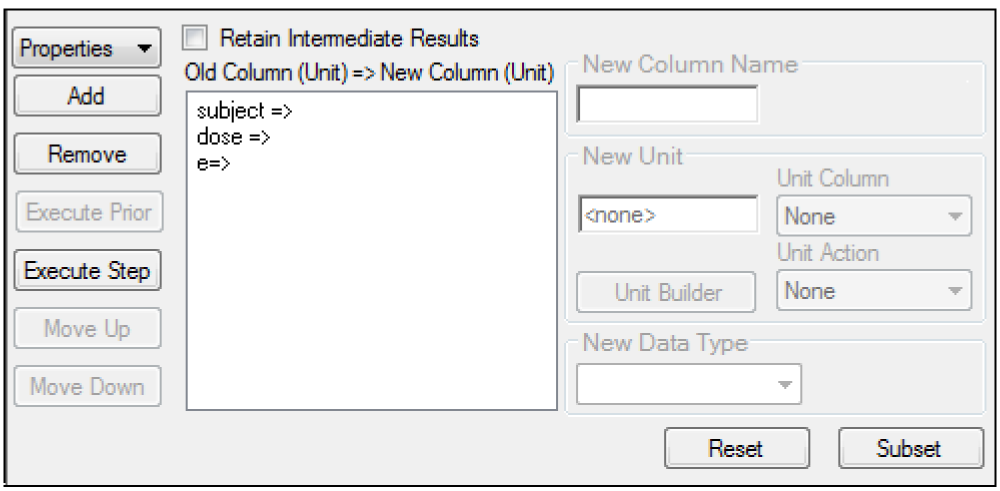
Main Mappings panel

Users must map a dataset to the Main Mappings panel when the first step is set up. All subsequent steps will automatically be mapped to the same dataset.

None: Columns mapped to this context are simply included in the output.
Sort: Sort variables used to define individual profiles.

Options tab

The Options tab lists all the column headers in a worksheet and any associated units. The column headers and units are displayed in the columns list in the Options tab.



To change column header properties:

Select a column header in the columns list to change its properties.

In the **New Column Name** field, type a new column header name.

Phoenix does not allow spaces in column headers and will substitute an underscore (_) for a space.

A column name can only consist of alphanumeric characters and underscores, and cannot start with a number.

The constraints on column names exist because spaces and other characters in column names can cause filter and sort functions to not work correctly.

In the **New Unit** field, type a new unit for the new column.

Alternatively, click **Units Builder** to use the *Units Builder* dialog to change column units. The Units Builder can be used to specify new units or convert existing units.

In the **Unit Action** list, select the action desired: **Specify**ing the unit or **Convert**ing units. See “Using the Units Builder” for more details on this tool.

Each column in a worksheet can use different units. The units are displayed in parentheses in the column header, and can be used in calculations. If the units are not standard or recognizable, Phoenix displays them in braces: {mmHg}. Nonstandard units are carried throughout any operations but are not used in any calculations. For a list of valid units and prefixes, see “Valid units and prefixes in Phoenix”.

Caution: If it is possible, units are automatically converted when the new column unit does not match the old column unit. Make sure the old and new column units match if unit conversion is not necessary or wanted.

In the **New Data Type** menu, select **Text** or **Numeric** to change the data type of the selected column.

Changing a column from text to numeric deletes any non-numeric values in the column. Changing a column from numeric to text does not delete any values.

Data type refers to column data types. There are two kinds, numeric and text. Numeric columns contain only numeric values, and Phoenix treats the values in a numeric column as numeric data.Text, or string-type, columns can contain mixed numeric and text values, but Phoenix treats values in a text column as non-numeric values that cannot have certain operations performed on them, such as an arithmetic transformation.

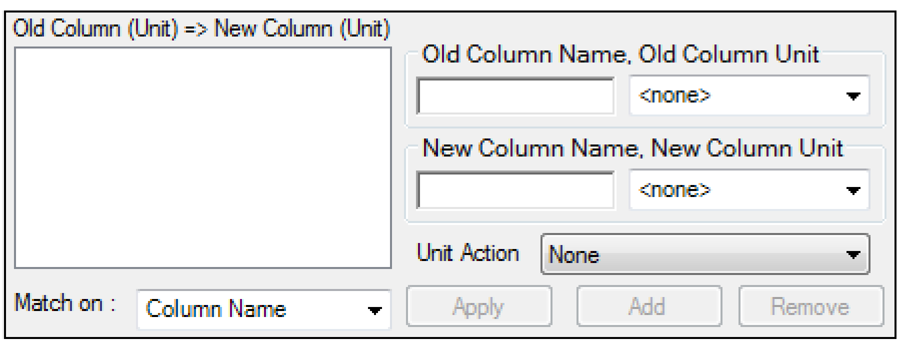
Select another column header in the columns list to change its properties.

For a list of valid units and prefixes, see “Valid units and prefixes in Phoenix”.

Defaults tab

The Defaults tab is used to automatically change column properties. Users can specify new column names and units for common columns like Time or Concentration.

Caution: Defaults must be specified ***before*** a worksheet is mapped in the Properties operation.



When a worksheet is mapped to a Properties operation that has defaults set, any matching column headers and units are automatically changed or converted.

Defaults are listed on the default columns box.

To add new defaults

Type the column header name to be automatically converted in the **Old Column Name** field.

Select a unit, if applicable, in the **Old Column Unit** menu.

Type a new column name in the **New Column Name** field.

Select a new unit, if applicable, in the **New Column Unit** menu.

Caution: If it is possible, units are automatically converted if the new column unit does not match the old column unit. Make sure the old and new column units match if unit conversion is not necessary or wanted.

Click **Add** to add the new column header default to the default columns box.

The default column name can be edited after it is added.

Make any changes in the column name field and column units menus, and click the **Apply** button to apply the changes.

In the **Match on** menu, select whether or not to match the default column to input worksheet columns based on column name or column name and unit.

Select a default in the default columns box and click **Remove** to remove the column default.

Add another default by typing another column header name in the **Old Column Name** field and repeating the previous instructions.

Transformation operation

The **Transformation** operation creates a new column in a worksheet that is the result of a transformation. Phoenix supports arithmetic, baseline, custom, and function transformations. All data in the source column are transformed regardless of exclusions, which are carried over to the new column.

The **Transformation** user interface consists of two main parts, the Setup tab and the Options tab.

Main Mappings panel
Options tab

Main Mappings panel

Users must map a dataset to the Main Mappings panel when the first step is set up. All subsequent steps will automatically be mapped to the same dataset. Required input will be highlighted orange in the interface.

Users can select to assign the units of an input (mapped) column to a new column created via a transformation. If the Output Column **Unit** selection is mapped, the column mapped to that context will have its unit used in the new output column.

Context associations for a **Transformation** object change depending on which transformation type is selected in the Options tab.

Arithmetic transformation mappings

None: Columns mapped to this context are simply included in the output.
x Column and **y Column**: Columns in a worksheet used in an arithmetic transformation.

Output Columns:
None: Units of columns mapped to this context are not used in the new output column.
Unit: The column whose units are to be used in the new output column.

Baseline transformation mappings

None: Columns mapped to this context are simply included in the output.
x Column: The independent variable that is used to compute the baseline values.

Sort: Sort variable(s) used to define individual profiles.
Time: Time values that are used to compute the baseline values.

Output Column:
None: Units of columns mapped to this context are not used in the new output column.
Unit: The column whose units are to be used in the new output column

Custom transformation mappings

Output Column:
None: Units of columns mapped to this context are not used in the new output column.
Unit: The column whose units are to be used in the new output column.

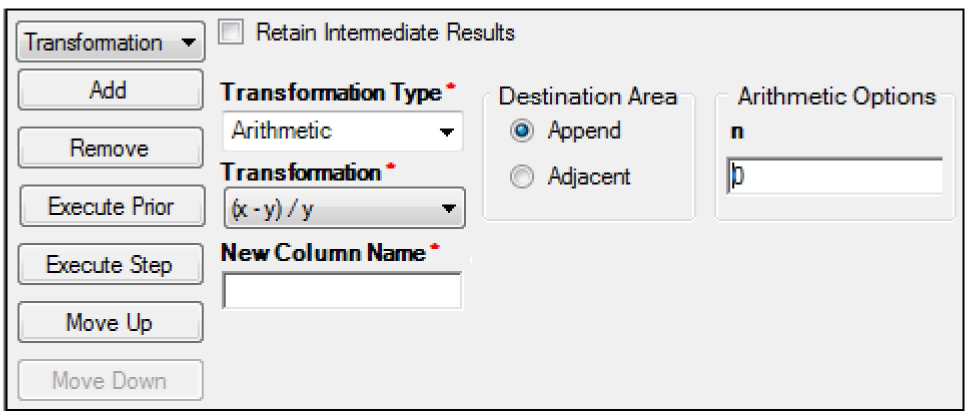
Other mapping contexts are defined in the Formula field.

Function transformation mappings

None: Columns mapped to this context are simply included in the output.
x Column: The independent variable that is used to provide the values for the function transformations.

Output Column:
None: Units of columns mapped to this context are not used in the new output column.
Unit: The column whose units are to be used in the new output column.

Options tab



The Options tab is used to select the transformation type and specify options for each transformation type. The Options tab also allows users to specify the sequence of the operations in the Data Wizard.

Phoenix supports the following types of transformations:

Arithmetic: (x – y)/y, (x + y)/y*100, x – n, x – y, x*n, x*y, x/n, x/y, x^n, x^y, x + n, x + y

Baseline: % Change from Baseline, Change from Baseline, Ratio from Baseline

Custom: Custom Function, see “Example custom functions”.

Functions: 1/x, Absolute value(x), e^x, LN(x), Log10(x), Square root(x)

In the Arithmetic and Functions options, **x** and **y** are columns in a worksheet, in the Arithmetic options, **n** is a number, and in the Functions options **e** is the base of the natural logarithm (2.718281828).

Note: Blank cells are treated as zero when operated on with cells that contain numbers.

In the **Transformation Type** menu, select one of four transformations: **Arithmetic**, **Baseline**, **Custom**, **Functions**.

Arithmetic options

In the **Transformation Type** menu, select **Arithmetic**.

In the **Transformation** menu, select the arithmetic transformation type.

If one of the **x** and **y** transformations are selected, the **x Column** and **y Column** mapping contexts are made available in the Main Mappings panel.

Use the option buttons to map data types in the worksheet to the **x Column** and **y Column** contexts. If one of the **x** and **n** transformations are selected, then a value for **n** must be specified.

In the **Arithmetic Options** field, type a value for **n**.

In the **New Column Name** field, type a name for the column used to contain the transformed values.

In the Destination Area, select one of the option buttons.

Append places the new column after the last column in the dataset.

Adjacent places the new column to the right of the data type mapped to the x Column context.

Baseline options

Users can choose whether to specify sort variables for baseline transformations. Sort variables define unique profiles that are used to compute change from baseline separately for each profile. Typically, a single variable representing subject IDs is sufficient. Other data may require more than one variable, such as Subject and Period. The baseline transformation sorts the output worksheet in alphabetical or numerical order, based on the sort variables.

Rules for using datasets in a baseline transformation:

By default, Phoenix uses the value corresponding to time=0 as the baseline for each unique profile. If a profile has more than one value at time zero, Phoenix uses the first value as the baseline.

If a zero time value is not in the dataset, the time value to use for the baseline value (normally the lowest time) must be specified, or the user must choose to use the minimum time for each group, in order to generate the baseline transformations.
Enter the lowest (or other) time value in the **Fixed Value** field or
Select **MinimumPerGroup** in the **Starting Point** dropdown menu.

If the columns mapped to **x Column** has a zero or missing value at the time specified for the baseline, then the **% Change from Baseline** and **Ratio from Baseline** options will produce empty results. An alternate baseline time value or the **MinimumPerGroup** option may be used.

To create a baseline transformation

In the **Transformation Type** menu, select **Baseline**.

In the **Transformation** menu, select the baseline transformation type.

If **% Change from Baseline** is selected, Phoenix performs a transformation on a column by calculating the percent change between each value and either a fixed baseline value or the minimum value for each distinct profile.
result=(x – baseline)/baseline*100

If **Change from Baseline** is selected, Phoenix performs a transformation on a column by calculating the change between each value and either a fixed baseline value or the minimum value for

each distinct profile.
result=x – baseline

If **Ratio from Baseline** is selected, Phoenix performs a transformation on a column by determining the ratio to either a fixed baseline value or the minimum value from each distinct profile.
result=x/baseline

In the Main Mappings panel, click the option buttons to specify the **x Column**, the **Sort** column(s), and the **Time** column.

Users can map multiple or no columns in a worksheet to the Sort context. Each column mapped to the Sort context creates a unique profile. Baselines are calculated on a per profile basis.

In the **New Column Name** field, type a name for the column that will contain the transformed values.

In the **Starting Point** menu, select **Fixed Point** or **Minimum per Group**.

If **Minimum per Group** is selected, the lowest time point in each profile is used to generate the baseline transformation. Selecting this option means that the baseline transformation uses a different starting point for each profile defined by the sort key(s).

If **Fixed Point** is selected, users can enter custom starting time value in the **Fixed Value** field.

In the **Fixed Value** field, type a time value for a time column in Numeric format or in Text format.

If a time column is in Text format, users must type fixed time value in the same format used to enter the time values in the worksheet. For example, if the first time point used as the baseline is 1:00, then 1:00 must be typed in the Fixed Value column. For acceptable dates and times in Text format, see “Date and time formats”.

The default is zero, because Phoenix, by default, evaluates the change from baseline at time=0. If a value is entered that is higher than the highest time value, then no output values are produced in the new column.

In the **Treat Time Values as** menu, select the format used by the time column.

Numeric Format means the Time column is in Numeric format.
Date\Time Format means the Time column is in Text format. If selected, the **Time Units** menu is made available. The selected units are applied to the transformed time column, and are converted if they do not match the source time column units.

In the **Time Units** menu, select the units to use in the transformed time column.

If **Date\Time Format** is selected, the **Create Transformed Time Column** checkbox is made available.

Check the **Create Transformed Time Column** box to create a Numeric time column in the output that is based on the values in a Text time column or clear the checkbox to not create a transformed time column.

In the **Destination Area**, select one of the option buttons.

Append places the new column after the last column in the dataset.
Adjacent places the new column to the right of the data type mapped to the x Column context.

Custom options

Users can create a custom transformation that transforms one or more columns in a worksheet using the functions provided by Phoenix.

To create a custom transformation

In the **Transformation Type** menu, select **Custom**.

Custom Function is selected by default in the **Transformation** menu. There are no other options in the menu for custom functions.

In the **New Column Name** field, type a name for the column that will contain the transformed values.

In the **Formula** field, type a custom function or use the pointer to select a function name in the **Function List** and drag the function name to the **Formula** field.

Custom functions can be defined, edited, and combined in the **Formula** field. The **if** custom function allows users to create a compound function using the logical operators & (and) and | (or). For example, `if((col1=1) & (col2=2), 1, 0)`. Each condition in the **if** statement must be placed in parentheses. The function name must be followed immediately by the left parenthesis, there cannot be a space.

See "Example custom functions" for a list of all possible functions and examples of how to use them. The same information is also listed in the Function List in the Options tab.

In the Main Mappings panel, click the option buttons to specify the mapping contexts created by the custom function.

Functions options

To find the absolute value, logarithmic values, or square root

In the **Transformation Type** menu, select **Functions**.

In the **Transformation** menu, select the function transformation type.

Use the option buttons to map a column in the worksheet to the **x Column** context.

In the **New Column Name** field, type a name for the column used to contain the transformed values.

In the **Destination Area**, select one of the option buttons.

Append places the new column after the last column in the dataset.
Adjacent places the new column to the right of the data type mapped to the x Column context.

Note: Using the Data Wizard, it is easy to create a sequence of operations, whether transformations or combinations of the other Wizard operations.

Example custom functions

Below are some common functions that may be helpful.

`substitute(conc,"BQL",0.1,0)`
In the mapped column "conc", replace each cell value found to be equal to BQL with 0.1 in the new column.

`substitute(CobsPop, 0.1,"BQL",0)`
In the mapped column “CobsPop”, replace each cell value found to be 0.1 with “”BQL” in the new column.

`if(CobsPop==0.01, 1, 0) or;`
Note: There are 2 equal signs.
If any cell in the mapped column “CobsPop” is equal to 0.1, then enter a 1 in the new column; otherwise enter a 0.

`if(CobsPop = 0.01, 1, 0)`
Note: When using a single equal sign, spaces are needed before and after the equal sign.
If any cell in the mapped column “CobsPop” is equal to 0.1, then enter a 1 in the new column; otherwise enter a 0. (Same as previous function.)

`if(CobsPop = 0.1, 1, if(CobsPop < 1, 2, 0))`
Note: You need spaces before and after the < sign or use two << signs without spaces.
Embedded ifs. If any cell in the mapped column “CobsPop” is equal to 0.1, then enter a 1 in the new column; if it is less than 1, enter a 2; otherwise enter a 0.

`if(CobsPop = 0.1, 1, if(id==1, 2, 0))`
Embedded ifs with different vars. If any cell in the mapped column “CobsPop” is equal to 0.1, then enter a 1 in the new column; if the mapped column “id” is equal to 1, enter a 2; if none of these conditions are met, enter a 0.

`replace(conc,2,2,"LQ")`
Starting at number 2 position in the mapped column “conc”, replace the string with 2 letters “LQ”. This is useful for converting BQL to BLQ, but notice that it does not discriminate, so a number 1.537753 ends up being 1LQ37753 (position 2 and 3 replaced). Use with caution!

`Ln(conc)`
Write the natural log of the value in the mapped column conc in the new column.

Custom functions list

`abs`: Return the absolute value of the supplied parameter.

```
abs(-12)=12;
abs(ColumnA)
```

`acos`: Return the inverse cosine of parameter1.

```
acos(-0.5)=2.094395
```

`acosh`: Calculate the inverse hyperbolic cosine of parameter1.

```
acosh(10)=2.99322
```

`asin`: Calculate the inverse sine of parameter1.

```
asin(-0.5)= -0.5236
```

`asinh`: Calculate the inverse hyperbolic sine of parameter1.

```
asinh(-2.5)= -1.6472311
```

`atan`: Calculate the inverse tangent of parameter1.

```
atan(1)=0.785398
```

`atan2`: Calculate the arc tangent of two coordinates.

```
atan2(x coord, y coord);
atan2(-1,1)= -2.3561945
```

`atanh`: Calculate the inverse hyperbolic tangent of a value.

```
atanh(0.76159416)=1
```

`average`: Return the average of the supplied parameters.

```
average(A1:A10);
average(12, 5, 7, 8, 11.4)
```

`ceiling`: Return the smallest integer value greater than, but not equal to, the value supplied.

```
ceiling(12.5)
```

`chiinv`: Calculate the inverse chi-square distribution

```
chiinv(p, df)
```

`clean`: Clean text of non-printable characters.

```
clean("string with non-printable chars");
clean(A1)
```

`concatenate`: Combine two or more strings into one string.

```
concatenate(A1:A5);
concatenate(ColumnA, "& ", ColumnB)
```

`cos`: Calculate the cosine of parameter1.

```
cos(1.047)=0.50017107
```

`cosh`: Calculate the hyperbolic cosine of parameter1.

```
cosh(4)=27.30823
```

`count`: Return the number of values in a list, including empty cells.

```
count(A1:A5)
```

`counta`: Return the number of non-empty cells in a given range.

```
counta(A1:A5)
```

`date`: Return the sequential serial number that represents a particular date.

```
date(2007, 11, 27)=39411
```

`datevalue`: Use datetime to return the serial number of the date represented by date_text. Use this function to convert a date represented by text to a serial number. If time is associated with the date, then the serial date will be a decimal and not a whole number.

```
datevalue("11/27/2017")=39411
```

`day`: Return the day of a date, represented by a serial number. The day is given as an integer ranging from 1 to 31.

```
day(serial_time);
day(39411)=27
```

`even`: Return the smallest even integer greater than the argument.

```
even(12.1)
```

`exp`: Return e raised to the power of the supplied parameter.

```
exp(3);
exp(ColumnA)
```

`fact`: Return the factorial of the supplied parameter.

```
fact(3)
```

`Finv`: Calculates the quantile of F-distribution and returns the absolute value.

```
Finv(p,df1,df2);
Finv(0.7, 1, 10) = 1.194776
```

`floor`: Return the largest integer less than the supplied parameter.

```
floor(12.9)
```

`format`: Format a string using .NET string formatting commands.

```
format(ColumnA, “G8”);
format(“.12345”, “G8”)
```

`geomean`: Return the geometric mean of a range of positive data.

```
geomean(A1:A15)
```

`geovar`: Return the geometric variance of a range of positive data.

```
geovar(A1:A15)
```

`harmean`: Return the harmonic mean of a range of data.

```
harmean(A1:B32)
```

`harmvar`: Return the harmonic variance of a range of data.

```
harvar(A1:C33)
```

`hour`: Return the hour of a time value. The hour is given as an integer, ranging from zero (12:00 A.M.) to 23 (11:00 P.M.).

```
hour(serial_time);
hour(38711.06302)=1;
hour(37811.27135)=6
```

`if`: Return true if conditional argument is true; false otherwise.The `if` function also supports using & (and) and **|** (or) in statements, and supports nested `if` statements.

Note: parameter 1 (logical test) must return true or false; place a space between cell reference and '='

```
if((Time=1) & (Conc>2),…);
if((Time=1) | (Conc>2),…);
if(trt=”Reference”, “R”, “T”);
if(CVWR<=30, ‘125.00’,
if(CVWR<=50, 100*exp(+0.76*sqrt(Estimate)), 143.19))

if((A1=0.25), 1, 0)
```

`IsNull`: Return true if value of cell is NULL (empty).

```
IsNull(ColumnA)
```

`left`: Return the specified number of characters (from left to right) of a string.

```
left(“This is a test”, 1)=T;
left(“This is a test”, 3)=Thi; left(A1, 3)
```

`length`: Return the length of a string.

```
length("this is a test")=14;
length(A1)
```

`ln`: Return the natural log of the supplied parameter.

```
ln(2.3);
ln(ColumnA)
```

`log`: Return the log of the first parameter to the base of the second parameter.

```
log(number, base);
log(5,3)
```

`log10`: Return the log base 10 of the parameter.

```
log10(5);
log10(ColumnA)
```

`lower`: Return the supplied string as lower case.

```
lower("This Is A Test")="this is a test";
lower(A1)
```

`mid`: Return a specific number of characters from a string from a given position and length parameters.

```
mid(text, start pos, distance);
mid("This is a test", 2, 3)=his
```

`minute`: Return the minutes of a time value. The minute is given as an integer, ranging from zero to 59.

```
minute(serial_time);
minute(38711.06302)=30
```

`mod`: Return the remainder after parameter1 is divided by parameter2.

```
mod(number, divisor);
mod(12,2)
```

`month`: Return the month of a date represented by a serial number.
The month is given as an integer, ranging from **1** (January) to **12** (December).

```
month(serial_time);
month(39411)=11
```

`now`: Return the current date and time as a double (serial date/time).

```
now()=current date
```

`odd`: Return the smallest odd integer greater than the supplied parameter.

```
odd(13.1)
```

`pi`: Return the value of pi.

```
pi()
```

`product`: Return the product of a list of real numbers.

```
product(A1:Z88)
```

`rand`: Return a random number based on a lower limit, an upper limit, and a seed.

```
rand(,);
rand(0,1,92756)
```

`replace`: Replace a sub-string with another string.

```
replace(text, start pos, distance, replace with);
replace("T_%_025", 2, 3, "-")=T-025;
replace(ColumnA,1,4,"")
```

`right`: Return a specific number of characters from a string starting from the right and moving left.

```
right("This is a test", 3)="est"
```

`root`: Return the root of a parameter1, using parameter2/parameter3.

```
x^(a/b);
root(x, a, b);
root(2, 3, 4)
```

`round`: Round parameter1 to the number of decimal places defined by parameter2.

```
round(12.345, 2)=12.35;
round(ColumnA,1)
```

`roundsig`: Round parameter1 to the number of significant digits defined by parameter2. Note that Phoenix worksheets do not support displaying trailing zeros in decimals, so not all significant digits will be displayed in this case.

```
roundsig(12.234, 3)=12.3
```

`search`: Return the one-based starting position of a substring within a larger string. The third argument is the one-based starting position for the search. The function returns –1 if there is no match.

```
search("Phoenix", "oe", 1)=3
```

`second`: Return the seconds of a time value. The second is given as an integer in the range zero to 59.

```
second(38711.06302)=44
```

`sign`: Determine the sign of a number. Returns 1 if the number is positive, 0 if the number is zero, or –1 if the number is negative.

```
sign(-12);
sign(0);
sign(200)
```

`sin`: Calculate the sine of parameter1.

```
sin(1)=0.84147098
```

`sinh`: Calculate the hyperbolic sine of parameter1.

```
sinh(1)=1.175201194
```

`sqrt`: Return the square root of parameter1.

```
sqrt(9)
```

`stdev`: Estimate standard deviation based on a range of data.

```
stdev(A1:C1)
```

`strcmp`: An integer indicating the case sensitive lexical relationship between the two comparands.

Value condition < zero, stringA is < stringB
Value condition = zero, stringA = stringB
Value condition > zero, stringA is > stringB

```
strcmp(stringA, stringB)
```

`substitute`: Substitute new text for old text in a text string and optionally [for a given instance]. [] is optional but the preceding comma is required; `substitute(ColumnA,"_%_","",)`

```
substitute(text, target text, replacement text, [instance])
```

`sum`: Return the sum of the specified values.

```
sum(A1:A12);
sum(1,2,3,4,5)
```

`sumsq`: Return the sum of the squares of the arguments.

```
sumsq(C1:C33)
```

`tan`: Calculate the tangent of parameter1.

```
tan(0.785)=0.99920399
```

`tanh`: Calculate the hyperbolic tangent of parameter1.

```
tanh(-2)= -0.96403
```

`time`: Return the decimal number for a particular time.

```
time(hour, min, sec);
time(12,2,3)=0.50142361
```

`timevalue`: Use datetimes to return the decimal number of the time represented by a text string, with precision up to the second.

```
timevalue("2:24 AM")=0.1
```

`tinv`: Calculate the inverse t distribution and returns absolute value.

```
tinv(p, df);
tinv(0.7, 10)=tinv(0.3, 10)=0.541528
```

`today`: Return the serial number of the current date.

```
today()=current date as serial time
```

`trim`: Remove all spaces from text except for single spaces between words.

```
trim("      this is     a test")="this is a test"
```

`trunc`: Truncate a real number to an integer by removing the decimal places.

```
trunc(number);
trunc(12.1234)
```

`upper`: Return parameter1 in upper case.

```
upper("this is a test")="THIS IS A TEST"
```

`var`: Return the variance of a set of real numbers.

```
var(A1:A5)
```

`weekday`: Return the day of the week corresponding to a date. The day is given as an integer, ranging from 1 (Sunday) to 7 (Saturday).

```
weekday(serial_time);
weekday(39411)=Monday (Sunday is the first day)
```

`year`: Return the year corresponding to a date. The year is returned as an integer in the range 1900–9999.

```
year(39411)=2007
```

Filter operation

The **Filter** operation allows users to search for values in a dataset, specify if only matching data are returned (include), if the matches are filtered out (exclude), or replaced with another value. Additional options allow users to choose if the entire dataset is to be searched or just a particular column and if the entire row containing a matching cell is filtered or just the matching cell.

Main Mappings panel
Options tab

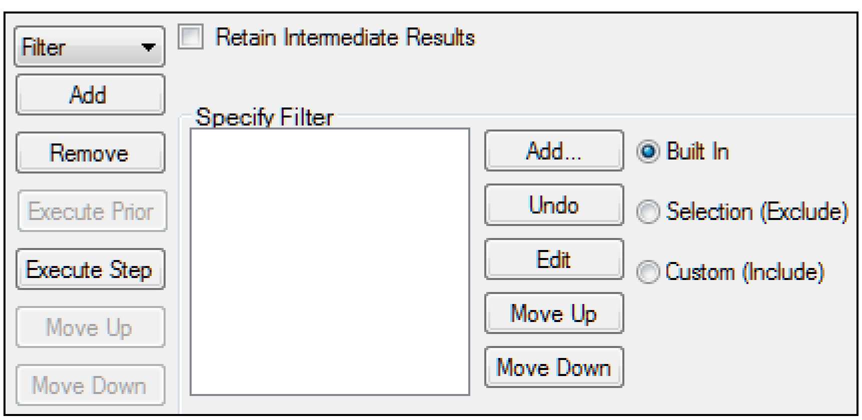
Main Mappings panel

Users must map a dataset to the Main Mappings panel when the first step is set up. All subsequent steps will automatically be mapped to the same dataset.

Use the Main Mappings panel to specify which input variables are filtered. Main Mapping input variables to context associations is optional.

None: Columns mapped to this context are simply included in the output.
Exclude: Columns mapped to this context are excluded in the result worksheet.

Options tab



To specify the type of filter

Select one of the option buttons to choose the filter type.

Built In – Use the Filter Specification dialog to add a filter.
Selection (Exclude) – Use the Filter Selection dialog to exclude part of a dataset.
Custom (Include) – Use the Custom Filter Entry dialog to specify a custom filter.

Click **Add** to add a filter.

The **Specify Filter** field lists all added filters. Select a filter to remove, edit, or move it.

Filters are executed in the order they are listed.

Click **Undo** to remove the last filter created from the list.

Click **Edit** to edit a filter.

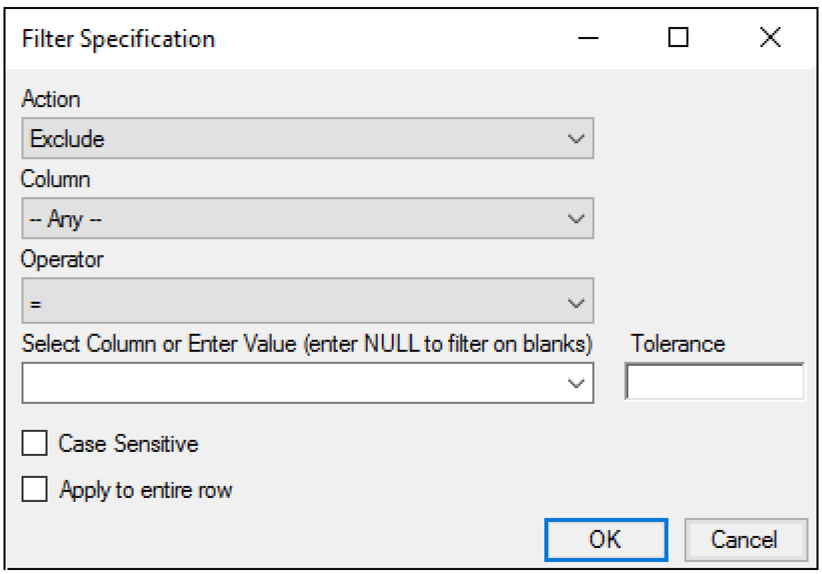
Click **Move Up** to move a filter to top of the list.

Click **Move Down** to move a filter to the bottom of the list.

Note: If a **User Selection** filter is defined and listed in the Specify Filter field, the **Move Up**/**Move Down** buttons in the Data Wizard are disabled.

Filter Specification dialog

When the **Built In** option is selected in the Options tab, clicking **Add** displays the *Filter Specification* dialog.



In the **Action** menu, select a filter action.

Exclude: Filter out cells/rows that match the filter criteria.
Include: Keep only the cells/rows that match the filter criteria.
Replace: For each cell that matches the filter criteria, replace it with a specified value.

From the **Column** menu, select the column to which the filter criteria is to be applied.

From the **Operator** menu, select an operator.

=: equal to the search string
<: less than the search string
>: greater than the search string
≤: less than or equal to the search string
≥: greater than or equal to the search string
≠: not equal to the search string

Note: To exclude (include) "not equal" values, instead include (exclude) equal values.

Select the name of an existing column from the **Select Column or Enter Value** pull-down menu to compare its cell values with those in the column chosen in the **Column** pull-down menu.
Or
Type a value directly into the field to search for that value in the column selected in the **Column** pull-down menu.

If **Exclude** or **Include** is the action, check the **Apply to entire row** box to exclude/include the entire row when the filter criteria is matched. or clear the checkbox (the default) to exclude or include a cell that matches the criteria.

If **Replace** is the action:

In the **Replace with** field, type the value to place in a cell that matches the filter criteria.

Check the **Replace All** box to replace all instances where the criteria is matched in the specified column (or in all columns if **Any** is specified). Clear the checkbox to only replace the first match in the specified column (or first match in each column if **Any** is specified).

Type a value in the **Tolerance** field to search for values within a range of a numeric search value.

The **Tolerance** field is only available when a numerical value is entered in the **Value** field and is used to find values not different from the numeric search value by more than the tolerance value. This function is optional.

Numeric values that are +/- the tolerance of the search value are considered to match the search value. If a non-numerical value is entered in the **Find** field, then the **Case Sensitive** checkbox is made available.

Select the **Case Sensitive** checkbox to search for strings that match the capitalization used in the search string.

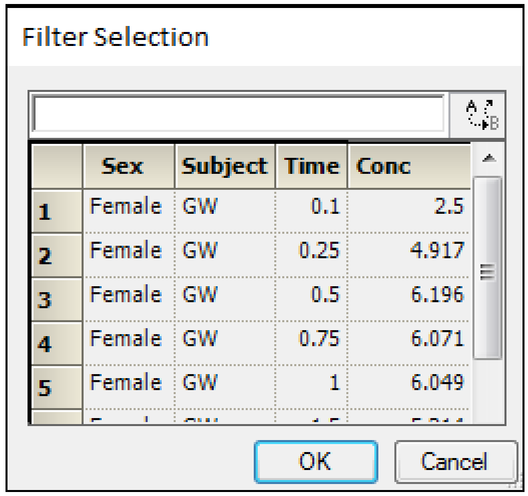
Built-in filter rules:

Blank cells can be filtered by using the term ‘NULL’ in the filter expression to represent the blank cells.

Users can filter cells that contain values with leading single quotes by typing an additional single quote before the value in the *Filter Specification* dialog. For example, to filter a value like ‘000123’, users need to type “`000123`” in the Custom Filter Entry dialog.

Filter Selection dialog

When the **Selection (Exclude)** option is selected in the Options tab, clicking **Add** displays the *Filter Selection* dialog.



Note: If this table is blank, click **Cancel**, check the **Retain Intermediate Results** checkbox in the Options tab, and then click **Add**. The table will be populated.

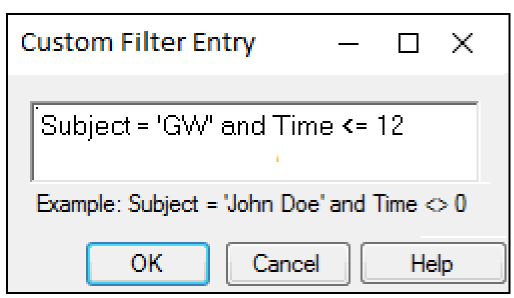
Use the pointer to select part or all of a worksheet.

Click **OK** to exit the *Filter Selection* dialog, or click **Cancel** to exit the dialog without excluding the selected cells.

Note: Adding a **User Selection** filter to the list in the Specify Filter field results in the **Move Up**/**Move Down** buttons in the Data Wizard becoming disabled.

Custom Filter Entry dialog

This section contains the syntax and some of the codes that can be used to create custom inclusion filters for a worksheet. Any standard SQL syntax can be used. Custom filters are defined in the *Custom Filter Entry* dialog.



In the *Custom Filter Entry* dialog, type the custom filter.

Click **OK** to add the filter or click **Cancel** to exit the dialog without adding the filter.

Only one filter can be added at a time in the *Custom Filter Entry* dialog.

Custom filter syntax:

```
[Column name] [Expression] [Value] [Logical operator][Column name]
[Expression] [Value]
```

Example: `Subject='GW' AND Time <= 12`

Logic operators:

Statement grouping is done using the Boolean AND, OR, and NOT operators. Use parentheses to group clauses and force precedence. The AND operator has precedence over other operators.

Example: `(Subject='JDW' OR Subject='LEJ') AND Conc > 1`

When creating comparison expressions, the following operators are allowed:

=: Equals
<>: Not equals
<: Less than
<=: Less than or equal
>: Greater than

Custom filter rules:

- User-defined values can be used in expressions to compare against column values.
  Example: `Effect <= 75.00`
- String values must be enclosed in single quotes.
  Example: `Subject='JDW'`
- String values and column names are not case sensitive.
- Date values should be enclosed with pound signs (#).
  Example: `Date > #12/01/2008#`
- Decimals and scientific notation are permitted for numerical values.
- Blank cells can be filtered by using the term 'NULL' in the filter expression to represent the blank cells.
- A wildcard can be specified by a percent sign with the operator 'like'.
  Example: `Analyte like 'Metabolite%'`

Results

Note: Any step in the Data Wizard can be revisited, revised, and re-executed. All of the steps performed are described carefully in the Summary part of the Output.

All of the steps in the Data Wizard generate output. The output forms specific to a particular kind of operation are specified below. In general, each step in the Data Wizard will create the following output:

Result: The final result of all operations in the step.
Summary: Listing of all steps in the Data Wizard.
Settings: The settings used in all steps.

Additional output when intermediate results are retained.

Final Results: The Results, Summary, and Settings that represent all steps.
Secondary: Non-empty intermediate results that are not used in the final results above.

Additional output when intermediate results are retained

Final Results: The Results, Summary, and Settings that represent all steps.
Intermediate Results: All non-empty intermediate results generated by the steps.

Ratios and baseline adjustments example

This example demonstrates some frequently used calculations, including:

Computing ratios
Creating a baseline-adjusted variable

Most Phoenix objects require the same basic steps for their use. However, there may be multiple paths to accomplishing a step (e.g., main menu, right-click menu, drag-and-drop, etc.). For simplicity, only one is listed here.

Note: Any object added to a project can be viewed in its own window by selecting the object in the Object Browser and double-clicking it or pressing **ENTER**. All instructions for setting up and executing an object are the same whether the object is viewed in its own window or in Phoenix's viewing.

The completed project (`Transformations.phxproj`) is available for reference in …`\Examples\Data and Plots`.

Computing ratios

Phoenix can compute derived parameters as ratios of modeling output parameters. This functionality has been designed specifically for the computation of F (fraction of oral dose absorbed) and for the calculation of metabolite to parent drug ratios.

This example will demonstrate the computation of F. Metabolite to parent drug ratios would be calculated in the same manner.

Two datasets are needed for this example: one with AUC from IV data for 24 subjects, and another with AUC from oral data from the same 24 subjects. These datasets are provided in the Phoenix example subdirectory as `IV.csv` and `Oral.csv`. During the following steps, these datasets will be merged into one dataset, F will be computed for each subject, followed by calculations of the summary statistics for F.

1. Create a new project named `Transformations`.
2. Import …`\Examples\WinNonlin\Supporting files\IV.csv` and `Oral.csv`.
3. Click the **Next Arrow** button and then click **Finish** in the *File Import Wizard* dialog.
4. Right-click the **IV** in the Data folder and select **Send To > Data Management > Join Worksheets**.
5. In the Mappings panel, map the data types as follows:
   Subject to the **Sort** context.
   Form to the **Source Column** context.
   AUC to the **Source Column** context.
6. Select **Worksheet 2** in the Setup list.
7. Drag the **Oral** worksheet from the Data folder to the Worksheet 2 Mappings panel.
8. Map the data types as follows:
   Subject to the **Sort** context.
   Form to the **Source Column** context.
   AUC to the **Source Column** context.
9. Click  (**Execute** icon) to execute the object.

	Subject	Form	AUC	Form_1	AUC_1
1	1	IV	1410.122	Oral	1120.591
2	2	IV	1374.091	Oral	1113.876
3	3	IV	1405.321	Oral	1120.407
4	4	IV	1428.506	Oral	1118.816
5	5	IV	1408.36	Oral	1151.663
6	6	IV	1431.353	Oral	1114.848

Figure 26-1. Portion of Join Worksheets Result worksheet

Calculate F (fraction of oral dose absorbed).

1. Right-click **Workflow** in the Object Browser and select **New > Data Management > Data Wizard**.
2. In the Options tab, select **Transformation** from the **Action** menu.
3. Click the **Add** button.
4. In the Mappings panel for the Data Wizard (Step 1: Transformation), click (**Select Source** icon).
5. In the dialog, select the Join Worksheets object's **Result** worksheet and click **OK**.
6. **Arithmetic** is automatically selected in the **Transformation Type** menu. Do not change this setting.
7. Select **x/y** in the **Transformation** menu.
8. In the **New Column Name** field type `Fraction`.
9. Map the data types as follows:
   AUC_1 to the **y Column** context.
   AUC_2 to the **x Column** context.
10. Execute the object.

Calculate descriptive statistics

1. Right-click **Workflow** in the Object Browser and select **New > Computation Tools > Descriptive Statistics**.
2. Click the **Select Source** icon.
3. Select the Data Wizard object's **Result** worksheet and click **OK**.
4. Map the data types as follows:
   Fraction to the **Summary** context.
   Leave all other data types mapped to **None**.
5. In the Options tab, check the **Confidence Intervals** and **Number of SD Statistics** checkboxes, but do not change the default values for these two items.
6. Check the **Other Statistics** checkbox.
7. Execute the object.

The Statistics worksheet results are shown below:

	Variable	N	NMiss	NObs	Mean	SD	SE	Variance	CV%	Min
1	Fraction	24	0	24	0.79899307	0.016351252	0.003337685	0.00026736343	2.0464823	0.76386828

Median	Max	Range	Mean Log	SD Log	Geometric Mean	Geometric SD	Geometric CV%
0.79959515	0.82030833	0.056440052	-0.22460449	0.02052611	0.7988321	1.0207382	2.0528272

CI 95% Lower	CI 95% Upper	CI 95% Lower Mean	CI 95% Upper Mean	CI 95% Lower Var	CI 95% Upper Var
0.76516793	0.83281821	0.79208854	0.80589759	0.00016150381	0.000526101

CI GEO 95% Lower	CI GEO 95% Upper	CI 95% Lower GEO Mean	CI 95% Upper GEO Mean	Lower 1SD	Upper 1SD
0.76562255	0.83348215	0.79193821	0.80578601	0.78264181	0.81534432

GEO Upper 1SD	Sum	Harmonic Mean	Skewness	Skewness Pop	Kurtosis	Kurtosis Pop	Pseudo SD	KS PValue
0.81539846	19.175834	0.79867053	-0.28376537	-0.26571283	-376.25732	-0.92552059	0.01644706	0.77891952

Creating a baseline-adjusted variable

In many cases it is useful to fit a model to a variable with some endogenous or baseline level, for example, blood pressure or estrogen levels. The calculation of these PK parameters would generally be done on the baseline-adjusted observation values. This example will compute the change from baseline in a response variable, creating an analysis-ready new column of data.

Compute the change from baseline using a column transform.

1. Import …`\Examples\WinNonlin\Supporting files\endogenous.dat`.
   Click **Finish** in the *File Import Wizard* dialog.
2. Right-click **Workflow** in the Object Browser and select **New > Data Management > Data Wizard**.
3. In the Options tab, select **Transformation** as the **Action** and click **Add**.
4. Drag the **endogenous** worksheet from the Data folder to the Data Wizard 1 object Main Mappings panel.
5. Select **Baseline** in the **Transformation Type** menu on the Options tab.
6. Select **Change from Baseline** in the **Transformation** menu.
7. In the **New Column Name** field type `Change`.
8. In the Main Mappings panel, map the data types as follows:
   Time to the **Time** context.
   Conc to the **x Column** context.
9. Execute the object.

	Time	Conc	Change
1	0	10.02	0
2	1	52.4991	42.4791
3	2	63.048	53.028
4	3	61.5303	51.5103
5	4	80.7451	70.7251

Figure 26-2. Part of Column Transformation Result worksheet

The Change column is added to the dataset and is ready for use in modeling.

10. Right-click the project and select **Close Project**.

This includes the Transformations — Ratios and Baseline Adjustments example.

Descriptive Statistics

Phoenix can compute summary statistics for variables in any worksheet. This feature is frequently used to create data to plot means and standard errors, for preclinical summaries, to summarize modeling results, or to test for normal distribution of data. Separate statistics for subgroups are obtained through the use of one or more sort variables.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Computation Tools > Descriptive Statistics**.
Or Main menu: **Insert > Computation Tools > Descriptive Statistics**.
Or right-click menu for a worksheet: **Send To > Computation Tools > Descriptive Statistics**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

This section includes information on the following:

User interface description
Statistical results and computational formulas
Weighted summary statistics

User interface description

Main Mappings panel
Options tab

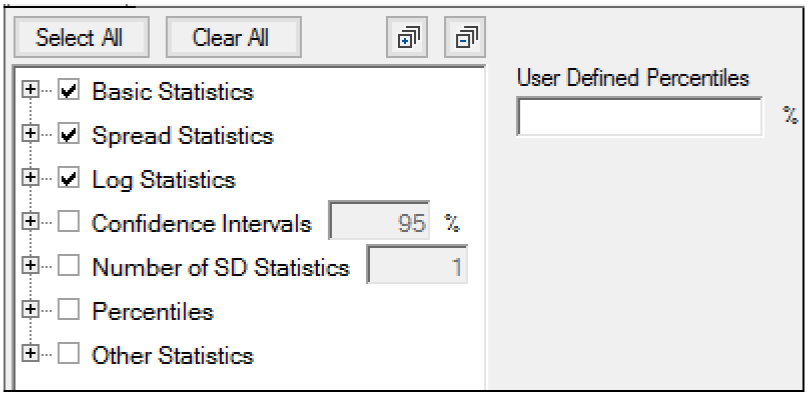
Main Mappings panel

Use the Main Mappings panel to identify which variables are used to compute statistics or weight the data. Required input is highlighted orange in the interface.

None: Data types mapped to this context are not included in any computation or output.
Summary: The variable(s) for which statistics are computed.
Sort: Categorical variable(s) identifying individual data profiles, such as subject ID or gender. Separate statistics are computed for each unique combination of sort variables.
Weight: If a weight variable is present in the dataset, it can be used to weight the summary statistics. If a weight is non-numeric or missing, the observation is excluded from the analysis. If a weight is negative, it is changed to zero (0) upon execution.

Options tab

See “Statistical results and computational formulas” for a full list of the available statistics.



Use the tree on the right to select the statistics to compute and include in the report by checking the corresponding checkboxes.

> The available statistics are grouped into categories and checking/unchecking a category checkbox controls all of the checkboxes for statistics within that category. For example, unchecking the **Spread Statistics** checkbox unchecks the **Min**, **Median**, **Max**, and **Range** checkboxes.
>
> Click the **Select All** or **Clear All** buttons to quickly check/uncheck all checkboxes in the list, respectively, with a single click.
>
> Click the  button to expand all categories in the tree. Click the  button to collapse all categories in the tree.

There are a number of preset percentiles available in the **Percentiles** category (1, 2.5, 5, 10, 25, 50, 75, 90, 95, 97.5, 99). However, if you wish to include other percentiles, enter them as a comma-separated list in the **User-specified percentiles** field.

To generate confidence interval statistics, type the desired confidence interval in the **Confidence Interval** field.

> Check the **Confidence Intervals** checkbox to compute all statistics in that category or expand the category to select a subset of the statistics

To generate standard deviation statistics, type the desired number of standard deviations in the **Number of SD Statistics** field. The value must be greater than 0 and less than or equal to 10.

> Check the Number of SD Statistics checkbox to compute all statistics in that category or expand the category to select a subset of the statistics.

Statistical results and computational formulas

The Descriptive Statistics object creates a Statistics worksheet and a Settings text file in the Results tab. The Statistics worksheet includes summaries of all statistical computations. The Settings file contains user-specified settings.

CI GEO X% Lower: Lower limit of an X% confidence interval for the logs of the data, back-transformed to original scale:

$$\exp(Mean\_Log - t_{\alpha/2} \times SD\_Log)$$

CI GEO X% Upper: Upper limit of an X% confidence interval for the logs of the data, back-transformed to original scale:

exp($Mean\_Log + t_{\alpha/2}$ x SD_Log)

where (1 – α)*100 is the percentage given for the confidence interval
and $t_{\alpha/2}$ is from the t-distribution with N–1 degrees of freedom.

CI X% Lower: Lower limit of an X% confidence interval for the data (i.e., confidence interval that tells the range that is expected to have X% of the data)

$Mean$ – ($t_{\alpha/2}$ x SD)

CI X% Lower GEO Mean: Lower limit of an X% confidence interval for the Geometric Mean:

$$\exp\left(Mean\_Log - t_{\alpha/2}\frac{SD\_Log}{\sqrt{N}}\right)$$

(equivalently, exp of the lower CI for $Mean\_Log$).

CI X% Lower Mean: Lower limit of an X% confidence interval for the mean (i.e., the confidence interval in which the mean exists with X% certainty)

$$Mean - t_{\alpha/2}\frac{SD}{\sqrt{N}}$$

CI X% Lower Var: Lower limit of an X% confidence interval for the variance (i.e., the confidence interval in which the variance exists with X% certainty):

$$\frac{(N-1) \times Variance}{\chi_U^{\ 2}}$$

where χ_u^2 is from the χ^2-distribution with N–1 degrees of freedom.

χ_u^2 cuts off an upper tail of area α/2 where (1–α)*100 is the percentage for the confidence interval.

CI X% Upper: Upper limit of an X% confidence interval for the data:

$$Mean + t_{\alpha/2}SD$$

where (1–α)*100 is the percentage given for the confidence interval,
and $t_{\alpha/2}$ is from the t-distribution with N–1 degrees of freedom.

CI X% Upper GEO Mean: Upper limit of an X% confidence interval for the Geometric Mean:

$$\exp\left(Mean\_Log + t_{\alpha/2}\frac{SD\_Log}{\sqrt{N}}\right)$$

where (1 – α)*100 is the percentage given for the confidence interval,
and $t_{\alpha/2}$ is from the t-distribution with N – 1 degrees of freedom.

CI X% Upper Mean: Upper limit of an X% confidence interval for the mean:

$$Mean + t_{\alpha/2}\frac{SD}{\sqrt{N}}$$

where $(1-\alpha)*100$ is the percentage given for the confidence interval,
and $t_{\alpha/2}$ is from the t-distribution with $N-1$ degrees of freedom.

Thus, a 95% confidence level indicates that $\alpha=0.05$. Note that for $N>30$, the t-distribution is close to the normal distribution.

CI X% Upper Var: Upper limit of an X% confidence interval for the variance:

$$\frac{(N-1) \times Variance}{\chi_L^{\ 2}}$$

where χ_L^2 is from the χ^2-distribution with $N-1$ degrees of freedom.

χ_L^2 cuts off a lower tail of area $\alpha/2$ where $(1-\alpha)*100$ is the percentage for the confidence interval.

CV%: Coefficient of variation: $(SD/Mean)*100$

GEO Lower XSD and GEO Upper XSD: Range determined by adding or subtracting "X" log standard deviations from the log-mean, back-transformed to original scale:

$$\exp(Mean\_Log \pm X(SD\_Log))$$

When X=1, this range is equivalent to: ($Geometric\_Mean$/exp(SD_Log) and $Geometric\_Mean$*exp(SD_Log))

Geometric CV%: Geometric coefficient of variation:

$$\sqrt{\exp((\mathrm{SD\_log})^2) - 1} \times 100$$

Geometric Mean: N^{th} root of the product of the N observations. Equivalently, the exponential of the $Mean\_Log$. Each value must be > zero:

$$\sqrt[n]{X_1 X_2 X_3 \ldots X_n}$$

$$\exp\left(\frac{1}{n}\sum_{i=1}^{n} \ln X_i\right)$$

Geometric SD: Geometric standard deviation of the natural logs of the observations exp (SD_Log)

Harmonic Mean: Reciprocal of the arithmetic mean of the reciprocals of the observations:

$$\frac{N}{\sum_{i=1}^{N} \frac{1}{x_i}}$$

IQR: Interquartile range is the difference between the first and third quartiles (i.e., the middle 50% of the data). IQR is only included in the output when the **Include Percentiles** checkbox is checked.

KS PValue: Kolmogorov-Smirnov normality test ρ value. This quantifies the distance between the empirical distribution function of the data and the cumulative distribution function of the Normal distribution. The empirical distribution function F_n for n independent and identically distributed observations X_i is defined as:

$$F_n(x) = \frac{1}{n}\sum_{i=1}^{n} I_{X_{i \le x}}$$

where $I_{X_{i \le x}}$ is the indicator function and = 1 if $X_i \le x$, otherwise 0.

The Kolmogorov-Smirnov statistic for a given cumulative distribution function $F(x)$ is:

$$D_n = \sup_x |F_n(x) - F(x)|$$

where $\sup x$ is the supremum of the set of distances. A ρ-value is then computed to determine the significance of D_n.

Kurtosis: Sample coefficient of excess (sample excess kurtosis):

$$\left(\frac{(N-1)}{(N-2)(N-3)}\right)\left[(N+1)\left(\frac{(\Sigma(x_i-\bar{x})^4)/N}{[\Sigma(x_i-\bar{x})^2/N]^2}-3\right)+6\right]$$

Sample Excess Kurtosis=[Population Excess Kurtosis*(N+1)+6]*(N–1)/[(N–2) x (N–3)]

Kurtosis Pop: Population coefficient of excess (population excess kurtosis):

$$\frac{\Sigma(x_i-\bar{x})^4/N}{[\Sigma(x_i-\bar{x})^2/N]^2}-3$$

Population Excess Kurtosis=((Sample Excess Kurtosis x (N–2) x (N–3)/(N–1)) –6)/(N+1)

Lower XSD and Upper XSD: Range determined by adding or subtracting X standard deviations from the mean $Mean$ +/– $X*SD$

Max: Maximum value

Mean: Arithmetic average

$$\frac{\sum_{i=1}^{N}(X_i)}{N}$$

Mean log: Arithmetic average of the natural logs of the observations

$$\frac{\sum_{i=1}^{N}\ln(X_i)}{N}$$

Median: Median value — from the percentiles computations, 50^{th} percentile.

Min: Minimum value.

N: Number of observations with non-missing data (i.e., numeric observations).

NMiss: Number of observations with missing data (i.e., non-numeric observations such as text or blanks).

NObs: Number of observations (i.e., $N+NMiss$)

P(ercentiles): The P^{th} percentile divides the distribution at a point such that P percent of the distribution are below this point. For a sample size of n, the quantile corresponding to the proportion p ($0<p<1$) is defined as:

$Q(\mathrm{p})=(1-f)*x(j)+f*x(j+1)$

where:
$j = \mathrm{int}(p*(n+1))$, (integer part)
$f = p*(n+1) - \mathrm{j}$, (fractional part)
$x(j)$ = the j-th order statistic

The above is used if $1 \leq j < n$. Otherwise, the empirical quantile is the smallest order statistic for j=0 or the largest order statistic for j=n.

(Definition 6 in Hyndman and Fan, "Sample Quantiles in Statistical Packages", American Statistician, Nov 1996. Equivalent to SAS PCTLDEF 4, Excel PERCENTILE.EXC, and NIST Engineering Statistics Handbook, Section 7.2.6.2, Percentiles.)

Pseudo SD: Jackknife estimate of the standard deviation of the harmonic mean. For n points, x_1, … x_n, the pseudo standard deviation is:

$$\sqrt{(n-1)\sum_{i=1}^{n}(\overline{H}_i-\overline{H})^2}$$

where:

$$\overline{H} = \frac{1}{n}\sum_{i=1}^{n}\overline{H}_i$$

and:

$$\overline{H}_i = \frac{(n-1)}{\frac{1}{x_1}+\frac{1}{x_2}+\ldots+\frac{1}{x_{x-1}}+\frac{1}{x_{x+1}}+\ldots+\frac{1}{x_n}}$$

$$= \frac{(n-1)}{\left(\sum_{i=1}^{n}\frac{1}{x_i}\right)-\frac{1}{x_i}}$$

Range: Range of values (maximum value minus minimum value).

SD: Standard Deviation:

$$\sqrt{\quad}$$

SD Log: Standard deviation of the natural logs of the observations:

$$\sqrt{\frac{\sum_{i=1}^{N} (\ln(X_i) - MeanLog)^2}{N-1}}$$

SE: Standard Error:

$$\frac{SD}{\sqrt{N}}$$

Skewness: Sample coefficient of skewness (sample skewness):

$$\left(\frac{\sqrt{N(N-1)}}{N-2}\right)\left(\frac{\Sigma(x_i - \bar{x})^3 / N}{[\Sigma(x_i - \bar{x})^2 / N]^{3/2}}\right)$$

Sample Skewness=Population Skewness*sqrt(N*(N–1))/(N–2)

Skewness Pop: Population coefficient of skewness (population skewness):

$$\frac{\Sigma(x_i - \bar{x})^3 / N}{[\Sigma(x_i - \bar{x})^2 / N]^{3/2}}$$

Population Skewness=Sample Skewness*(N–2)/sqrt(N*(N–1))

Sum: Sum of the values in the column mapped to Summary:

$$\sum_{i=1}^{N} x_i$$

Variance: Unbiased sample variance:

$$\frac{\sum_{i=1}^{N} (X_i - \bar{X})^2}{N-1}$$

Units

When summary statistics are calculated for a variable with units, some of the output will have units. Assuming that the variable summarized is x and has x-$units$ specified, the units for the summary statistics are:

N, **NMiss**, **NObs**: No units
CV%, **Geometric CV%**: No units
Skewness, **Skewness Pop**, **Kurtosis**, **Kurtosis Pop**, **KSP Value**: No units
Mean Log, **SD Log**: No units
Variance: x-unit^2
CI Lower Var, **CI Upper Var**: x-unit^2
Everything else: x-unit

If more than one Summary variable is mapped, with at least two of those variables having units in the input dataset, and the units differ, a stacked Units column is displayed in the Statistics output worksheet that reports the units of the Summary variables. In cases where the input data does not have units, or the units are all the same, then the units of the statistics are displayed in the column headers.

Weighted summary statistics

Summary statistics can be weighted by selecting a column in the dataset in the Main Mappings panel to provide weights. If a weight is non-numeric or missing, the observation is excluded from the analysis. Weighted descriptive statistics output also includes a text file called Settings that contains user-specified settings. Some summary statistics and all percentiles are excluded in weighted output.

Results and computational formulas for weighted calculations

The output for weighted summary statistics contains a column indicating the summary variable(s), one for each sort variable, and the statistics listed below.

CI X% Lower: Lower limit of an X% confidence interval for the weighted data:
$$\textit{Weighted Mean} - t_{\alpha/2} \times \textit{Weighted SD}$$

CI X% Lower Mean: Lower limit of an X% confidence interval for the weighted mean.

CI X% Lower Var: Lower limit of an X% confidence interval for the weighted variance.

CI X% Upper: Upper limit of an X% confidence interval for the weighted data:
$$\textit{Weighted Mean} + t_{\alpha/2} \times \textit{Weighted SD}$$

CI X% Upper Mean: Upper limit of an X% confidence interval for the weighted mean.

CI X% Upper Var: Upper limit of an X% confidence interval for the weighted variance.

CV%: Weighted coefficient of variation:
$$(\textit{Weighted SD}/\textit{Weighted Mean})*100$$

Kurtosis Pop: Weighted coefficient of excess (population excess kurtosis):

$$\frac{\dfrac{\Sigma w_i (x_i - x_w)^4}{N}}{\left[\dfrac{\Sigma w_i (x_i - \bar{x}_w)^2}{N}\right]^2} - 3$$

Lower XSD and **Upper XSD**: Range determined by adding or subtracting X weighted standard deviations from the weighted mean:
$$\textit{Weighted Mean} +/- X*\textit{Weighted SD}$$

Max: Maximum value

Mean: Weighted arithmetic average:

$$\frac{\Sigma w_i \times x_i}{\Sigma w_i}$$

Min: Minimum value

N: Number of non-missing observations (including those with weights=zero)

NMiss: Number of observations with missing data

NObs: Number of observations (including observations with weights=zero)

Range: Range of values (maximum value minus minimum value)

SD: Weighted standard deviation:

$$\sqrt{Weighted\ Variance}$$

SE: Weighted standard error:

$$\frac{Weighted\ SD}{\sqrt{N}}$$

Skewness Pop: Weighted coefficient of skewness (population skewness):

$$\frac{\Sigma w_i(x_i - \bar{x}_w)^3 N}{[\Sigma w_i(x_i - \bar{x}_w)^2 / N]^{3/2}}$$

Sum: Weighted Sum:

$$\Sigma w_i \times x_i$$

Variance: Weighted variance:

$$\frac{\Sigma w_i(x_i - \bar{x}_w)^2}{N - 1}$$

where $\bar{x}_w$ is the weighted mean.

ggquickeda

The ggquickeda object provides access to the ggquickeda R shiny application, which is an interface to ggplot2/table1. The application enables quick exploration of data to detect trends on the fly. You can do scatter plots, dot plots, box plots, bar plots, histograms, densities, and summary statistics tables.

The ggquickeda object requires:

- Installation of R: It is recommended that the version of R required to run the ggquickeda package be verified by looking at the ggquickeda documentation on the cranr-project.org website.
- Configuration of the Phoenix R plugin: Use the Phoenix *Preferences* dialog (**Edit > Preferences**) to set the location of the R executable.
- Installation of the R package ggquickeda: Use R package installation process (e.g., `install.packages("ggquickeda")`). All other R packages required to run ggquickeda will also be installed. For a list of these additional packages, see the ggquickeda documentation on the cranr-project.org website.

Information on using the ggquickeda package can be found at
https://cran.r-project.org/web/packages/ggquickeda/vignettes/ggquickeda.html
and
https://cran.r-project.org/web/packages/ggquickeda/vignettes/AdditionalPlotsStats.html

Use one of the following to add the object to a Workflow:

Right-click menu for a worksheet: **Send To > External Software > ggquickeda**.
Right-click menu for a Workflow object: **New > External Software > ggquickeda**.
Main menu: **Insert > Open External Software > ggquickeda**.

Note: A dataset must be mapped to the object before the ggquickeda interface is displayed. To do this, use the **Select Source** button in the area to the right of the Object Browser. If you use drag and drop instead, be sure to drag to the top area near the **View Source** button on the right until the mouse cursor changes from unavailable to available and then release the mouse button (otherwise, the dataset will not be mapped and the interface will not open).

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Once you have executed the ggquickeda object, import the results into Phoenix to continue your analysis.

Integral

Integral is a database system for secure storage of study data and analyses. Integral provides a secure data management system with complete auditing capabilities. The combination of Integral and Phoenix provides an effective means to share source data, models, scripts and results among the members of a drug development team. The combination also supports compliance with the U.S. Food and Drug Administration's 21 CFR Part 11 regulation.

Phoenix can work in conjunction with Integral for secure storage and change tracking for data and analyses. This section covers the use of Phoenix as an Integral client: loading Integral data to Phoenix and saving data from Phoenix as Integral projects and experiments. Integral can also be accessed by way of a Web interface, which provides additional operations. The Integral functions and operations are covered in the Certara Integral documentation.

This section contains the following topics:

Accessing the Integral browser

Note: Connection to Integral from Phoenix requires the setting of some preference options. Refer to "Setting up a connection" for more information.

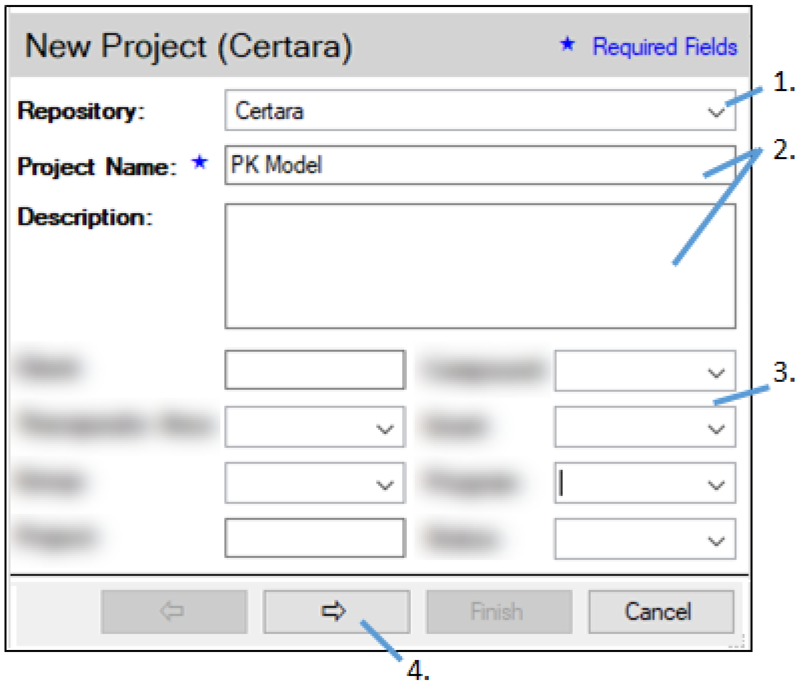
Selecting **Integral > Browser** from the main Phoenix menu displays the login page of Integral. Once credentials are verified, the Integral interface is presented. For details on using this interface, go to Certara Integral documentation.

Use the red X button to close the Integral browser dialog when finished.

Adding a project to Integral

Note: Connection to Integral from Phoenix requires the setting of some preference options. Refer to "Setting up a connection" for more information.

An Integral project can be created from a project loaded in Phoenix. With the project selected in the Object Browser, select **Integral > Save to New Project** (or right-click a project in the Object Browser and select **Save to New Project in Integral**). If a connection to Integral has not been established, you will be asked to enter your log in credentials first.



1. All of the repositories to which you have been permitted access are listed in the **Repository** pull-down menu. Select the one to which the project is to be saved.
2. Enter the name (**Project Name**) and a description (**Description**) of the project.
3. Use the remaining fields and pull-downs to enter additional information.

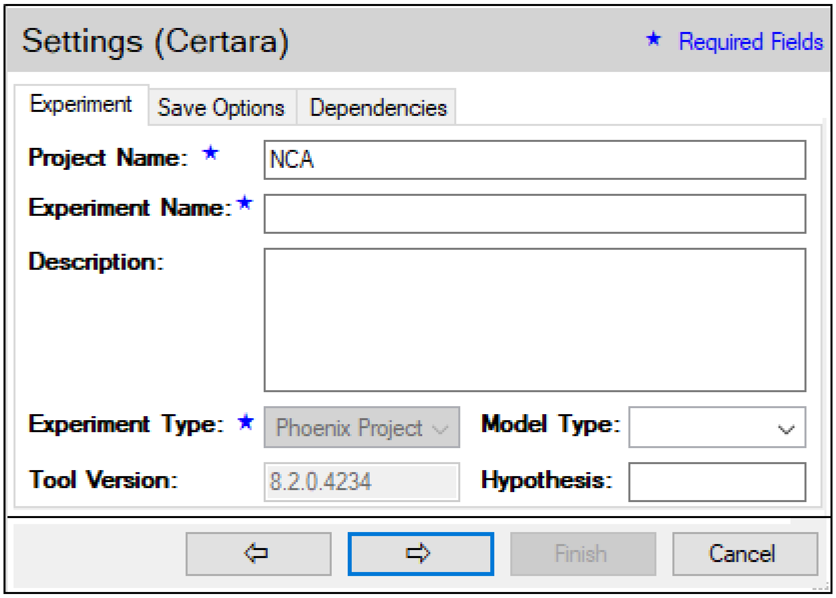
   The options available in the dialog are controlled by the administrator.
4. When finished, click **Next Arrow** button to continue to the Settings page (see "Defining the settings for a project").

Defining the settings for a project

The settings for a project are divided into three separate tabs:

- Experiment tab
- Save Options tab
- Dependencies tab

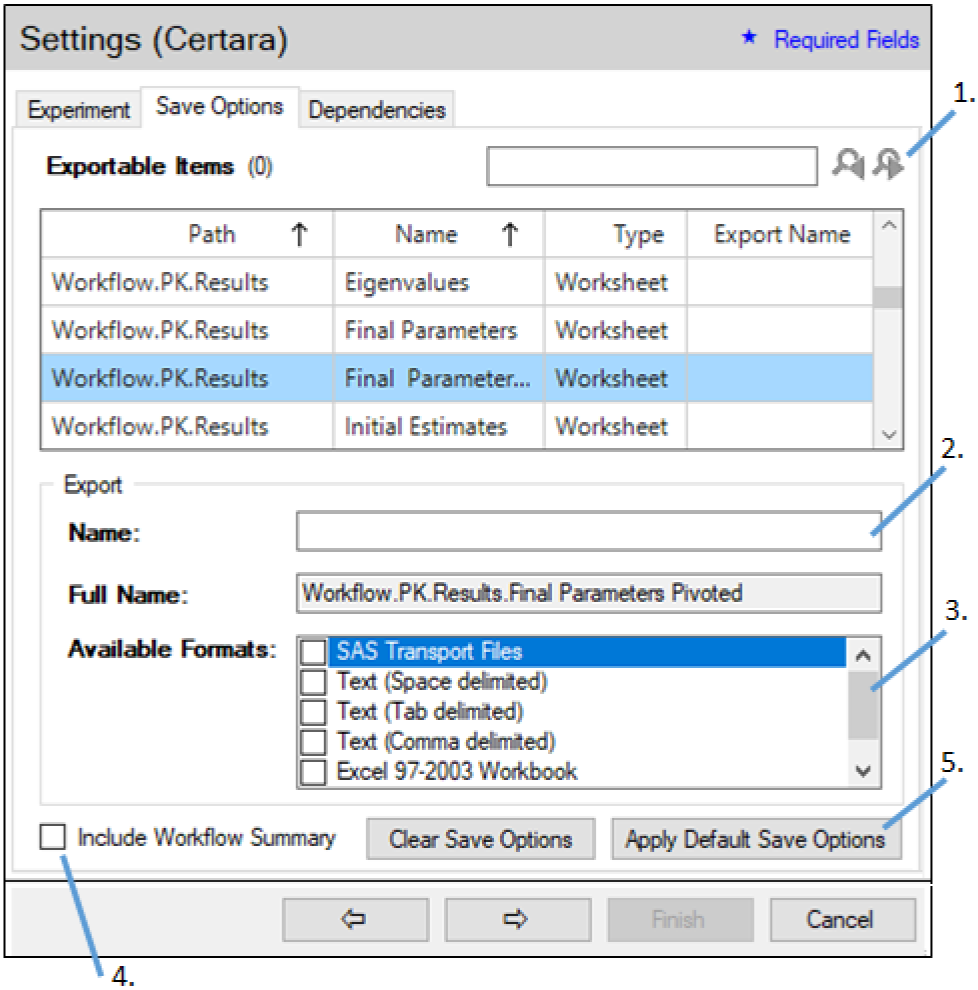
Experiment tab



In the **Experiment** tab, define an experiment in the project using the available fields and menus. The options available are set up by the administrator.

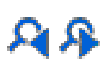
Save Options tab

Click the **Save Options** tab to set up what and how the project items will be saved to Integral.



In the **Save Options Settings** tab, each item available for export listed.

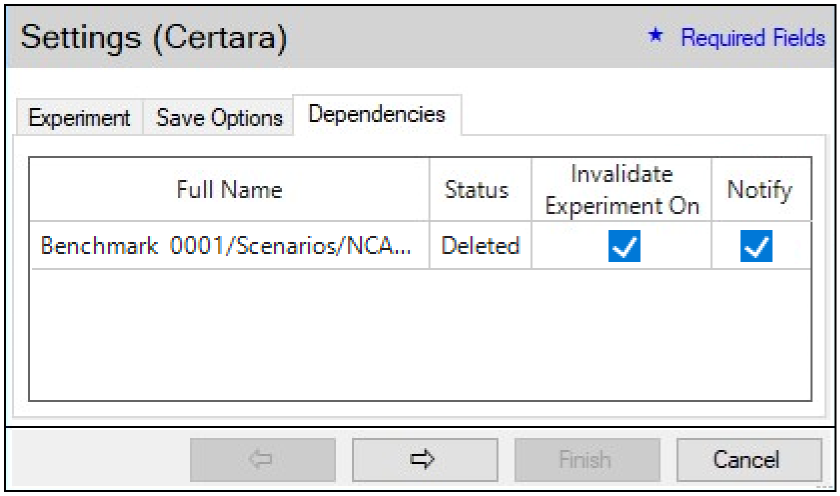
1. Search through the list by entering the query in the field above the list and using the following buttons to find the next or previous instance of the query.

2. If a name other than the one assigned by Phoenix (shown in the **Full Name** field) is to be used when exporting an item, select the item and enter the new name in the **Name** field.
3. Select the format(s) in which to export the item by checking the box(es) in the **Available Formats** list.
4. If the **Include Workflow Summary** box is checked, a `Workflow Summary.zip` file is saved in the project.
5. Use the **Clear Save Options** button to remove any user-entered names or format settings. Use the **Apply Default Save Options** button to use the default settings for the data type of the selected item. See "Configuring default save options" for details on setting up default save options.

Dependencies tab

Click the **Dependencies** tab to set dependency tracking options.



Objects loaded from Integral into the current project are listed in the Dependencies tab, along with their current status.

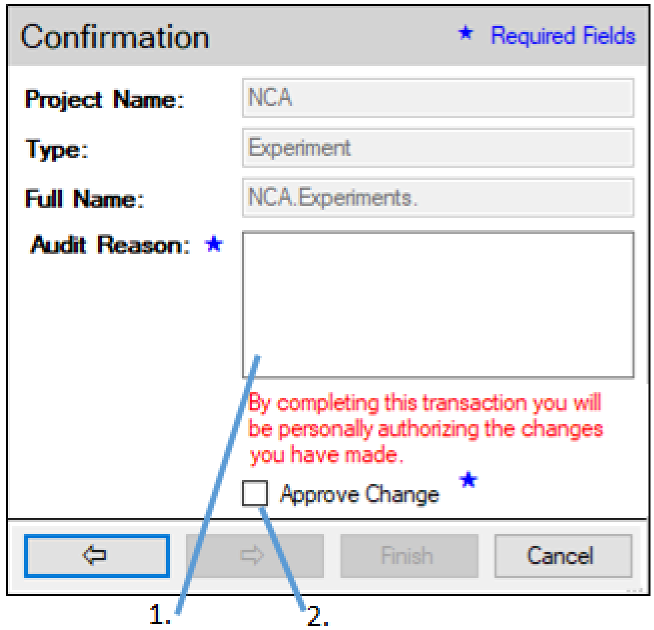
Checking the **Invalidate Scenario On** box for a dependency causes experiments that reference the object to be marked as out-of-date (i.e., invalidated) when a different version of the object is saved to Integral. Clearing the checkbox will result in an experiment not being marked out-of-date when a new version is saved to Integral.

Check the **Notify** box to send the user a message when the experiment is invalidated.

After setting the experiment properties, save options, and dependency customizations, click **Next Arrow** button to continue to the Confirmation page (see "Confirming changes").

Objects loaded from the Integral into Phoenix projects have their dependencies maintained.

Confirming changes



1. In the Confirmation page, enter a statement regarding the new project being added to Integral in the **Audit Reason** field.
2. Check the **Approve Change** box to authorize submission to Integral.
3. Click **Finish**.

The saving process begins and a progress dialog is displayed. Once the Phoenix project has been saved to Integral, the progress dialog goes away.

Note: When a Phoenix project is loaded into Integral for the first time, a SavePoint (i.e., a snapshot of the experiment) will not be registered. Only after it is loaded into Phoenix from Integral and saved back will SavePoints and versions be registered.

Saving updated projects to Integral

The Integral **Save** and **Save As** options are enabled when a project that has already been saved in Integral is loaded into the Object Browser. These options are located in the **Integral** menu or on the right-click menu for a project in the Object Browser as **Save to Integral** and **Save As to Integral**.

Using the **Save** option creates a SavePoint for the experiment in Integral. A SavePoint is essentially a snapshot of the experiment as it currently exists. At any point in the future, you are able to take the experiment back to a prior state by loading the corresponding SavePoint.

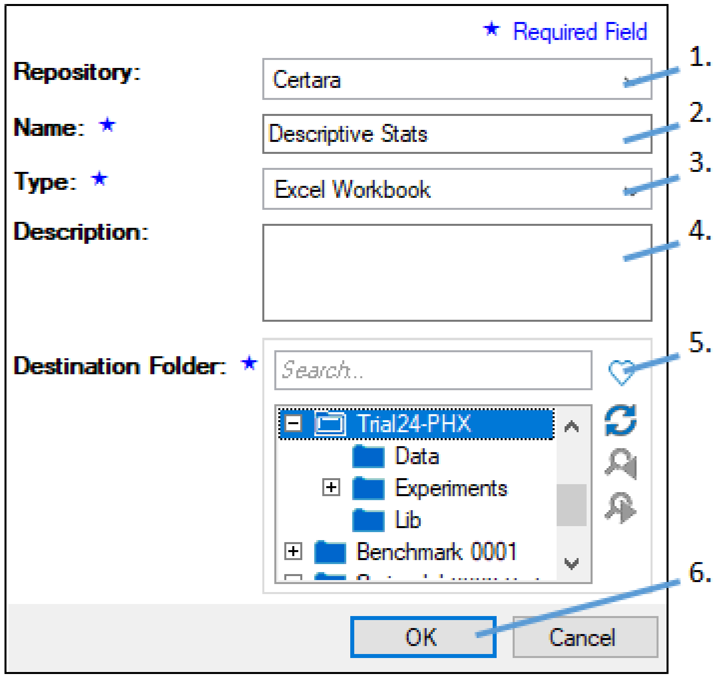
Once you load an experiment from Integral into Phoenix, create a SavePoint before making any changes. You can then easily return to the starting point as needed. If you try to create a SavePoint after making changes to the experiment, you are warned about the changes and asked to choose to either save the changes as a new experiment (**Save As**) or discard the changes and load the latest saved version from Integral (**Get Latest**).

Using the **Save As** option, as mentioned in the previous paragraph, creates a new experiment.

Selecting either **Save** or **Save As** takes you to the *Settings* dialog, where you can make the necessary modifications before saving to Integral. See "Defining the settings for a project".

Adding items to Integral

With the item to save selected in the Object Browser, select **Integral > Add Selected Item** (or right-click the item in the Object Browser and select **Add Selected Item to Integral**).



1. All of the repositories to which you have been permitted access are listed in the **Repository** pull-down menu. Select the one to which the item is to be saved.
2. Enter a name (**Name**) for the item or use the default name.
3. Select the type of the item being added from the **Type** pull-down.
4. Enter a description (**Description**) of the item.
5. Select the Integral folder in which to save the item from the list.
   To search through the list:

   -Enter the query in the field above the list.

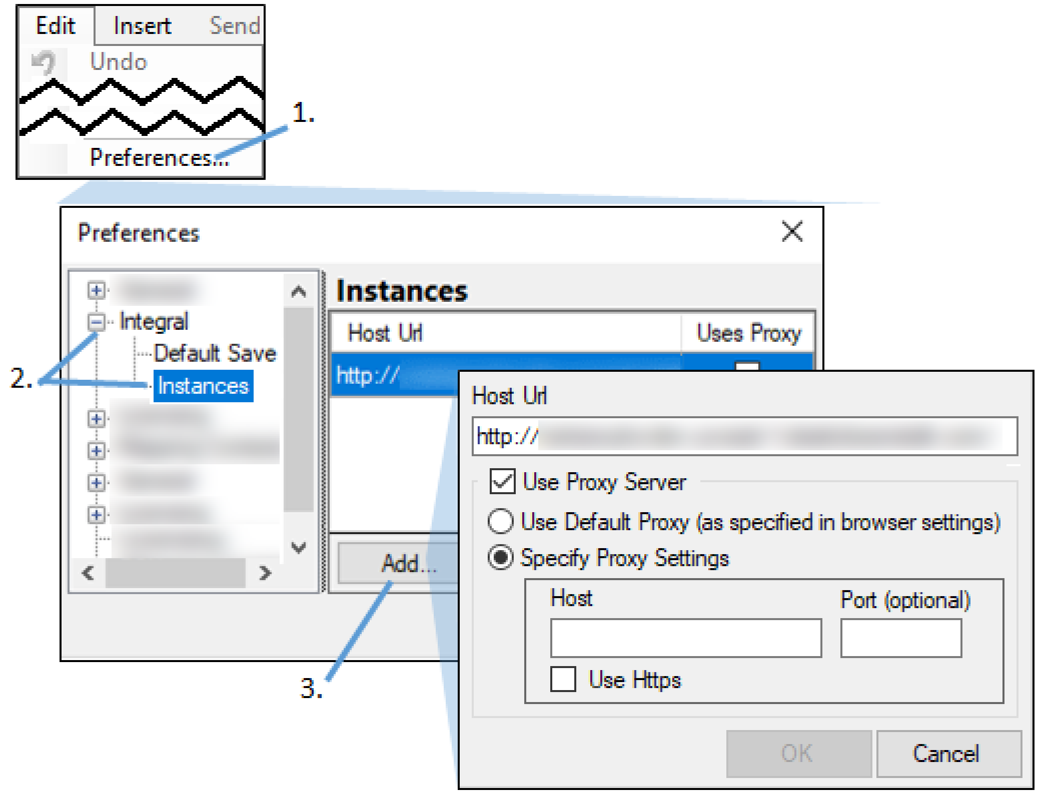
   -Use to find the next or previous instance of the query.

   - Load a list of favorite locations in Integral by clicking .

   - To refresh the list, click .
6. Click **OK** to add the item to Integral.
7. Use the Integral browser to view the newly added item.

Setting up a connection

The Integral connection information must be provided before Phoenix can connect to Integral.



1. Select **Edit > Preferences.**
2. In the *Preferences* dialog, click the (**+**) sign beside Integral and select **Instances**.
3. Click **Add** to display the *Integral Configuration* dialog and enter the configuration properties.

   To connect directly, enter the address to the web site in the **Host Url** field.

   To connect via proxy, check the **Use Proxy Server** box and then choose whether to **Use Default Proxy** or **Specify Proxy Settings** by entering the **Host** and **Port** information to access a different proxy. (Check the **Use Https** box if this is an HTTPS proxy server.)
4. Click **OK** to save the new Integral instance.

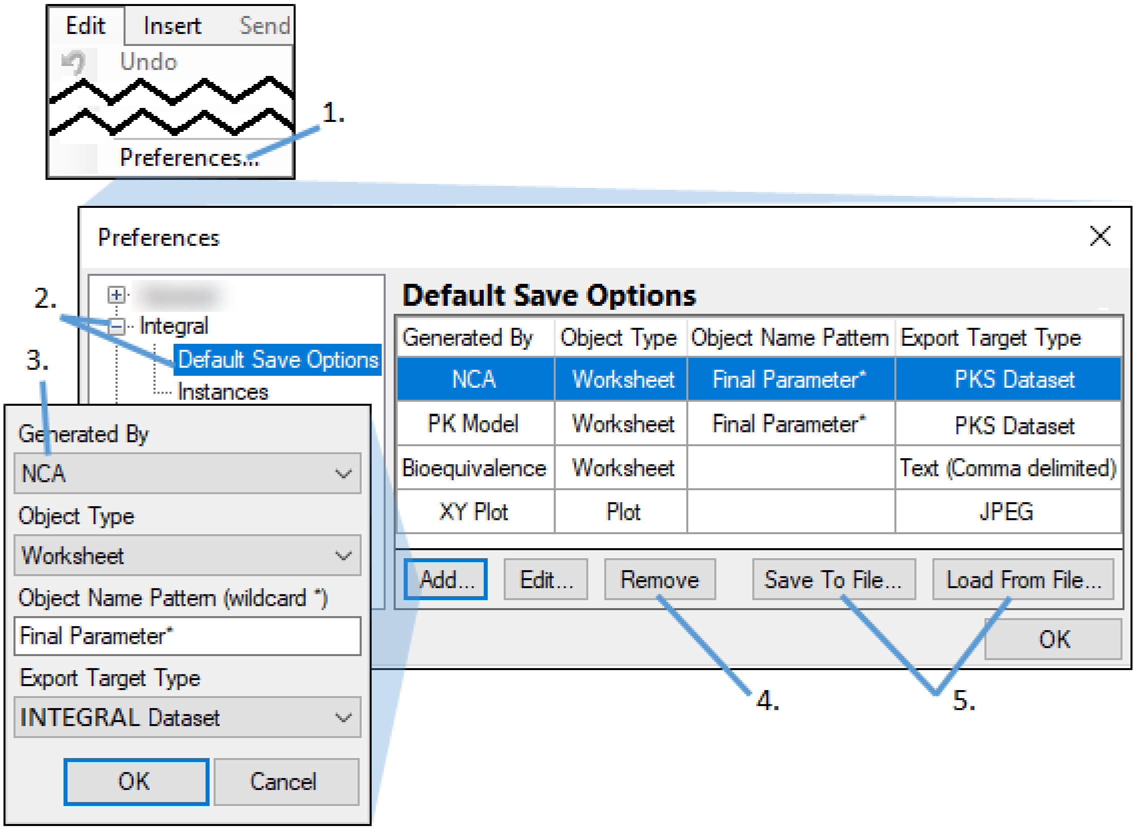
To edit an existing Integral instance definition, select it in the *Preferences* dialog and click **Edit**. Then make the modifications in the displayed dialog.

To delete the instance definition, select it in the *Preferences* dialog and click **Remove**.

Note: Users cannot edit or remove instances to which they are currently connected.

Configuring default save options

The default save options can be configured in the Integral section in the *Preferences* dialog. The default save options determine how operational object output is displayed in Integral. An operational object's output should be displayed when it is useful for data mining or reports, or if the output is loaded individually into another project to be re-used or shared.



1. Select **Edit > Preferences**.
2. In the *Preferences* dialog, select **Integral > Default Save Options**.
3. To add a default save option, click **Add**.
   To edit an option, select it and click **Edit**.

   In the *Default Save Option* dialog, use the pull-down menus and field to define a save option. For example, the previous image shows a new default save option being defined involving NCA. When the program encounters an NCA generated worksheet with a name that starts with “Final Parameter”, it is to be exported to Integral as an Integral Dataset.
4. To remove a save option, select the option and click **Remove**.
5. To save the defined options to an XML file, click **Save to File**, then select a location and enter a filename in the dialog. To load options from a file, click **Load from File**.

Saving the default save options to a file is a useful way of synchronizing settings across an organization.

Using PKS scenarios and Integral

If you have the legacy PKS plugin, you can continue to use it to update data and scenarios. Any changes made through the PKS plugin will be synced with the information in Integral. However, the reverse situation is not true. Change made through Integral will not be synced to PKS.

PKS scenarios can be opened in Phoenix through the Integral plugin by going to the corresponding project and loading the desired scenario. Phoenix will open the scenario as a project. Note that a new version of the scenario cannot be saved, but it can be saved as a new project in Integral. (Right-click the scenario in the Object Browser and select **Save to New Project in Integral**.)

NONMEM Shell

The NONMEM object runs NONMEM models by using NONMEM control files and datasets. The results are returned to Phoenix.

Note: Phoenix program plugins, such as the NONMEM object, assume that the corresponding third party software is installed and running properly.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > External Software > NONMEM Shell**.
Or Main menu: **Insert > External Software > NONMEM Shell**.
Or right-click menu for a worksheet: **Send To > External Software > NONMEM Shell**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

This sections contains information on the following topics:

Setting up preferences

Global preferences are available to the user. Some third party tool objects require certain global settings to be specified prior to use. There are optional settings to enable editing of scripts in external programs from within Phoenix. Some optional preferences can streamline the workflow by automatically filling in or setting options in the object's UI with information entered by the user in the *Preferences* dialog.

To set up access to the external program

Select **Edit > Preferences**.

In the *Preferences* dialog, select the **NONMEM** in the menu tree.

Enter the path to the batch file in the first field or click **Browse** to locate and select the file/directory.

Click **Test** to make sure the correct file is selected.

To specify a development environment

There is a Development Environment section available on the preference pages. When the development environment is defined in this section, users can access that environment from the NONMEM object's Options tab with the **Start** button. This allows users to edit scripts in other specified environments, and then pull the updated scripts back into Phoenix, at which time, the script can be executed from Phoenix and the output processed through the normal Phoenix workflow.

In the **Command** field, enter the directory path to the executable or click **Browse** to locate and select the file.

In the **Arguments** field, enter any arguments/keywords to use when starting up the environment.

To define a default output location

Setting the output folder in the *Preferences* dialog eliminates the need to enter the information in the Options tab for each run. The fields will automatically be filled with the paths entered here.

Enter the directory path in the **Default Output Folder** field or use the **Browse** button.

Note: If the user specifies a default output location, the user must ensure that they have write access.

Turn on the **Create a unique subfolder for each run** checkbox to generate and then store the output from each run in a new subfolder of the output folder.

User interface description

Setup tab
Options tab
Result Filters tab

Setup tab

The **Setup** tab allows mapping of datasets and control files to the object. The Mappings panel(s) of the Setup tab displays the column headers specified in the control file. The Text panel allows users to map a control file to the object and view the contents.

Context associations for NONMEM objects change depending on the column headers, or input, defined in the control file. Some common mapping contexts associated with NONMEM are listed in "Common NONMEM context definitions".

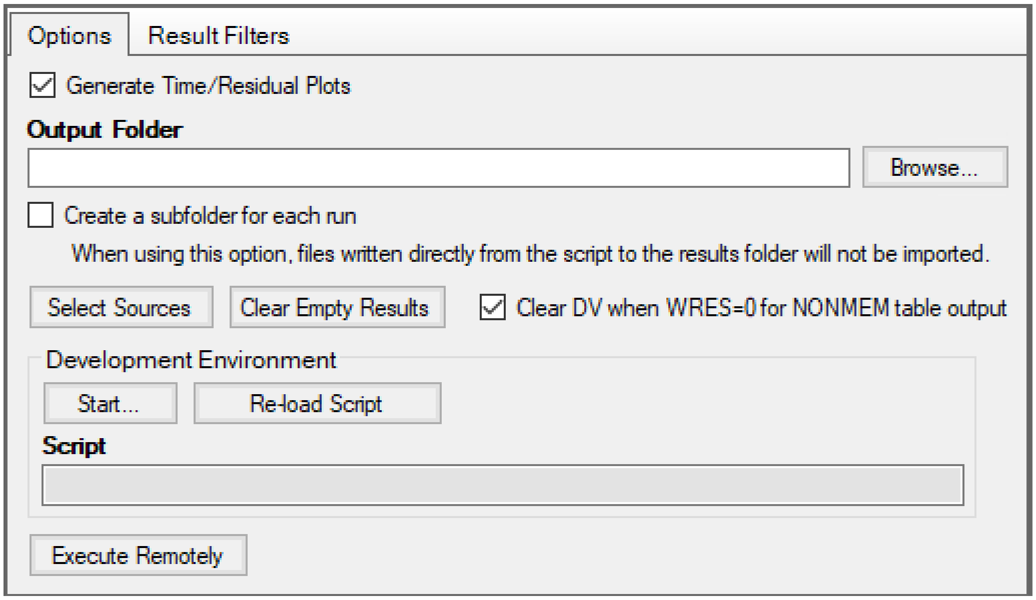
Common NONMEM context definitions

The following context definitions are common NONMEM variable names. They are not representative of all NONMEM variable names. Required context mappings are colored orange in the Mappings panel.

None: Exclude data type from analysis and output.
ID: Subject identification number.
AMT: Dose given at dosing time or time zero for observation records.
DOSE: Dose given to each subject.
TIME: Blood sampling times.
When using the Dose-Effect model, TIME is required as an input field in data, even though it is not used in analysis. You can create a dummy TIME column and map it work around this restriction.
CONC_DV: Typically drug concentration in plasma, but can be any dependent variable.
MDV: Missing dependent variable.
AGE: Age in years.
WT: Weight in kilograms.
ISM: Is male or is not male. In the column, 1=male, and 0=female.
CLCR: Creatinine clearance in mL per minute.

Options tab

The Options tab is used to define a location for the output, access development environment, and start a remove execution.



Entering an output location is optional. If a directory is not specified then Phoenix places output in a temporary folder that is deleted after Phoenix is closed. This may be preferred when sharing third party tool projects with other users, as the output folder is machine specific and may not exist on other machines. If users want to save the results from a third party tool object run to a disk, then they must either specify an output folder or manually export each result to disk.

Enter the output folder path in the field or click **Browse** to specify the output folder location.

Turn on the **Create a subfolder for each run** checkbox to add a new results folder in the specified output location each time the object is executed.

This option prevents the output from being overwritten with each run, especially if the default output folder option, under **Edit > Preferences**, is being used.

Click **Select Sources** to include additional files along with the mapped input.

As an example, if a NONMEM object creates an MSF file that contains the estimates to full precision, then a second NONMEM object can use the MSF file as an Input File source.

Note: The **Select Sources** button in a NONMEM object's Options tab can only access workflow objects. To access items in the Data or Code folders, use the **Select Source** icon in the Setup tab toolbar.

Click the **Clear Empty Results** to remove any results published by the object that are empty.

Turn on the **Clear DV when WRES=0 for NONMEM table output** checkbox to clear the cell in the DV column for rows where the WRES column value equals 0.

To start the development environment, click **Start** in the Development Environment section of the Options tab.

The development environment as configured in the *Preferences* dialog is started. (See "To specify a development environment".)

Note: NONMEM requires that a dataset be mapped to the object before the development environment will start.

When script work is completed, click **Reload Script** to bring the modified script into Phoenix for use in the next execution of the object.

The following are available only for a NONMEM object:

Select the version of NONMEM to use when the object is executed. The versions are defined in the *Preferences* dialog, see "To set up access to the external program".

Use the **Generate Time/Residual Plots** checkbox to control which plots are generated. These plots are required for some types of comparisons. In other cases, the type of model and data are not appropriate for the automatically generated plots, and can cause errors during the execution, in which case the user can uncheck this option.

Result Filters tab

See the "Result Filters tab" description for the PsN object.

Importing/Writing the code to access the external program

The NONMEM object must have code that will allow it to initiate the external program and submit jobs. The code can be stored as a control file, imported into the project, and mapped to the object, or the code can be directly entered into the object.

Import and map file containing code
Write code in the Text panel
Adding shortcuts in scripts
Filtering results by size

Import and map file containing code

The process is the same as for many other Phoenix objects. Refer to "Importing datasets" common task description.

Write code in the Text panel

Instead of importing and mapping a control file, users can write their own code or copy and paste code from another source. (For more information, see the "Write code in the Text panel" section for the PsN object.

Below are additional notes for NONMEM.

- Changes made to the `$INPUT` record are reflected in the Dataset Mappings panel. Changes made to a mapped control file do not change the control file in the Code folder.
- Any blanks or tabs before statements should be removed prior to executing in Phoenix. Otherwise, the statement will be ignored.
- Use only upper case when the specifying PHXTBL in the control file. Otherwise, duplicate NONMEM output files will result since Phoenix generates a file named "PHXTBL" by default for use with the NONMEM Comparer object.

- Input statements should not contain equal strings. For example, $INPUT ID TIME DV=DROP LNDV=DV MDV AMT RATE EVID DOSE should be changed to $INPUT ID TIME DV MDV AMT RATE EVID DOSE and the column LNDV mapped to DV.
- If a NONMEM control statement calls to perform more than one fit, the control statement should be split and the models run in sequence. For example, it should not be used with multiple $PROB input files, superproblems, or $PRIOR routines.

  In order for NONMEM to call Ifort variables within Phoenix the setup of `nmfe7.bat` needs to be modified to support specific compilers. The modifications needed are:

  ```
  set F77HOME=C:\Program Files\Intel\Compiler\Fortran\10.1.011
  if '%F77VERHOME%==' set F77VERHOME=%F77HOME%
  call "%F77VERHOME%\Ia32\bin\ifortvars.bat"
  ```
- If NONMEM is installed on the same server as Phoenix, edit the path in the system environment so that gfortran comes ahead of the Certara software (i.e., edit the path so that `C:\Program Files\gfortran\libexec\`… comes first in the path, before `C:\Program File s(X86)\Certara\Phoenix\MinGW`…) to avoid issues where NONMEM errors out.

Adding shortcuts in scripts

The input can be defined within the script as a shortcut by adding `;PHX_SHORTCUT` to the end of the `$DATA` statement.

```
$DATA FILE [OPTIONS];PHX_SHORTCUT
```

`FILE` will be replaced with the path to the file.

Filtering results by size

See the "Filtering results by size" section for the PsN object.

Executing the NONMEM object

Click  (**Execute** icon) or click **Execute Remotely** in the Options tab to run the job remotely.

Executing a third party tool object remotely sends the job to the server that is defined in the *Preferences* dialog (**Edit > Preferences > Remote Execution**). See "Phoenix Configuration" for instructions. The project is saved automatically.

The project must have been saved at least once prior to executing on RPS, otherwise execution will not pass validation and a validation message will be generated.

At this point, the step being executed on RPS, along with any dependent objects, has been locked. It is now safe to close the project or to continue working in Phoenix.

Results

The results are displayed on the Results tab. The output falls into the following categories:

Output Data: Datasets in tabular form
Text Output: Settings files, log files, and other text output
Other: Other kinds of files, for example: documents, export files, binary files, etc.
Images: Graphs or other images in recognized image formats (jpg, tiff, emf, etc.)

The NONMEM object generates the following output:

PHXTBL: Summary of ID, TIME, CWRES, DV, PRED, RES, and WRES. The table is generated by default even if there is no TABLE statement in the control file. (Do not use the name PHXTBL (lowercase, uppercase, or mixed case) for any other table, since the name is in use.)

Summary: Contains the total number of observations, total number of subjects, lengths of theta, minimum objective function value, total number of parameters, AIC, BIC, and the conditions for estimation.

GFCOMPILE: List of Digital FORTRAN compiler messages created during NONMEM execution.

FCON: NONMEM control stream file.

FDATA: Dataset used with NONMEM.

FREPORT: List of subroutines that generate commands used to create the NONMEM model.

FSTREAM: NONMEM file control stream.

FSUBS: List of generated FORTRAN subroutines.

PRDERR: List of errors encountered during execution of the PRED subroutine.

Raw_Output: Unparsed output from NONMEM.

Settings: Input worksheet used and the options selected.

stdout: Warnings and errors (if any) for problems.

If a NONMEM control file has a $COV statement then the total number of parameters in the model are calculated in the Summary table. If there is no $COV statement, then users can specify the number of parameters in the control file by adding this comment prior to the $EST statement:

```
;  #parameters= X
```

where X is an integer.

If the control file contains several $EST statements the number of parameters comment preceding the estimate statement(s) would be used.

If the number of parameters is available then AIC and BIC are calculated:

```
AIC=Min. Val. Of Obj. Func+2*(Tot. #Params)
BIC=Min. Val. Of Obj. Func+(Tot. #Params*Loge(Tot.#obs))
```

Note: To correctly read in TABLE files generated by NONMEM, the `ONEHEADER` command must be present in the control file as part of the TABLE statements.

Additional NONMEM parameter data tables

Sigma SE: Standard error(s) of the observation error variance estimates if the $COV statement is in the control file.

Theta: Fixed effect estimates.

Omega: Estimates of the elements of the random effect(s) covariance matrix.

Sigma: Estimates of the observation error variance(s).

Table 1: NONMEM generated table files.

COVARIANCE MATRIX OF ESTIMATE: Covariance matrix for the model parameter estimates if the $COV statement is in the control file.

CORRELATION MATRIX OF ESTIMATE: Correlation matrix for the model parameter estimates if the $COV statement is in the control file.

Theta SE: Standard errors of the fixed effect estimates (thetas) if the $COV statement is in the control file.

Omega SE: Standard errors of the random effect covariance matrix element estimates (omegas), if the $COV statement is in the control file.

(Optional) File name of the TABLE statement: NONMEM generated table files.

Users can double-click any plot in the Results tab to edit it. (See the "Options tab" description for plots for more details.) Plot edits are maintained during consecutive NONMEM modeling runs.

Plots

DV VS PRED: Dependent variable in the X-axis and predicted variable in the Y-axis. Generated by default.

PRED VS CWRES: Predicted variable in the X-axis and conditional weighted residuals in the Y-axis.

PRED VS RES: Predicted variable in the X-axis and residual variable in the Y-axis. Generated by default.

PRED VS WRES: Predicted variable in the X-axis and weighted residuals in the Y-axis. Generated by default.

TIME VS DV: Time in the X-axis and dependent variable in the Y-axis. Generated by default.

TIME VS CWRES: Time in the X-axis and conditional weighted residuals in the Y-axis.

TIME VS PRED: Time in the X-axis and predicted variable in the Y-axis. Generated by default.

TIME VS RES: Time in the X-axis and residual variable in the Y-axis. Generated by default.

TIME VS WRES: Time in the X-axis and weighted residuals in the Y-axis. Generated by default.

(Optional) Plot names in the $SCAT statement: NONMEM generated plots. SCAT statements in NONMEM code will only automatically generate a plot in Phoenix if there is a TABLE statement in NONMEM that contains the variable being plotted. Third party tool objects generate a TABLE statement automatically for ID, TIME, DV, PRED, RES, and WRES and thus, SCAT statements involving these variables will be created. If other variables are required by the SCAT statement, the user must specify them in an appropriate TABLE statement.

The **Settings** text file is generated and contains the updated concentration column.

NONMEM Comparer

The NONMEM Comparer object allows users to compare the output of NONMEM models.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > External Software > NONMEM Comparer**.
Or Main menu: **Insert > External Software > NONMEM Comparer**.
Or right-click menu for a worksheet: **Send To > External Software > NONMEM Comparer**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

This section contains information on the following:

User interface description
Results

User interface description

Setup tab
Options tab

Setup tab

Note: Although there are no icons in the Setup tab for importing/saving/loading object settings, these operations are still available using the **File > Import** menu, and right-clicking the object in the Object Browser or in the workflow diagram.

Models in the Setup tab are listed using the object name as seen in the object browser. If a NONMEM model was created by making a copy of a previous NONMEM model, then the copy is nested underneath the first model in the Comparison. The original model is the root model, and the copied model is the child.

Model copies that are nested underneath the original model will typically have additional parameters that are compared against the original model, which has fewer parameters.

To change the hierarchical relationship between root and sub-models

Use the pointer to select a model in the Setup tab and drag the model on top of another model.

Click **Yes** in the *Move* confirmation dialog.
The selected model is nested underneath the selected root model.

To move a child model back to the root level, right-click the child model and select **Orphan Model**.

Click **Yes** in the *Move* confirmation dialog.
The model is moved back to the root level in the Setup tab.

To exclude/include a model in the comparison

In the Comparison tab, users can select or clear the **Hide** or **Compare** checkboxes to exclude or include a model in the comparison.

If the **Hide** checkbox is checked, then the model is considered "hidden" and is removed from any comparisons.

If the **Compare** checkbox is checked, then the selected model is included in comparisons.

Options tab

The Options tab can be used to add or remove columns, worksheets, and plots used for comparisons.

In the Columns list, clear checkbox to ***remove*** that column from the comparison. Removed columns are not included in the output worksheets.

In the Worksheets and Plots lists, clear the checkbox to ***exclude*** that worksheet or plot from the results.

In the Plot Options area, select the height, width, and graphic format for the output plot.

If a NONMEM model is marked as hidden, then check the **Hide Selected** checkbox to ***remove*** the model from the Setup tab and the comparison. (The hidden model is not used in any comparisons.)

Check the **Full Names** checkbox to ***display*** the full name of a model. The full name includes the name of the workflow containing the model.

Use the buttons in the **Selections** area to select or hide several models at once. Multiple rows in the Comparison panel must be selected to use these buttons.

Select multiple rows in the Comparison panel to use the buttons in the Selections area.

Click **Check Hide** to ***hide*** the selected models.
Click **Check Compare** to ***include*** the selected models in the comparison.
Click **Un-Check Hide** to ***not hide*** the models.
Click **Un-Check Compare** to ***remove*** the models from the comparison.

Results

Worksheets

Correlation Matrix of Estimate: Estimates of the correlation of model parameter estimates listed for all the models being compared.

Covariance Matrix of Estimate: Variance-covariance matrix for model parameter estimates listed for all the models being compared.

Omega: Estimates of the random effect variance-covariance matrix (Omega) and standard errors of omega elements listed for all the models being compared.

Overall: Stacks the table 'Summary' result for each individual run but doesn't present any comparison calculation. Columns include:

NAME: The name of the NONMEM object being compared
Tot. # Obs: total number of observations
Tot. # Individuals: Total number of individuals
Length of Theta: Total number of fixed effects variables
Min. Val Of. Obj. Func: Is the minimum value of the objective function for each NONMEM run
AIC: Akaike Information Criterion for each model run

BIC: Bayesian Information Criterion for each model run
Conditions of Estimation: is the $EST statement of each control file

Residuals: Stacked results from PHXTBL created for each individual NONMEM run with the addition of Model name. It contains columns for NAME (Model names being compared), ID, TIME, CWRES, DV, PRED, RES, and WRES.

Sigma: Estimates and standard errors of the observation error variance-covariance matrix (Sigma) for all models being compared.

Theta: Estimates and standard errors of the observation error variance-covariance matrix (Sigma) for all models being compared.

Summary: Estimates and standard errors of the fixed effect parameters (Theta) for all models being compared. Models are shown across the top. Columns include:

NAME: The name of the NONMEM object being compared
Method: The $EST statement of each control file
Lineage: List the 'parent' (i.e. reduced model) if the current model is a 'child' (derived from but with additional parameters) of another model
Min. Val Of. Obj. Func: The minimum value of the objective function for each NONMEM run
AIC: Akaike Information Criterion for each model run
BIC: Bayesian Information Criterion for each model run
–2(LL)Delta: Difference in Min. Val Of Obj. Func. for nested models only (Lineage-Child model)
AICDelta: Difference in AIC values. for nested models only (Lineage-Child model)
BICDelta: Difference in BIC values for nested models only (Lineage-Child model)
#params: Number of model parameters
#obs: Number of observations
#Subj: Number of subjects
p-value: Chi-Square p-value based on the Likelihood Ratio Test for nested models only

The Plot Table is generated and illustrates all the selected plots in rows for each model being compared (columns). This plot table is not editable and it places side by side the plots from the individual runs for easy visualization. Any changes done to the individual run plots will be reflected in this Plot table. This table can be exported or printed using the right-click menu options.

The Settings text file is generated and contains the list of current columns, plots, and models being compared.

ODBC

Note: The ODBC user interface is only available when using the 32-bit version of Phoenix.

Phoenix can exchange data with Open Database Connectivity (ODBC) compliant databases such as Oracle and SAS. For example, Phoenix can read rows of PK data from an ODBC-compliant database, and save analysis output back to a table in that database. This is done using the ODBC import and export functionality in Phoenix.

This section contains the following topics:

Establishing a connection

The first step in an ODBC import or ODBC export is to establish a connection to a specific database.

Creating a new connection string creates a new connection string, defining the database type and location. This connection string may be saved as part of an import or export settings file for re-use.

Loading a saved connection extracts the connection string from a previously-saved import or export file. This establishes a link to the database, to be used with a new or saved query or export.

Creating a new connection string

To define the database type and location for ODBC import or export

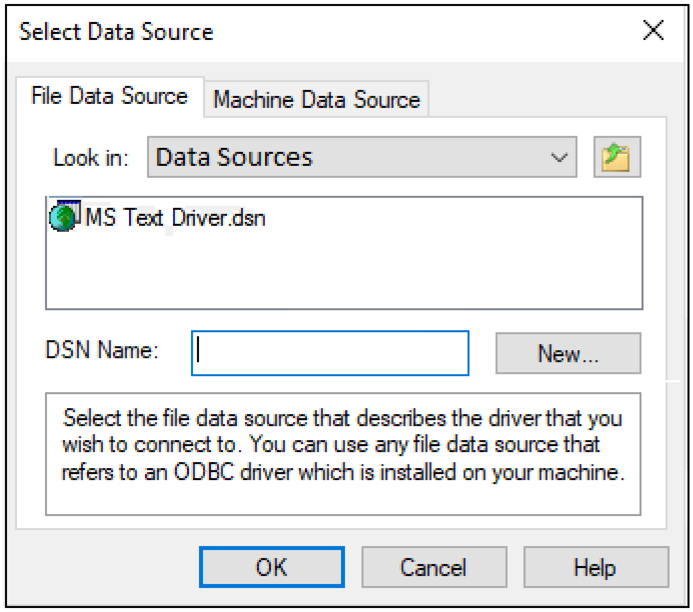
Select **File > ODBC > Import (or Export) > Legacy WnI**.

Select the **Create a new Import** (or **Export**) option button in the *ODBC Import* (or *Export*) dialog.

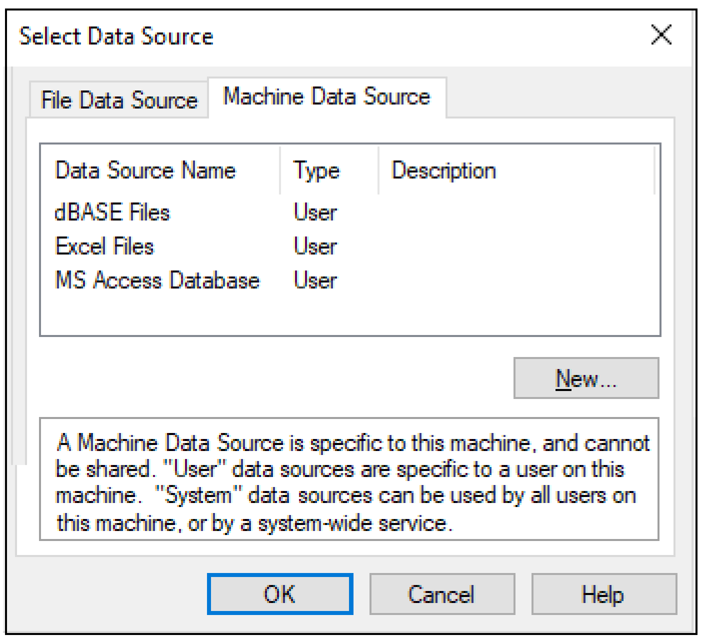
Click **Next**.

Select the **Create a new connection** option button and click **Next**.

Click **New** to set up new File or Machine data sources or select a data source from one of the two tabs in the *Select Data Source* dialog. (See Microsoft Windows documentation for details on creating new data sources.)



The File Data Source tab lists all file Data Source Names (DSNs) and subdirectories on the system. These are file-based data sources that can be shared among all users who have the same ODBC drivers installed. The data sources do not need to be dedicated to a single user or local to a specific computer.



The Machine Data Source tab uses information stored in Window's registry, which provides the majority of the connection string information.

Click **OK**.

If a log in dialog appears, enter the appropriate login ID and password for the data source and click **OK**.

ID and password are set up by the Database Administrator or Information Technology personnel.

A connection string may be saved along with a import query or export definition in an import (*.imp) or export (*.exp) settings file for re-use. This is done at the conclusion of building the import query or export definition. A connection string can also be saved by itself and loaded separately during the import/export setup process.

The next step is to set up a query (see “Specifying the Query”) to pull the desired data from the database, or create an export definition (see “Creating a new export”) to map Phoenix data columns to database fields.

Loading a saved connection

Once a connection string is saved in an import (*.imp) or export (*.exp) file, it can be loaded for use with different import queries or export definitions.

Select **File > ODBC > Import > Legacy Wnl or File > ODBC > Export > Legacy Wnl**.

Select the **Create a new Import** (or **Export**) option button in the *ODBC Import* (or *Export*) dialog and click **Next**.

Select the **Load an existing connection** option button and click **Next**.

In the *Open* dialog, select the import file (*.imp) or export definition file (*.exp) containing the connection string for the desired database and click **Open**.

Proceed with the import or export, as detailed under “Specifying the Query” for imports or “Creating a new export” for export.

ODBC import

Use ODBC Import to load data from an ODBC-compliant database directly to a worksheet. An import involves establishing a connection to the database, then defining a query to draw specific fields and records from it.

Database connection: Both ODBC import and export use a connection string that defines the database type and location. This string can be created by pointing to the database type and file, or loaded from a previously-saved import or export as detailed under “Establishing a connection”.

Query: Once the database connection is established, an import requires a query to set which data table, field(s) and records to import. The query can be created in the or loaded from a previously-saved import as described under “Specifying the Query”. Phoenix translates the query into Structured Query Language (SQL), which can be edited before executing the import.

The query settings can be saved with a connection string to an import specifications file (*.imp), for later re-use. The query settings can also be saved without the connection string and loaded for use with other databases via different connection strings.

Phoenix also provides a Custom Query Builder for creation of dynamic link library (DLL) files that can access additional data source types, including Watson version 7.x DMLIMS. See “Using the custom query builder”.

Note: If an error is encountered when using ODBC Import, try setting the permissions of the `C:\Windows\SysWOW64\comdlg32.ocx` file (`C:\Windows\SysWOW64\comdlg32.ocx` for 32-bit systems) to Read-Execute and Read for Everyone user.”

Specifying the Query

Once a database connection string is established (see "Establishing a connection"), ODBC import requires a query specifying the data table, field(s) and records to be imported. There are two ways to specify a query:

Building a query
Loading a saved query

Building a query

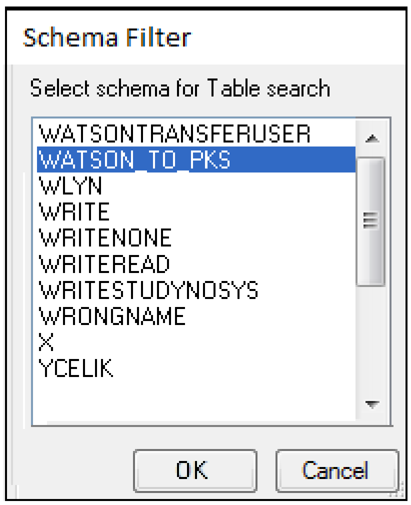
Select **File > ODBC > Import > Legacy WnI**.

Select the **Create a new Import** option button in the *ODBC Import* dialog and click **Next**.

Create a new or load a saved connection string, as detailed under "Establishing a connection".

Select the **Build a Query** option button and click **Next**.

The Phoenix Query Builder accesses the database, and loads a list of the available tables. If the appropriate ODBC drivers are available, the *Schema Filter* dialog is displayed. It provides a means to filter the available database tables by schema, a metadata organizational tool. The schema are created by the database administrators.



If the *Schema Filter* dialog is displayed, select the schema to use in filtering the list of data tables, then click **OK**.

In the Source Table list, select a table from which to import data.

Click **Next** to continue with selecting the fields to import or click **Done** to load all fields in the table.

To select a field(s) to import:

Click a field in the list to select it for import. (Clicking a field a second time, deselects it.)

Click **Select all** to select all fields. (Click **De-Select all** to clear all field selections.)

Click **Next** to continue with filtering the records or click **Done** to import all records in the selected fields.

To create the record filter:

In the **Field Name** menu, select a field name used to filter queries.

In the **Operator** menu, select a comparison or logical operator.

Note: The logical operator **like** means true if the operand matches a pattern.

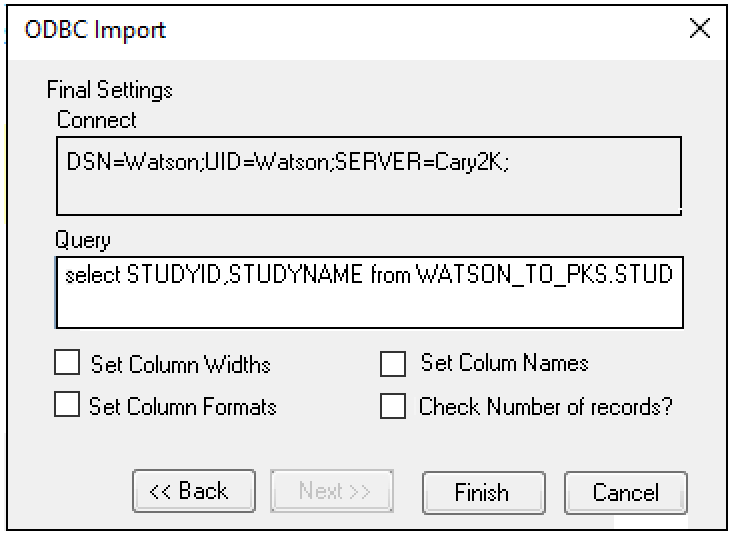
Enter a value in the **Field Value** field or click **List Distinct Values** to select from all existing values for the selected field.

Click **Add** to set the filter.

To apply more than one filter, select the **And** or **Or** option buttons and return to create another filter. Filters are applied in the order they are created.

Click **Done** when all filters are entered.

In the *ODBC Import: Final Settings* dialog, confirm/edit the connection string and query SQL.



Check the **Set Column Widths** checkbox to adjust the destination worksheet's columns to match the widths of the fields in the database.

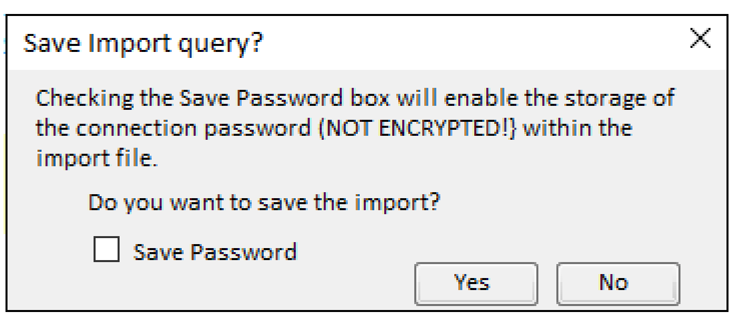
Check the **Set Column Names** checkbox to adjust the destination worksheet to have the same column names as the source fields.

Check the **Set Column Formats** checkbox to apply the appropriate number formats to columns containing times, currency, and dates.

Check the **Check Number of records?** checkbox to provide a count of filtered records prior to the import, and the option to return and edit the query if needed.

Click **Finish** to import the selected data to a Phoenix worksheet.

If **Check Number of Records?** is checked, a message is displayed that states the number of records returned by the query. Click **Yes** to continue.



In the *Save Import query?* dialog, check the **Save Password** checkbox to save the database username, password, and connection string in the import file.
Saving all three pieces of information in the import file allows users to connect to a database.

Caution: The import file is not encrypted, so the saved password is not secure.

Click **Yes** to save the import file.

In the *Save As* dialog, select a directory in the **Save in** field, type a file name in the **File name** field, and click **Save**.

If a user clicks **Cancel** in the *Save As* dialog the worksheet is still imported into Phoenix, but the import file is not saved.

The size of the worksheet Phoenix can import depends on the amount of memory in the computer running Phoenix. The list below shows memory requirements and cell limitations. ODBC drivers might impose additional limits.

For 1 gigabyte of RAM, there is a limit of 2 million worksheet cells
For 2 gigabytes of RAM, there is a limit of 4 million worksheet cells
For 3 gigabytes of RAM, there is a limit of 6 million worksheet cells

Loading a saved query

A saved import specifications file (*.imp) may or may not contain the connection string, depending on what options were specified during saving.

Select **File > ODBC > Import > Legacy Wnl**.

In the *ODBC Import* dialog, select the **Load an existing Import** option button and click **Next**.

In the *Open* dialog, select the import (`*.imp`) file and click **Open**. The *ODBC Import: Final Settings* dialog appears with all settings for that import loaded.

Makes changes as needed in the *Import: Final Settings* dialog or by using the **Back** button.

When the settings are correct, click **Finish**. The data from the database are then loaded into a Phoenix worksheet.

Be aware that, once a connection string (new or existing) is established, any saved query can be loaded so long as it uses the tables, fields, and record types in the database to which Phoenix is connected.

Using the custom query builder

The Custom Query Builder provides a means to build custom dynamic link library (DLL) files that access additional data source types, including Watson version 7.x DMLIMS. Further, Phoenix provides templates for creating the DLL files to access custom data sources.

Select **File > ODBC > Import > Legacy Wnl**.

Select **Use Custom Query Builder** and click **Next**.

The *Select a Builder* dialog is used to set the data resources to access. If the Custom Query Builder has not been used before, this dialog may be empty.

To add resources to the Query Builder, click **Add**, then double-click the appropriate DLL file such as `WatsonLIMS.dll`.

To configure the Watson DMLIMS custom resource to make sure that data are imported correctly:

Select that item and click **Edit**.

In the *Configuration* dialog, enter the name of the Watson LIMS tables' owner.

Enter the full directory path for the Watson templates or click **Browse** to locate the directory on your local machine or on a network server.

Click **OK** to close the *Configuration* dialog.

Highlight **Watson DMLIMS** (or another custom query builder) in the *Select a Builder* dialog and click **OK**.

The dialog asks whether to load a query.

To load a saved query, click **Yes**. In the *Open File* dialog, select an existing query (file type `*.wts` for Watson LIMS) and click **Open**.

If no query has been saved for this builder, click **No** and proceed with the following steps.

In the log in dialog, enter user name, password, and database alias, and click **OK**.

Note: The user name, password, and alias for any custom database system (such as the Watson DMLINS) are set by the database administrator or IT personnel. Request this information from that person or department.

In the *Study Selection* dialog, select a study by clicking on the row and then click **Next**.

Use the **Order Study By** field to sort any category, such as study number or ID, study director, etc., in order to find a listing more quickly.

Note: If no projects are listed in this dialog, contact your IT department.

In the *Import Data Variables* dialog, select the desired variables.

If all available variables are desired, click **Select All**.

For a subset, drag each variable to the **Selected Variables** field.

A particular combination of variables can be saved as a template. To create a new template drag the variables for the template to the **Selected Variables** field and click **New**. Then enter a name for the template.

The fields will be imported in the order shown in the Selected Variables list.

Click **Next** to continue with data filtering or click **Done** to import all data in the selected fields.

Define a filter in the *Filter* dialog:

Select the field to filter on from the **Field** box.

Choose an operator.

Either enter a value in the **Field Value** field or click **List Distinct Values** to select from all existing value for the selected field.

Click **Add** to set the filter.

Use the **And**/**Or** operators to create compound filters such as Age>12 and Gender=Male.

Click **Done** to load the data into a Phoenix worksheet. If **Check # of rows returned** checkbox was selected, Phoenix reports a count of records returned.

ODBC export

Phoenix can export selected worksheet columns to specific fields within a table in any ODBC-compliant database. Like ODBC import, the export requires a connection string defining the database type and location. It also requires an export definition to map columns in the source worksheet to fields in the target database table.

Database connection: Both ODBC import and export can use the same connection string to define the database type and location. This string is created in the ODBC Export wizard or loaded from a previously-saved import or export as detailed under "Establishing a connection".

Export definition: Once the database connection is established, an export requires a mapping of columns from the Phoenix worksheet to fields in the target database table. This export definition may be created in the ODBC Export wizard or loaded from a previously-saved export as shown under "Creating a new export".

The export definition can be saved with a connection string to an export definition file (*.exp), for later re-use. The export definition can also be saved without the connection string and loaded for use with other databases via different connection strings.

See the following topics for more information:

Creating a new export
Loading a saved export

Creating a new export

In the Data folder, select a worksheet to export.

Select **File > ODBC > Export > Legacy Wnl**.

In the *ODBC Export* dialog, select the **Create a new Export** option button and click **Next**.

Create a new or load a connection string as detailed in "Establishing a connection".

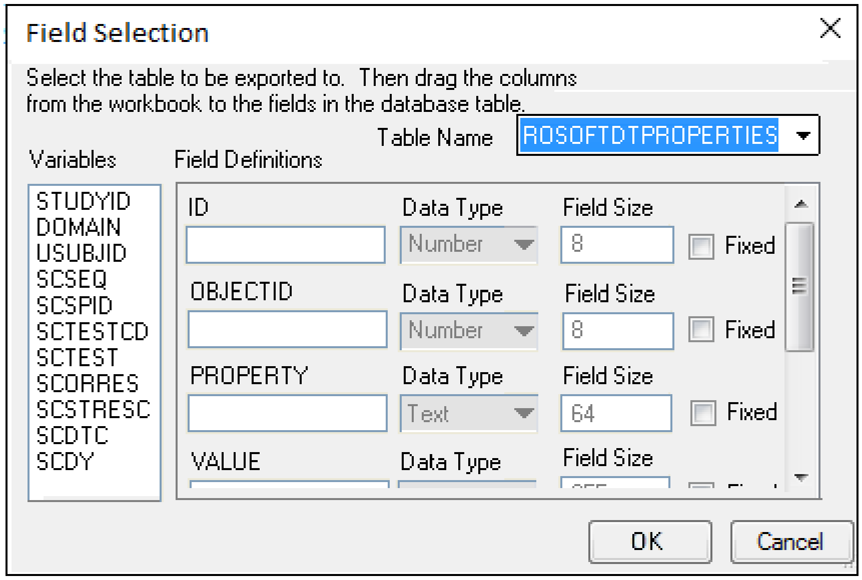
In the *ODBC Export Definition* dialog, select the **Build a Definition** option button and click **Next**.

As with the ODBC import, the schemas used to select the data variables can be specified. The *Schema Filter* dialog displays available schemas, if any were created by the database administrators.

If the *Schema Filter* dialog is displayed, select a schema and click **OK**.

Using schema filters can speed up export operations by using saved export files.

In the **Table Name** menu of the *Field Selection* dialog, select the database table to receive the exported data.



Drag the variables from the **Variables** list to the appropriate database fields under **Field Definitions**.

To export one constant value for all records in a given field, check the **Fixed** checkbox for a variable and enter a value in the field name.

This method can be used to differentiate one export from another. The data type and field size are set by the database administrator.

Click **OK**.

In the *Save Export?* dialog, check the **Save Password** checkbox to save the database username, password, and connection string in the export file.

Saving all three pieces of information in the import file allows users to connect to a database. The export definition file contains all information needed to reproduce the same export, excluding any constants in fixed fields.

Note: The import file is not encrypted, so the saved password is not secure.

Click **Yes** to display the *Save As* dialog for specifying the location and file name.

If you click **Cancel** in the *Save As* dialog, the worksheet is still exported into the database, but the export file (*.exp) is not saved.

Loading a saved export

A saved export file (*.exp) may or may not contain the connection string, depending on what options were specified during saving. The field mappings in any ODBC export definition can be re-used with any database connection, assuming the field and table names in the export file exactly match a table in the selected database.

Select the dataset to export in the Data folder.

Select **File > ODBC > Export > Legacy Wnl**.

In the *ODBC Export* dialog, select the **Load an Export** option button and click **Next**.

In the *Open* dialog, select the export file (`*.exp`) and click **Open**. (Log on to the data source, if necessary.)

If the *Schema Filter* dialog is displayed, use the **Schema Filter** option to narrow the set of available data tables (optional) and click **OK**.

Users can select **All schemas** in the *Schema Filter* dialog.

Make any adjustments needed in the *Field selection* dialog and click **OK** to complete the export.

Pharsight Knowledgebase Server

The Pharsight Knowledgebase Server (PKS) is a database system for secure storage of study data and analyses. The PKS provides a secure data management system with complete auditing capabilities. The combination of the PKS and Phoenix provides an effective means to share source data, models, scripts and results among the members of a drug development team. The combination also supports compliance with the U.S. Food and Drug Administration's 21 CFR Part 11 regulation.

Phoenix can work in conjunction with the Pharsight Knowledgebase Server (PKS) for secure storage and change tracking for data and analyses. This chapter covers the use of Phoenix as a PKS client: loading PKS data to Phoenix and saving data from Phoenix as PKS studies and scenarios. The PKS can also be accessed by way of a Web interface, which provides additional operations, and an XML API. The PKS functions and operations are covered in the *Pharsight Knowledgebase Server User's Guide.*

This section contains the following topics:

The PKS information structure

Phoenix is an object (text, chart, model, data) based application. Those objects fit into specific niches in the PKS data structure. PKS saves observations and related data as a PKS study. Analysis settings and output are added to the study as scenarios. Non-Phoenix documents, such as analysis output, reports, and graphics that are related to the study, can be loaded into the PKS and associated with a scenario.

Studies

The basic unit of information in the PKS is a ***study***. A study starts with a collection of raw data that must include longitudinal observations, observation times and subject identifiers, and may include dosing and subject demographics. A study must have all of these data characteristics if data is mapped to PKS internal structures, but the study can contain any type of data if stored in the study library. Studies can be created with data mapped to the PKS data structures, or they can contain file-based data, maintained in the study library. As analyses are performed on these data, the analyses, including model settings and results, can be added as scenario(s) within the study.

A PKS study requires specific fields. First, a study must include at least one column containing subject identifiers. A collection of fields taken together can be used for subject identification. For example, first name, last name.

A study can include, but is not required to have, multiple columns of ***subject data***: time-invariant, subject-specific information such as body weight or gender, that is, baseline covariates.

A study can include time-dependent observation and dosing data. Observation data can include records of concentration, measurements of blood pressure, heart rate, etc. Each data collection point can have multiple observations. In this case, a sampling variable is used to differentiate the samples.

If the observation data includes multiple, concurrent measurements for any subject, for example, multiple assays performed on a given sample or multiple samples during a given visit, the dataset must include a variable that differentiates the measurements, that is, values 1, 2, 3 for the 1^{st}, 2^{nd} and 3^{rd} samples.

Time fields

Because a study generally includes time-dependent observation data, a study must include relative nominal time, indicating the times at which observations and doses if included, were scheduled in the protocol. This is in contrast to relative actual time, representing the times that observations or doses really happened. ***Relative time*** is time elapsed since the start of the study, period or phase. If the data uses infusion dosing, the relative nominal end time must be identified as well. If only the Relative Nominal Time is defined in the dataset, a duplicate column is created for the actual times.

Note: To create a study that does include longitudinal observation data, include a dummy time column, with values for each row as placeholders, in the study.

Valid relative time units in PKS are: sec, min, hr, day, weeks, years. This restriction only applies to the nominal time, nominal end time, relative time, and relative end time. Other data elements can have any units (times, concentrations or other measurements).

Study metadata

When a study is created, information about the study can be entered in the *Create Study* dialog. This dialog includes information about the study: Study Name, Portfolio, Project, Indication, Study Type, Study Design, Compound, etc. The metadata provides ways to search and filter the data within the database. The metadata are saved with the study. See "Creating a PKS study" for more information about study metadata.

Scenario

When an analysis is performed on a PKS study, the combination of source data, model, and results data can then be saved in the PKS as a ***scenario*** of the original study. A ***scenario*** can include a structural model, initial parameters, and/or statistical tests to be applied to a particular dataset for fitting or analysis, as well as any derived output from those tests or analysis. Scenarios are roughly comparable to the Phoenix concept of a project in that it is possible to save, in one place and under one name, related work: the data source, a model with model parameters, dosing, other model settings, and the analytical output. There is also a file created when the scenario is saved that contains all of the History entries for the scenario at the time of the save. Scenarios are associated with, that is, they are the children of a particular study data source, although it is possible to create further scenarios from a study or from an existing scenarios. See "Creating a Scenario" for more information.

Note: Loading a PKS scenario and submitting the workflow to the JMS for processing can prevent the scenario from being saved if the PKS middle-tier URL has changed since the scenario was last saved. If this occurs, run the scenario locally and save it to the PKS again.

Global Library objects

The PKS can store documents, or library objects, such as study reports, SAS or NONMEM code files, or a graphic created by saving a Phoenix chart to an image file. Sets of documents can be associated with scenarios. See “Global Library objects” for more information.

Dosing

Dosing information is a special case of study data. Dosing is generally saved as part of a PKS study and it is preferable to have the dosing data in the same worksheet as the observations, though it is not required.

If dose data is in a separate worksheet, it can be added to a study by loading it during study creation and its variables assigned as part of mapping the study variables. See “Creating a PKS study” for more information.

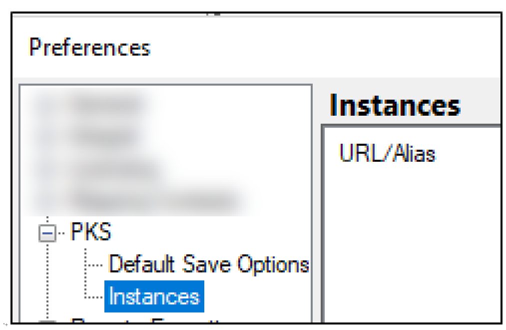
The dosing worksheet must contain, at a minimum, subject identifiers, dose amounts, and relative nominal dose times. It must contain the sort variables required to distinguish profiles. The worksheet can contain columns for more than one analysis scenario. Users can select which dose columns to use for a given scenario. See “Creating a Scenario” for more information.

To append dosing data to an existing PKS study, import a worksheet containing the dose information. Use the PKS Append/Update feature to map the new data columns to PKS study fields. See “Editing study data” for more information.

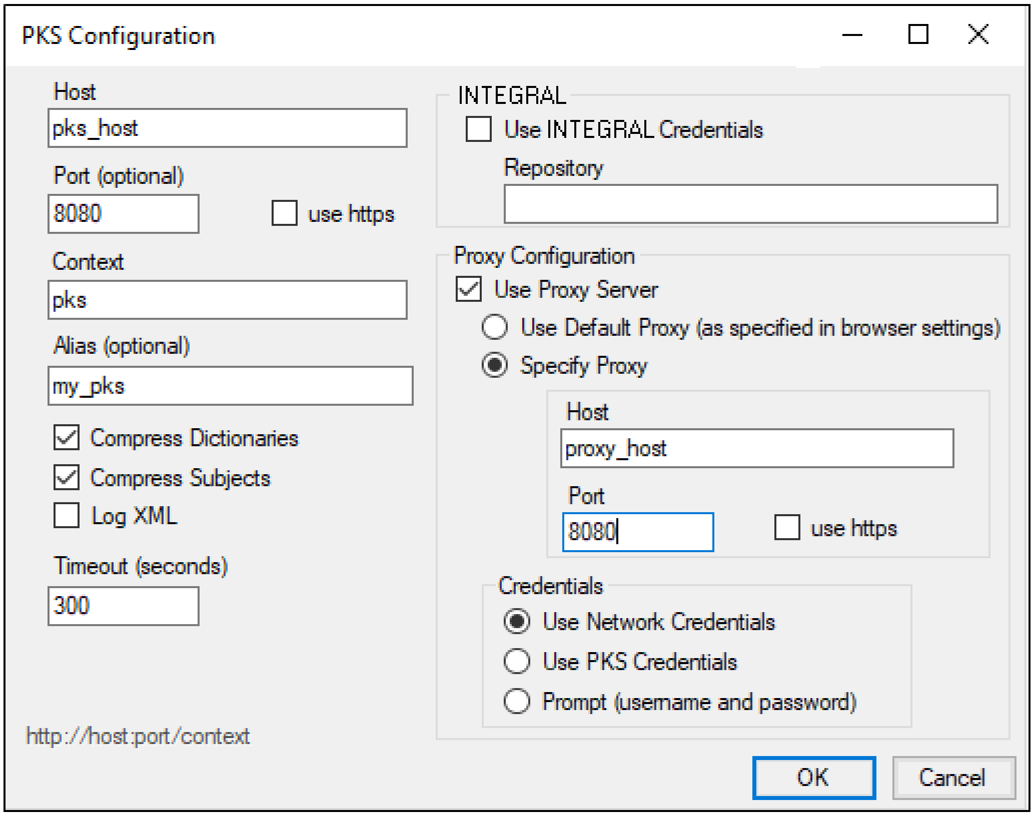
Setting up a PKS connection

The PKS connection information must be provided before Phoenix can connect to PKS installations.

- Select **Edit > Preferences**.
- Click the (**+**) sign beside PKS and select **Instances**.



- Click **Add**. The *PKS Configuration* dialog is displayed.



- Enter the requested configuration properties.
- Leave the **Compress Subjects** checkbox selected to improve performance by compressing study data per subject as it is transmitted to the PKS.
  - Clearing the **Compress Subjects** checkbox is only recommended for diagnostic purposes.
  - Selecting the **Log XML** checkbox is only recommended for diagnostic purposes.
- To use your Integral login information, check **Use Integral Credentials** and enter the web location for the repository in the field.
- To connect via proxy from the Phoenix PKS Plugin, configure the proxy information with the specific instance.
- Check the **Use Proxy Server** checkbox.
  If this checkbox is not checked, the controls inside the proxy configuration settings are disabled, and no proxy will be used.
- Select **Default Proxy** or click **Specify Proxy** to enter the **Host** and **Port** information to access a different proxy.
- Three **Credentials** or authentication methods are available for passing credentials to the proxy server. Select one of the credential methods:
  Use Network Credentials: The system passes the credentials used to access the network.
  Use PKS Credentials: The user name and password specified for the PKS connection are passed to the proxy by the system. (Users who have also configured PKS with LDAP authentication may want to select this option.)
  Prompt (username and password): The system prompts for the proxy user name and password.
- Click **OK** to save the new PKS instance.
- Click **OK** to close the *Preferences* dialog.

Users can edit PKS instances after they are created. In the Instances page in the *Preferences* dialog, select a PKS instances and click **Edit** to edit it and **Remove** to remove it.

Users cannot edit or remove instances to which they are currently connected.

PKS Browser

Most interactions with PKS occur through the PKS Browser. The PKS Browser displays a list of studies in the system and their contents on the left. The table in the right panel allows sorting and searching of the studies. All of the study information on the left is available in the table on the right.

A study contains libraries, scenarios, and views. Selecting one of these "collection" nodes in the left panel will list the items in that collection in the right panel. Selecting one of the items in the list will display the properties for that item in the right panel. Selecting the study itself provides an opportunity to edit some of the study properties and post them to the system. The Custom Attributes tab lists any custom attributes that are defined for a study through the PKS Web Interface. Selecting a particular scenario displays several tabs of information: properties, custom attributes, dependencies (such as a study view, other scenario object, or global library), list of objects that are saved within the scenario.

The contents displayed in the PKS Browser are limited by the logged in user's security permissions and by any applied filters.

The PKS Browser also has a toolbar that allows users to perform several common PKS functions, including: switching between library and study views, refreshing the browser contents, setting display options, filtering PKS contents, toggling study and object property displays, creating new scenarios, study views, and new study object, and editing, appending, and updating study data.

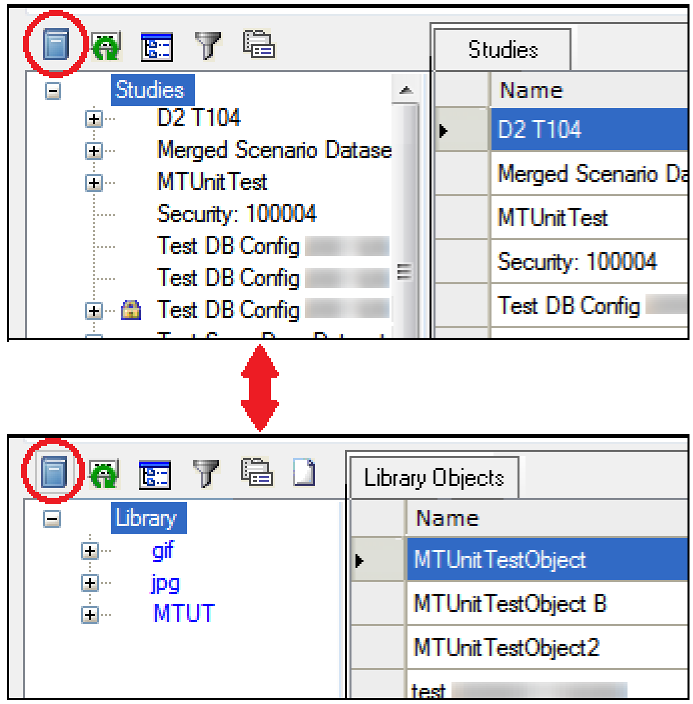
The PKS Browser includes the following capabilities:

Viewing the Global Library
Refreshing the browser view
Displaying options
Filtering based on properties
Viewing Study and Study Object properties
Creating a Scenario
Creating a Study View
Loading existing scenarios/creating new scenario versions
Creating a new Study Library object
Editing study data
Appending data

Viewing the Global Library

The PKS Global Library can be used to store documents, models, scripts, images, and other binary files that can be re-used across many projects or analyses. The PKS Browser can be toggled back and forth between viewing the Global Library contents and viewing the Study menu tree.

- Click  (**Library** icon) in the PKS Browser toolbar to toggle between the Global Library and Study views.



Refreshing the browser view

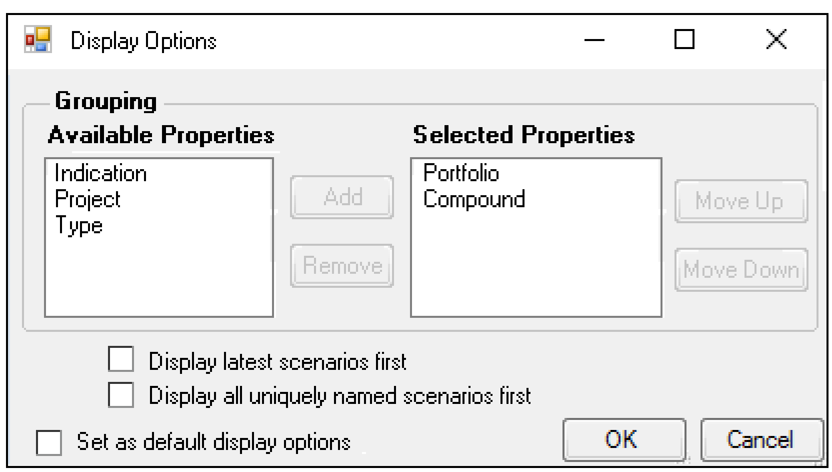
PKS contents can change as a result of actions from other users. The changes might not be immediately reflected in the PKS Browser.

- Click **Refresh** to load the current contents of the PKS.

Displaying options

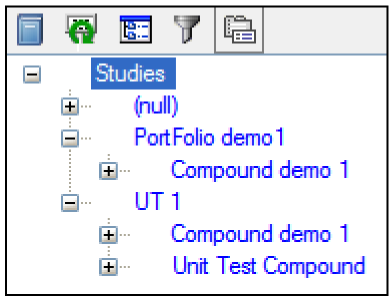
In the PKS Browser, the studies are listed in alphabetical order by default. They can also be grouped by indication, project, portfolio, compound and type.

- Click  (**Display Options** icon) to set the browser display options.



- Use the pointer to select one or more of the properties in the **Available Properties** list and click **Add** to move properties to the Selected Properties list. (Use the **Remove** button to move properties back to **Available Properties** list.

- Change the display order of selected properties by selecting a property and doing any of the following:
  - Click the **Move Up** and **Move Down** buttons.
  - Select the **Display latest scenarios first** checkbox (displays the scenarios in reverse order of derivation).
  - Select the **Display all uniquely named scenarios first** checkbox (displays all uniquely named scenarios at the root level).
    This option can be useful when multiple branches of a scenario, such as a new version with a different name, exist.
- To use the current settings in the dialog as the default display options, turn on the **Set as default display options** checkbox.
- Click **OK** to change the view of the studies and/or scenarios.

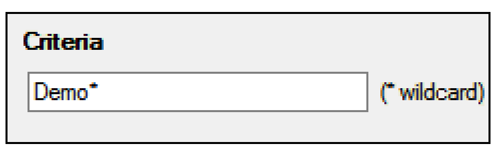


Filtering based on properties

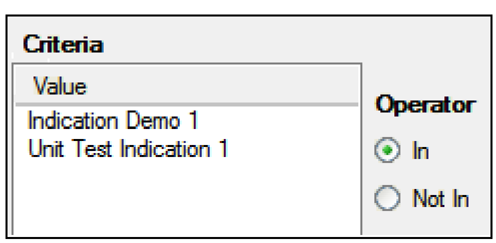
Filter criteria can be created based on the properties of a study, scenario, or Global Library objects. Filter specifications can be saved and reused, and a filter specification can be set as the default filter.

- Click  (**Filter** icon), which displays the *Filter PKS Contents* dialog.
- In the **Category** menu select **Study** or **Scenario**.
- Select a study or scenario property in the Property List.
- For some properties, text values must be specified in the **Criteria** field.

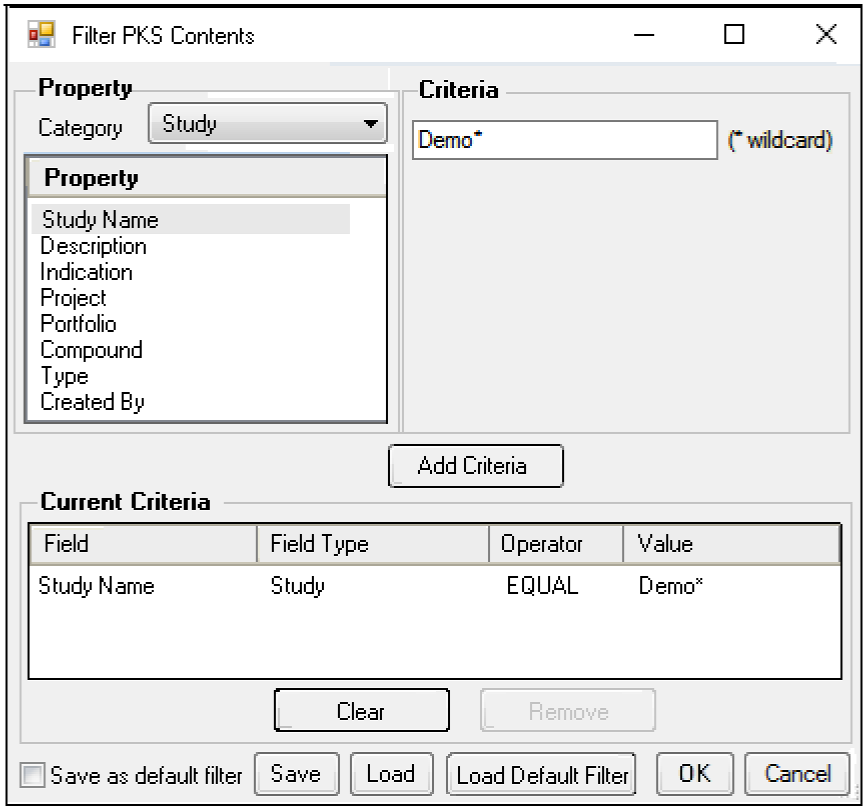
  An asterisk can be added to act as a wildcard for the filter criteria.



- For some properties users must select criteria based on existing values in the PKS database.



- Click **Add Criteria**, which adds the filter criteria to the filter in the **Current Criteria** list.



- Click **Add Criteria** to continue adding other criteria.
- Click **OK** to apply the filter criteria. The **Clear Filter** icon  (**Clear Filter** icon) is added to the PKS Browser toolbar.

  – Click **Clear** to clear all criteria from the Current Criteria field.
  – Select a criteria and click **Remove** to remove the criteria from Current Criteria field.
  – Click **Save** to save the filter criteria as an `.xml` file.
  – Click **Load** to load a saved filter criteria file.
  – Select the **Set as default filter** checkbox before saving the filter to set it as the default filter.
  – The default filter can be loaded by clicking **Load Default Filter**.
  – To clear the default filter, click **Clear**, select the **Set as default filter** checkbox and click **OK**.
  – To remove a filter applied to the PKS Browser, click the **Clear Filter** icon in the PKS Browser toolbar.

Viewing Study and Study Object properties

The PKS Browser allows users to view and modify the current study and scenario properties.

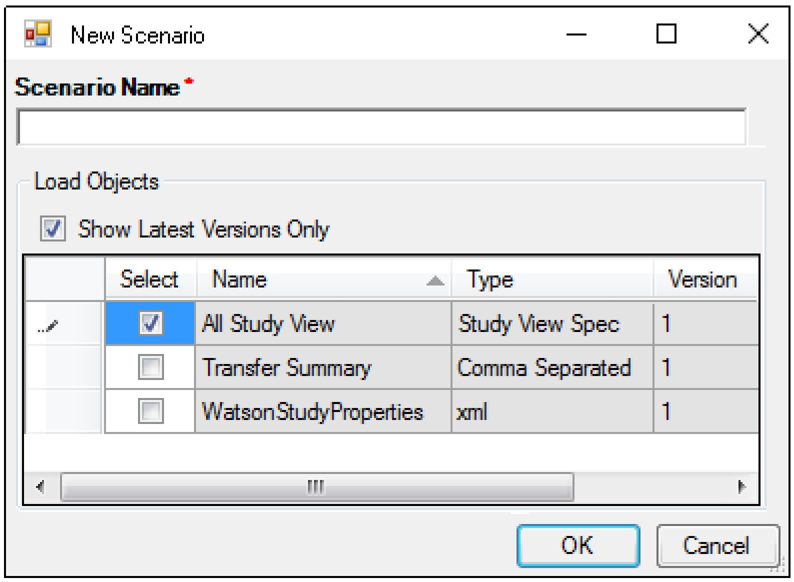
– Click  (**Show Properties** icon) to toggle the study properties view on and off.
– Select a study to view its Study Properties tab.
– Edit the study properties using the property menus that define the study.
– Edit the study description.
– Click **Apply** to save the changes to the PKS.

Creating a Scenario

Each PKS Scenario is treated as a Phoenix project. Scenarios can be created containing dependencies on multiple PKS objects stored in the parent study, or in other studies or scenarios, or in the Global Library.

If a study only contains study library objects, those objects can be loaded directly into a project. However, if data is mapped to PKS data structures, then a study view must be generated before creating a scenario. When the new scenario is created, the data can be analyzed, modified and then saved to the PKS as a scenario for the selected study.

- Select a study and then click (**New Scenario** icon) in the toolbar or **Action > New Scenario** from the menu.
  Or right-click a library or view object and select **New Scenario**.



- Type a scenario name in the **Scenario Name** field.
- Clear the **Show Latest Versions Only** checkbox to display all objects that can be loaded. If the scenario being created is the first version, then no additional objects are displayed.
  - Check the checkbox beside an object to include the object in the new scenario.
  - Select as many objects as needed to create the new scenario.
- Click **OK** to create the scenario. A message is displayed when the scenario project is created.

  If any errors were encountered during scenario creation they are displayed in a separate message.

  New scenarios typically contain the contents of one or more study views.

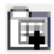
  After a scenario is created, additional objects can be loaded into the scenario by opening the PKS Browser, selecting an object, and clicking (**Load Object** icon).
- Click **Close** to close the PKS Browser.
- Use Phoenix to edit data, add or update models, or make any other changes before saving the new scenario to the PKS.

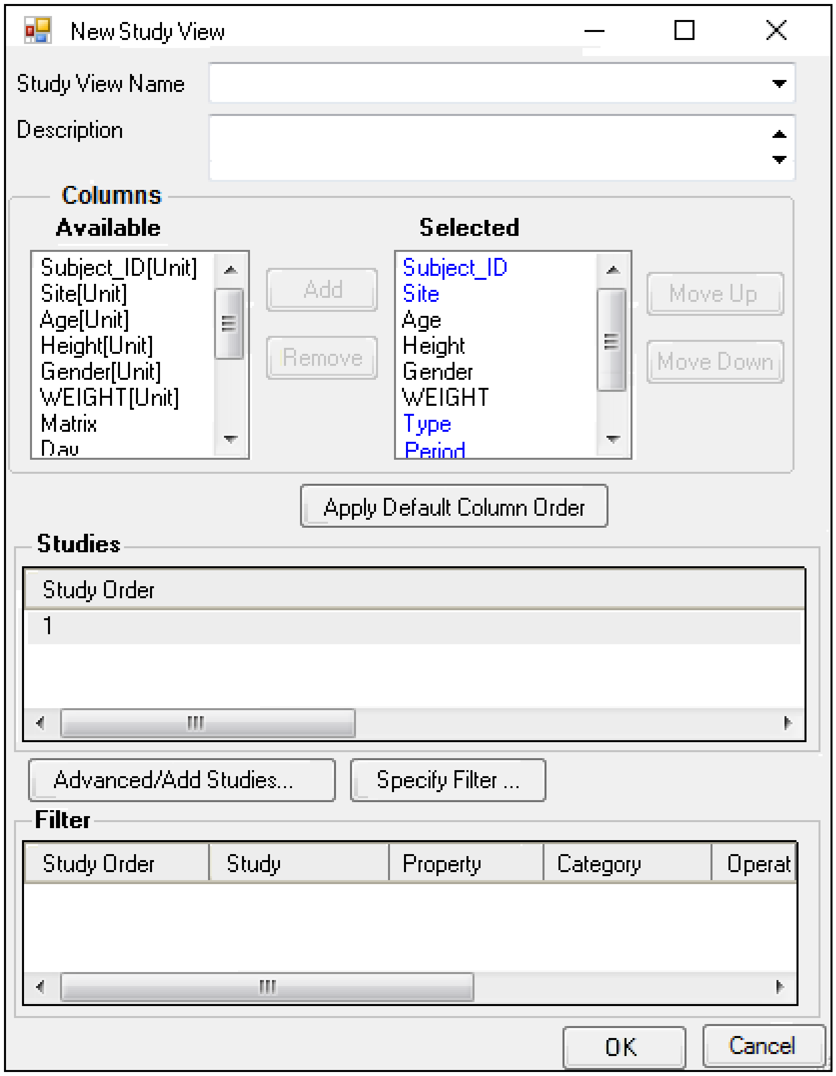
See "PKS Save and Save As options" for instructions on saving the scenario to the PKS.

Creating a Study View

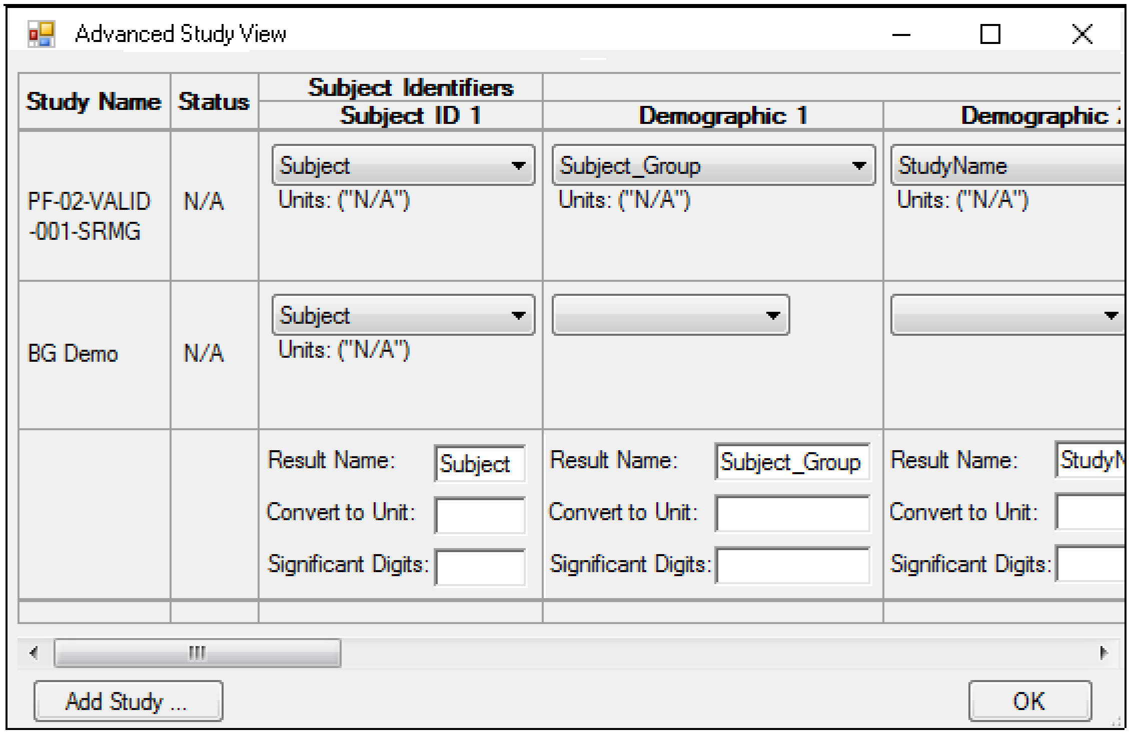
Study views define how to extract data from the PKS. Most commonly, views are specified to extract a subset of data (columns or rows) from the currently selected study. More complex views can be created to extract subsets of data from multiple studies.

Study views provide critical information necessary to reproduce datasets as they exist over time, and they provide for more granular status tracking of dependent analyses.

- Select a study and click  (**New Study View** icon).



- Type the study view name in the **Study View Name** field.
- Specify the columns to include in the view and their order.
  - Select a column in the Available list and click **Add** to move the column to the Selected list for inclusion in the study view.
    (Click **Remove** to move the column back to the Available list).
  - Select a column in the Selected list and click **Move Up** and **Move Down**.
- Use the *Advanced Study View* dialog to add studies to the new view and adjust the column associations and settings.
  - Click **Advanced/Add Studies**, which displays the *Advanced Study View* dialog.



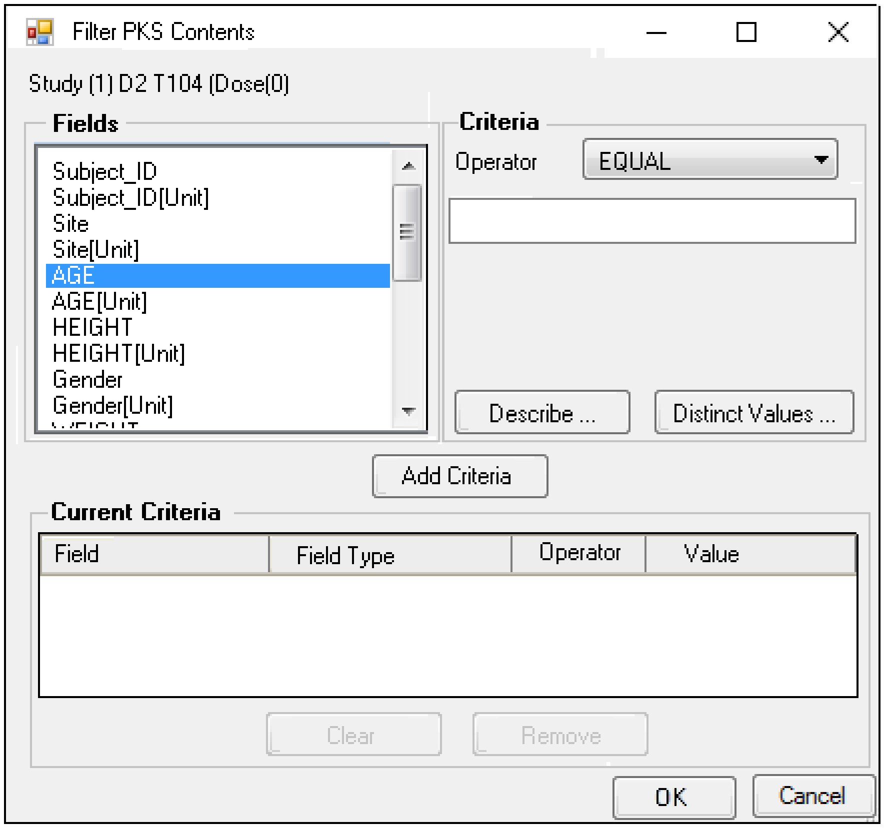
- Click **Add Study** to open the PKS Browser.
- Select a checkbox beside one or more studies and click **Select** to add them to the study view.

The new study information in displayed in the *Advanced Study View* dialog.

Depending on how the data source associated with a study is mapped, users can make changes to columns mapped to four areas: Subject Identifiers, Subject Demographics, Data Collection Point, and Observations.

- Use the menus in the Subject Identifiers, Subject Demographics, and Observations sections to change column mappings.
- Enter a new result name in the **Result Name** field or accept the default name.
- If a column has an associated unit, convert it by entering a conversion unit in the **Convert to Unit** field.
- Enter a new significant digit value in the **Significant Digits** field or accept the default value.
- In the **Data Collection Point** section, users can modify the nominal and relative time units, or leave the default settings.
- Click **OK** to close the *Advanced Study View* dialog.

- Click **Specify Filter**, which displays the *Filter PKS Contents* dialog.



- Select a field in the **Fields** list.
- In the **Operator** menu, select boolean operator to specify the criteria.
- In the **Criteria** field, enter a filter criteria for the selected field.

OR

- Click **Distinct Values** to display all distinct values in the selected field.
- Select a value and click **Select** to add the value to the Criteria field.
- Click **Add Criteria** to add the filter criteria to the Current Criteria list.
- Select a field and click **Describe** to open the Data Description window.
- Click **OK** to close the Data Description window.
- Click **Clear** to remove ALL of the filter criteria in the Current Criteria list.
- Select a filter criteria and click **Remove** to remove only that criteria from the Current Criteria list.

- Click **OK** in the *Filter PKS Contents* dialog to save the filter criteria. The filter criteria are displayed in the Filter list in the *New Study View* dialog.
- Click **OK** in the *New Study View* dialog to display the *PKS Save* dialog.
- Enter an Audit Reason in the **Audit Reason** field and enter your password in the **Password** field.
- Click **OK** to have the PKS process the new study view.

Loading existing scenarios/creating new scenario versions

- Select an existing scenario in the PKS Browser.
- Open the scenario in one of three ways:
  Double-click the scenario
  Or right-click the scenario and select **Load Scenario to Project**.
  Or click  (**Load Object** icon) in the toolbar.

  If the scenario has out of date dependencies, users are prompted to load current objects. If the latest versions are not loaded, use the **Refresh from Source** button to get the latest version of the dependent objects.

  Users can choose to load the scenario in its existing state or to get the most recent versions of dependent objects.

  Updated versions of individual PKS objects can be retrieved from the PKS.

- Select a scenario in the Object Browser. Right-click the scenario and select **Refresh from Source** to update the scenario from the PKS.

  When work is complete on the loaded scenario, it can be saved as a new version to the PKS.

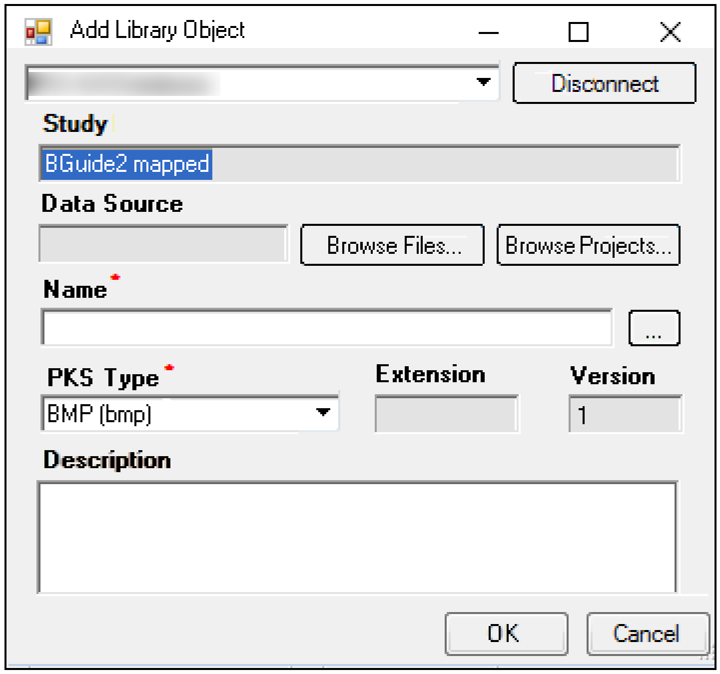
- Select **PKS > Save** to save the scenario.
- Select **PKS > Save As** to save the scenario as a new branch.

  Work can continue on scenarios between Phoenix and PKS sessions. Changes can be saved back to the PKS at any time.

Creating a new Study Library object

PKS supports storage and version history of objects, such as files or binary objects, at the study level. These objects can include documents, scripts, rule sets, or other files useful for the reporting or analysis of study data.

- Select a study to which to add a library object and then click the **New Study Object** icon  (**New Study Object** icon).



To load a file from a disk:

- In the *Add Library Object* dialog, click **Browse Files**.
- In the *Open* dialog, search for and select a file and click **Open**.
  The directory path is displayed in the **Data Source** field. The file name is listed in the **Name** field.

  Change the file name by typing a new file name in the **Name** field.
  Or select a name by clicking **[…]** to open the PKS Global Library browser.
- Select a library object and click **Select**.
- The object name is displayed in the **Name** field.

To load an object from an opened project or projects:

- Click **Browse Projects** to open the *Select Object* dialog.
- Select an object in an open project and click **Select**.
- In the *Add Library Object* dialog, use the **PKS Type** menu to assign a different type to the object.

  Some objects have only one PKS type. The PKS type default and options are based on the object file type.
- Enter a description for the object in the **Description** field.
- Click **OK**, which displays the *PKS Save* dialog.
- Enter an Audit Reason in the **Audit Reason** field.
- Enter your password in the **Password** field.
- Click **OK** to create a Global Library object in the PKS.

To create a new version of an existing study library object:

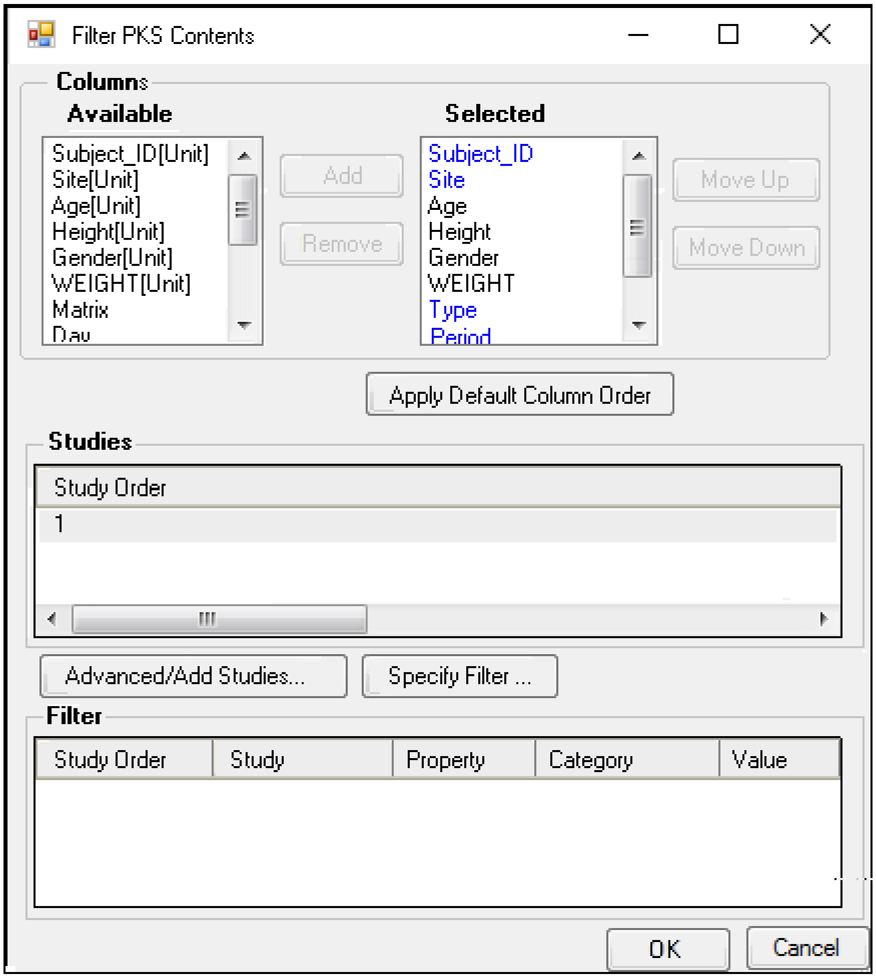
- Select the object in the PKS Browser.
- Click the **New Study Object** icon. The *Add Library Object* dialog is displayed.

- Make any necessary changes in the *Add Library Object* dialog.
- Update the library object by selecting a newer version from a saved file or an open project.
- Click **OK** to update the object.

  In the PKS Browser, the updated version is listed beneath the previous version.

Editing study data

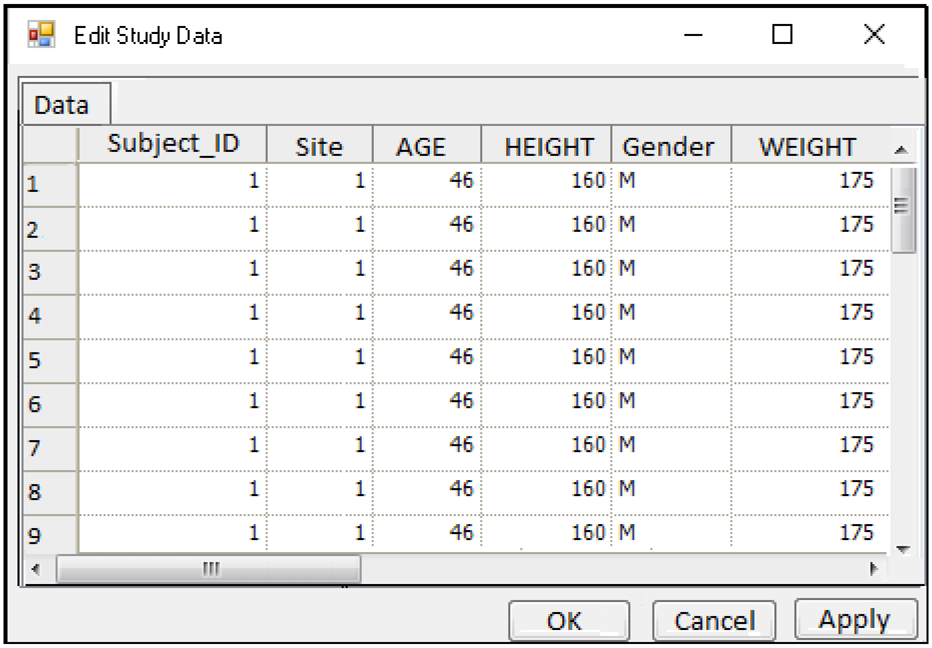
- Select a study to edit in the PKS Browser.
- Click (**Edit Study Data** icon) (or right-click the study and select **Edit Study Data**).



  - In the *Load Study Data* dialog, accept the default study data columns in the **Selected** field.

  OR

  - Select a column in the Available list and click **Add** to move the column to the Selected list.
  - Remove a column from the selected list by selecting it and clicking **Remove**.
  - Change the column order in the Selected list by selecting a column and clicking the **Move Up** and **Move Down** buttons.
  - To specify a filter to return desired subset of data, click **Specify Filter** to add a filter.
- Click **OK** to retrieve the data and display it in the *Edit Study* dialog.



	Subject_ID	Site	AGE	HEIGHT	Gender	WEIGHT
1	1	1	46	160	M	175
2	1	1	46	160	M	175
3	1	1	46	160	M	175
4	1	1	46	160	M	175
5	1	1	46	160	M	175
6	1	1	46	160	M	175
7	1	1	46	160	M	175
8	1	1	46	160	M	175
9	1	1	46	160	M	175

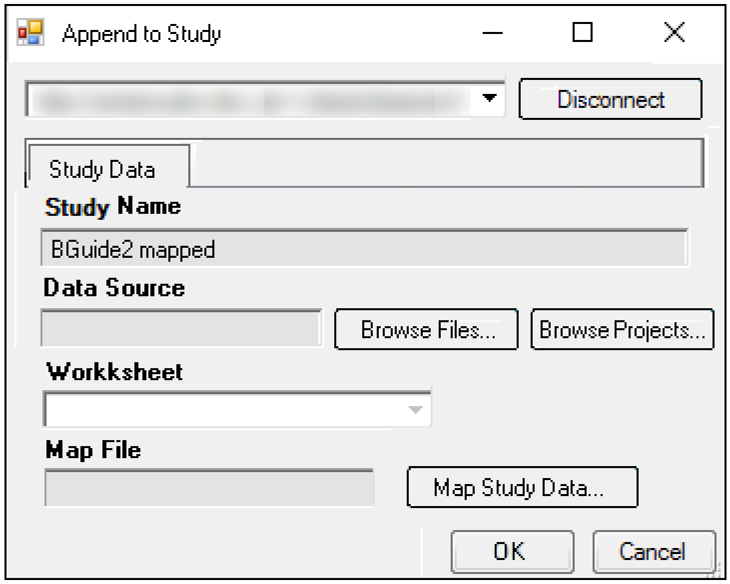
- Edit or insert values as needed.

- Click **Apply**, which displays the *PKS Save* dialog.
- Enter an Audit Reason in the **Audit Reason** field.
- Enter your password in the **Password** field.
- Click **OK**, which displays the PKS Process Manager.
- Click **Close** in the *Process Manager* dialog.
- Close the *Edit Study Data* dialog.

Appending data

Data can only be appended to a study that already has been added to the PKS.

- Select a study to append data to in the PKS Browser.
- Click  (**Edit Study Data** icon) (or right-click the study and select **Append/Update Study Data**).



- In the *Append to Study* dialog, select a data source by selecting a file or by selecting a dataset in a currently opened project.
  To learn more about Study Data, see "Selecting a data source".
  - If the there are multiple worksheets, select the one to use as the source for creating the study.
    If the selected data source is a workbook/worksheet, the *File Import Wizard* is displayed.
    If a data source from a project is selected, the *Select Object* dialog is displayed.
  - Select a worksheet in the *Select Object* dialog and click **Select** to add the worksheet as a data source.
- Click **Map Study Data**.
- In the *Study Mapping* dialog, assign the source columns to the appropriate tab.

  See "Mapping study data" for instructions on using the *Study Mapping* dialog.

  Users can load study mappings from a file. See "Loading a study map from a file" for instructions on loading a `.map` file.

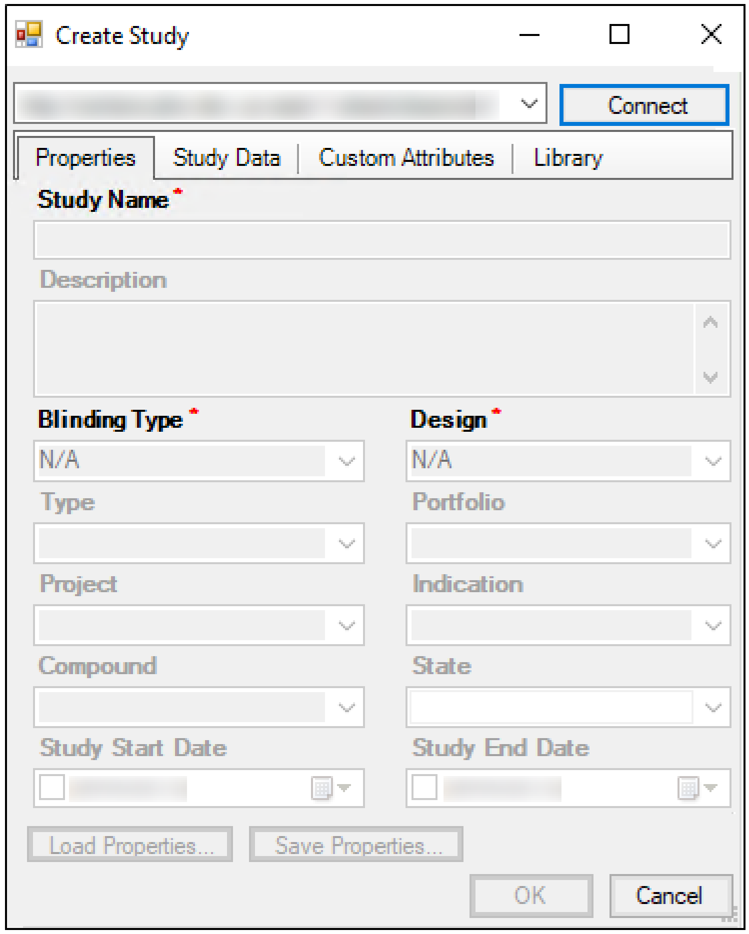
  Users can also load study mappings from the PKS. See "Loading a study map from PKS" for instructions on loading mappings from the PKS.
- Click **OK** to close the *Study Mapping* dialog.
- Click **OK** in the *Append Study* dialog, which displays the *PKS Save* dialog.
- Enter an Audit Reason in the **Audit Reason** field.
- Enter your password in the **Password** field.
- Click **OK**, which displays the PKS Process Manager.
- Click **Close** to close the PKS Process Manager window.

  The additional study data is incorporated into the first project.

Creating a PKS study

Studies are the fundamental unit of PKS organization. A PKS study stores raw data to be modeled and analyzed in one or more scenarios.

- A study can be created from a project loaded in Phoenix (**PKS > Save Project as PKS Scenario**) or from scratch (**PKS > Create Study**). In either case, the *Create Study* dialog is used to define the study components.



If a connection to an instance of PKS is not established, the fields and menus are unavailable in the *Create Study* dialog.

- To establish a PKS connection, select a PKS instance in the instance menu in the *Create Study* dialog. The selected PKS instance is used to create a new study.
If no instance is available, configure the PKS connection settings as described in “Setting up a PKS connection”.
- Click **Connect** and enter your user name and password in the *Connect to PKS* dialog and click **OK**.

If the **Prompt** option for credentials is selected in the *PKS Configuration* dialog, the *Connect to PKS* dialog will display prompting for the PKS user name and password and a user name and password for the proxy connection.

The metadata fields in the *Create Study* dialog are made available:

Study Name: Used to identify and locate a study in PKS; must be unique within the PKS database; typed entry; 50 character max. (Required field)

Description: Text describing the study; press Ctrl+Enter for line breaks; typed entry; 2000 character max.

Blinding Type: Blinding level for the study; typed or selected from list of prior values; 30 character max. (Required field)

Design: Experimental structure, e.g., parallel or crossover; typed or selected from list of prior values; 30 character max. (Required field)

Type: Type of study; typed or selected from list of prior values; 30 character max. (Required field)

Portfolio: Development portfolio to which the study belongs; typed or selected from list of prior values; 50 character max.

Project: Development project to which the study belongs; typed or selected from list of prior values; 100 character max.

Indication: Primary indication(s) for the study; typed or selected from list of prior values; 50 character max.

Compound: Main drug compound(s) under development; typed or selected from list of prior values; 50 character max.

State: Whether the study will be locked against changes or not; selected entry: normal or locked.

Study Start Date: Date on which the study began; typed or selected from the calendar popup; YYYY.MM.DD format.

Study End Date: Date on which the study concluded; typed or selected from the calendar popup; YYYY.MM.DD format.

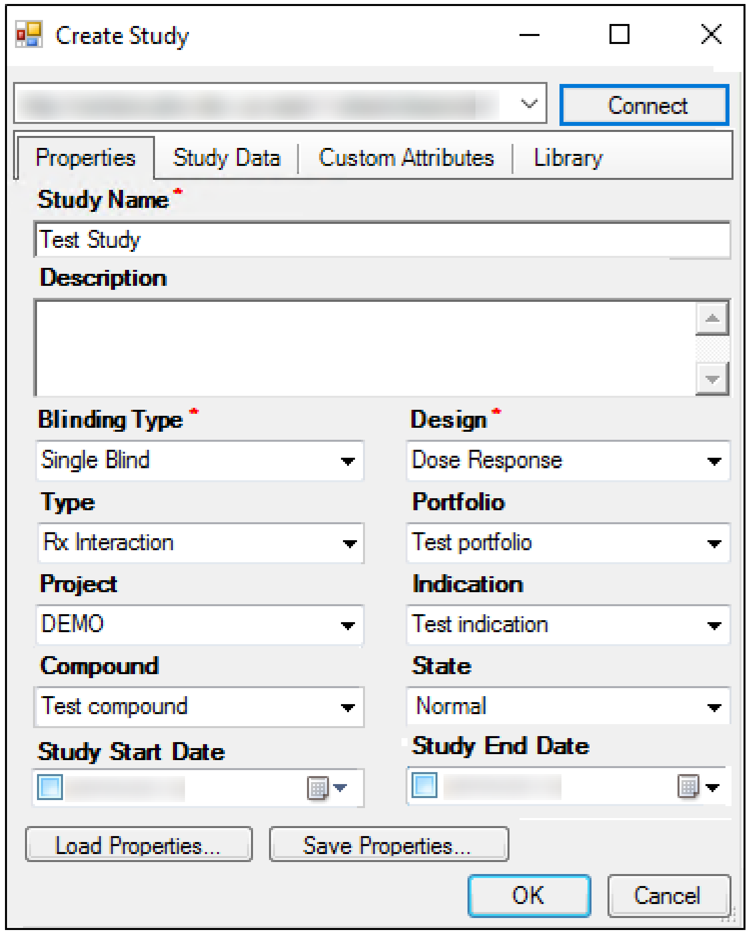
- In the Properties tab, enter the study name and a description of the study.
- Use the menus in the *Create Study* dialog to select blinding type, design type, study type, portfolio, etc.
- To save the study properties, click **Save Properties**.
- Type a name in the File name field and click **Save**.

The study properties are saved as a `.map` file.

Load study properties from a file

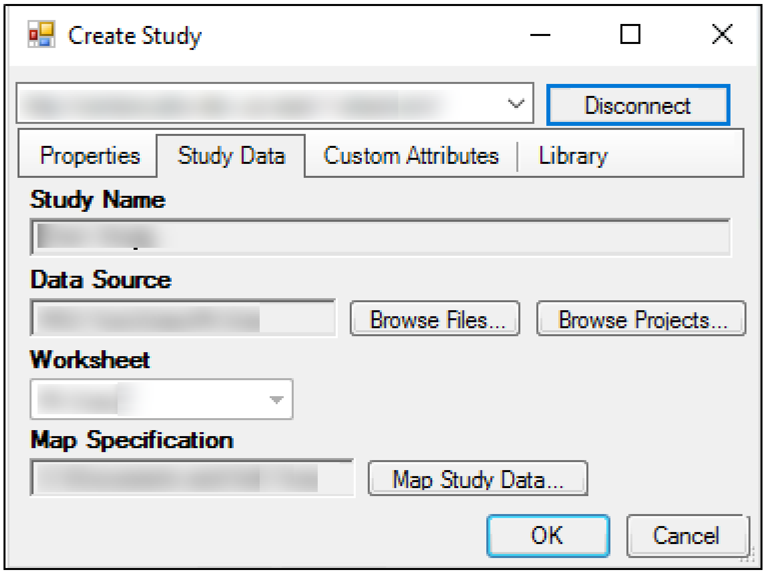
- Click **Load Properties**. The *Open* dialog is displayed.
- In the *Open* dialog, select the directory that contains the study properties file.
- In the **Files of type** menu, select one of three study property file types:
  Map (`*.map`)
  XML (`*.xml`)
  WNL Map (`*.pks`)
- Select the file and click **Open** to load saved study properties.

To learn more about creating and loading properties, see "PKS study properties".

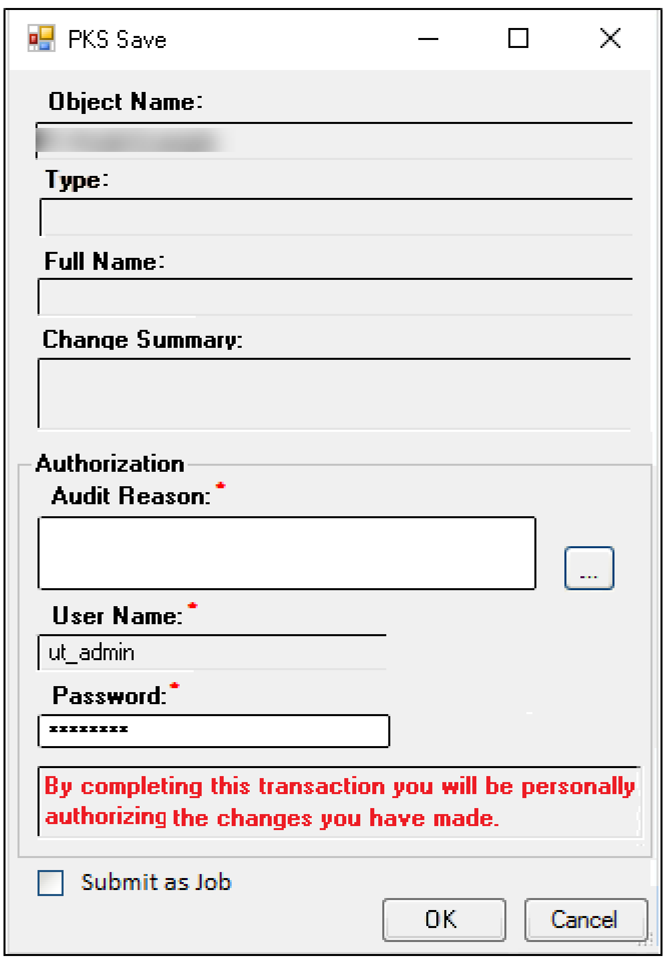


- Select the Study Data tab.
- Click **Browse Files** to select a data source from a file.

  Column names in the data source cannot include an apostrophe as it can lead to errors when the data is added to the mapped columns.
- Click **Browse Projects** to select a data source from an open Phoenix project.
- Use the *Select Source* dialog to navigate to a data source in Phoenix.
  For more on Study Data, see "Selecting a data source".
  - If the selected data source contains multiple worksheets, the *File Import Wizard* is displayed.
  - In the *File Import Wizard*, select the worksheet to use as the source for creating the study.
  - Additional worksheets can be appended to the study using the **Append/Update** feature.
- Click **Map Study Data** and then:
  - Create a new study mapping as detailed in "Creating and saving a .map file".
  - Load a map from file as detailed in "Loading a study map from a file".
  - Load map from PKS as detailed in "Loading a study map from PKS".
- Click **OK**, which saves the map settings to the study.

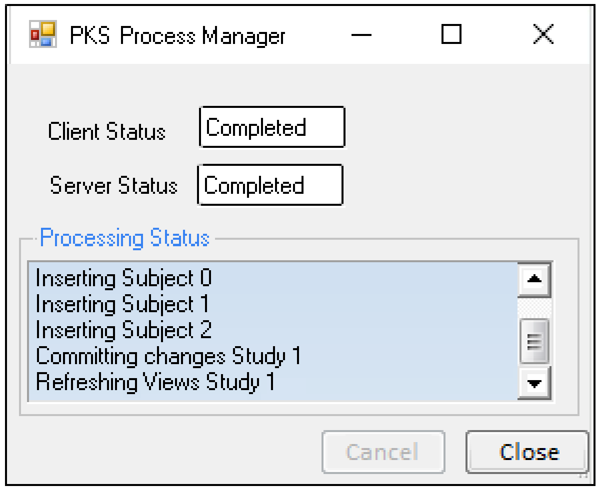


- Select the Custom Attributes tab and check the boxes of the custom study attributes to include in the study.
- Check **OK** in the *Create Study* dialog to display the *PKS Save* dialog.



- Enter an Audit Reason in the **Audit Reason** field.

- Enter your password in the **Password** field.
- Click **OK**, which displays the PKS Process Manager.



- Click **Close**, which saves the study to the PKS.

The study can also be submitted as a job after which the Phoenix session can be terminated and the processing will continue on the server processed later.

- Select the **Submit as Job** checkbox to process.
- When the PKS has received the job information the *PKS Process Manager* can be closed.
- Use the *PKS Job Viewer* to monitor the processing status.

PKS study properties

Properties can be entered once or saved for future use. Once a properties file has been saved, the file can be loaded during any study creation. Saving the properties file is helpful if multiple projects have the same properties or if you create a study in PKS from this project multiple times. The saved properties can be modified once they have been loaded.

This section covers the following topics:

Creating and Saving Properties to a file
Loading properties files

Creating and Saving Properties to a file

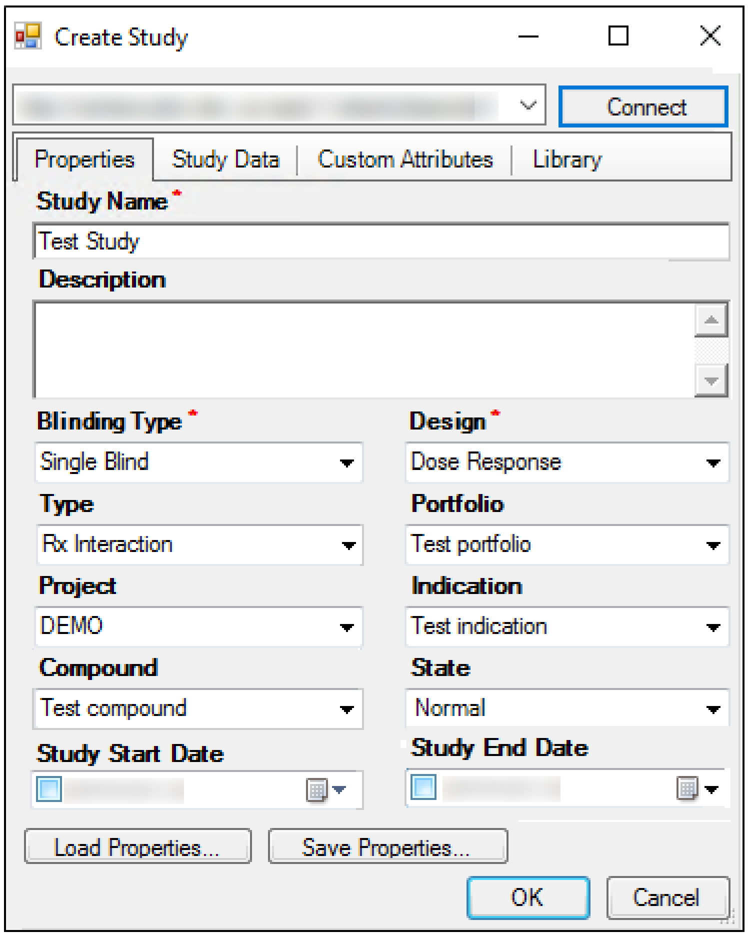
- Load a Phoenix project file (*`.phxproj`) or create a new project.
- Select **PKS > Create Study**.
- If Phoenix is not already connected to PKS, click **Connect** and enter your login credentials in the *Connect to PKS* dialog.
- In the **Study Name** field, type a study name.
- Enter a description in the **Description** field.
- Use the menus in the *Create Study* dialog to specify Blinding Type, Design, Type, Portfolio, etc. A red asterisk (*) denotes a required study property.
- Click **Save Properties** to save the study properties.
- In the *Save As* dialog, enter a file name and select a location in which to save the `.map` file.

- Click **Save** to save the `.map` file.

Loading properties files

- Load a Phoenix project file (*`.phxproj`) or create a new project.
- Select **PKS > Create Study**.
- If Phoenix is not already connected to PKS, click **Connect** and enter your login credentials in the *Connect to PKS* dialog.
- Click **Load Properties** to load a file with saved study properties.
- In the *Open* dialog, select a `.map` file or a `.pks` file.

  Phoenix WinNonlin study properties are saved as a `.map` file.
  WinNonlin 5.3 study properties are saved as a `.pks` file.
- Click **Open**, which loads the study properties.



- If necessary, users can further modify study properties after the properties are loaded.
- Enter a new name or description in the Study Name and Description fields, or use the menus to modify study properties such as Blinding Type, Design, Type, etc.

PKS study data

If study files are saved to the study library, no mapping is necessary. However, if a study is going to be saved to the PKS from Phoenix, the data source and its columns must to be mapped before creating the study in the PKS. Only one data source needs to be selected. The data source can be imported from a disk or selected from an open project.

Once a data source is selected the observation data, demographic data, and other data must be mapped to the appropriate columns. A `.map` file can be created and saved or properties can be loaded from a previously created `.map` file.

Note: If a sample, dose, or demographic source field contains multiple values, use one of the following options to prevent leading zeros or commas from being stripped:
– include a space between the values (e.g., “01, 2, 3”)
– include quotes in the value, so in a CSV file, it would be “”01,2,3””
– include any non-numeric characters in the value

Selecting a data source

- Load a Phoenix project file (*`.phxproj`) or create a new project.
- Select **PKS > Create Study**.
- If Phoenix is not already connected to PKS, click **Connect** and enter your login credentials in the *Connect to PKS* dialog.
- In the Properties tab, make sure the study property fields contain the appropriate selections.
- Select the Study Data tab.

There are two ways to add a data source: selecting a file from a disk or selecting a worksheet in a Phoenix project.

- To select a file from a disk:
  - Click **Browse Files**.
  - In the *Open* dialog, select a worksheet or workbook then click **Open**.
  - In the **Options** area of the *File Import Wizard*, specify any additional import options.
  - Click **Finish** to add the worksheet or workbook.
- To select a file from a Phoenix project:
  - Click **Browse Projects**.
  - In the *Select Source* dialog, click the (**+**) signs beside workbooks and operational object results to locate a data source.
  - Use the pointer to select the data source.
  - Click **Select**.

The *Select Object* dialog closes and the selected data source is listed in the **Data Source** field.

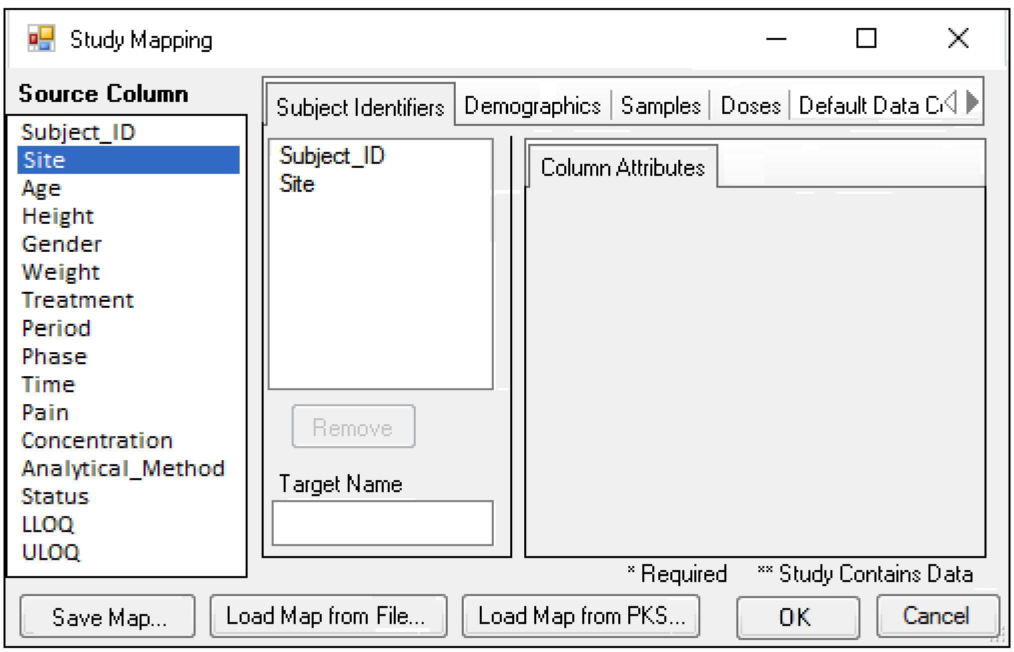
Mapping study data

Study data can be mapped to PKS structures and saved as a `.map` file, loaded from an existing map file on a disk, or loaded from an existing `.map` file in the PKS.

Creating and saving a .map file

- Load a Phoenix project file (*.`phxproj`) or create a new project.
- Select **PKS > Create Study**.
- In the *Create Study* dialog, select the **Study Data** tab.
- In the Study Data tab, select a data source and click **Map Study Data**.

  In the *Study Mapping* dialog, all the source columns in the worksheet are listed on the left. All of the different contexts for mapping are shown as tabs on the right.
- To map a column to a Subject Identifier, Demographic, Samples, or Doses context, click and drag the source column from the list on the left to the list in the context tab. For example, drag the column that uniquely identifies subjects from the Source Column list to the list in the **Subject Identifiers** tab.



  - Use the **Remove** button to unmap a selected column.
  - Enter an alternative name for the selected column by typing it in the **Target Name** field.
  - Select the mapped column in the list to display attributes that can be modified.
- Specify column attributes and defaults for data collection points or treatments.
  - If the attribute values are in a separate column, click and drag that column to the attribute field.
    (For example, if units are recorded as a separate column in the data source, click and drag that column name from the Source Column list to the **Units** attribute text field.)

- If the attribute value is always the same (i.e., static), enter that value and select the **Static** checkbox.

The Demographics tab maps subject data such as demographics and covariates.The selected demographic columns must contain values that exist once per subject. That is, the values are not time or visit dependent.

The Samples tab is for mapping time-dependent sample results and contains the following column attributes.

Unit: Units of measurement.

Status: Indicates data status, for example, below a limit of quantification (BQL), or missing due to dropout or non-adherence. Valid data are finite. The list of statuses is defined by a PKS administrator.

Sample_Number: Sample identifier.

Sample_Matrix: Identifier for the sample matrix.

Sample_Description: Further information about the sample.

Analytical Method: Assay or technique used to obtain the sample data.

LLOQ: Lower limit of quantification for the assay. A numerical value.

ULOQ: Upper limit of quantification for the assay. A numerical value.

The Doses tabs contain the following column attributes.

Unit: Units of measurement.

Status: Indicate data status, for example, below a limit of quantification (BQL), or missing due to dropout or non-adherence. Valid data are finite. The list of statuses is defined by a PKS administrator.

Sample_Number: Sample identifier.

Sample Description: Text information about the sample.

Route: Variable identifying route, oral, IV, IM, etc., for each dose.

The Data Collection Point tab (and Default Data Collection Point tab) is used to specify columns that contain data used to uniquely identify events where samples were collected or doses were administered. The mappings can be overridden per dose or sample. The following column attributes are available on the Data Collection Point tab:

Period: Identifier for the period of the study.

Phase: Identifier for phase of the study.

Matrix: Matrix value, if study involves a matrix of analyte and concentration combinations.

Day: Number of days after the study, phase, period started.

Visit: Identifier for the visit during which observation was made/sample was taken.

Analyte: ID of the analyte used.

DCP Description: (Data Collection Point description) use this field for variables that distinguish different measurements stored a single observation column, for example, an indicator variable noting whether a given record contains a measurement of plasma concentration or pain score.

Relative_Nominal_Time: Scheduled time of observation or sampling since last dose.

Nominal_Time_Unit: Sample identifier.

Relative_Nominal_End_Time: Identifier for the sample matrix.

Relative_Actual_Time: Further information about the sample.

Relative_Actual_End_Time: Assay or technique used to obtain the sample data.

Actual_Clock_Time: Lower limit of quantification for the assay. A numerical value.

The Treatment tab (and Default Treatment tab) is used to specify columns that uniquely identify administered treatments. Treatment information is combined with data collection point information to uniquely identify events where samples were collected or doses were administered. The following column attributes are available on the Treatment tab:

Treatment: Variable identifying the treatment.

Treatment_Description: Additional descriptive field.

Route: Variable identifying route, oral, IV, IM, etc., for each dose.

Regimen: Variable identifying dose regimen.

Fasted_Fed: Variable identifying whether subject ate before dosing.

Formulation: Variable identifying drug formulation for each dose.

State: Additional descriptive field.

The Default Treatment mappings can be overridden per dose or sample.

- Click **OK**. The *Save As* dialog is displayed.
- Select a directory in which to save the `.map` file and type a name in the **File name** field. Click **Save**.
- Click the **OK** in the *Study Mapping* dialog.

The map file is used to create the study.

Loading a study map from a file

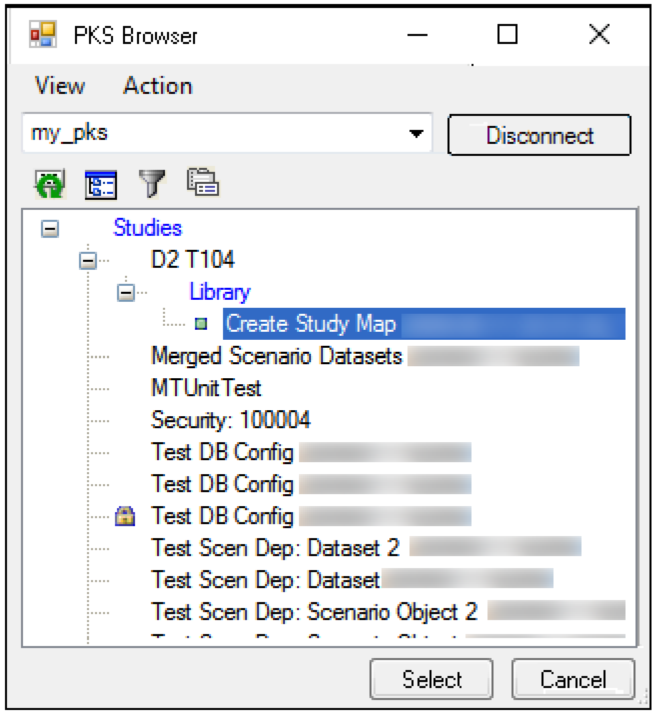
- In the **Study Data** tab of the *Create Study* dialog, select a data source and click **Map Study Data**.
- Click **Load Map from File**. which displays the *Open* dialog.
- In the *Open* dialog, search for and select the `.map` file.
- Click **Open** to load the `.map` file.
- Click **OK** to close the *Study Mapping* dialog.

The loaded mappings are applied and attached to the study.

The mappings are applied to the selected data source as closely as possible. Phoenix displays warning messages if there are any problems with the mappings.

Loading a study map from PKS

- In the **Study Data** tab of the *Create Study* dialog, select a data source and click **Map Study Data**.
- Click **Load Map from PKS**.



- In the PKS Browser, click the (**+**) sign beside the study that contains the mappings and select the map file.
- Click **Select** to load the map file.
  The loaded mappings are applied and attached to the study.

  The mappings are applied to the selected data source as closely as possible. Phoenix displays warning messages if there are any problems with the mappings.
- (Optional) Click through the study mapping tabs to make any changes.
- Click **OK** to close the *Study Mapping* dialog.
- In the *Save As* dialog, save the mapping file.

Detaching PKS objects from source

Objects loaded from PKS can be detached from their PKS source. Detaching an object from its source allows the objects to be edited without a link to a specific PKS source.

To detach a project, select the project in the Object Browser and then select **PKS > Detach PKS Settings from Project** or right-click the project object in the Object Browser and select **PKS > Detach Object**.

The PKS source information is removed from all items in the project and are editable.

To detach an individual item within a project, right-click the item in the Object Browser and select **PKS > Detach Object**.

The PKS source information is removed from the selected item in the project and is editable.

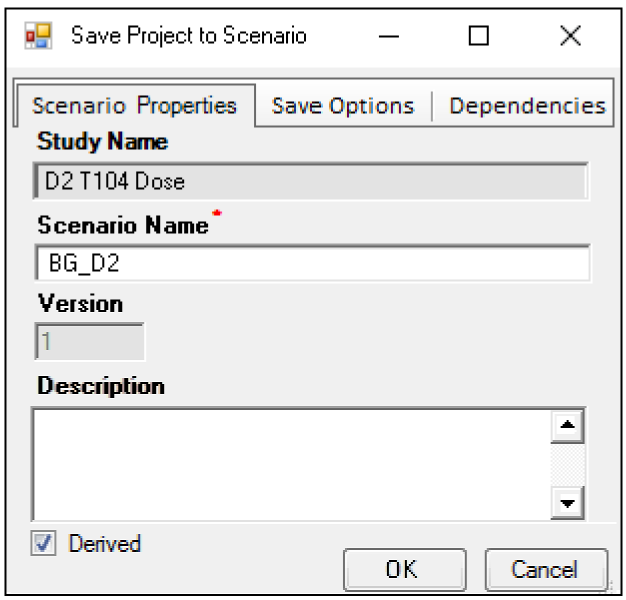
PKS Save and Save As options

The PKS Save option is enabled when a scenario is created or loaded into the Object Browser. The PKS Save As option is used to save a scenario with a new name in order to create a new branch.

Note: Windows has a maximum file path limit of 255. PKS operations involve creating projects/objects based on names generated from the study and scenario names. These object/projects will be saved to disk using the temp paths. This combination can result in file names (path+filename) that exceeds the Windows limit of 255 characters. To avoid potential issues with Phoenix operations due to exceeding this limit, maintain smaller study and scenario names, and/or change the tmp/temp environment variables to a shorter path (i.e. C:\tmp).

Load a scenario as a project from PKS into Phoenix and make any changes to the project using the instructions in "Creating a Scenario".

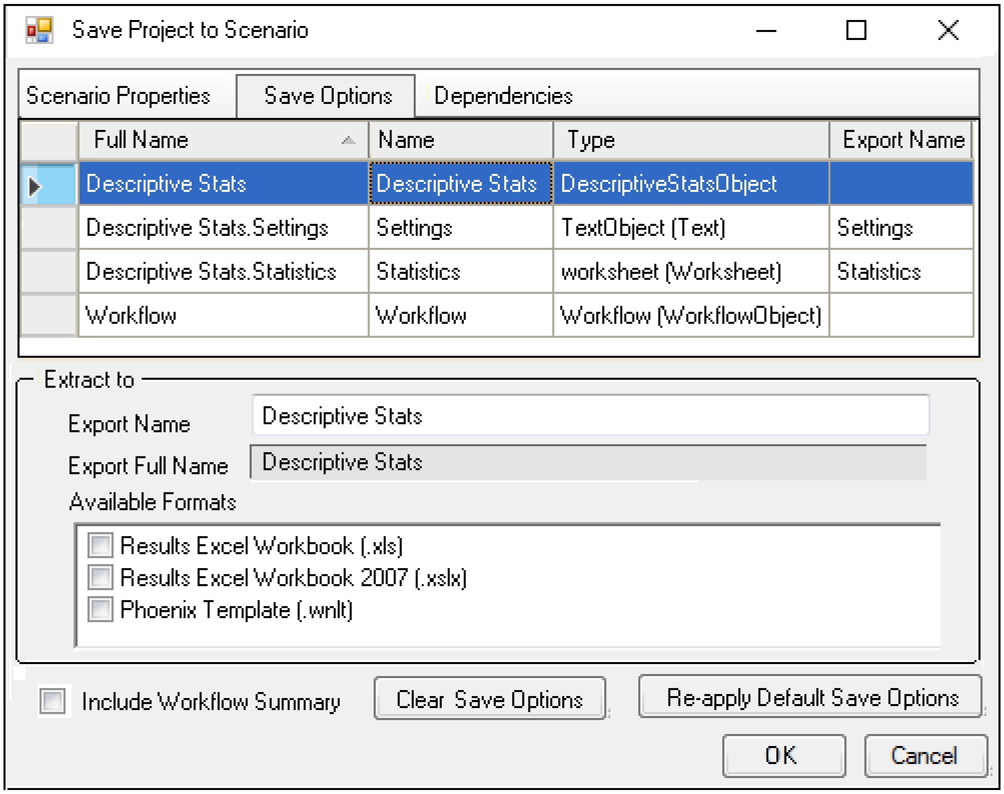
- Select the scenario in the Object Browser.
- Select **PKS > Save** or **Save As**.



- In the Scenario Properties tab of the *Save Scenario* dialog, the Study Name and Scenario Name are already entered, based on the project information.
- Accept the default scenario name or type a new name in the Scenario Name field.
- Enter a description in the Description field, or leave the default description.
- Clearing the **Derived** checkbox allows the users to enter a new name for the scenario and save it as version one of a new scenario. Checking this box saves the scenario as a subsequent version of an existing scenario.
- Select the **Save Options** tab.

  In existing scenarios, users can modify save options in the Save Options tab, or apply default save options.

  - Click **Re-apply Default Save Options** to apply the default settings as set in the PKS Preferences.

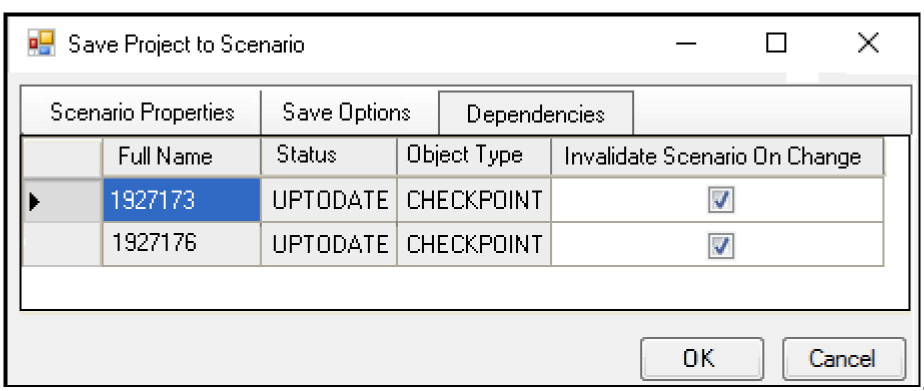


The Save Options tab displays objects in the current scenario that can be exported or saved to additional formats in the PKS.

Exporting objects using the **Save** and **Save As** functions allows objects to be viewed in the PKS Web interface, shared in other PKS Scenarios, and referenced by reports or queries.

Default save options are applied to new scenarios. See “Configuring default save options” for instructions on setting default save options.

- Select an object in the Save Options tab.
  - In the **Export Name** field, type a new name.
  - In the **Available Formats** field, check the format to be assigned to the selected object.
- Check the **Include Workflow Summary** box to save the `Workflow Summary.zip` file in the scenario.
- Select the **Dependencies** tab. The Dependencies tab allows users to set dependency tracking options.



Objects loaded from the PKS into the current scenario are listed in the Dependencies tab.

The default setting for each dependency is **Invalidate Scenario On Change**, which causes the scenario to be marked as out-of-date if or when a different version of the object is saved to the PKS. Clear the **Invalidate Scenario on Change** checkbox to not mark scenarios as **Out-of-Date** if or when a new version of the object is saved to the PKS.

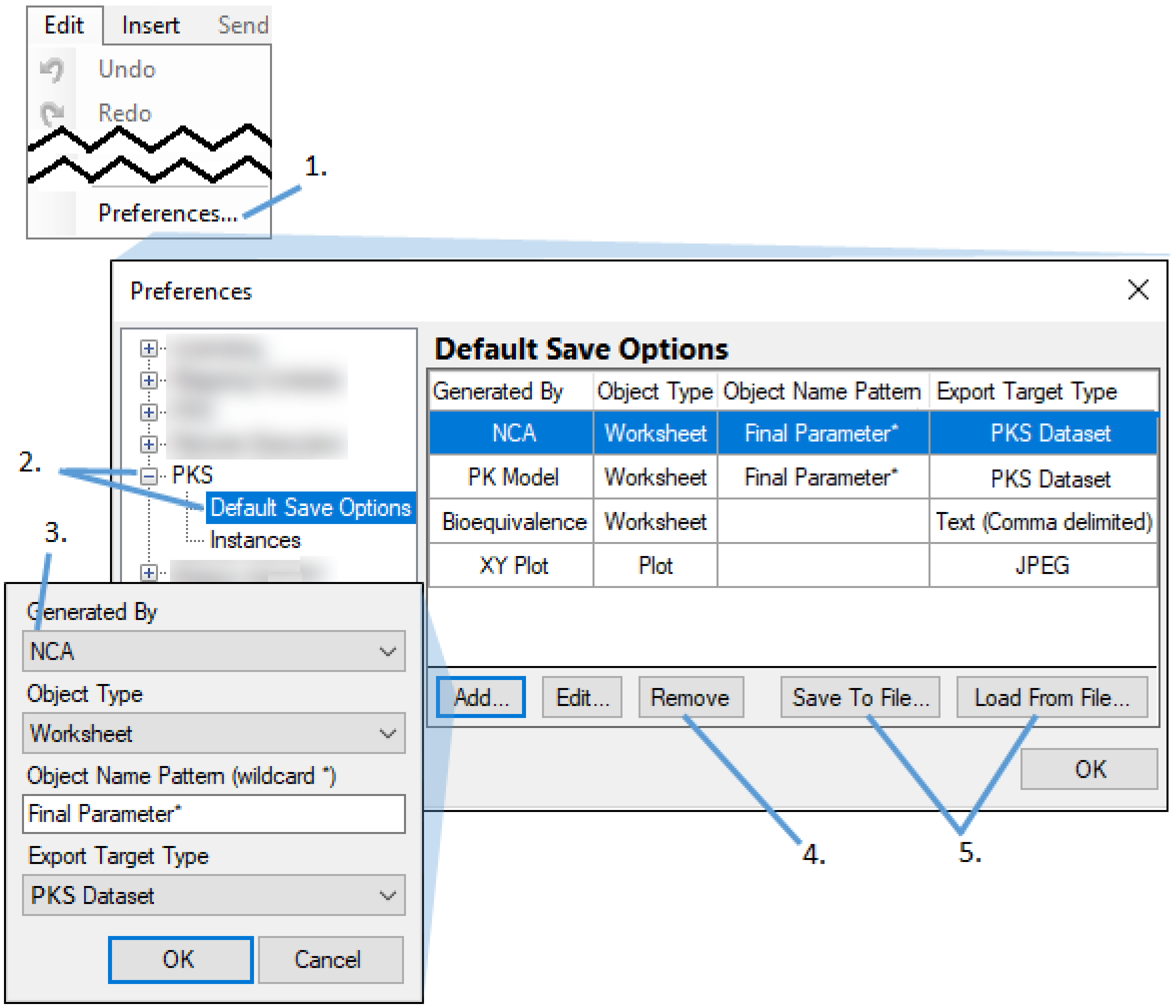
- After setting the scenario properties, save options, and dependency customizations, click **OK**.
- In the *PKS Save* dialog, enter an Audit Reason in the **Audit Reason** field.
- Enter your password in the **Password** field.
  - Check the **Submit as Job** checkbox to submit the job.
    (You can continue working in Phoenix or close it and the job will continue to run until completion.)
  - Use the PKS Job Viewer to monitor the status of submitted jobs.
- Click **OK** to save the scenario.

  The PKS Process Manager is displayed and shows the save progress.
- When the processing is complete or the job is submitted, click **Close** to close the PKS Progress manager.

Note: Loading a PKS scenario and submitting the workflow to the JMS for processing can prevent the scenario from being saved if the PKS middle-tier URL has changed since the scenario was last saved. If this occurs, run the scenario locally and save it to the PKS again.

Configuring default save options

The default save options can be configured in the PKS section in the *Preferences* dialog. The default save options determine how operational object output is displayed in the PKS. An operational object's output should be displayed when it is useful for data mining or reports, or if the output is loaded individually into another project to be re-used or shared.



1. Select **Edit > Preferences**.
2. In the *Preferences* dialog, select **PKS > Default Save Options**.
3. To add a default save option, click **Add**.
   To edit an option, select it and click **Edit**.

   In the *Default Save Option* dialog, use the pull-down menus and field to define a save option. For example, the previous image shows a new default save option being defined involving NCA. When the program encounters an NCA generated worksheet with a name that starts with "Final Parameter", it is to be exported to PKS as a PKS Dataset.
4. To remove a save option, select the option and click **Remove**.
5. To save the defined options to an XML file, click **Save to File**, then select a location and enter a filename in the dialog. To load options from a file, click **Load from File**.

Saving the default save options to a file is a useful way of synchronizing settings across an organization.

Loading and exporting multiple PKS objects

Multiple PKS objects can be loaded from Scenarios, Study Libraries, and from the Global Library

- In the PKS Browser, select the scenario or library to load.
- Click **Load Selected Objects**.

The **Load Selected Objects** button is available on the Scenario Objects tab, Study Library tab, and Library Objects tab.

The **Custom Load** button allows the user to load system objects, scenario objects, and study objects without using the default import handler for the object type. For example, `.xml` files can be loaded without Phoenix assuming it is a settings file. Pressing the **Custom Load** button displays a dialog showing the same options when the **File > Custom Import** menu option is used.

To export multiple PKS objects from Scenarios, Study Libraries, Global Libraries, and Study Views directly to disk as a zip file:

- In the PKS Browser, select the objects to export.
- Click **Export Selected Objects**.

The **Export Select Objects** button is available on the Scenario Objects tab, Study Library tab, Library Objects tab, and Views tab.

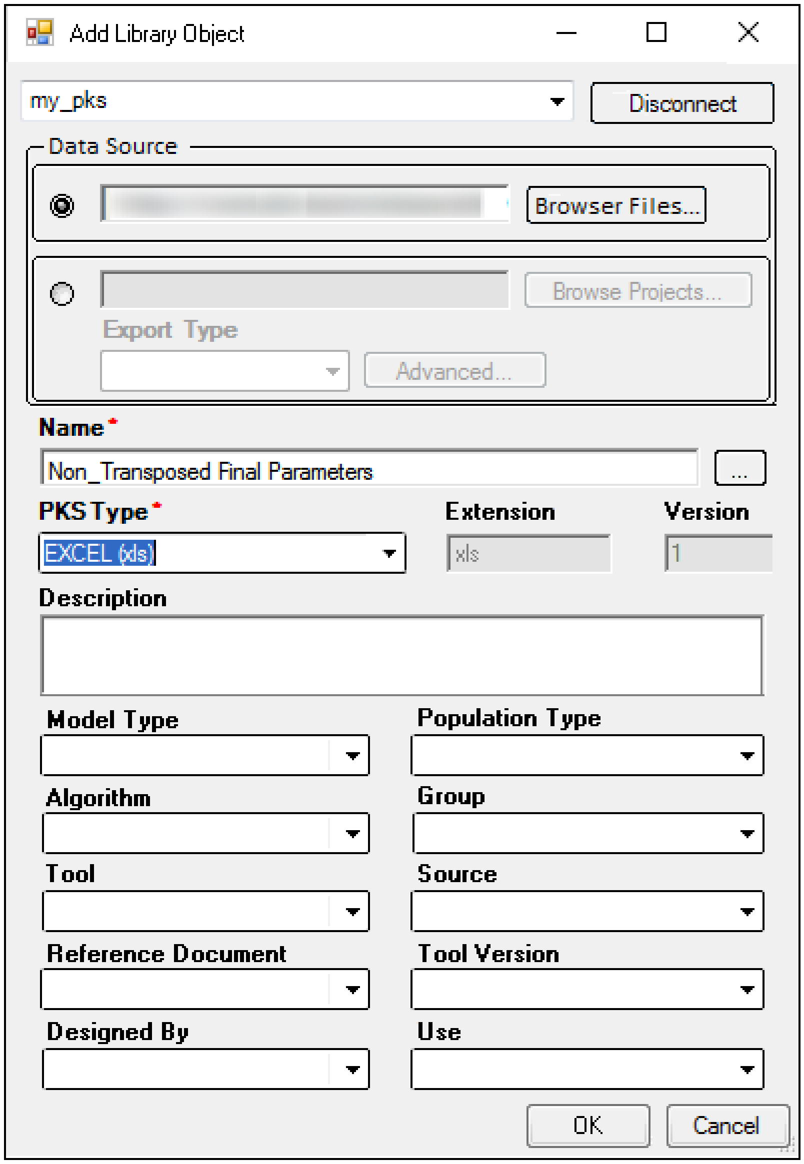
Ctrl+click to select the objects to export or use Ctrl+A to select all objects.

PKS datasets and study views are saved as `.csv` files with the units row included. If a selected file does not have an extension or it is not recognized, then the file is saved with a `.unknown` extension.

Global Library objects

The PKS Global Library can be used to centralize storage of objects that can be re-used across many projects. Objects loaded from the Global Library into Phoenix projects have their dependencies maintained.

- Select **PKS > Add to Library**. The *Add Library Object* dialog is displayed.



To select a file from disk:

- Click **Browse Files**.
- Use the *Open* dialog to search for, select, and open a file.
- The directory path is displayed in the Data Source field. The file name is listed in the Name field. Change the file name by typing a new file name in the **Name** field. Or select a name by clicking **[…]** to open the PKS Global Library browser.
- Select a Global Library object and click **Select**. The object name is displayed in the **Name** field.

To select a file from a Phoenix project:

- Click **Browse Projects**.
- In the *Select Object* dialog, use the pointer to select a data source and click **Select**.

  In the *Export* dialog, the type of file to export the object in the **Save as type** menu. Most non-dataset objects have no export options other than the file name and where to save the file.

  A few of the file types lead to additional dialogs of export options. For example, if a plot is specified, the *Image Settings* dialog is displayed; for an Excel file the *Excel Export Options* dialog is displayed; for an SAS Transport file, the *Rename Columns* dialog is displayed; for plain data files (CSV, DAT, or TXT formats), the Data *Export Options* dialog is displayed.
  - Make any changes in the dataset export dialogs and click **OK**.

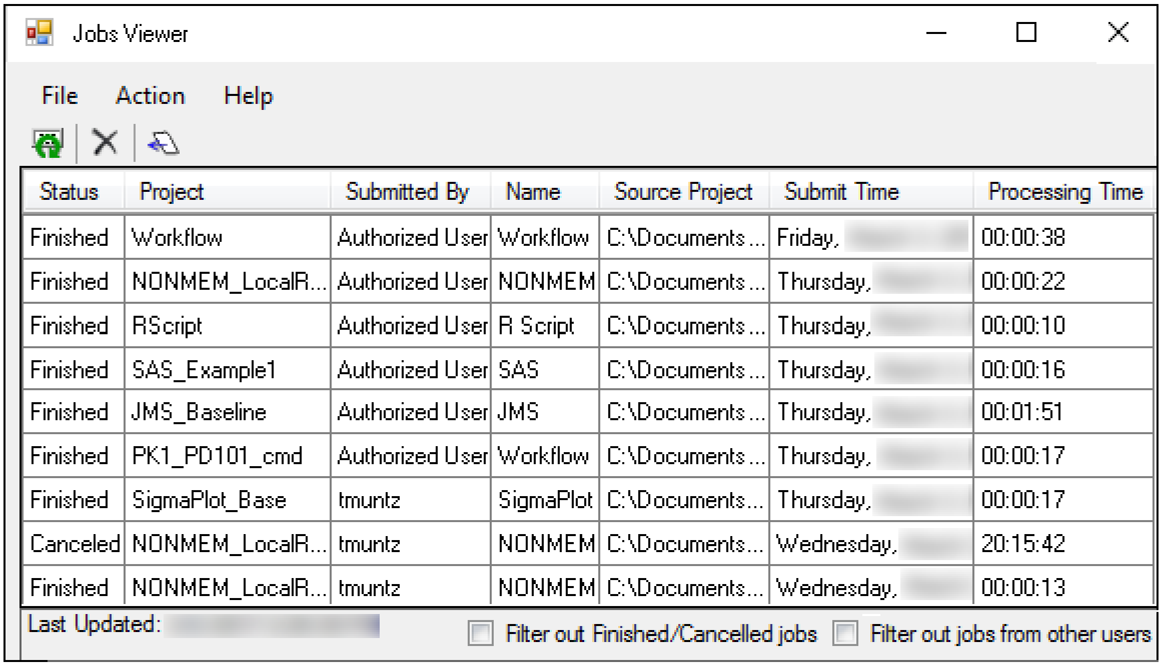
  The file is saved and the *Add Library Object* dialog displays the new file information.
- Use the **PKS Type** menu to assign a different type to the object.

  Some objects have only one PKS type. The PKS type default and options are based on the object file type.
- Enter a description for the object in the **Description** field.
- Use the attribute menus (Model Type, Population Type, etc.) to select different attributes for an object, or leave the default selections.
- Click **OK**, which displays the *PKS Save* dialog.
- Enter an Audit Reason in the **Audit Reason** field.
- Enter your password in the **Password** field.
- Click **OK** to create a Global Library object in the PKS.
- Use the **PKS Browser** to view the newly added Global Library object.

PKS Job Viewer

The *PKS Job Viewer* displays all jobs submitted by the current user within a specified time frame.

- Select **PKS > Job Viewer**. The *Job Viewer* dialog is displayed.



- In the **Time Frame** menu select a time range to use to display submitted job history.
- Click **Refresh** to refresh the *Job Viewer* and get the current status of submitted jobs.
- Check/uncheck the **Auto-refresh** checkbox to toggle automatic refreshing of the *Job Viewer* using the selected **Interval**.
- If the **Auto-refresh** checkbox is checked, use the **Interval** pull-down to adjust the time between refreshes: **5**, **10**, **30**, or **60** seconds.
- Select a job that is not completed and click **Terminate** to cancel the job.

Note: When terminating a job or reviewing the job list, it is recommended that the user turn off the **Auto-refresh** checkbox.

Plotting

Phoenix includes several plot objects. These can be used to create plots using imported datasets, or output data from an analysis. Users can choose from:

Bar Plot object: To display the numeric values of categorical data. The data values of each series are represented as horizontal bars, which are plotted along the vertical axis at equally spaced intervals.

Column Plot object: To display the numeric values of categorical data. The data values of each series are represented as vertical columns, which are plotted along the horizontal axis at equally spaced intervals. Error bars can be added when no Groups are used.

Box Plot object: To graphically represent groups of numerical data through their five-number summaries, which include the smallest observation, the lower quartile (Q1), the median (Q2), the upper quartile (Q3), and the largest observation.

Histogram object: To create a graphical display of a frequency distribution. Bars are used to show a count of the data points that fall into various ranges.

XY Plot object: To create scatter or line plots. It can also be used to create overlaid plots. Regression lines and error bars can be added to XY plots.

QQ (quantile-quantile) Plot object: To display the quantiles of numeric data along with a comparison distribution which is the Standard Normal, to determine how closely the data fits the normal distribution. A quantile is the percent of data points below a given value.

Scatter Plot Matrix object: To shows a correlation between two or more variables. The Scatter Plot Matrix object contains all the pair-wise scatter plots of the variables on a single page in a matrix format.

X-Categorical XY Plot object: To create scatter plots when X is discrete data. It can also be used to create overlaid plots. Profile data, the independent variable, and the dependent variables can also be mapped to the Grouping context. For example, if time data is mapped to the X context, it can also be mapped to the Group context. If the time data is also mapped to the Group context, and concentration data is mapped to the Y context, then the plot displays the time and concentration data points using different markers for the data points.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Plotting > [plot object name]**.
Or Main menu: **Insert > Plotting > [plot object name]**.
Or right-click menu for a worksheet: **Send To > Plotting > [plot object name]**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Additional information is available on the following topics:

Terminology of a plot display
Plots user interface
Plotting results
Error bars and overlaying plots example

Terminology of a plot display

Before describing the individual controls, it will be helpful to understand the terminology used when discussing the areas of a plot displayed in the Phoenix user interface.

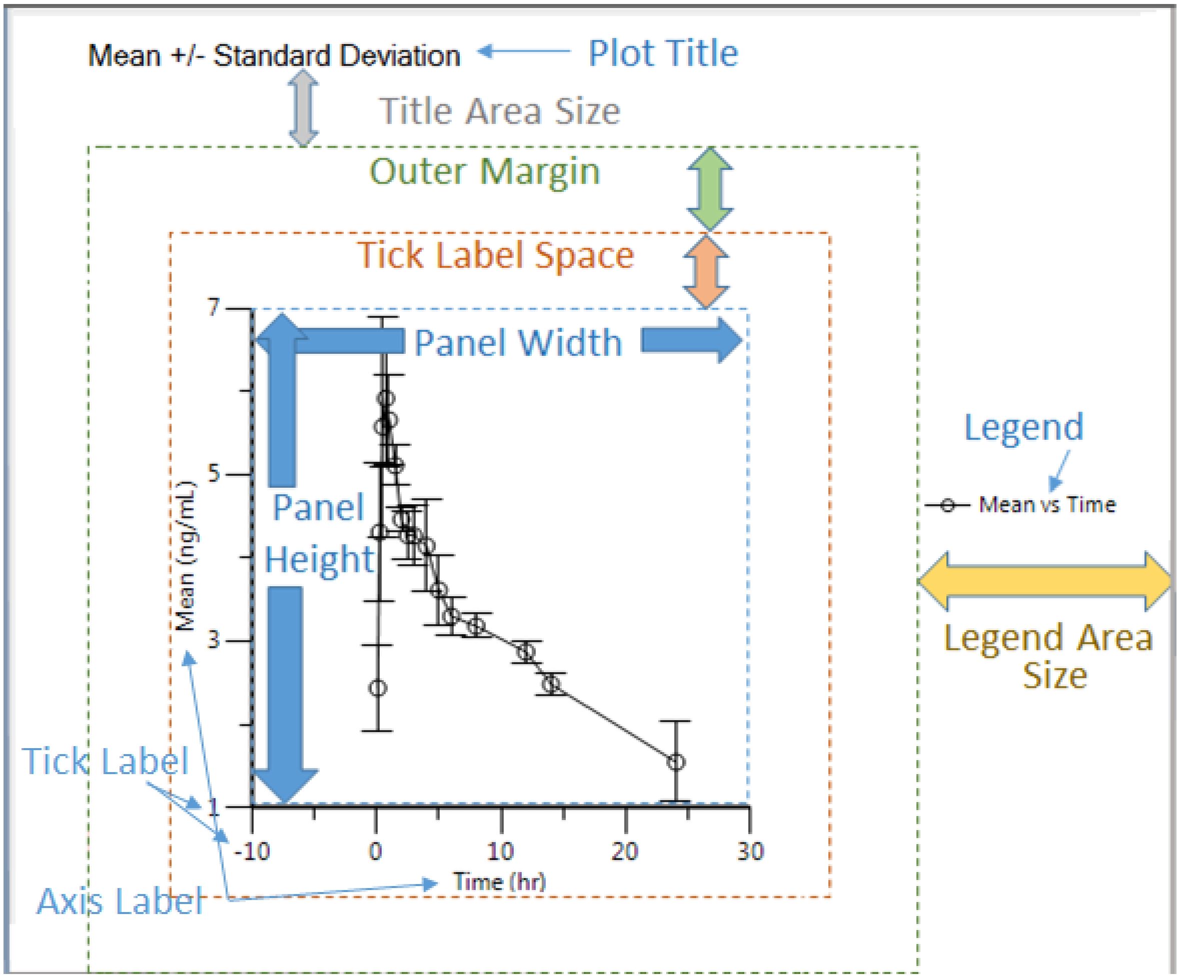


Figure 46-1. Anatomy of a Phoenix plot

- The center of the display is the actual plot or graph, itself. This includes the plotted data points, any regression lines or error bars, and the axes lines. Adjusting the panel height and width options will change the size of this area.
- The area that encompasses the tick marks, tick labels, and labels for the axes is called the axis and tick label space.
- The outer margin area extends beyond the axis and tick label space area and provides white space around the plot.
- The legend area is where the plot's legend is displayed, if specified.
- The space between the area where the plot's title is displayed and the outer margin area is referred to as the title area size.
- The area between the individual plots that make up a lattice is called chart spacing. For non-latticed plots, it is the area around the plot.

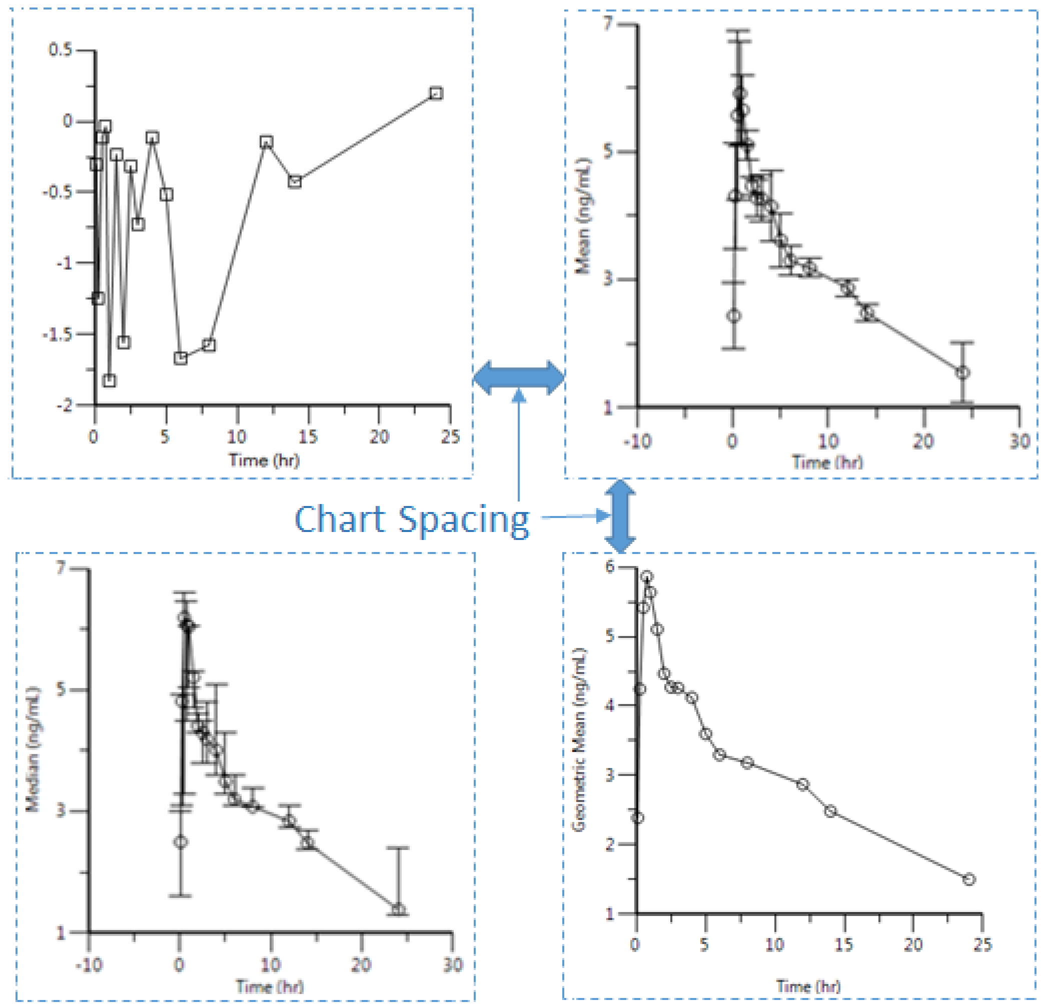


Figure 46-2. Chart Spacing is the white space between plots in a lattice

Adjusting the sizes of these areas is available in the Options tab below the display area, select the **Layout** under the **Plot** node. There are also controls for setting the appearance of different labels used in a plot. If you find a particular set of values that you would like to use as the default settings, they can be entered in the Plotting Defaults page of the *Preferences* dialog (**Edit > Preferences**). See "Plotting defaults" for more details.

Plots user interface

Plot objects in Phoenix share a set of common controls that allow users to configure the plot display. Plot options are located in the Options tab, which is located underneath the Setup tab. Users can select one of five main categories in the navigation tree to display the corresponding group of display options. The categories are the same for all plots except Scatter Plot Matrix (which does not have **Legend** or **Reference Lines** options).

Most menu options in the Options tab can be used to format the plot display before or after the plot object is executed. Options that do not automatically update the plot display are noted.

Data Mappings panel

Use the Data Mappings panel to identify how input variables are used in a Plot object. Separate plots can be created for each profile. Required input is highlighted orange in the interface.

None: Data types mapped to this context are not included in the output.

X: The independent variable axis. Note that, for Bar plots, this axis is the vertical axis. A single X mapping is required for Column, Bar, XY, and X-Categorical XY plots.

Y: The dependent variable axis. A single Y mapping is required for Box and QQ plots. Mapping of either **Y** or **Y2** is also required for XY, X-Categorical XY, Bar, and Column plots.

Y2: The secondary dependent variable axis. This axis is displayed on the top of each plot.

Included: Variables used to create a Scatter Plot. At least two variables must be mapped to this context.

Data Label: Labels for data points on the X axis.

Distribution: Variable used to create the Histogram plot quartiles. A single Distribution mapping is required.

Group: Only for Bar, Column, Box, and XY plots. Groups the X axis based on the selected variable.

Grouping: Only for X-Categorical XY plots. **None**: Data types mapped to this context are not grouped. **Grouping Group**: Displays the data points using different data point markers based on the variable mapped to this context. Any data type in a dataset can be mapped to Group even if it is also mapped to the independent and dependent variables contexts.

Lattice Conditions: **Row**: Separates the plots into multiple rows based on the selected variable or variables. (See “More on latticed plots in Phoenix”.) Not available for Scatter Plots. **Column**: Separates the plots into multiple columns based on the selected variable or variables. Not available for Scatter Plots. **Page (Sort)**: Separates the plot by page based on the selected variable. Allows users to sort a plot by a variable or variables.

Error Bars: Error bars represent the overall distribution of the data and are used to indicate how closely the means of the data reflect the true values. Error bars are only available for XY, and X-Categorical XY plots, and for Column plots that have no Group mapping. (See “Set up error bars".) **Lower Error Bar**: Error bar lengths or coordinates down the Y-axis. **Upper Error Bar**: Error bar lengths or coordinates up the Y-axis. Different variables in a dataset can be mapped separately to the Lower and Upper Error Bar contexts.

More on latticed plots in Phoenix

Latticing data is a way of arranging a plot display based on a sort key. For example, if a dataset contains columns for subjects, time of dose, and concentration, it is possible to create a graph that displays time versus concentration for each subject if subject is selected as a sort key.

There are two ways to arrange a latticed graph: by row and by column. If a graph is latticed by subject, and there are three subjects in the dataset, Phoenix can create three graphs on one page that are displayed as either three rows or three columns.

The Lattice Titles window allows users to map a title to the columns in the source dataset that are used as lattice values. Users can map a separate worksheet to Lattice Titles, or use the source dataset if it contains titles for the latticed variables. The lattice titles worksheet must contain the data that are used as the sort key or keys for the latticing, as well as one column that contains the title for the latticing sort keys.

For example, if a user wanted to create a graph that was latticed by subject, he or she would need a second worksheet that contains the subject IDs in one column, and the title for the subject IDs in another column. That worksheet would then be mapped to the Lattice Titles window.

Lattice conditions

- Variables mapped to **Lattice Conditions Row** create a single column of plots in the Results tab. For example, if a dataset contains 10 subjects and the subject variable is mapped to Lattice Conditions Row, then a column of 10 rows (one row per subject) with a separate plot in each row is created in the Results tab.
- Variables mapped to **Lattice Conditions Column** create a single row of plots in the Results tab. For example, if a dataset contains 10 subjects and the subject variable is mapped to Lattice Conditions Column, then a row of 10 columns (one column per subject) with a separate plot in each column is created in the Results tab.
- Variables mapped to **Lattice Conditions Page (Sort)** create a separate plot per page in the Results tab. Each page is located on its own tab in the Results tab.
  For example, if a dataset contains 10 subjects and the subject variable is mapped to Lattice Conditions Page (Sort), then 10 separate plots are created on 10 separate page tabs in the Results tab.

Lattice Titles panel usage

If a variable in a dataset is mapped to any of the Lattice Conditions, then the Lattice Titles panel is displayed in the Setup tab list. Users can map a worksheet to the Lattice Titles page to add titles to the variable mapped to a Lattice Condition. Scatter Plot Matrix objects do not have a Lattice Titles panel.

- Import a worksheet that contains the titles associated with the variable or variables mapped to a lattice condition.
- Use the pointer to drag the worksheet from the Data folder to the Lattice Titles panel.
  If the worksheet mapped to the plot Data Mappings panel contains the title column, drag the same worksheet to the Lattice Titles panel.
- Select the **Title** option button to map the title column to the Title context.
  The Lattice Condition selected in the plot Data Mappings panel must also be selected in the Lattice Titles panel. The column in the dataset that contains the title for the variable mapped to a Lattice Condition must be mapped to the Title context.

Plot Options tab

Select **Plot** in the menu tree to access the following tabs:

Content tab, see “Define display sets”

Appearance tab, see “Set plot background and border”

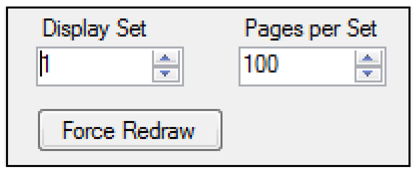
Title tab, see “Define plot title”

Graphs tab, see “Add or remove plots”

Define display sets

Select **Plot > Layout** in the tree, then click the Content tab.

Phoenix has a maximum limit of 100 page tabs per plot display panel. This is only a limit on the number displayed, all plots are created, and, if an export is requested, all plots are exported. If a dataset contains more than 100 profiles mapped to a lattice condition, then plots 101 to 200 are contained in the second display set, etc. The Plot Content tab provides controls for switching between display panels (i.e., display sets) and for adjusting the number of tabs available at one time in a display panel.



In the **Display Set** box, single-click the up and down arrows to view switch to a different set of page tabs (i.e., a different display set).

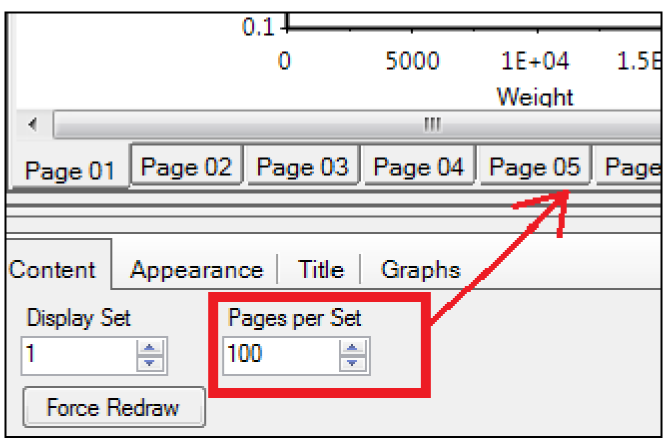
In the **Pages per Set** box, select or type the number of plot page tabs per display set.

The default and maximum number of page tabs per display set is 100.

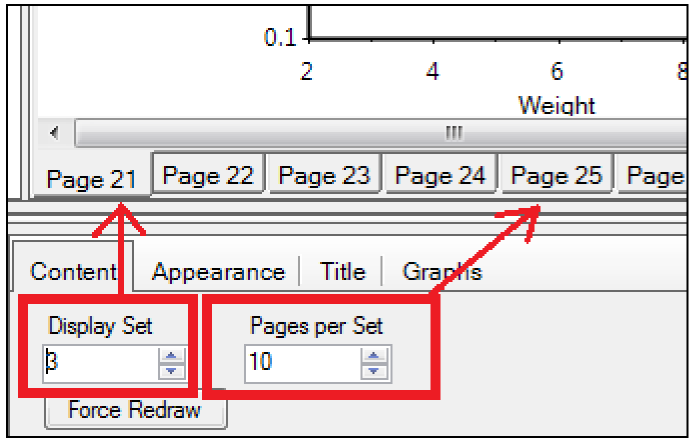
Change the **Pages per Set** value to display less page tabs in the plot display panel.

Click the **Force Redraw** button to apply any changes made to the settings on this tab. (Clicking in another field or pressing the **Enter** key after changing the value in a field also triggers a redraw.)

The example below uses the default settings for the Content tab. The first 100 pages of the latticed results are available in Display Set 1.



The figure below shows that the third display set has been selected for display and that the number of pages per set has been lowered to 10. Pages 21 through 30 are available when Display Set 3 is selected.



Set plot background and border

Select **Plot > Layout** in the tree, then click the Appearance tab.

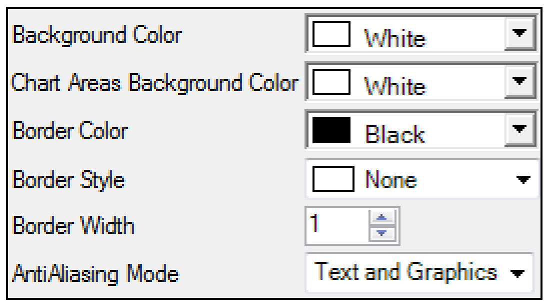


Figure 47-1. Plot Options — Appearance tab

In the **Background Color** menu, select the background color used in the plot display panel by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

In the **Chart Areas Background Color** menu, select the background color used as the background for each plot by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color

In the **Border Color** menu, select the background color used in the plot display panel by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

In the **Border Style** menu, select the border style to display around each graph.

In the **Border Width** field, select or type the width for the plot borders. Users can select up to a 20 point border width.

In the **AntiAliasing Mode** menu, select the part of the plot to be smoothed through anti-aliasing. Anti-aliasing options include:

None (default)

Text: smooth the lines in text only

Graphics: smooth the lines in the graphs only

Text and Graphics: smooth all lines (text and graphs)

Note that anti-aliasing can slow down performance.

Define plot title

Select **Plot > Layout** in the tree, then click the Title tab.

The Title menu item displays the title text field to enter a title for the plot. The tab also contains traditional Windows text formatting tools for defining the appearance of the title.

In the **Text** field, type a title.

Use the formatting controls above the **Text** field to modify the title's appearance.

Add or remove plots

Select **Plot > Layout** in the tree, then click Graphs tab.

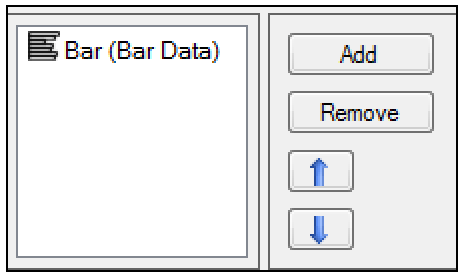


Figure 47-2. Plot Options — Graphs tab

Not all plot objects support adding multiple graphs to one plot object. If a plot object supports this feature, the Graphs tab instructions are included in that plot's section.

Note: Users cannot add additional plots to Box, Histogram, or QQ plot objects, so the Graphs tab controls are unavailable for those plots.

Click **Add** to add another plot to the Plot object. An additional plot is added to the plot list in the Graphs tab and an additional plot input is added to the Setup tab list.

Map a dataset to the additional plot object using the same steps listed under "Data Mappings panel".

Remove a plot by selecting a plot in the plot list in the Graphs tab and clicking **Remove**.

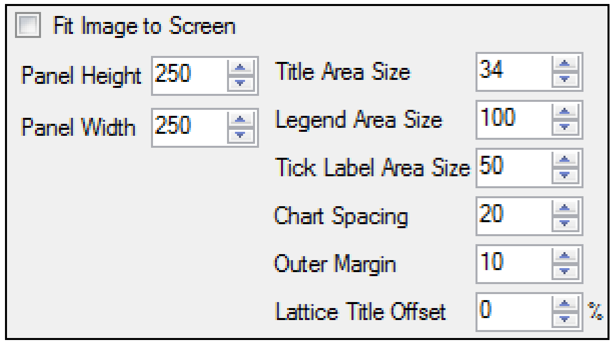
Change the order of the plots by selecting a plot in the plot list in the Graphs tab and clicking the up or down arrow buttons.

Note: Plots are given a default name based on the variables mapped to the **X**, **Y**, and **Y2** contexts.

Plot Layout Options tab

Select **Plot > Layout** in the tree.

Refer to "Terminology of a plot display" for a review of the various areas that make up a plot.



Select the **Fit image to screen** checkbox to force the plot image to fit the current size of the right viewing panel.

Note: Selecting **Fit image to screen** disables all other options in the Layout tab.

In the **Panel Height** field, select or type the number of pixels used to specify the plot height.

In the **Panel Width** field, select or type the number of pixels used to specify the plot width.

> If a value is entered that is larger than what can be used in the plot display panel, then Phoenix automatically changes the value to maximum possible. Selecting more pixels than can be used to create the plot automatically changes the title, legend, axis and tick label space, chart spacing, and margin values.

In the **Title Area Size** field select or type the number of pixels used for the title area of the plots. Setting the value too low can cause the title to get cropped.

In the **Legend Area Size** field select or type the number of pixels used for the legend area. The Scatter Plot Matrix object does not use the **Legend Area Size** control.

In the **Tick Label Area Size** field select or type the number of pixels used for the tick labels.

In the **Chart Spacing** field select or type the number of pixels used to specify the distances between plots.

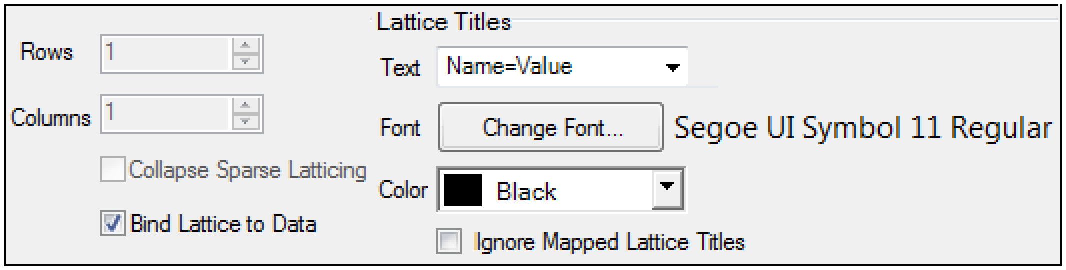
In the **Outer Margin** field select or type the number of pixels used to specify the margin around the plots.

In the **Lattice Title Offset** field select or type the number of pixels used to offset the lattice title from the plots.

Plot Lattice Options tab

Select **Plot > Lattice** in the tree.

The default lattice setting for a plot with a study variable mapped to one of the lattice conditions is **Bind Lattice to Data**. This setting automatically displays multiple plots per page (maximum is 15 by 15 plots per page). If a variable with more than 225 values is mapped to any lattice condition, Phoenix cannot automatically create the graph and lattice options must be set manually.



Clear the **Bind Lattice to Data** checkbox to specify lattice display options.

In the **Lattice Rows** box, select or type the number of rows used to lattice the plot.

In the **Lattice Columns** box, select or type the number of columns used to lattice the plot.

Select the **Collapse Sparse Latticing** checkbox to remove empty plots.

> If multiple variables are mapped to lattice conditions and one variable does not contain as many data points as the others, some empty plots are created. Complete plots are only created when all variables mapped to lattice conditions contain the same number of values. Selecting the **Collapse Sparse Latticing** checkbox removes the empty plots.

The **Text** menu controls the part of the plot title that comes from the data on which the lattice depends (e.g., the variable mapped to the Lattice Condition). Select the format for displaying this information in the title of each latticed plot. Options include:

Name: displays the name of the mapped variable.

Value: displays the value of the mapped variable.

Name - Value: displays the name and value of the mapped variable.

None: no information about the mapped variable is included in the title.

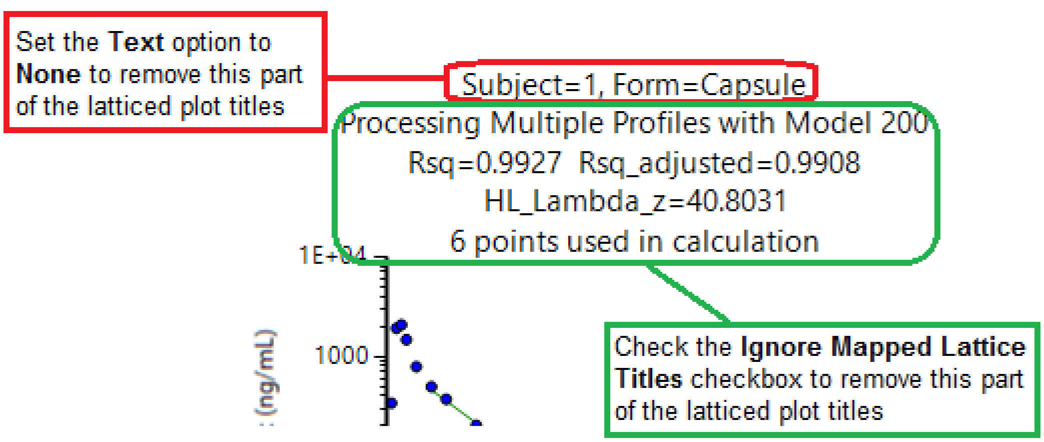
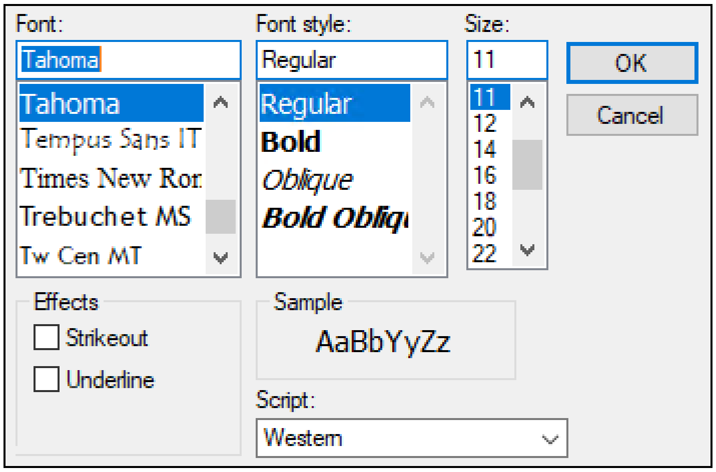


Figure 47-3. Controlling the content of latticed plot titles

Click the **Change Font** button to open the *Font* dialog and change the lattice title font.



Select the font type, style, size, effect, and script. Click **OK** to accept the changes or **Cancel** to leave the font the same.

In the **Color** menu, select the lattice title color by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

Check the **Ignore Mapped Lattice Titles** box to hide the portion of the latticed plot titles derived from the worksheet being plotted.

Axes Options tab

The X, Y, and Y2 menu items set the appearance of the plot axes. The Box Plot and Histogram objects only have a Y context, but they do have X and Y axes. Select the X or Y menu items to set the appearance of the plot axes. The Scatter Plot object will list an axis item for each variable mapped to the **Included** context.

Select one of the axis menu items to access the following tabs:

- Content tab, see:
  "Set the axis range"
  "Set the axis scale"
- Appearance tab, see "Define axis and tick mark appearance"
- Axis Label tab, see "Format the axis label"
- Order tab, see "Order categorical axes"

Set the axis range

Select **Axes > X**, **Y**, or **Y2** in the tree, then click the Content tab.

Options for setting the range are fairly consistent across plot objects.

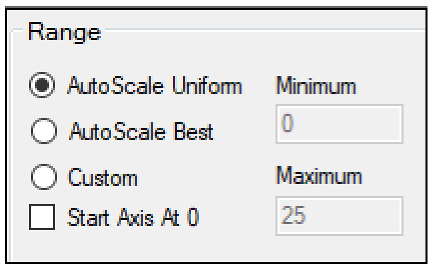


Figure 48-1. Axis Options — Content tab

There are two autoscaling methods available for determining the axis range.

AutoScale Uniform creates a uniform axis scale across all plots when multiple pages, rows, or columns are used to show the plots. This is the default setting. Note that, in some plots, this option can cause the axis to extend past the highest data point or below the lowest point, since the largest range needed is used. (This option does not apply to Scatter Plot Matrix.)

AutoScale Best allows Phoenix to determine the best axis scale based on the number of data points and the values used to create each individual plot. This is the default setting for the X-axis when the X-axis is categorical (X-Categorical XY, Box, Bar, and Column plot objects).

Note: Both Auto-scale options use the highest and lowest data points mapped to the axis to create the scale, where the first option uses the highest and lowest points from all plots in the lattice, and the second option uses the highest and lowest points for each individual plot.

For axes that are continuous, if either auto-scale option is selected and **Linear** scaling is specified, the **Start Axis At 0** checkbox becomes available. When checked, this option forces the axis numbering to start at 0, regardless of the data being plotted.

A **Custom** option allows manual entering the range for the axis. This option is available for the Y- and Y2-axes for all plot objects and the X-axis for QQ, Scatter Plot Matrix, and XY Plots.

- Enter the starting point (i.e., the lowest value on the axis) in the **Minimum** field.
- In the **Maximum** field, type the end point (i.e., highest value on the axis).

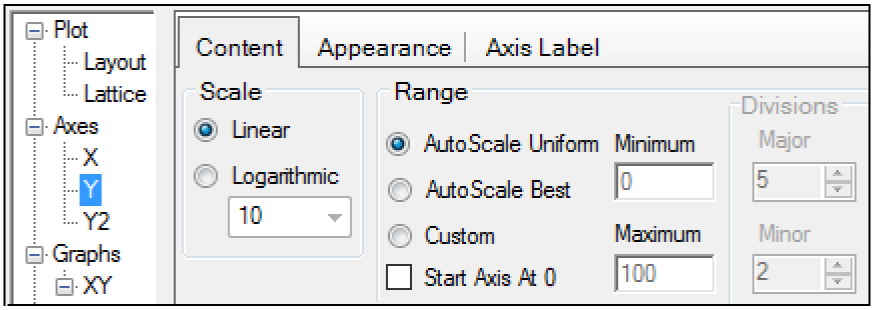
- Use the **Divisions** options to specify the number of tick marks that appear on the axis.

  In the **Major** field, enter the number of numerically-labeled tick marks to display on the axis. In the **Minor** field, enter the number of unlabeled tick marks to appear the axis.

Set the axis scale

Select **Axes > X**, **Y**, or **Y2** in the tree, then click the Content tab.

Scaling is available for the X-. Y- and Y2-axes for all plot objects and the X-axis for QQ, Scatter Plot Matrix, and XY Plots.



Select whether to perform **Linear** (default) or **Logarithmic** scaling of the axis.

If **Logarithmic** is specified, select the logarithmic base. Options include: **2**, **10**, **e** (base of the natural logarithm).

Define axis and tick mark appearance

Select **Axes > X**, **Y**, or **Y2** in the tree, then click the Appearance tab.

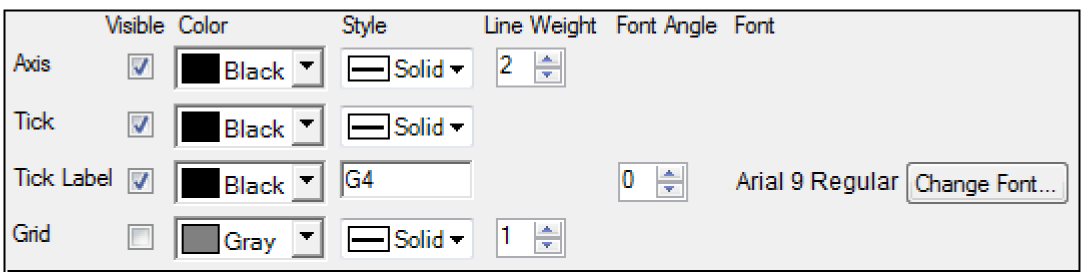


Figure 48-2. Scatter Plot Axis Options — Appearance tab

Clear the **Visible** checkbox to remove the corresponding item from the plot.

> Clearing this checkbox for Axis disables all other axis and tick mark formatting controls in the Appearance tab.

Use the **Color** menu to set the color. Choose one of the color scheme tabs: **Palette**, **Named**, or **System** and click the color.

Select the line style for the axis, ticks, and grids from the **Style** menu

Enter the format for the tick label in the **Tick Label Style** field.

> The default is **G4**. G is the Microsoft .NET general format used for displaying real numbers in decimal form. Using the G format converts a number to either fixed-point or scientific notation, depending on the length of the number and the specified precision. The **4** indicates that four numbers can be displayed on axis tick marks.
>
> Users can enter their own custom format using the following characters:

G4: The default format. Can be changed to display numbers longer than four digits. (Usage: G5, G6, etc.)

0: Displays the whole number. (Usage: 0)

0.00: Displays the whole number plus two decimal places. (Usage: 0.00)

#: The pound sign is used as a digit placeholder. The digit is displayed if it exists, and is blank otherwise. 0 and # can be combined, 0 for required digits and # for optional digits. (Usage: #.##, 0.0####)

.: Decimal point. (Usage: #.##)

,: Thousand separator. (Usage: #,###.##; #,##0; #,##0.00)

%: Percentage sign. (Usage: #.##%; 0%; 0.0%)

E0; **E+0**; **E–0**: Entering any of these characters will cause the scale ticks to be formatted using scientific notation. (Usage: #.##E0; #.##E+0; #.##E–0)

ABC: Plain text characters are displayed literally. (Usage: Hello world)

Note: Standard and custom .NET numeric formats are supported for labels. Full specifications can be found at:
– Standard numeric format strings: https://docs.microsoft.com/en-us/dotnet/standard/base-types/standard-numeric-format-strings
– Custom numeric format strings: https://docs.microsoft.com/en-us/dotnet/standard/base-types/custom-numeric-format-strings

---

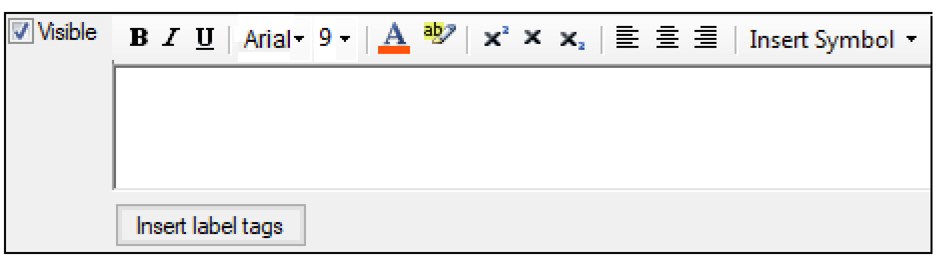
Select or type the thickness of the axis or grid lines in the **Line Weight** field.

For tick labels, use the **Font Angle** field to specify how far to rotate the tick labels (in degrees). The range of valid angle values is from **–90** to **90**.

For axis and tick labels, click the **Change Font** button to open the *Font* dialog. Select the font type, style, size, effect, and script for the label and click **OK**.

Format the axis label

Select **Axes > X**, **Y**, or **Y2** in the tree, then click the Axis Label tab.



Clear the **Visible** checkbox to remove the axis label from the plot.

Type a title for the axis in the text field. Axis titles are automatically assigned based on the column header and units of the variable mapped to the axis.

Use the tools to customize the format of the text.

In the **Insert Symbol** menu, select Greek letters to insert in the axis title. Users can select any lowercase or uppercase Greek letters except zeta, eta, kappa, xi, rho, and upsilon.

Click the **Insert label tags** button to enter place holder text into the label which Phoenix will replace with the mapped value. The place holder labels are:

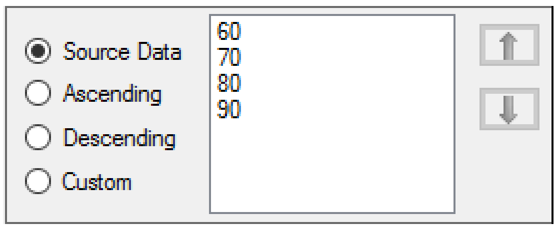
<x:#> for the x column names
<xunit:#> for the x column units
<y:#> for the y column names
<yunit:#> for the y column units

The # is replaced by the number corresponding to the graph (generally one unless the user has overlaid multiple graphs).

Order categorical axes

Select **Axes > X** in the tree, then click the Order tab.

Note: The Order tab is available only for the X axis of X-Categorical XY, Bar, Column, and Box plots.



The available X axis values are displayed in the list. The order in which the values appear along the X axis of the plot is specified by selecting one of the following:

Source Data: Order the values as they appear in the source data.
Ascending: Order the values from least to greatest.
Descending: Order the values from greatest to least.
Custom: Select a value and use the arrows to arrange the values to the desired order.

Graphs Options tab

All plot object except Scatter Plot, have a Graphs menu that lists all plots in the object. Many objects have plots with names based on the variables that are mapped to the X, Y, or Y2 contexts. For example, if Time is mapped to the X axis and Concentration is mapped to the Y axis, the plot is named Concentration vs Time.

Graphs menu options also change depending on whether or not a variable is mapped to the **Y2** axis, multiple variables are mapped to the Y axis, **Data Label**, **Group**, or one of the **Lattice Conditions** contexts.

Y2: If a variable is mapped to the Y2 axis, then two plots are listed under Graphs. For example, if Time is mapped to the X axis and Effect is mapped to the Y2 axis, the second plot is named Effect vs Time.

Multiple **Y**: If more than one variable is mapped to the Y axis, then a separate plot for each mapped variable is listed under Graphs.

Data Label: If a variable is mapped the Data Label context and no variables are mapped to the Y2 axis or the Group contexts, then only one plot is listed under Graphs.

Group: If a variable is mapped to the Group context, then all variable values are listed under the plot name in the Graphs menu. For example, if Subject is mapped to the Group context, then all Subject identifiers are listed under the plot name. If multiple variables are mapped to the Group context to create unique profiles, then each profile is listed under the plot name.

Lattice Conditions: If a variable is mapped to one of the Lattice Conditions contexts and no variables are mapped to the Y2 axis or the Group contexts, then only one plot is listed under Graphs.

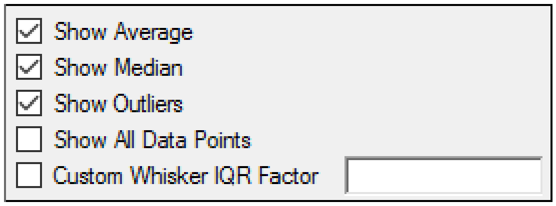
For Scatter Plots, there is no list of graphs, only a single Graph item that, when clicked, provides access to the Appearance tab for the plot.

Selecting a particular plot under the Graphs menu provides access to the following tabs of controls (tab and option availability depend on the plot type).

- Content tab
  Define data display and how quartiles and whiskers are generated
  Set up histogram bins
  Sort X values and specify offsets for multiple XY plots
  Set up regression lines for XY plots
  Set up error bars
- Appearance tab
  Specify appearance of data labels
  Specify appearance of bars
  Specify appearance of borders
  Specify appearance of markers
  Specify appearance of data labels
  Specify appearance of scatter plot diagonal labels
  Specify appearance of lines
  Specify appearance of error bars
  Specify appearance for Group variables
- Quick Styles tab: quickly switch the XY plot between a line and a scatter plot and set Group options

Define data display and how quartiles and whiskers are generated

Select **Graphs >** <box graph name> in the tree, then click the Content tab.



Use the **Show Average** checkbox to toggle display of the line indicating the average value of the data in the box plot.

Use the **Show Median** checkbox to toggle display of the line indicating the median value of the data in the box plot.

Use the **Show Outliers** checkbox to toggle display of the outliers in the plot display panel.

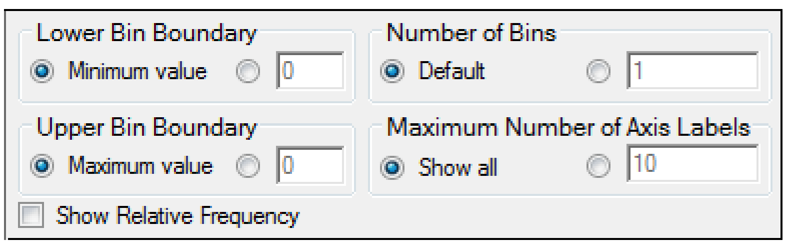
Use the **Show All Data Points** checkbox to toggle display of all data points in the plot display panel.

Check the **Custom Whisker IQR Factor** box to enter a custom value used to calculate the IQR (inter-quartile range).

In the **Custom Whisker IQR Factor** field, type the value to use as a multiplier used to determine how far to extend both the top and bottom whiskers.

Set up histogram bins

Select **Graphs >** <histogram graph name> in the tree, then click the Content tab.



In the **Lower Bin Boundary** area, select **Minimum value** to use the lowest value of the variable mapped to the **Distribution** context as the minimum value, or select the option button beside the field and enter a value.

In the **Upper Bin Boundary** area, select **Maximum value** to use the highest value of the variable mapped to the **Distribution** context as the maximum value, or select the option button beside the field and enter a value.

In the **Number of Bins** area, select **Default** to use the default number of bins, or select the option button beside the field and enter the number of bins.

In the **Maximum Number of Axis Labels** area, select **Show all** to display all axis labels, or select the option button beside the field and type the maximum number of axis labels to display.

Check the **Show Relative Frequency** box to display the relative frequency on the Y axis. The default frequency display is a simple frequency.

Sort X values and specify offsets for multiple XY plots

Select **Graphs >** <graph name> in the tree, then click the Content tab.

These options are available for the output plots for the XY and X-Categorical XY Plot objects.

Figure 49-1. Graphs Options — Content tab for XY plots

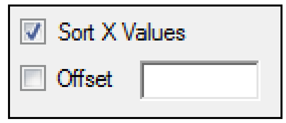


Figure 49-2. Offset option available for second and subsequent plots in a multi-plot graph

To control sorting of plots

Clear the **Sort X Values** checkbox to disable automatic sorting. When checked, the **Sort X Values** option sorts data in ascending X axis order before creating the plots. Clear this option when creating plots with a hysteresis curve.

To shift the first plot

For XY and X-Categorical XY Plot objects, when multiple columns are plotted on a single graph (e.g., predicted and observed results), each plot can be shifted to the left or right.

Shifting the first plot requires adjusting the X-axis range. Note that changing the range also affects the other plots, so it is recommended that you position the first plot, if desired, before setting the offsets for the other plots.

Select **Axes > X** in the tree, then click the Content tab.

Select the **Custom** option and adjust the values in the **Minimum** and **Maximum** fields.

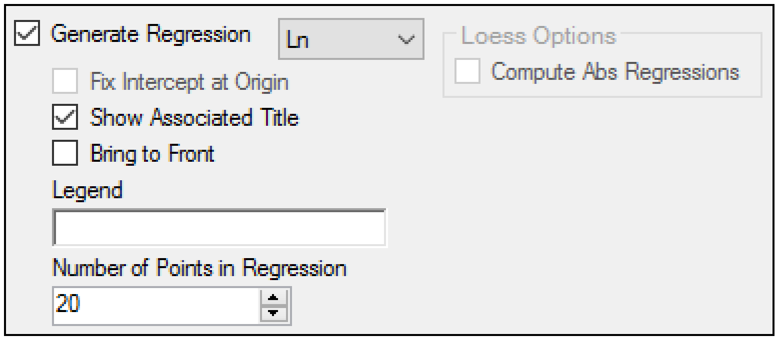
To offset subsequent plots

Select the name of the plot to offset under the Graphs menu item.

On the Content tab check the **Offset** box and enter the number of units (for the XY Plot object) or pixels (for the X-Categorical XY Plot object) that the plot should be shifted. Entering a positive value moves the plot to the right, a negative value moves it to the left.

Set up regression lines for XY plots

Select **Graphs >** <XY graph name> **> Regression** in the tree, then click the Content tab.



Check the **Generate Regression** box to display a regression line on the plot.

Select the type of regression line to display.

Ln (log base e)

Linear

LOESS (LOcally wEighted Scatter plot Smoothing)

If selected, the **Loess Options** group is made available

Note: If a regression line is selected, the values used to create the line are displayed across the top of the plot.
Ln: the log of the Y slope and the values of a and b.
Linear: The R-squared, intercept estimate, and slope estimate values are displayed.
LOESS: Nothing is displayed.

Select the **Compute Abs Regressions** checkbox to fit a LOESS regression to the absolute values of the dependent variable, in addition to the normal LOESS regression that does not take absolute values. The reflection of the absolute value fit through the X-axis is also included. This is useful when the magnitudes of the dependent variable are more important than the signed values, for example, weighted residuals.

Select the **Fix Intercept at Origin** checkbox to fix the intercept of a linear regression line at the plot's origin. This option is only available when Linear regression is specified, as Ln and LOESS do not use intercept values.

Clear the **Show Associated Title** checkbox to not include the regression line equation in the title of the plot.

Check the **Bring to Front** checkbox to display the regression line in front of the data points.

In the **Legend** field, type a name for the regression line so it is displayed in the plot legend.

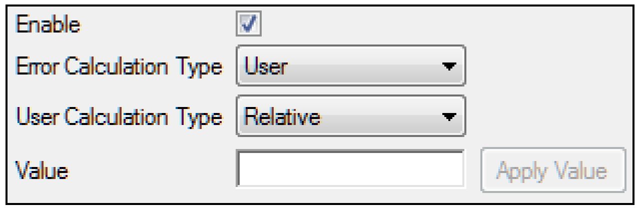
The **Number of Points in Regression** field controls the display of the regression line plot, by setting the number of points at which to evaluate and plot the regression line.

Set up error bars

Special note for X-Categorical plots: For X-Categorical XY Plot objects, use the Descriptive Statistics object to compute data for the error bars. The Descriptive Statistics results worksheet will be used as input for a second plot, with the Mean column being mapped to the Y axis and the SD column mapped to the Error Bars context. Use the **Offset** option in the Content tab for the second plot to shift the error bars as desired. See the example “Multiple profile analysis using NCA”.

Select **Graphs >** <graph name> **> Error Bars** in the tree, then click the Content tab.

Error bars are available for an XY Plot, X-Categorical XY Plot, or a Column object that has no Group mapping.



Clear the **Enable** checkbox to disable error bars. Check to enable, but additional mappings or settings are required before error bars will display.

In the **Error Calculation Type** menu, select the calculation type used to create the error bars.

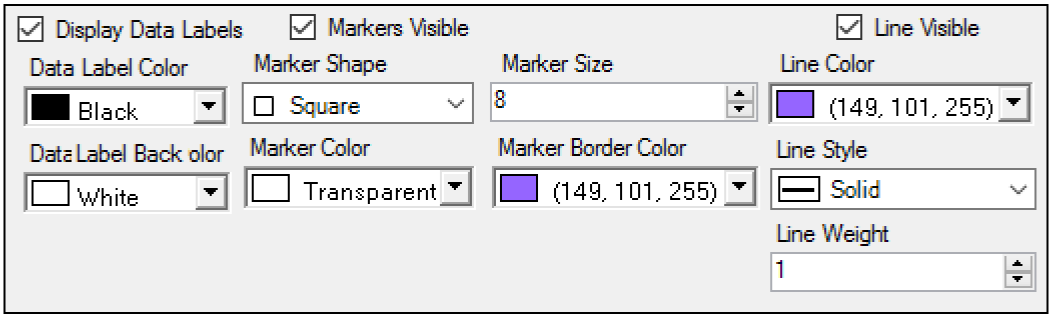
> **FixedValue**: Use the value entered in the **Value** field as the length of the lower and upper bars. Phoenix ignores the variable or variables mapped to the error bar contexts.
>
> **User**: Apply the method selected in the **User Calculation Type** menu to the error bar mapped columns in the Data Mappings panel. Choose from:
>
> **Absolute**: The mapped columns are Y-axis coordinates. Values mapped as **Lower** are the Y-axis coordinates for the ends of the lower error bars, and values mapped as **Upper** are the Y-axis coordinates for the ends of the upper error bars. The error bars display only when the mapped data values for **Lower** are below the corresponding plotted points or when the mapped data values for **Upper** are above the corresponding plotted points.
>
> **Relative**: The mapped columns are error bar lengths. Values mapped as **Lower** are the lengths from the plotted points to the lower ends of the error bars, and values mapped as **Upper** are the lengths from the data points to the upper ends of the error bars.

Click **Apply Value** to use the typed value in the display of the error bars.

Specify appearance of data labels

For all plots except box plots, the display of labels for the data can be controlled. The background color for data labels can be set for scatter plots and grouped XY plots. Grouped XY plots also have a setting for the label color.

Select **Graphs >** <graph name> in the tree, then click the Appearance tab.



Check the **Display Data Labels** box to display variable values beside the bars/points.

In the **Data Label Color** menu, select the color for the data label by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

In the **Data Label Back Color** menu, select the background color for the data label by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

Specify appearance of bars

Bar appearance options are only available for Bar, Column, Box, and Histogram objects.

Select **Graphs >** <graph name> in the tree, then click the Appearance tab.

In the **Bar Width** box, select or type the width of the bars. (This option is only available for Bar and Column objects.)

In the **Fill Color** menu, select the color for the bar by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

Specify appearance of borders

Border appearance options are only available for Bar, Column, Box, and Histogram objects.

Select **Graphs >** <graph name> in the tree, then click the Appearance tab.

Select the color for the border by selecting a color scheme tab: **Palette**, **Named**, or **System** n the **Border Color** menu and clicking the color.

In the **Border Style** menu, select the style for the border.

In the **Border Width** box, select or type the width of the borders.

Specify appearance of markers

Marker appearance options are only available for Box, XY, QQ, Scatter Plot and X-Categorical XY Plot objects.

Select **Graphs >** <graph name> in the tree, then click the Appearance tab.

Check the **Markers Visible** box to display plot markers.

Select the shape to use as a data point marker from the **Marker Shape** menu.

In the **Marker Color** menu, select the color for the marker by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

In the **Marker Size** box, select or type the size of the data point markers.

In the **Marker Border Color** menu, select the color for the marker border by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

Specify appearance of data labels

Data label options are available for all plot objects except Box Plot objects.

Select **Graphs >** <graph name> in the tree, then click the Appearance tab.

Use the **Display Data Labels** checkbox to toggle the display of data point labels.

Turning on the checkbox adds the following two controls:

In the **Data Label Color** menu, select the color for the label by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

In the **Data Label Back Color** menu, select the background color for the label by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

Specify appearance of scatter plot diagonal labels

Diagonal labels are only applicable to Scatter Plot objects.

Select **Graph** in the tree.

In the **Appearance** tab, use the **Display Diagonal Labels** checkbox to toggle the display of labels along the diagonal.

Turning on the checkbox adds the **Change Font** button to the tab. Click to access tools for adjusting the label font, size, style, and effects.

Specify appearance of lines

The options described below can be used to change the appearance of lines in all groups by selecting the XY Plot or X-Categorical XY Plot in the tree. To only change the line appearance in an individual group, select that group in the tree.

To change the line display, click the plot node in the navigation tree. For regression lines, expand the plot node in the navigation tree and click **Regression**. If **Compute Abs regressions** is selected in the Regression Content tab, users can also format the LOESS absolute regression line display using the controls in the **Abs Loess Lines** area.

Select **Graphs >** <graph name> in the tree, then click the Appearance tab.

Check the **Line Visible** box to display a line connecting the points (this option is not available for regression lines).

In the **Line Color** menu, select the color for the line by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

In the **Line Style** menu, select the style for the line.

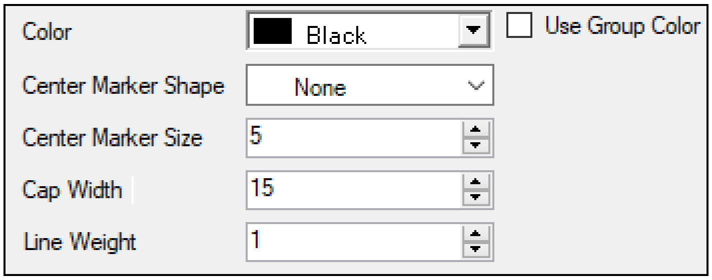
In the **Line Weight** box, select or type the weight of the line.

Specify appearance of error bars

Select **Graphs >** <graph name> in the tree, then click the Appearance tab.

Expand the plot node in the navigation tree and click **Error Bars**.

Click the **Appearance** tab.



In the **Color** menu, choose the color used to display the error bars center point marker by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

Check the **Use Group Color** checkbox to use the **Line Color** specification in the plot's Appearance tab to color the error bars.

In the **Center Marker Shape** menu, select the shape of the marker used to indicate the center point of the error bars. The default marker shape is **None**.

In the **Center Marker Size** field, type or use the arrows to change the size of the marker.

In the **Cap Width** field, type or use the arrows to change the width of the top and bottom bars.

In the **Line Weight** field, type or use the arrows to change the thickness of the error bar lines.

Specify appearance for Group variables

Several Plot objects contain a Group context. If one or more variables are mapped to the Group context, then the variable values are listed under **Graphs >** <graph name> in the tree.

Note: The plot object must be run before users can view Group variables in the Graphs menu.

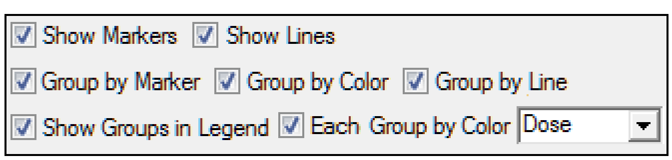
Select a Group value to access its Appearance tab. The Group variables Appearance tab controls are the same as those in the XY plot Appearance tab (see "Specify appearance of data labels" and subsequent sections) with one extra field, **Legend Text**.

In the **Legend Text** field, type a label for the Group value in the legend.

Quick Styles tab

The Quick Styles tab allows users to quickly switch the XY plot between a line and a scatter plot. Users can also use the tab to quickly update the plot display. The Quick Styles tab is only available in the XY Plot object.

Select **Graphs >** <graph name> in the tree, then click the Quick Styles tab.



Options include:

Show Markers toggles display of markers. If at least one sort variable is mapped to the **Group** context, each profile is assigned its own unique marker shape and color combination, otherwise, all markers are the same by default. Clearing this option automatically clears the **Group by Marker** checkbox and all profiles are assigned the same marker shape.

Show Lines toggles displaying the plot as a line plot or as a scatter plot.

Group by Marker toggles displaying all markers as the same shape or by group. This option is only available when at least one variable is mapped to the **Group** context.

Group by Color toggles coloring all lines and markers the same (black by default) or by group. This option is only available when at least one variable is mapped to the **Group** context.

Group by Line toggles using the same style (solid by default) for all lines or style by group. This option is only available when at least one variable is mapped to the **Group** context.

Show Groups in Legend toggles the display of profiles in the plot legend. This option is only available when at least one variable is mapped to the **Group** context. Clearing this checkbox also clears and makes unavailable the **Group by Marker**, **Group by Color**, and the **Group by Line** checkboxes.

Each Group by Color toggles using the same color for each level (i.e., value) of the Group variable selected from the pull-down menu, when two or more variables are mapped to the Group context. Only the line color and the marker color will change, styles remain unchanged. If the user changes either a marker color or a line color for an individual member of the group (individual members are listed below Error Bars in the tree on the left), then that color change is applied to all the individuals members in the same group.

Legend Options tab

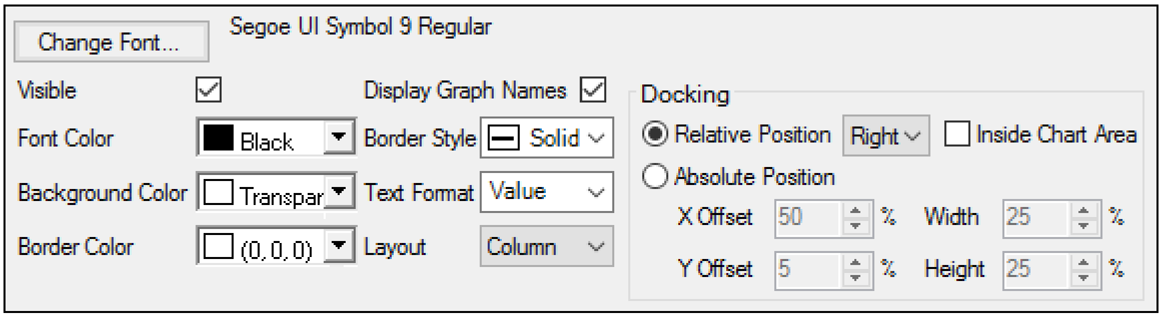
The Legend menu allows users to change the formatting and display properties. A legend is created in the plot display panel for each plot page tab.

Selecting the Legend menu provides access to the following tabs of controls.

Appearance tab
Order tab

Appearance tab

Select **Legend** in the tree to access the legend Appearance tab.



The Legend Appearance tab allows users to specify how the legend is displayed for each plot or group of plots. All plot objects share a common set of legend formatting controls.

Click the **Change Font** button to open the *Font* dialog and change the legend font.

Use the **Visible** checkbox to toggle display of the legend in the plot.

In the menus for **Font Color**, **Background Color**, and **Border Color**, use one of the three tabs (**Palette**, **Named**, or **System**) to select the color.

Use the **Display Graph Names** checkbox to toggle display of plot names in the Legend.

If no variable is mapped to the Group context, then the only information in the Legend is the plot name. In this case, clearing the **Display Graph Names** checkbox has the same effect as clearing the **Visible** checkbox because the legend is removed from the plot display panel.

In the **Border Style** menu, select the legend border line style.

In the **Text Format** menu, select the legend label format:

Value: Only values of variable(s) mapped to the Group context are displayed in the legend.

Name: Value: The name of variable(s) mapped to the Group context is displayed with the corresponding value in the legend.

In the **Layout** menu, select the how the legend items are to be listed:

Column: List all legend items as a single column.

Row: List all legend items as a single row.

Table: List legend items as a table (multiple rows and columns).

In the **Docking** area, select whether to use relative or absolute positioning to place the legend with respect to the plots.

Relative Position: Use the menu to specify the relative position (**Top**, **Right**, **Bottom**, **Left**). Check the **Inside Chart Area** checkbox to move the legend inside the area defined by the two axes.

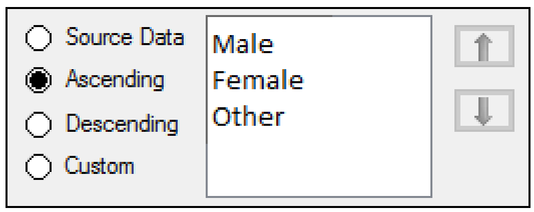
Absolute Position: Enter the percentage from the left edge of the display (**X Offset**) and from the top edge of the display (**Y Offset**) to position the legend. Use the **Width** and **Height** fields to adjust the size of the legend area as a percentage of the display area.

Note: The **Inside Chart Area** checkbox and **Absolute Position** options are not available for latticed plots, unless latticed only by page (one plot per page).

Order tab

The Order tab is available only when at least one Group is mapped for an XY, X-Categorical XY, Bar, Column, or Box plot.

Select **Legend** in the tree to access the legend Order tab.



The available Group values are displayed in the list. The order in which the values appear in the legend is specified by selecting one of the following:

Source Data: Order the values as they appear in the source data.

Ascending: Order the values from least to greatest.

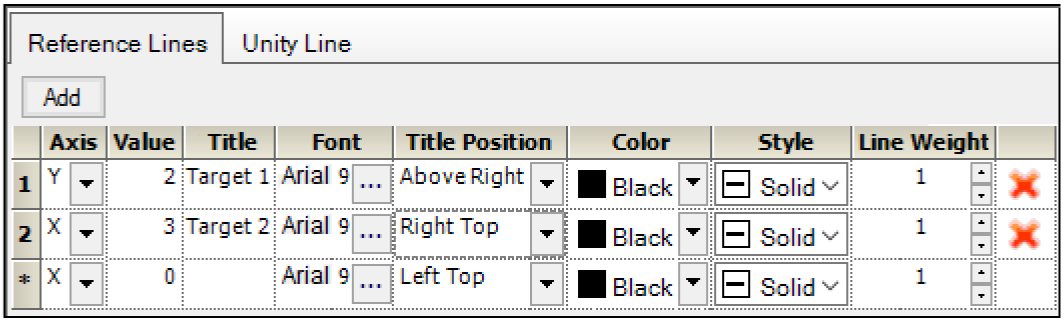
Descending: Order the values from greatest to least.

Custom: Select a value and use the arrows to arrange the values to the desired order.

Reference Lines Options tab

The Reference Lines menu allows users to add reference lines to the X, Y, or Y2 axes of a plot. Reference lines are useful for highlighting base lines or therapeutic ranges in a plot. Added reference lines are listed in the table.

Select **Reference Lines** in the tree and then click the Reference Lines tab.



Click **Add** to add a row in the table.

Use the **Axis** column drop-down menu to select the axis to use for the reference line.

In the **Value** column, type the axis value on which to place the reference line.

In the **Title** column, type a title for the reference line (optional).

Click **[…]** in the **Font** column to display the *Font* dialog for changing the format of the text (font, font size, font style, and effects).

In the **Title Position** column, select the location where the title is to be displayed relative to the axis.

In the **Color** menu, select the reference line color by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

In the **Style** menu, select the reference line style.

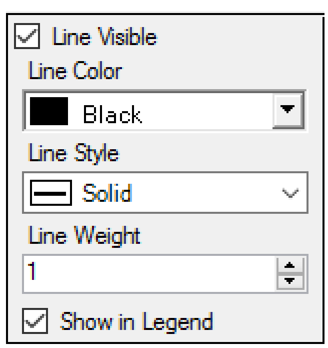
In the **Line Weight** box, select or type the reference line weight.

To remove a reference line, click the red **X** in the corresponding row in the table.

Line of unity

For XY and QQ Plot objects and the Levy plot generated by the IVIVC object, options are available on the Unity Line tab for the line of unity, where Y=X. The two axes must use the same scaling (i.e., both are linear or both are logarithmic) for the options to be active.

Select **Reference Lines** in the tree and then click the Unity Line tab.



Check the **Line Visible** box to add a unity line in the plots and enable the Line of Unity settings. Uncheck the box to hide the unity line.

In the **Line Color** menu, select the unity line color by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

In the **Line Style** menu, select the unity line style.

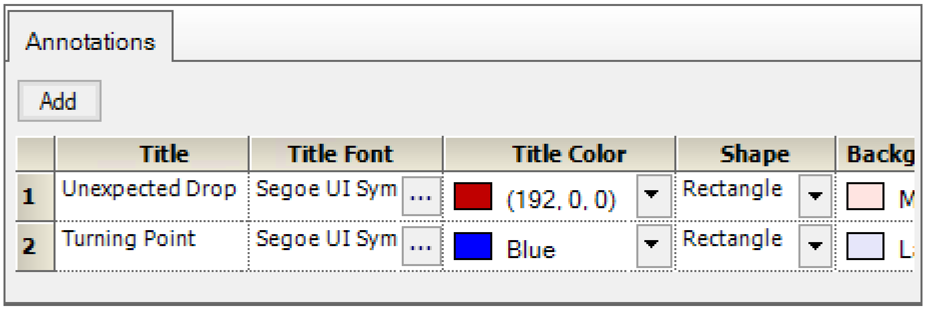
In the **Line Weight** box, select or type the weight of the unity line.

Select the **Show in Legend** checkbox to include the unity line in the legend.

Annotations Options tab

The Annotations tab allows users to annotate the graph. Annotations can be dragged and dropped anywhere within the graph area.

Select **Annotations** in the tree to access the Annotations tab.



Click **Add** to add a row in the table.

In the **Title** column, type the annotation text.

Click **[…]** in the **Font** column to display the *Font* dialog for changing the format of the text (font, font size, font style, and effects).

In the **Title Color** menu, select the annotation color by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

In the **Shape** column, select shape to use for the annotation text area.

In the **Background Color** column, select the color behind the annotation text by selecting a color scheme tab: **Palette**, **Named**, or **System** and clicking the color.

In the **Border Style** menu, select the style of border for the annotation area.

In the **Border Color** column, select the color for the annotation border.

In the **Border Width** column, select or enter the width of the annotation border.

To remove an annotation, click the red **X** in the corresponding row in the table.

Plotting results

The results are displayed on the Results tab. The option buttons selected in the Data Mappings panel and the options selected in the Options tab determine the number of plots that are created in the Results tab. A Settings file is also generated containing all selections made in the object interface.

A plot can be viewed and modified in its own window by selecting it in the Results list and double-clicking it or pressing **ENTER**. Once a result is displayed in its own window, the object can be re-executed by clicking  (**Re-execute Plot** icon) in the toolbar.

Double-clicking a point in an XY plot, bar plot, or scatter plot matrix plot opens the worksheet for that plot in a separate window, with the row corresponding to the double-clicked point highlighted.

For all plot types except scatter plot matrix, click various parts of the plot image to go to the options associated with that part of the plot output. (See "Plot Options tab" for more details on the options available.)

Click an axis to display the corresponding axis menu
Click the title to display the Title text field.
Click the legend to display the Legend menu
Click a bar, column, or marker to display the Graphs > Appearance tab.
Click a box, bin, or XY line to display the Graphs > Content tab.

Hover the cursor over part of a plot, such as a bar, marker, line, or part of a box or histogram, to view a popup showing the associated data.

Copy or export results

To copy a plot, select the **Plots > Output** item in the list on the Results tab. Then right-click the displayed plot and select either **Copy High Resolution Image (vector)** or **Copy Image (bitmap)**.

To export a plot, select the **Plots > Output** item in the list on the Results tab and then do one of the following:

Right-click the displayed plot.

Or right-click the **Plots > Output** item in the list.

Or click  (**Export** icon) above the Results list

Use the dialog tools to specify a location, file name, and format for exporting the plot. Use the Image Settings options in the dialog to control the size of the exported plot.

If a plot has more than one page, each page will be exported to a separate file. Phoenix supports exporting plots in EMF, BMP, GIF, JPG, PNG, and TIFF formats.

Additional information on Box Plot results

In the Box plot, the dashed line is the median; the solid line is the arithmetic mean. The ends of the "box" are the 25th and 75th percentiles, which are computed by the same method as in Descriptive Statistics. These are also referred to as the first and third quartiles. The whiskers show the lowest data value still within 1.5 IQR of the lower quartile, and the highest value still within 1.5 IQR of the upper quartile, where IQR is the interquartile range (the difference between the third and first quartiles, the middle 50%). **Custom Whisker IQR factor** option in the Content tab allows the user to change the multiplier of IQR to a value other than 1.5.

Data values that do not fall between the whiskers are plotted as outliers (markers outside of the whiskers). Profiles with fewer than five data points plot the data points directly with no box.

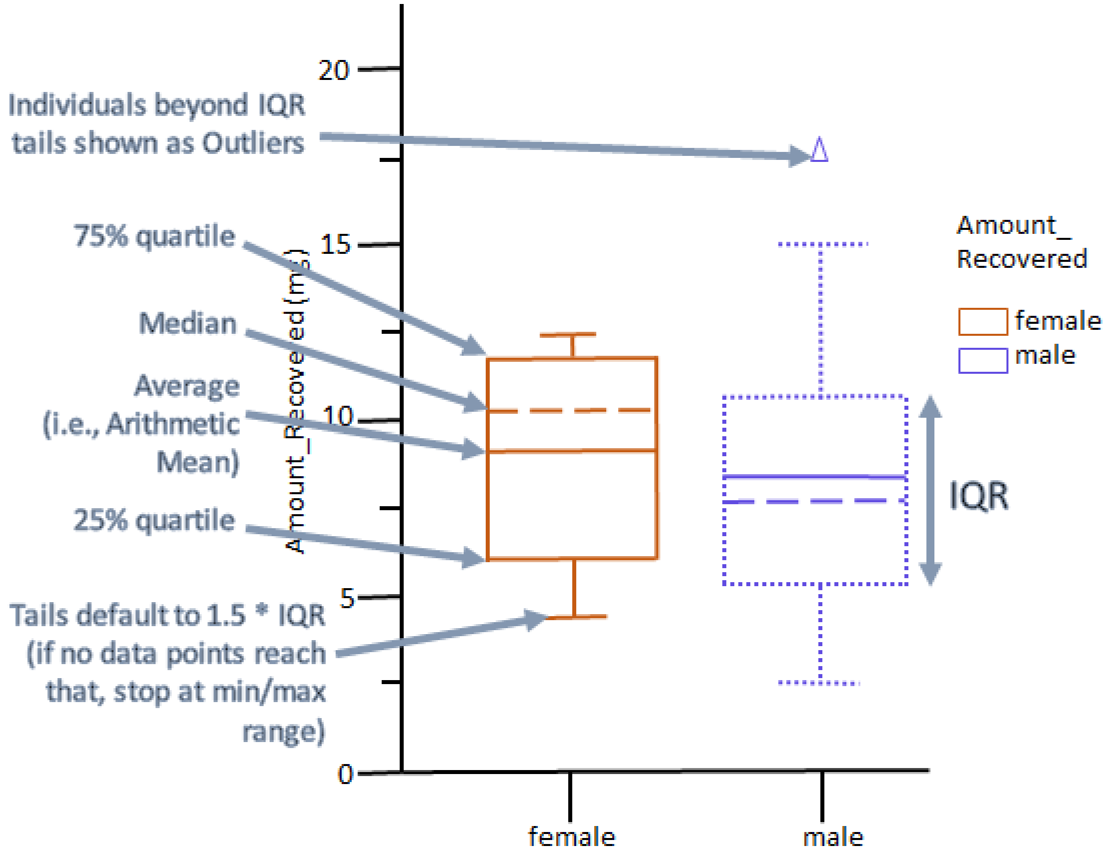


Figure 53-1. Interpreting a box plot with whiskers

Error bars and overlaying plots example

The first part of this example uses summary statistics and error bars to create two XY plots, one using relative error bars and the other using absolute error bars. Next, plot overlays are created to help with data comparison.

Most Phoenix objects require the same basic steps for their use. However, there may be multiple paths to accomplishing a step (e.g., main menu, right-click menu, drag-and-drop, etc.). For simplicity, only one is listed here.

Note: Any object added to a project can be viewed in its own window by selecting the object in the Object Browser and double-clicking it or pressing **ENTER**. All instructions for setting up and executing an object are the same whether the object is viewed in its own window or in Phoenix's viewing.

The completed project (`Plots.phxproj`) is available for reference in …`\Examples\Data and Plots`.

Set up the project

1. Create a new project called `Plots`.
2. Import the file …`\Examples\WinNonlin\Supporting files\Bguide2.dat`.
   Click **Finish** in the *Import File Wizard*.

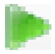
   Units must be added to the time and concentration columns before the dataset can be used to create plots.
3. In the Columns tab, below the displayed Bguide2 worksheet, select the **Time** column header in the Columns box.
4. Clear the **Unit** field and type `hr`.
5. Select the **Conc** column header in the Columns box.
6. Clear the **Unit** field and type `ng/mL`.
   Or click the **Units Builder** button and use the *Units Builder* dialog tools.

Note: Units added to ASCII datasets can be preserved when the datasets are exported to disk or a database. Phoenix adds the units to a row beneath the column headers. When importing a `.dat` or `.csv` file with units, select the **Has units row** option in the Options area in the *File Import Wizard* dialog.

Set up the Descriptive Statistics object

To create error data for the error bars, this example computes means and standard deviations for the concentration data at each time point.

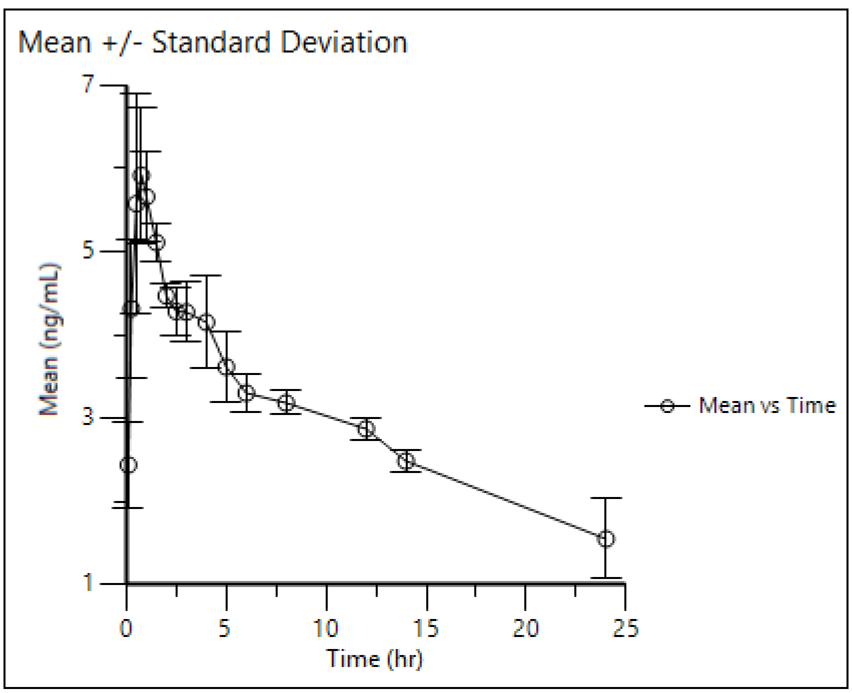
1. Right-click **Bguide2** in the Data folder and select **Send To > Computation Tools > Descriptive Statistics**.
2. Map the data types as follows:
   Sex mapped to **None**.
   Subject mapped to **None**.
   Time to the **Sort** context.
   Conc to the **Summary** context.

3. In the Options tab, check the **Confidence Intervals** and **Number of SD Statistics** checkboxes, but do not change the default values for these two items.
4. Click  (**Execute** icon) to execute the object.

Plot the mean +/- standard deviation using relative error bars

1. Right-click the Statistics worksheet in the Results tab and select **Send To > Plotting > XY Plot**.
2. Map the data types to the following contexts:
   Time to the **X** context.
   Mean to the **Y** context.
   SD to the **Lower** and **Upper Error Bars**.
   Leave all other data types mapped to **None**.
3. In the Options tab, click the **Title** sub-tab and type: `Mean +/- Standard Deviation` in the **Title** field.
4. Select **Graphs > Mean vs Time > Error Bars** in the Options tab list.

   User is the default Error Calculation Type and **Relative** is the default User Calculation Type. Do not change these settings. Using the **Relative** User Calculation Type causes Phoenix to add and subtract the errors from the mean.
5. Execute the object.

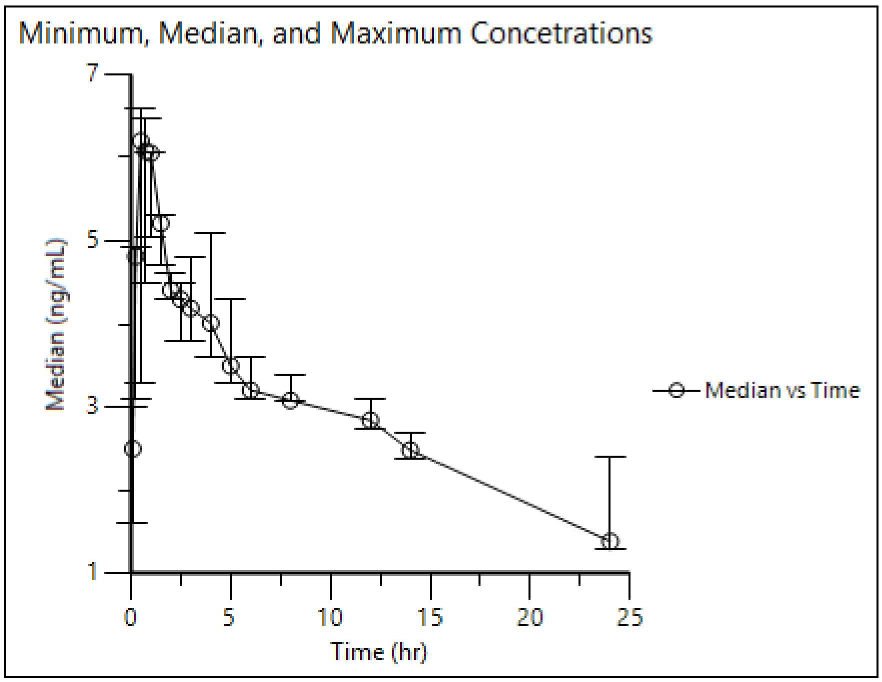


Plot the median, minimum, and maximum using absolute error bars

1. Right-click **Workflow** in the Object Browser and select the **New > Plotting > XY Plot** menu item.
2. In the XY Plot 1 XY Data Mappings panel click the **Select Source** icon to open the *Select Source* dialog.
3. Select the Descriptive Statistics object's **Statistics** worksheet and click **OK**.

4. Map the data types as follows:
Time to the **X** context.
Median to the **Y** context.
Min to the **Lower Error Bar**.
Max to the **Upper Error Bar**.
Leave all other data types mapped to **None**.
5. In the Options tab, click the **Title** sub-tab and type: `Minimum, Median, and Maximum Concentrations`.
6. Select **Graphs > Median vs Time > Error Bars**.
7. In the **User Calculation Type** menu select **Absolute**.

   Using the **Absolute** User Calculation Type instructs Phoenix to plot the Min and Max values on the Y axis, rather than to add and subtract them from the Median.
8. Execute the object.



Overlay multiple plots using variables from the same dataset

This example overlays data from separate columns in the same workbook.

1. Right-click **Workflow** in the Object Browser and select **New > Plotting > XY Plot**.
2. In the XY Plot 2 XY Data Mappings panel click the **Select Source** icon.
3. Select the Descriptive Statistic's **Statistics** worksheet and click **OK**.
4. Map the data types as follows:
Map **Time** to the **X** context.
CI 95% Lower Mean to the **Y** context.
CI 95% Upper Mean to the **Y2** context.
Leave all other data types mapped to **None**.
5. In the Options tab, click the **Title** sub-tab and type: `Overlay Charts`. Press **ENTER** to move to the next line and type: `Example 1`.

6. Select **Plot > Layout**.
7. Set the **Legend Area Size** field to `200`.
8. Select **Axes > Y** and then the **Axis Label** sub-tab.
9. In the field type `Confidence Interval` and click  to center the text.
10. Execute the object.

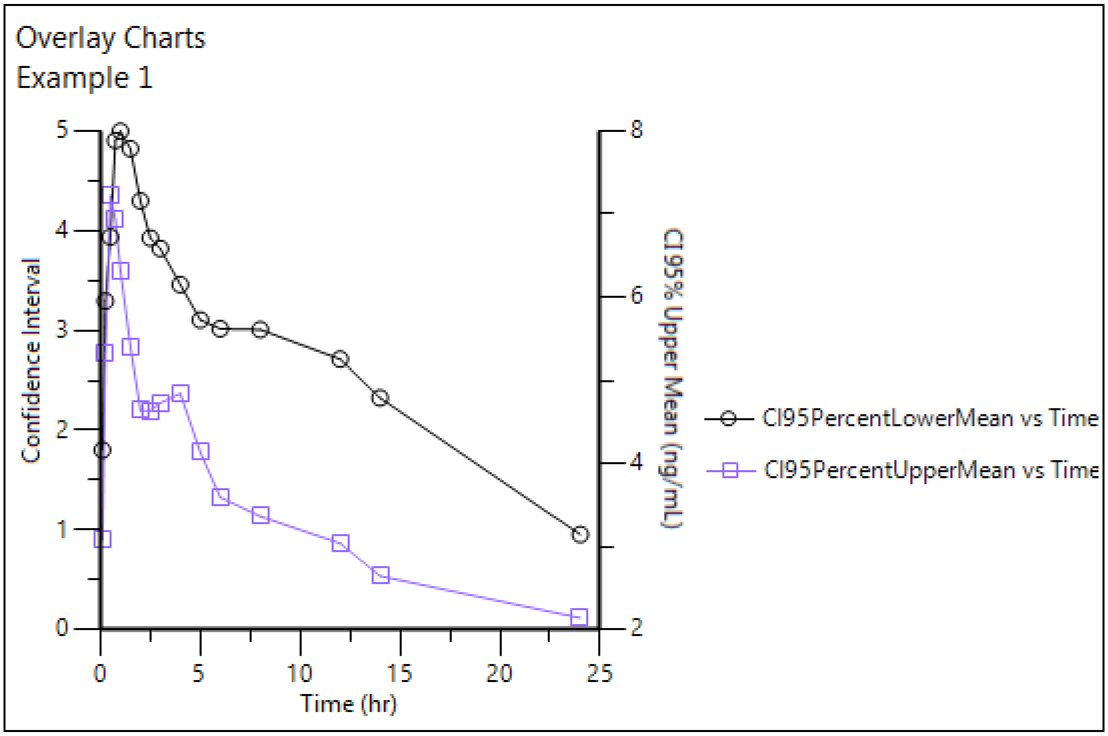


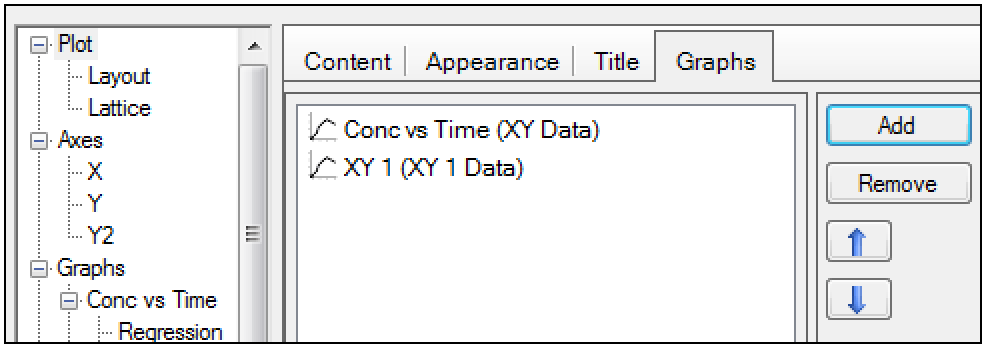
Figure 54-1. Overlaid charts

Note: If the data are stored in one column, it is also possible to create similar plots, without using the overlay feature, by assigning a variable or parameter to the Group context.

Overlay variables from multiple datasets

This part of the example plots the Observed and Predicted concentrations from a model fitting by using the exported output files from a PK Model object in a different project.

1. Import …`\Examples\Data and Plots\Supporting files\bg1 Sheet1.dat` and `Summary Table.dat`.
   Click the **Next Arrow** button and then click **Finish** in the *File Import Wizard* dialog.
2. Right-click **bg1 Sheet1** in the Data folder and select **Send To > Plotting > XY Plot**.
3. Map the data types as follows:
   Subject mapped to **None**.
   Time to the **X** context.
   Conc to the **Y** context.
4. Select the **Graphs** tab.
5. Click **Add**.



A second XY Plot input named XY 1 Data is added to the Setup list.

6. Select **XY 1 Data** in the Setup list.
7. In the Data Mappings panel click  (**Select Source** icon).
8. In the dialog, select **Summary Table** worksheet and click **OK**.
9. Use the option buttons in the XY 1 Data Mappings panel to map the data types to the following contexts:
   Map **Time** to the **X** context.
   Map **Predicted** to the **Y** context.
   Leave all other data types mapped to **None**.
10. In the Options tab, click the **Title** sub-tab and type: `Overlay Charts 2`.
    Press ENTER to move to the next line and type: `Example using two datasets`.
11. Select **Graphs > Conc vs Time**.
12. Select the **Appearance** tab.
13. Use the **Marker Color** menu to change the marker color to **Red**.
14. Execute the object.

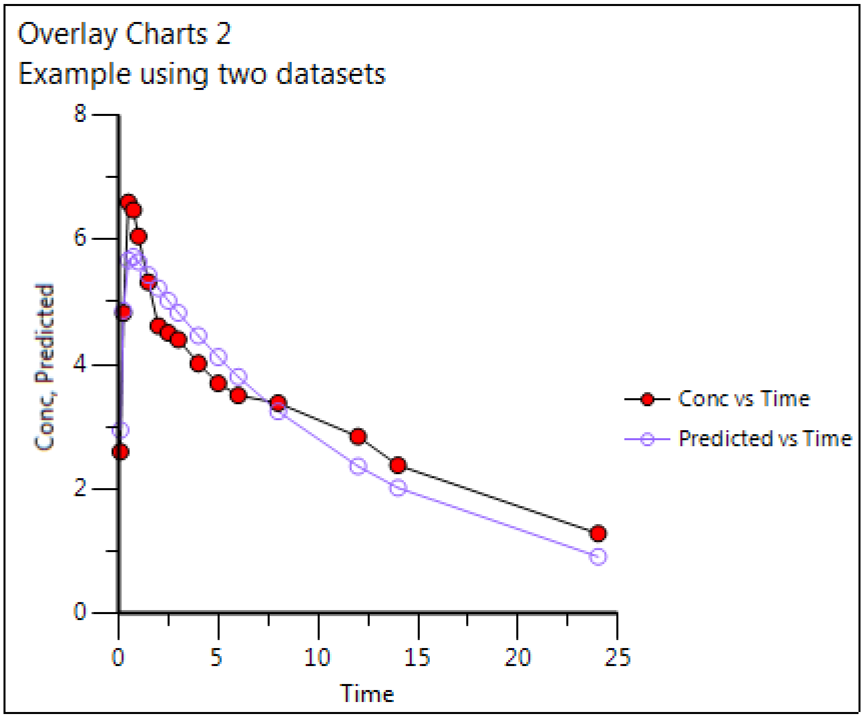


Figure 54-2. Chart of overlaid datasets.

15. Right-click the project and select **Close Project**.

This concludes the Error Bars and Overlaying Plots example.

PsN Shell

The PsN Shell object builds commands against Perl Speaks NONMEM and executes against multiple model files and datasets. The results are then returned to Phoenix.

Users build a list of command-line strings against these interfaces in the Phoenix UI and submit the strings of commands as a batch process to PsN on execution.

Note: Phoenix program plugins, such as the PsN Shell object, assume that the corresponding third party software is installed and running properly.

For PsN installation, consult the PsN installation documentation (https://uupharmacometrics.github.io/PsN/install.html). Guides on managing multiple versions of PsN, submitting to computer cluster environments, and general configuration of PsN can be found in the Documentation link on the PsN homepage (https://uupharmacometrics.github.io/PsN).

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > External Software > PsN Shell**.
Or Main menu: **Insert > External Software > PsN Shell**.
Or right-click menu for a worksheet: **Send To > External Software > PsN Shell**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Additional information is available on the following topics:

Setting up preferences
User interface description
Importing/Writing the code to access the external program
Executing a third party tool object
Results
PsN examples

Setting up preferences

Global preferences are available to the user. Some third party tool objects require certain global settings to be specified prior to use. There are optional settings to enable editing of scripts in external programs from within Phoenix. Some optional preferences can streamline the workflow by automatically filling in or setting options in the object's UI with information entered by the user in the *Preferences* dialog.

Setup access to the external program
Define a default working directory and output location

Setup access to the external program

Select **Edit > Preferences**.

In the *Preferences* dialog, select **PSN** in the menu tree.

Enter the directory path to the PsN configuration file in the first field or click **Browse** to locate and select the directory.

Upon selection, the file is parsed and the other fields are automatically populated if the information is present in the file. Otherwise, the user needs to specify the location of the Perl executable, PsN Utilities directory, and (optionally) the R executable.

To view and/or edit the PsN configuration file in a text editor, click **Open/Edit**.

For more information on the text editor, see http://www.syncfusion.com/products/user-interface-edition/windows-forms/edit/overview.

Click **Test** to make sure the correct file is selected.

In the PsN preference page, turn on the **Use Log Viewer** checkbox to display log information in a separate window during execution.

The **NONMEM Configuration(s)** list in the PsN page shows all of the configurations of NONMEM available for use as defined in the PsN configuration file.

Define a default working directory and output location

Setting the working directory or output folder in the *Preferences* dialog eliminates the need to enter the information in the Options tab for each run. The fields will automatically be filled with the paths entered here.

For PsN, enter the directory path in the **Default Working Directory** field.
Or click **Browse** to locate and select the directory.

Enter the directory path in the **Default Output Folder** field or use the **Browse** button.

Note: If the user specifies a default output location, the user must ensure that they have write access.

Turn on the **Create a unique subfolder for each run** checkbox to generate and then store the output from each run in a new subfolder of the output folder.

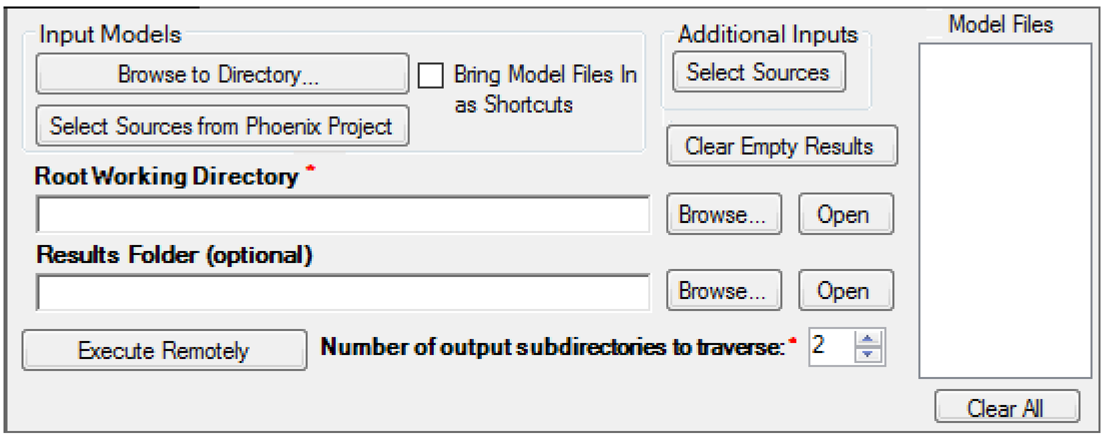
User interface description

Setup tab

The **Setup** tab allows mapping of model files to the object. The Mappings panel simply lists the columns found in the dataset. The Text panel allows users to map a model file to the object and view the contents.

Options and other tabs

The Options tab for the PsN Shell object is distinct in its functionality, relative to the other third party tool objects. The PsN Shell object also has a number of additional tabs related to specific commands that can be submitted to the PsN program.



To identify the model files

Access the model files using one of the following methods:

- To load model files from the file system, click **Browse to Directory Containing Model Files** to locate and select the folder containing the model file(s). The path to the model file cannot have spaces.

  Files with an extension of `.ctl` and `.mod` are recognized as model files. All models are brought into the Code folder of the Phoenix project and mapped to the PsN shell.

- If you want to create shortcuts to the model files in the file system instead of loading them into Phoenix, check the **Bring Model files In as Shortcuts** checkbox. (Turn off the checkbox to import the full model file as mentioned above.)

- If model files are already available in the project's Code folder, click **Select Sources from Phoenix Project** to select the desired model file.

The $DATA record for each model is parsed for the dataset name. The input specified for each unique dataset is published in the object. The names of the model files are added to the **Model Files** list on the rights side of the Options tab.

Caution: Clicking **Clear All** below the list of model files clears all of the entries in the Setup tab. All mappings to datasets, commands, and models are removed.

After the model file is parsed, the Setup tab will show a list of items that need to be mapped. Once the model files and dataset are specified and mapped, you can start building the command lines.

To start building the command lines

- Enter the path to the working directory in the **Root Working Directory** field or click **Browse** to locate and select the directory. (Click **Open** to display the contents of the directory in a separate window.)
- Enter the path to the folder where results are to be stored in the **Results Folder** field or click **Browse** to locate and select the folder. (Click **Open** to display the contents of the folder in a separate window.)
- Set the **Number of output subdirectories to traverse** field to identify the level of output subdirectories from which to retrieve results. The higher the number, the deeper into the output directories Phoenix will go to retrieve output.

Note: Setting the working directory and/or output folder in the *Preferences* dialog eliminates the need to enter the information in the Options tab for each run. The fields will automatically be filled with the paths entered as preferences. See "Define a default working directory and output location".

- Click **Select Sources** (under the Additional Inputs heading) to include additional files along with the mapped input. As an example, if a user wanted PsN to use a different configuration file than the default, they would:

  Import their configuration file into the project (it will be placed in the Code folder).

  Edit the commands so the `-config_file` option points to the name of their configuration file.

  Use the **Select Source** button in the Options tab to add their configuration file to the list in the Setup tab.

  When the object is executed, the user's configuration file will get copied to the working directory and the command that references that file will execute using that specified configuration file.
- Click the **Clear Empty Results** to remove any results published by the object that are empty.

Build the PsN command line

Use the Execute tab and the CDD, LLP, Bootstrap, SCM, SSE, VPC, and MCMP tabs to build the commands that will be submitted to PsN.

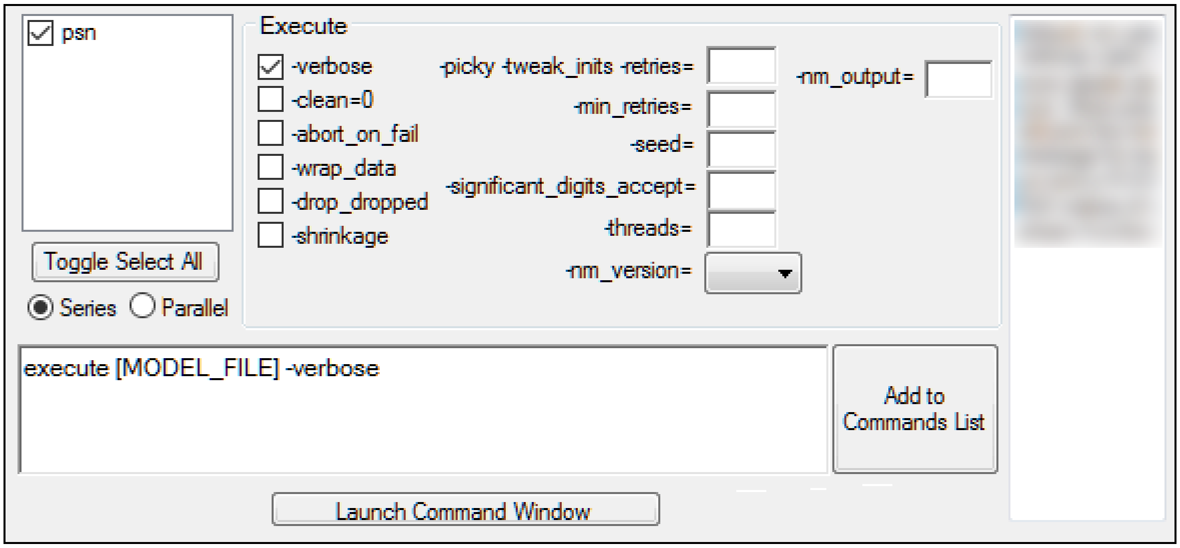


Figure 55-1. Execute tab for a PsN Shell object

Note: Spaces may be entered in the text entry fields, however, they must be enclosed in single or double quotes. If the space is not enclosed in quotes, the text is colored red and is not added to the command.

All of the tabs contain the following elements:

List of Available Models: Use the checkboxes to indicate which models to run the commands against. (Use the **Toggle Select All** button to quickly turn on or off all model checkboxes.)

Command Line Options: Turn on or off the checkboxes for the various tags to add/remove them from the command line. For options with fields, enter an appropriate value to add that option and its value to the command line. Clear the field to remove it. Invalid values will be colored red and not passed to command line.

Tooltip Viewer: Displays information regarding the item the cursor is hovering over.

Command Field: Displays the command line, with all of the options that have been checked or entered on that tab. The field itself is not editable.

Add to Commands List: Click this button to accept the command line as shown in the field and add it to the list of commands shown in the Setup tab. (Click the Commands node in the Setup tab to show list of commands as they will be submitted to PsN when the **Execute** button is clicked.)

If the **Series** option below the model list on the Execute tab is selected, then the command is added once for each model selected in the list.

If the **Parallel** option is selected, then the command is added once and contains all of the selected models explicitly listed in the command. NONMEM executes all the model files in parallel with this type of command.

Launch Command Window: Click this button to open a separate command line window for executing commands interactively.

- Turn on the checkboxes for the models to include in the execution.

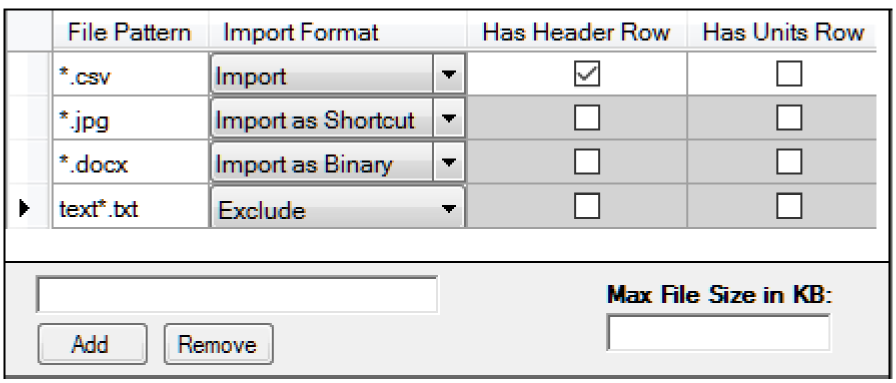
- Make the desired selections and value entries for the options on each command tab.
- When finished building a command, click **Add to Commands List**.

  The list of commands as they will be submitted to PsN when the **Execute** button is clicked can be viewed in the Commands List panel (click the **Commands** node in the Setup tab). The commands listed in this panel are directly editable.
- Type the commands directly in the panel or modify existing commands.

  Changes made directly in the panel are not automatically included in the execution. They must be applied first. A yellow bar at the beginning of a line indicates that a change has been made, but has not yet been applied.
- Click **Apply** to accept the changes made to the commands.

Result Filters tab

Allows specification of how different results files from the external program should be imported. Phoenix first looks for the first rule to match a file and uses that rule to import the object. The order of the rule matching is: **Always Import** (using normal import methods), **Max File Size** (will create a shortcut), **Shortcut Files**, **Binary Files** (using normal import methods). The user creates filter criteria based on filename patterns. If a maximum file size is specified, any file larger than the entered value will always be imported as a shortcut (unless the file matches filter criteria in the **Always Import** list).



Importing/Writing the code to access the external program

The PsN Shell object must have code that will allow it to initiate the external program and submit jobs. The code can be stored as a model file, imported into the project, and mapped to the object, or the code can be directly entered into the object.

Import and map file containing code
Write code in the Text panel
Filtering results by size

Import and map file containing code

- Select a project or workflow in the Object Browser and then select a third party tool object from the **Insert** menu.
- In the Options tab, click **Browse to Directory Containing Model Files**.
- In the *Browse for Folder* dialog, locate and select the directory containing the model file(s).

Imported PsN model files are added to the Code folder in the Object Browser and mapped to the PsN Shell. The $DATA record in each file is parsed for the name of the dataset and is added to Inputs in the PsN Shell.

Write code in the Text panel

Instead of importing and mapping a file, users can write their own code or copy and paste code from another source. (For more information on the text editor, see http://www.syncfusion.com/products/user-interface-edition/windows-forms/edit/overview.

- To enter the code manually, check the **Use internal Text Object** checkbox. If a script/control file is already mapped, a message is displayed that asks if the mapped file should be copied to the internal text editor.

  Click **Yes** to allow editing of the currently imported file.
  Click **No** to remove the imported control file.
- Type the code directly in the field.
- When entry or modifications are complete, click **Apply**.

Some important things to consider when entering code in the Text panel versus importing and mapping a script/control file are:

Apply must be clicked for the code entered or modified to be accepted.

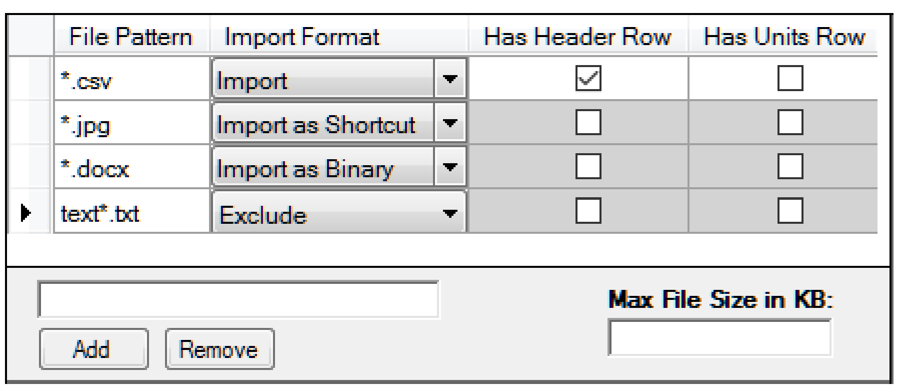
Changes made in the Text panel are not applied to the file on the disk.

The script can be modified either in the Code folder or in the object itself and these are kept in sync.

Once the user switches to **Use Internal Text**, any subsequent changes are not kept in sync with the script in the Code folder.

Filtering results by size

The Result Filters tab allows users to define filters that determine whether files of a certain name or size are returned to Phoenix as a shortcut, a binary file, a complete copy, or returned at all.



- Type the file pattern to serve as a filter into the field near the bottom of the tab and click **Add**. (Enter full file names or use the wildcard “*”, e.g., *.txt.)
- To remove a pattern from the list, select it and click **Remove**.
- For each pattern, select how files matching the pattern are to be handled:

  Import: Default file handling for imported data of that file type is used to import the file
  Import as Shortcut: The file itself is not imported, however, a shortcut is created that points to

the complete file
Import as Binary: The file is imported as a binary object, with no conversion to any specific Phoenix type
Exclude: The file is not imported

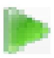
Should a file match several specified patterns, the precedence of processing is: **Exclude**, **Import**, **Shortcuts**, **Binary**.

For `.csv` and `.dat` output files, check the **Has Header Row** box to indicate that files matching the file pattern have a header row.

- For `.csv` and `.dat` output files, select the **Has Units Row** option to indicate that files matching the file pattern have a units row.
- Enter maximum size that an imported complete file can be in the **Max File Size in KB** field.

  Any file that exceeds this size is imported as a shortcut (unless the file matches a File Pattern whose Import Format is set to **Import**).

Executing a third party tool object

Click  (**Execute** icon).

Or, to run the job remotely, click **Execute Remotely** in the Options tab.

Executing a third party tool object remotely sends the job to the server that is defined in the *Preferences* dialog (**Edit > Preferences > Remote Execution**). See "Phoenix Configuration" for instructions. The project is saved automatically.

The project must have been saved at least once prior to executing on RPS, otherwise execution will not pass validation and a validation message will be generated.

At this point, the step being executed on RPS, along with any dependent objects, has been locked. It is now safe to close the project or to continue working in Phoenix.

In Phoenix, some objects in a workflow allow the user to click and execute the last object in a chain and it will re-run any necessary objects earlier in the workflow. This is true for the PsN Shell object.

Note: When executing PsN on JMS, the working folder must exist both on the client and on the JPS server or PsN will fail validation. Use a standard working folder location on all clients and make sure that the standard path also exists on all JPS servers.

Recovering from a failed PsN run

If a PsN run fails, do the following to attempt a restart of the job.

- In the Command List panel, type `::RECOVER` at the end of the command line whose execution failed. For example:

```
1 bootstrap “psn3” -verbose -sample=1000 ::RECOVER
```

Note: Do not change anything else in the command, just add the keyword.

- Click **Apply** and then execute the object .

PsN will go into the working directory and locate the latest output folder whose name matches the command signature (e.g., bootstrap_psn3_-verbose_sample_1000_…) and attempt to continue the processing that was done before.

Results

The results are displayed on the Results tab. The output falls into the following categories:

Output Data: Datasets in tabular form

Text Output: Settings files, log files, and other text output

Other: Other kinds of files, for example: documents, export files, binary files, etc.

Images: Graphs or other images in recognized image formats (jpg, tiff, emf, etc.)

During execution, the Log Viewer is displayed (if the **Use Log Viewer** checkbox in the PsN Preference page was turned on) and shows the standard output and standard errors from PsN. Click the **Pause** button to pause refreshing of the log so it can be reviewed at a particular point. The **Pause** button is renamed to **Resume** and clicking the button continues refreshing of the log. Click the checkbox to toggle showing and hiding the line numbers.

In the working directory, every command executed by PsN from Phoenix has a separate folder. The folder is named according to the signature of the command line followed by the date/time stamp (e.g., bootstrap_psn3_-verbose_sample_1000_20120210103030).

Output Data: Datasets in tabular form

Text Output: Settings files, log files, and other text output

Other: Other kinds of files, for example: documents, export files, binary files, etc.

Images: Graphs or other images in recognized image formats (jpg, tiff, emf, etc.)

Some results are duplicated in the Output Data and Text Output categories to allow users to view output in Phoenix Worksheet format as well as pass raw files to downstream objects.

PsN examples

This section contains step-by-step instructions for creating and executing a variety of third party tool projects.

Completed projects for these examples are available for reference in …\Examples\PsN. You can save a copy of the Examples directory (installed with Phoenix) to your Phoenix project directory via the Project Settings in the *Phoenix Preferences* dialog.

Note: All of these examples assume that the path to the psn.conf file has already been specified in Phoenix. (Select **Edit > Preferences > PsN** and enter/browse to the psn.conf file.)

Note: If all of the appropriate paths are set in this file (perl.exe, PsN utilities, R), Phoenix will populate the appropriate paths in this dialog. The available NONMEM configurations from psn.conf will be displayed for selection in the Options tab in the **-nm_version** pull-down.

PsN Shell object setup and execution example
Using shortcuts with the PsN Shell object
Using PsN Shell and R Shell objects to generate GOF and individual plots
Using PsN Shell and R Shell objects to generate VPC plots

PsN Shell object setup and execution example

The completed project (Ex01_PsN_Execute.phxproj) is available for reference in …\Examples\PsN.

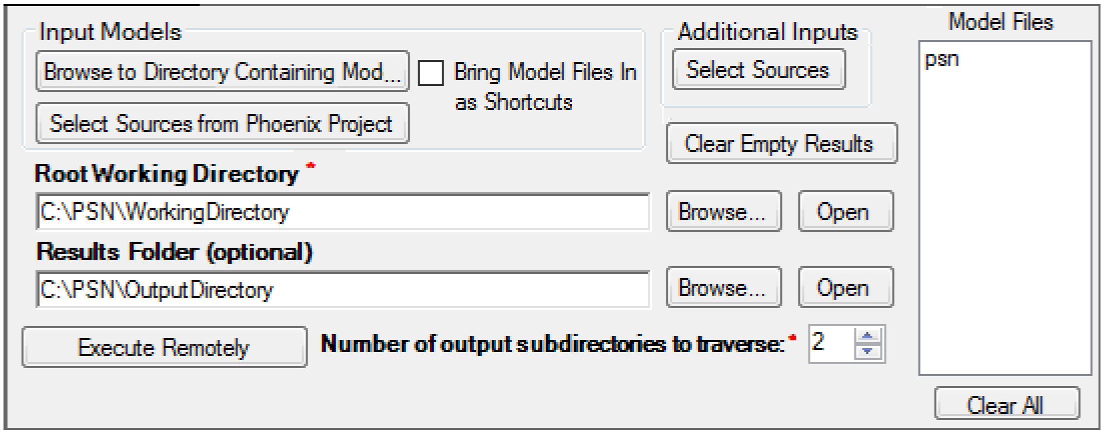
Set up the project and data

1. Create a new project named Ex01_PsN_Execute.
2. Import THEOPP.dat and the PsN control file psn.ctl from …\Examples\PsN\Example1.
3. In the *File Import Wizard* dialog, click **Finish**.

The THEOPP file is added to the project's Data folder and the psn.ctl control file is added to the Code folder.

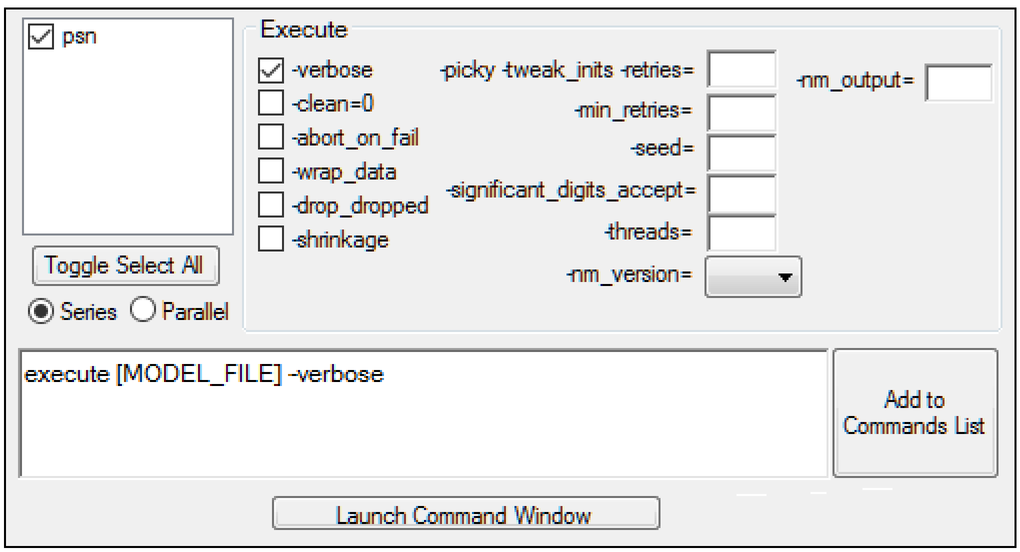
Set up the PsN Shell object

1. Select **Workflow** in the Object Browser and then select **Insert > External Software > PSN Shell**.
2. In the Options tab, click the **Select Sources from Phoenix Project** button.
3. In the *Select Sources* dialog, expand the Code folder, check the box for **psn**, and then click **OK** to specify the input model.
4. Click **THEOPP** in the Setup list, then drag the dataset **THEOPP** from the Data folder to the Mappings panel.
5. Specify the root working directory by typing the path to the desired folder in the **Root Working Directory** field or use the **Browse** button.
   This is where PsN will create run directories for each command executed (i.e., execute, bootstrap, etc.), so you must have write permission for the selected folder.



Execute the PsN Shell object

1. Click the Execute tab and build a command with the available command line options.
   Make sure the **psn** checkbox is checked in the model list.
   Check the **-verbose** checkbox.
2. Click **Add to Commands List** when finished building the command.



3. Click  (**Execute** icon) to execute the object.

This concludes the PsN Shell object setup and execution example. You may save the project, if you wish, or simply close it.

Using shortcuts with the PsN Shell object

The completed project (`Ex02_PsN_ExecuteWithShortcut.phxproj`) is available for reference in …`\Examples\PsN`.

The example control file is set up to look for the dataset source in `C:\temp`, so do ***either*** of the following:

Copy the `THEOPP` file from the …`\Examples\PsN\ExampleWithShortcut` folder to `C:\temp`.

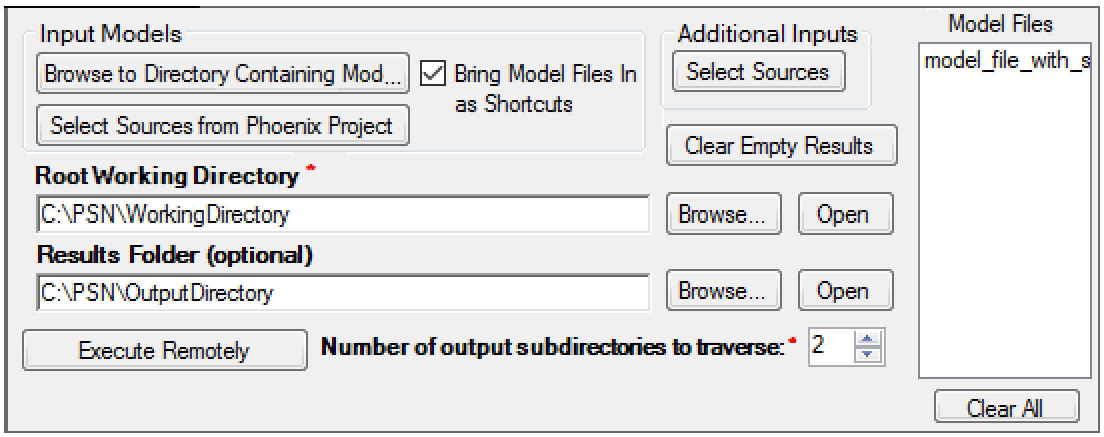
Or

Edit the `model_file_with_shortcut.ctl` file if another location is desired.

Set up the project and data

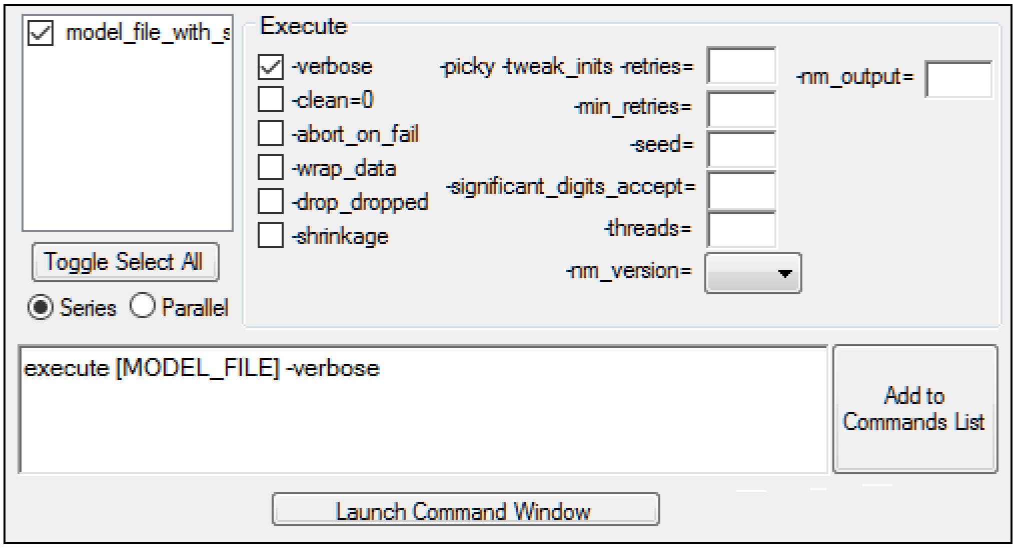
1. Create a new project named `Ex02_PsN_ExecuteWithShortcut`.
2. Select **Workflow** in the Object Browser and then select **Insert > External Software > PsN Shell**.
3. In the Options tab, check the **Bring Model Files in as Shortcuts** box.
4. Click the **Browse to Directory Containing Model Files** button and navigate to and select …`\Examples\PsN\ExampleWithShortcut`, then click **OK**.

   A link to the `model_file_with_shortcut.ctl` control file is added to the Shortcuts folder in the Phoenix project. A new item also appears in the Object list: model_file_with_shortcut.
5. Specify the root working directory, if one has not been specified already via the *Preferences* dialog, by typing in the path to the desired folder in the **Root Working Directory** field or use the **Browse** button. You must have write permission for the selected folder.



Execute the PsN Shell object

1. Click the Execute tab and build a command with the available command line options. Make sure the **model_file_with_shortcut** checkbox is checked in the model list. Check the **-verbose** checkbox.
2. Click **Add to Commands List** when finished building the command.



3. Execute the object.

This concludes the "Using shortcuts with the PsN Shell object" example. You may save the project, if you wish, or simply close it.

Using PsN Shell and R Shell objects to generate GOF and individual plots

This example involves the Xpose package for R. Make sure that this package is installed for R (http://xpose.sourceforge.net/docs_install.php).

The Xpose package uses the following tables (* is the run number):

`sdtab`* file (i.e., standard table file): This file contains columns such as ID, DV, PRED, IPRED, WRES, IWRES, RES, IRES, etc.

`patab`* file: This is a parameter table containing model parameters: THETAs, ETAs and EPSes. The correspondences between ETA and THETA can be defined within Xpose. EPS is optional in this table, it is mainly used to generate the parameter vs parameter plots and parameters vs covariates plots.

`catab`* Categorical covariates, e.g. SEX, RACE

`cotab`* Continuous covariates, e.g. WT, AGE

`extra`*, `mutab`*, `mytab`*, `xptab`*: Other variables that might be needed by Xpose (Xpose 4 and above can postulate all the other values from one table (`mytab1`), but it is always safer to have these plots).

`cwtab`*: The `cwtab` file is generated by Xpose. In NONMEM 7, the calculation of CWRES is built in.

`run*.mod`: Model specification file

`run*.lst`: NONMEM output

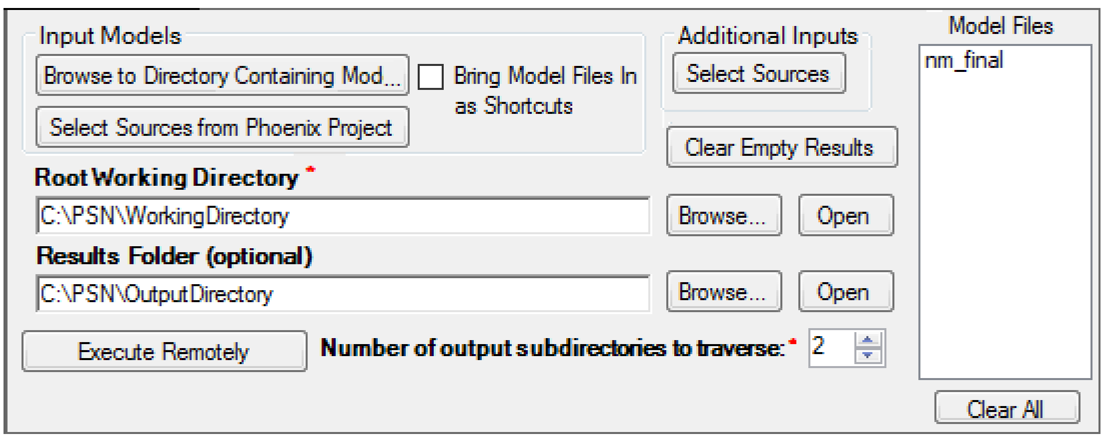
The completed project (`Ex03_PsN_Xpose_GOF.phxproj`) is available for reference in …`\Examples\PsN`.

Set up the project and data

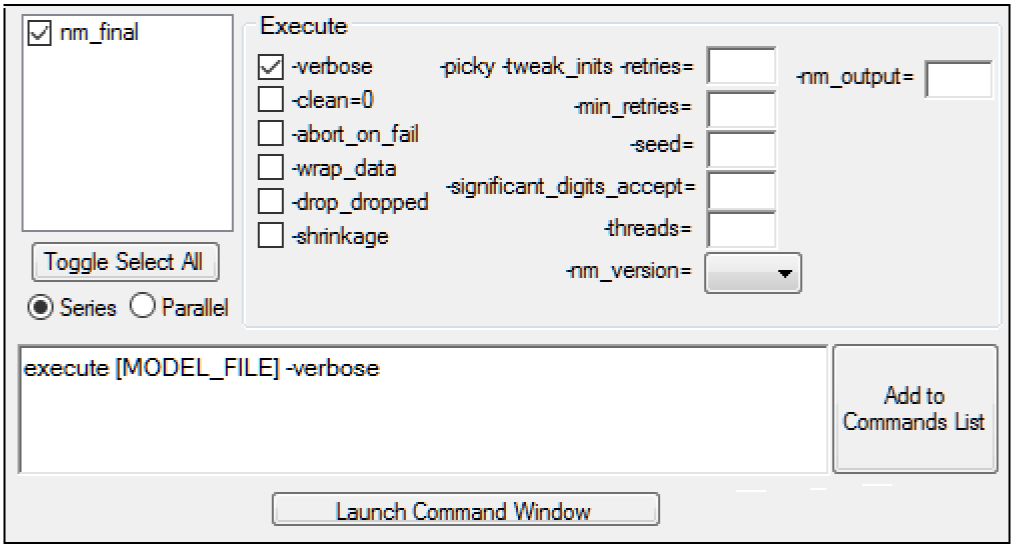
1. Create a new project named `Ex03_PsN_Xpose_GOF`.
2. Import the PsN control file `nm_final.ctl` and the dataset file `example.csv` from …`\Examples\PsN\Xpose_GOF_IND`.
3. In the *File Import Wizard* dialog, click **Finish**.

Set up the PsN Shell object

1. Select **Workflow** in the Object Browser and then select **Insert > External Software > PsN Shell**.
2. In the Options tab, click the **Select Sources from Phoenix Project** button.
3. In the *Select Sources* dialog, expand the Code folder, check the box for **nm_final**, and then click **OK**.
   A new item appears in the Object list, nm_final, and a dataset input is now available to the PsN shell, based on the dataset name in the control file (“example.csv”).
4. In the Setup tab list, click **EXAMPLE.CSV**.
5. Drag the **example** worksheet from the Data folder to the Mappings panel.
6. Specify the root working directory by typing the path to the desired folder in the **Root Working Directory** field or use the **Browse** button. You must have write permission to the selected folder.



7. Go to the Execute tab and build a command with the available command line options.
   Make sure the **nm_final** checkbox is checked in the model list.
   Check the **-verbose** checkbox.
8. Click **Add to Commands List** when finished building the command.



9. Execute the object.

Setting up the R Shell object

1. Import the R command file `Xpose_GOF_IND.R` from …`\Examples\PsN\Xpose_GOF_IND`.
2. Right-click **Xpose_GOF_IND** in the Code folder and select **Send To > External Software > R Shell**.
   An R Shell object is now in the workflow and has focus.
3. Specify the location to store results by typing the path to the desired folder in the **R Results Folder** field or use the **Browse** button. You must have write permission for the selected folder.
4. Click the **Select Sources** button on the Options tab and navigate to **Workflow > PsN Shell > Text Output**.
5. Check the boxes for **catab1**, **cotab1**, **patab1**, and **sdtab1**, then click **OK**.
6. Execute the R Shell and observe the goodness-of-fit and individual plots generated by Xpose.

This concludes the "Using PsN Shell and R Shell objects to generate GOF and individual plots" example. You may save the project, if you wish, or simply close it.

Using PsN Shell and R Shell objects to generate VPC plots

This example involves the Xpose package for R. Make sure that this package is installed for R (http://xpose.sourceforge.net/docs_install.php).

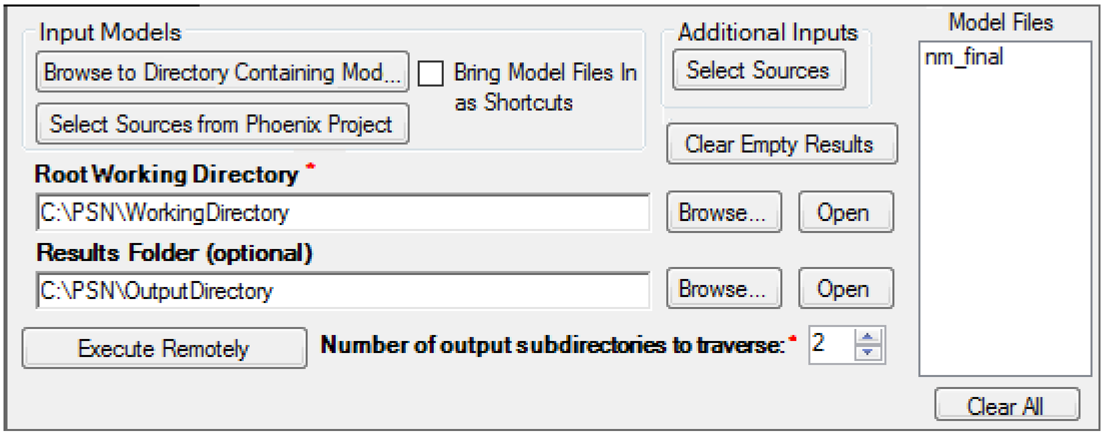
The completed project (`EX04_PsN_Xpose_VPC.phxproj`) is available for reference in …`\Examples\PsN`.

Set up the project and data

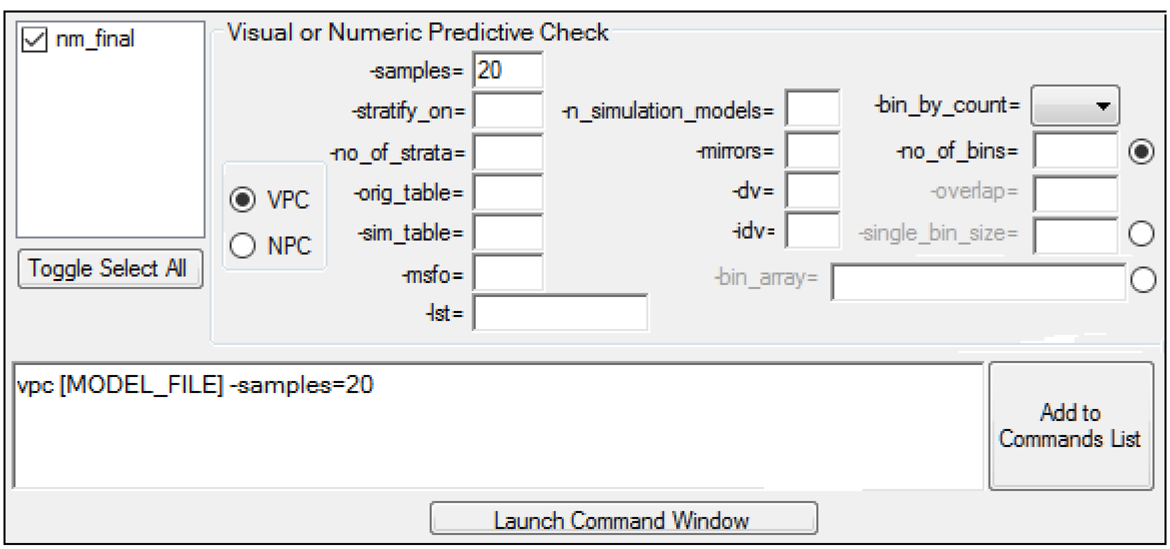
1. Create a new project named `Ex04_PsN_Xpose_VPC`.
2. Import the PsN control file `nm_final.ctl` and the dataset file `nonmem.csv` from …`\Examples\PsN\Xpose_VPC`.
   In the *File Import Wizard* dialog, click **Finish**.

Set up the PsN Shell object

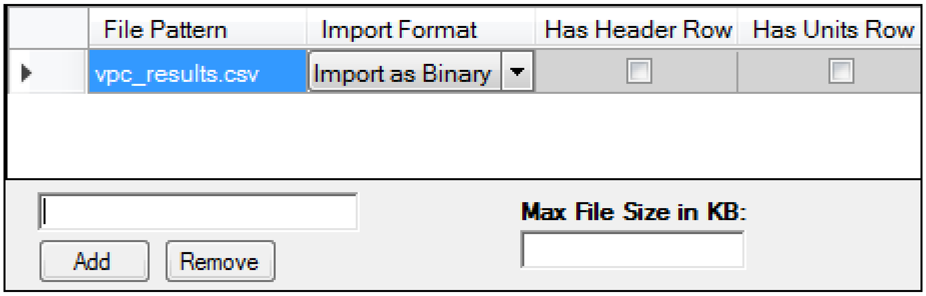
1. Select the workflow in the Object Browser and then select **Insert > External Software > PsN Shell**.
2. In the Options tab, click **Select Sources from Phoenix Project**.
3. In the *Select Sources* dialog, expand the Code folder, check the box for **nm_final**, and then click **OK**.
4. In the Object list in the Setup tab, click **NONMEM.CSV**.
5. Use the mouse pointer to drag the **nonmem** worksheet from the Data folder to the Main Mappings.
6. Specify the root working directory by typing the path to the desired folder in the **Root Working Directory** field or use the **Browse** button. You must have write permission for the selected folder.



7. Go to the VPC tab and build a command with the available command line options.
   Make sure the **nm_final** checkbox is checked in the model list.
   Keep the **-samples** option set to 20.
8. Click **Add to Commands List** when finished building the command.



9. Go to the Result Filters tab.
10. Type `vpc_results.csv` in the field and click **Add**.
11. Set the Import Format pull-down to **Import as Binary**.



12. Execute the object.

Set up the R Shell object

1. Import the R command file `Xpose_VPC.R` from …`\Examples\PsN\Xpose_VPC`.
2. Right-click **Xpose_VPC** in the Code folder and select **Send To > External Software > R Shell**.
3. Click the **Select Sources** button on the Options and navigate to **Workflow > PsN Shell**.
4. In the **Text Output** folder, check the box for **vpctab**.
5. In the **Other** folder, check the box for **vpc_results**, then click **OK**.
6. Execute the R Shell object and observe the VPC plots generated by Xpose.

This concludes the "Using PsN Shell and R Shell objects to generate VPC plots" example. You may save the project, if you wish, or simply close it.

Ratios and Differences

The Ratios and Differences tool in Phoenix is a data manipulation tool that is used to compare data from either one or two worksheets by computing ratios or differences. The computations are based on sort variables and on a variable that defines how data values are to be used as the X values and Y values of the ratios or differences. In Pharmacokinetics, ratios are often computed for observation data collected under two different scenarios and for resulting final parameters from two NCA or Modeling executions. For discrete final parameters or log-transformed observation data, differences may be applicable instead of ratios.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Computation Tools > Ratios and Differences**.
Main menu: **Insert > Computation Tools > Ratios and Differences**.
Right-click menu for a worksheet: **Send To > Computation Tools > Ratios and Differences**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Additional information is available on the following topics:

User interface description
Results

See “Analysis of three profiles using NCA” for an example of using the Ratios and Differences object.

User interface description

Worksheet 1 and 2 Mappings panel
Sort Map Mappings panel
Options tab

Worksheet 1 and 2 Mappings panel

Use the Worksheet Mappings panels to identify how input variables are used in the object.

Sort: (Optional) Categorical variable(s) identifying individual data profiles, such as subject ID or gender. Separate computations are computed for each unique combination of sort variables. When no Sorts are identified for a worksheet, the input is assumed to be from one profile.

Filter: (Optional) Column containing the X/Y filter value. This column is a special case of a sort variable that is used to split or filter the data into subsets, and the subsets are used to define which data (in another column) is to be used for X (the numerator in the case of ratios) and which data (in another column) is for Y (the denominator in the case of ratios). For example, a column named Day, which contains the values Day 1 and Day 14, is mapped as the Filter, and Day 14 will be used to filter for the rows where data in other columns will be used as numerator values, and similarly Day 1 will be used to filter for the rows where data in other columns will be used as denominator values. If **Filter** is not mapped, then only the **Sort**(s) are used to split the data.

Carry: (Optional) Columns from the source worksheet will be copied to the result worksheet.

Note: If no **Sort** or **Filter** is mapped, then this defines a special case where the X and Y columns will be required to be different columns (either on one worksheet or from two worksheets), and the Ratios and Differences object will compute the X/Y ratios (or differences) row-by-row.

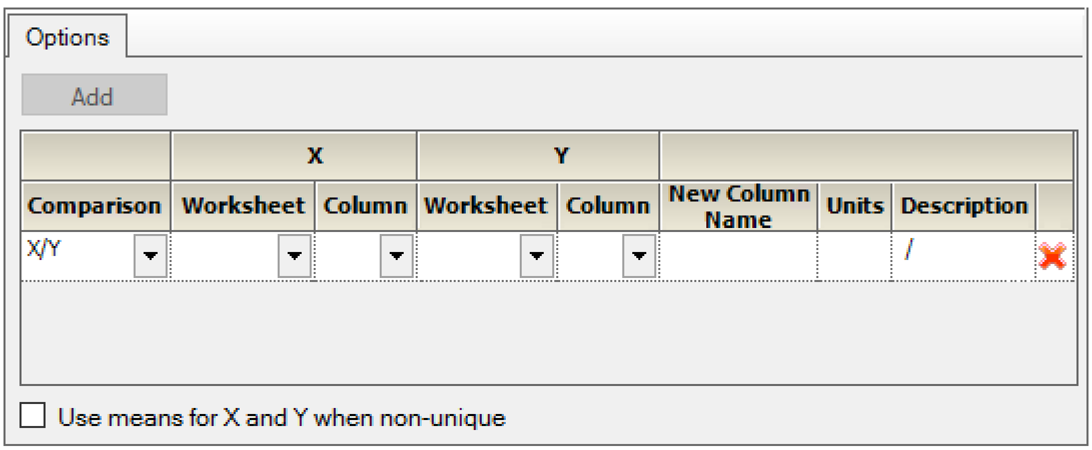
Sort Map Mappings panel

If a second worksheet is used, then the Sort Map worksheet may be needed to map the column names of Worksheet 1 and Worksheet 2, if they differ. This will allow rows in both worksheets to be merged based on their sort keys. The **Worksheet 1 Sort Keys** and **Worksheet 2 Sort Keys** pull-down menus are populated with the names of the columns defined as Sort keys on each worksheet's mapping panel. Required input is highlighted orange in the interface.

The Sort Map will automatically map columns of the same name. If there is not a matching name for a Worksheet 1 column, the Worksheet 2 column name will be blank.

Options tab

The Options tab is used to define the ratio and/or difference calculations that will be executed at run-time. Additional rows may be added by pressing the **Add** button, which becomes active once the input for Worksheet 1 is specified.



Comparison: The type of operation to be performed on X and Y, either X/Y or X – Y.

X or **Y Worksheet**: The worksheet to be used as the source for X or Y, respectively. Choose from either **Worksheet 1** or **Worksheet 2**. Only displayed if more than one worksheet is specified as input for the object.

X or **Y Column**: Name of the column in the **X** or **Y Worksheet** that contains the values to be used as X or Y, respectively.

X or **Y Filter Value**: If a column is mapped to the optional **Filter** context, select the value to use to filter for data values in other columns in order to find the X or Y values to use in the ratios. For example, a column named Day is mapped to the **Filter** context, which contains the values Day 1 and Day 14. The user selects Day 14 for the X option and Day 1 for the Y option in order to compute ratios of data on Day 14 over data on Day 1, for each **Sort** level.

The list of values to define X also includes **All**, which will create multiple sets of ratios or differences using all values in the X **Filter** column that are different from the specified **Y Filter Value**, to define the X's. Continuing the example, suppose the column Day contains Day 1, Day 14, and Day 28. The user selects **All** for the X option and Day 1 for the Y option. Ratios would be computed for each **Sort** level for Day 14 over Day 1 and for Day 28 over Day 1. Another example is comparing all metabolites to the parent drug.

New Column Name: Displays the name of the column that will contain the results of the specified operation on X and Y. The default name is created using the format:
[Ratio or Diff]_[X column name][X filter value]_[Y column name][Y filter value]

Units: The user-specified units of the comparison. ***Note:*** These units are ***NOT*** used during the calculation execution; they are only labels.

Description: A read-only textual representation of the calculation. The format is:
[Worksheet 1].[X column][where Filter=X filter value] [“/” | ”–”] [Worksheet 2].[Y column]][where Filter=y filter value]

Defined calculations can be deleted by pressing the red “X” on the row to be deleted.

If the Sort(s) and Filters do not split the X and Y data into unique values for X and Y, check the **Use means for X and Y when non-unique** box to calculate the mean of the X values and the mean of the Y values, and use the calculated means in the specified ratio or difference. If unchecked, and the values for a profile are not unique, an error message will be given.

Results

Worksheet output

In the stacked results worksheet(s), mapped columns are listed first, followed by parameter data columns used in the comparison computation, then the ratio/difference columns, and then the **Carry** variables.

Cells in the comparison columns will be empty for the X input worksheet data or if the Filter column is used and its value is the same as the X value.

The unstacked results worksheet(s), the X values, Y values, and ratios (or differences) are listed side-by-side, for each defined comparison, followed by the **Carry** variables.

Text output

Settings: The input worksheet used and the options selected.
Warnings and Errors: If any runtime errors are encountered, they are written to this file.

Reporter

The Reporter object generates and maintains clinical and pre-clinical study reports based on data and analyses resulting from the execution of Phoenix Workflow objects. It is designed to work with tables, graphs, text objects, and worksheets. For example, the Reporter object can take output from the AutoPilot Toolkit, PK tables and graphs and place them into final or interim reports.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Reporting > Reporter**.
Main menu: **Insert > Reporting > Reporter**.
Right-click menu for a worksheet: **Send To > Reporting > Reporter**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Additional information is available on the following topics:

Define the report content
Table options
Figure options
Pagination in the report
Captions
Footnotes
Report document setup
Handling lost connections
Object output
Setting up preferences

Define the report content

In the Setup tab, check item(s) in the hierarchical list to include them in the report. Selecting the top level node selects all child content below the node.

Uncheck item(s) in the hierarchical list to exclude them from the report. You can also click the red X next to the item in the lower list to delete it (the item is automatically unchecked in the top list).

Reporter is designed to recognize certain objects in a project as tables, figures, or lists and will add the appropriate form of content to the lower list.

Table: Added to the content list when any of the following are selected:

HTML (results of a Table object or from Tables folder of project)
Worksheets (from Data folder or results of object)
AutoPilot Toolkit spreadsheets
Comparer Plot table (from NONMEM Comparer or Maximum Likelihood Model Comparer)

Figure: Added to the content list when any of the following are selected:

Plots (from results of Plot objects or from plot results of objects)
AutoPilot Toolkit image (WMF, EMF, JPG)

Documents folder images (WMF, EMF, BMP, PNG, JPG)
Figures can be displayed in a grid or lattice, see "Report document setup" for instructions.

Listing: Added to the content list when any of the following are selected:

Text file (results of an object)
Code folder items

The lower list displays the selected content using the following naming convention: `ProjectName.Workflow.Object.Source.Name`. The items in this list can be reordered by dragging and dropping. Selecting an item in the list displays a preview in the panel on the right. (Note that any links displayed in the preview area, such as in the list of tables or figures, will not function until the document is exported.)

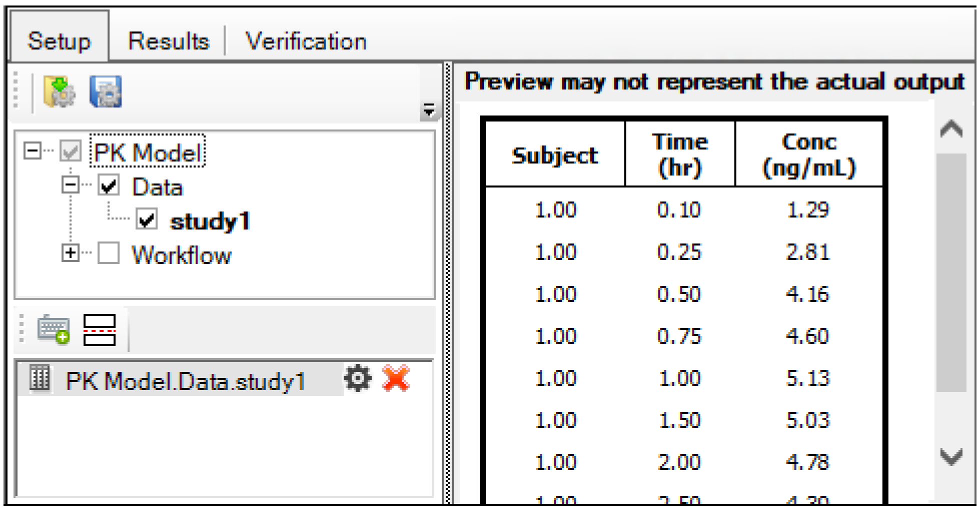


Figure 58-1. Setup tab showing preview of a mapped table

Add text to the report

Click (**Free Form** icon) in the toolbar of the lower list for direct entry of text to include in the report.

Any formatting, such as bold, italic, underline, superscript, subscript, use of symbols is preserved in the Reporter object's output document.

Order content

Items will appear in the output in the order they are shown in the lower list. To change the order, do either of the following:

Click an item and drag it to the new position in the list.
Ctrl or **Shift**+click to select multiple items and drag them to the new position.

Note that the order of the multi-selected items is maintained in the new location.

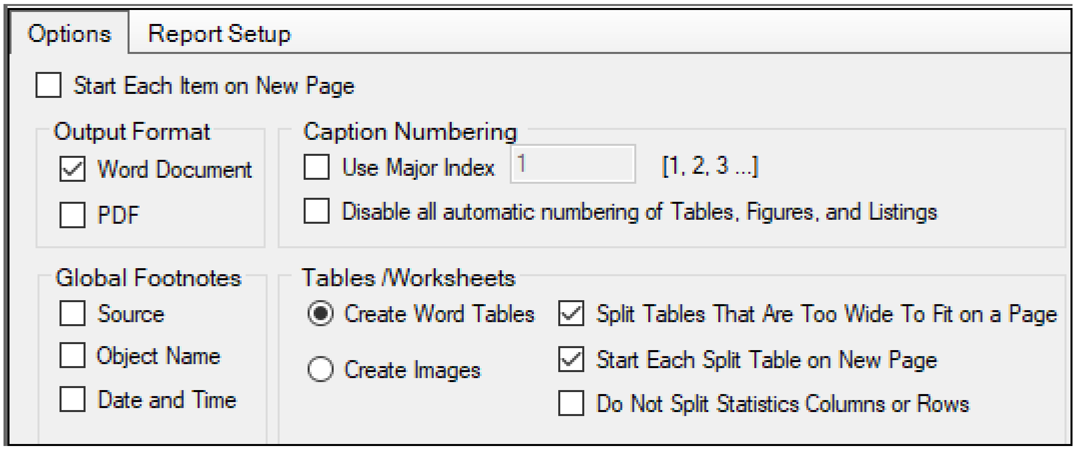
Table options

Choose the type of table

In the Options tab, specify the type of table to generate in the output:

Word table (**Create Word tables**): This is the default type. These tables can be modified using the tools in Word.

Image (**Create Images**): To prevent table contents from being modified, select this option and tables will be inserted as images in the output document.



Optimize table splitting

There are some tables generated by Phoenix and its modules that are too wide to fit on a single page of a report. Several options are available in the Options tab for setting how and when to allow splitting of such tables.

Split tables that are too wide to fit on a page controls splitting of tables. When unchecked, there is no table splitting, regardless of the table size.

The **Start each split table on new page** option becomes available when the **Split tables…** option is checked and, when selected, forces each split table to begin on a new page.

The **Do not split statistics columns or rows** option becomes available when the **Split tables…** option is checked and, when selected, prevents table splitting from occurring between statistics columns and/or rows.

Figure options

Set scale

- Click  (**Options** icon) next to the figure’s name in the lower list.
- Click the **Figure** tab in the dialog.
- Check the **Set Y-axis scale in report** box.
- Select **Linear** to output the figure with a linear scale.
- Select **Logarithmic** to output the figure with a log scale. Use the menu to select the type of logarithmic scale to use.

- Select **Linear and Logarithmic** to output the figure twice, with linear scale and log scale, stacking the figures vertically. Use the menu to select the type of logarithmic scale to use.

  If the **Arrange figures in a lattice** option is selected, then each log plot will be immediately after the corresponding linear plot, following the specified number of **Columns per row**.

Create a lattice of figures

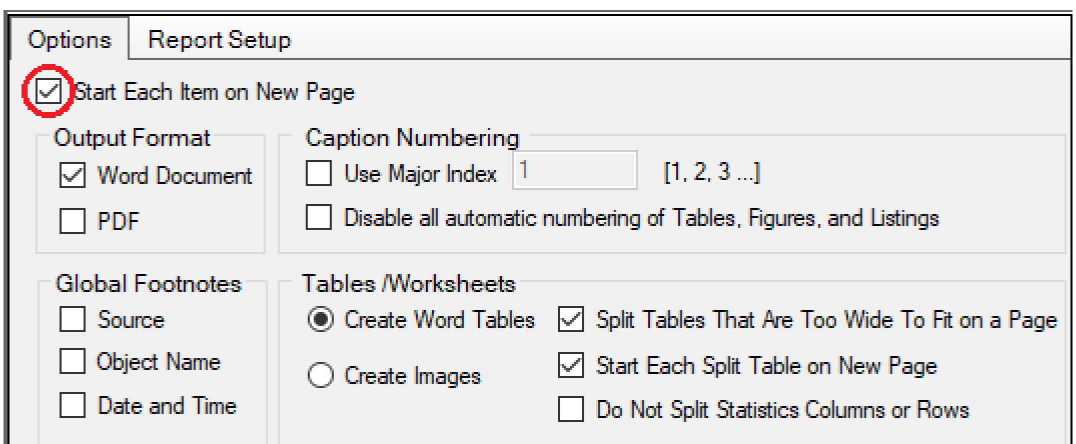
A lattice provides the opportunity to organize the display of multiple graphs in a grid layout.

- Click the **Reporter Options** icon next to a figure item in the lower list.
- Click the **Figure** tab in the dialog.
- Check the **Arrange figures in a lattice** box.
- Specify the number of columns in the lattice using the **Columns per row** option.
- Specify the number of rows in the lattice using the **Rows per page** option. (Select **To fit** to have as many rows in the lattice as will fit on the page.)
- To display borders for the rows and columns in the report, check the **Show grid lines** box.
- If the **Show figure numbers in lattice cells** box is unchecked, the individual figures in the lattice cells will not be numbered in the report (but the figure number will still be above the lattice).

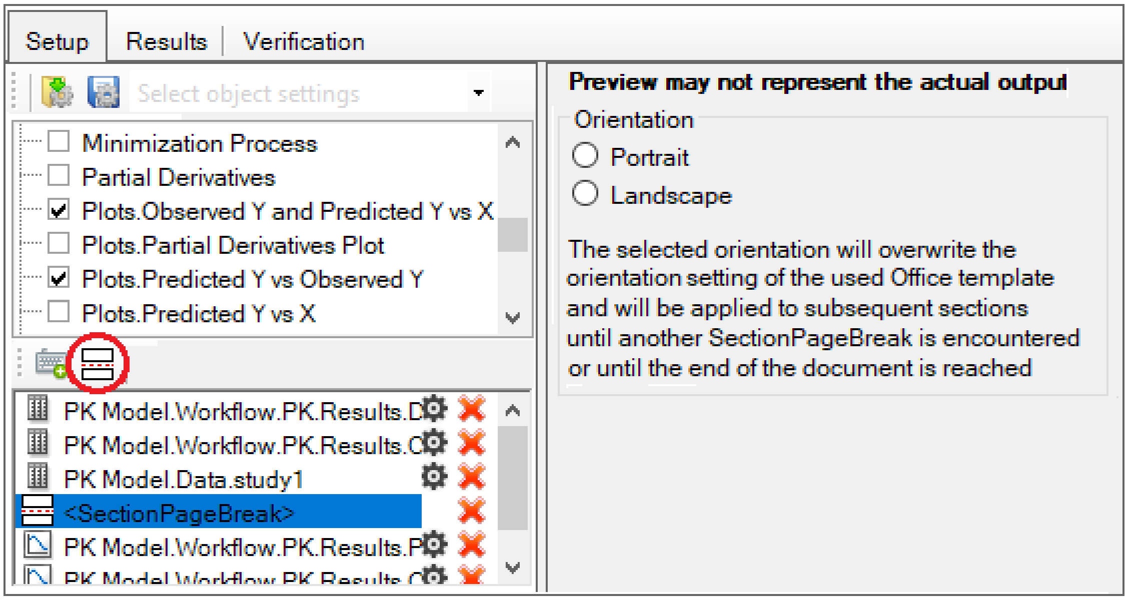
Pagination in the report

Indicating new pages in the report generated by the Reporter object can be accomplished in several ways.

- To place each Reporter item on a separate page, check the **Start each Item on New Page** checkbox in the Options tab.



- To insert a page break in between two particular Reporter items, click  in the lower list toolbar item. A Section Page Break is placed after the selected item in the lower list. (To specify the orientation of the page(s) in the section, select the Section Page Break item in the list and click **Portrait** or **Landscape** in the panel to the right of the list.)



- To avoid tables starting on a page with the previous item and then continuing on the next page, turn on the **Start each Split Table on New Page** checkbox in the Options tab.

Captions

Number items

All tables, figures, and listings are automatically numbered sequentially (e.g.,Table 1:, Table 2:, etc.). The same is true for figures and listings.

- To turn off the automatic numbering, check the **Disable all automatic numbering of Tables, Figures, and Listings** box.
- To use a specific primary number (e.g., Table 1.1, Table 1.2, etc.), in the Options tab, with the **Use Major Index** checkbox checked, enter the desired primary number in the field. Up to four numbers and three periods can be entered in the field, which would generate level five headings.

Latticed figures are automatically numbered sequentially within the lattice cells, using the figure number as the primary number (e.g., Figure 3.1, Figure 3.2, etc.), but this can be turned off by unchecking the **Show figure numbers in lattice cells** checkbox.

(Click the **Reporter Options** icon next to a figure item and select the Figure tab).

Add caption text

A caption can be defined for a table, figure, or listing item. Once defined, the caption can be saved, which adds it to the Caption tab's dropdown menu. Select the caption from the dropdown and reuse it within the same project or even across projects. See "Save and reuse captions" for more information.

- To create a caption, click the **Reporter Options** icon next to the item in the lower list.
- In the Caption tab, enter the text in the **Caption Text** field, or paste content from the Windows clipboard.

The text can be emboldened, italicized and superscripted/subscripted by selecting the text and clicking on the desired font style. To add a symbol, select it from the **Insert Symbols** pull-down.

If the entry mapped to the Reporter object is based on a worksheet, the **Source – Data Worksheet / Object Source** option will be active on the Caption tab, allowing data from the worksheet itself to be placed into the caption. The column names (and column units, if applicable) from the relevant worksheets are displayed on the right.

In the following figure, the text `Table results for Subject` has been typed into the **Caption Text** field and then the entry Subject has been added by dragging it from the list on the right.

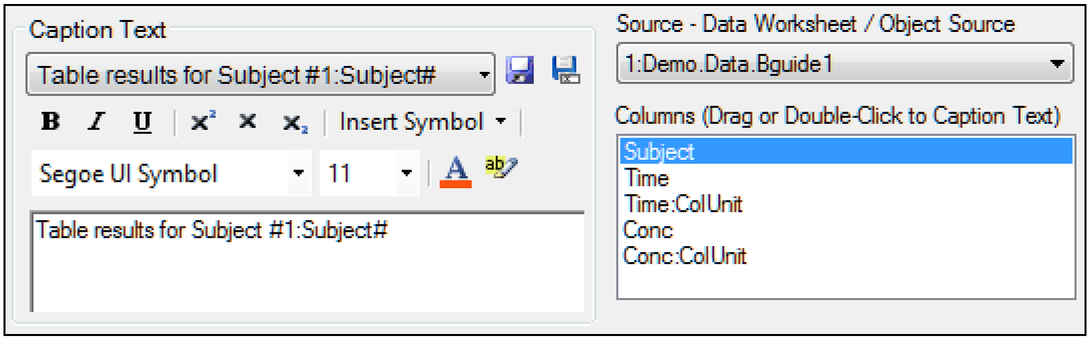


Figure 58-2. Caption tab with text entered

After execution of the Reporter object, the caption, as defined in the Caption tab, appears in the output above the associated table, figure, lattice, or list.

Optional text in captions

Optional text can be included in a caption. This text will appear in the caption in the generated tables or figures if at least one of the specified column(s) are present. When entering the caption in the **Caption Text** field, use double angle brackets before (**<<**) and after (**>>**) the text that is optional. For example:

```
PK Parameter table for subjects #1:Subject# <<having matrices
#2:Matrix#>>
```

When the Report object is executed, the appropriate worksheet will be checked to see if it includes a Matrix column. If the column is present, the portion of the caption within the double angle brackets will be included. If the worksheet does not contain a Matrix column, then the optional text will not be included.

Save and reuse captions

Commonly used captions can be saved and reused.

To add a new caption to the saved list

- Enter the caption text and adjust formatting as desired.
- If the **Caption Text** pull-down is blank, click on either (**Save**) or (**Save As**). A *Save As* dialog is displayed that lists any saved captions. Click **Save** to add the new caption to the saved list.
- If the **Caption Text** pull-down is not blank, click the **Save As** icon to display the *Save As* dialog and then click **Save**.

Captions are saved to the settings file specified in the *Preferences* dialog.

To edit a saved caption

- Select the saved caption from the **Caption Text** pull-down.
- Modify the text as desired and formatting as desired.
- Click the **Save** icon (this overwrites the saved caption).
  Or
  Click the **Save As** icon and select the saved caption to overwrite, then click **Save**.

The saved captions are accessible from the Caption tab for any item selected in the Setup panel.

Upon retrieval of the caption, the validity of the column pattern is checked. If the column name no longer exists, double angle brackets (**<< >>**) are inserted to surround the column pattern in the caption. If **<< >>** already exists, the column name is not checked until the Reporter object is executed.

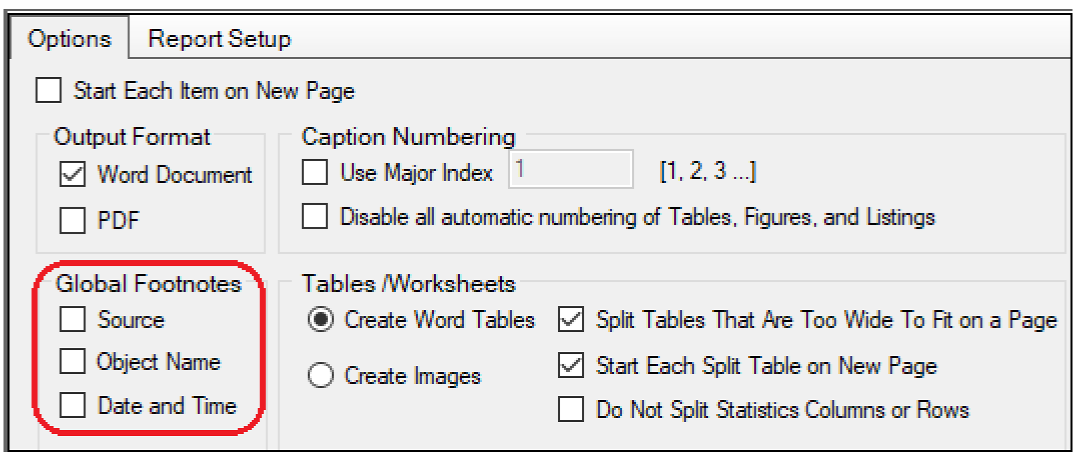
Deleting a saved caption must be done manually by editing the setting file.

Footnotes

Add footnotes

Footnotes can be defined as global or individual item footnotes. In addition, a contextual footnote may be created, see “Manage contextual footnotes” for more information.

A ***global*** footnote adds source information, object name, and/or a date-time stamp as a footnote to every individual table, figure, listing, and group member (time-concentration graphs only). This is accomplished by checking the Global Footnotes checkbox(es) on the Options tab.

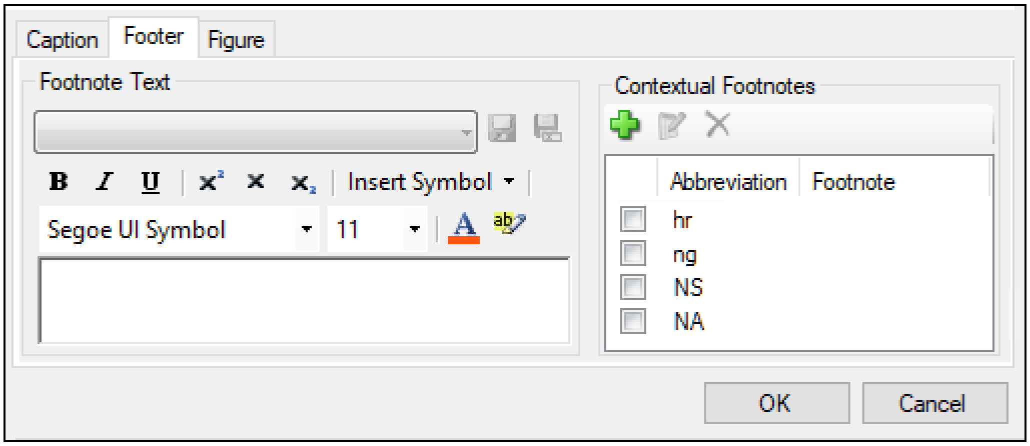


For a Worksheet, Table, Figure, or Listing result in the report, selecting the **Date and Time** global footnote option adds the date and time of execution for the object that generated that result. For items in the report that are not the result of an execution (e.g., data in the Data folder), the date and time of the last save of the project is used.

An ***individual item*** footnote can be defined for a table, figure, or listing. Once defined, the footnote can be saved, which adds it to the Footer tab’s dropdown menu. Select the footnote from the pull-down and reuse it within the same project or even across projects. See “Save and reuse footnotes” for more information.

- To create a footnote, click the **Reporter Options** icon next to the item in the lower list.
- In the Footer tab, enter the text in the **Footnote Text** field, or paste content from the Windows clipboard.

The text can be emboldened, italicized and superscripted/subscripted by selecting the text and clicking on the desired font style. To add a symbol, select it from the **Insert Symbols** pull-down.



After execution of the Reporter object, the footnote, as defined in the Footer tab, appears in the output below the associated table or figure.

Save and reuse footnotes

Commonly used footnotes can be saved and reused.

To add a new footnote to the saved list

- Enter the footnote text and adjust formatting as desired.
- If the **Footnote Text** pull-down is blank, click on either the **Save** icon or the **Save As** icon. A *Save As* dialog is displayed that lists any saved footnotes. Click **Save** to add the new footnote to the saved list.
- If the **Footnote Text** pull-down is not blank, click the **Save As** icon to display the *Save As* dialog and then click **Save**.

Footnotes are saved to the settings file specified in the *Preferences* dialog and will be added to the list in the Footnote panel pull-down.

To edit a saved footnote

- Select the saved footnote from the **Footnote Text** pull-down.
- Modify the text as desired and formatting as desired.
- Click the **Save** icon (this overwrites the saved footnote).
  Or
  Click the **Save As** icon and select the saved footnote to overwrite, then click **Save**.

The saved footnotes are accessible from the Footnote tab for any item selected in the Setup panel.

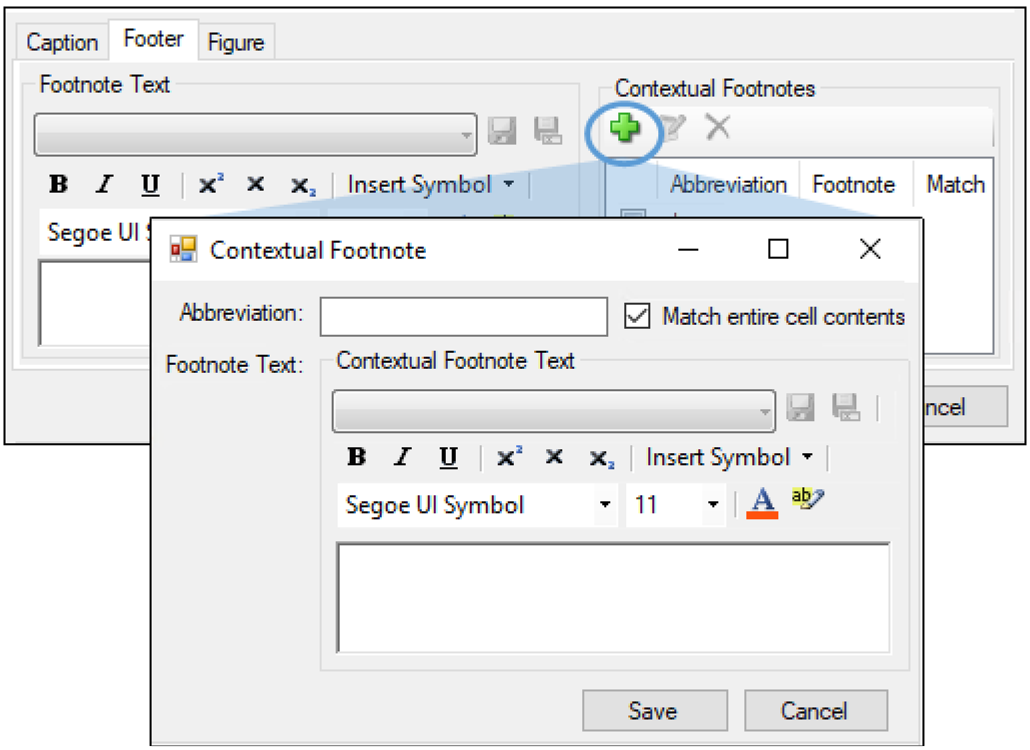
Deleting a saved individual item footnote must be done manually by editing the actual settings file.

Manage contextual footnotes

Contextual footnotes may be added to Table items to clarify abbreviations that appear as cell values in the table. The footnote will be added only if the specified abbreviation is found within the generated table.

To add a contextual footnote

- Click (**Add Footnote** icon).
- In the *Contextual Footnote* dialog, enter the text to search for in the **Abbreviation** field.
- Use the **Match entire cell contents** checkbox to toggle between performing an exact match or partial match search for the abbreviation.
- In the **Footnote Text** field, type the text to display as a footnote below the table if the abbreviation is found.



- Click **Save** to add the contextual footnote information to the Footnote panel.
- Use the checkboxes in the Contextual Footnote list to indicate the abbreviations to search for within the selected Table item.

When the Reporter object is executed, the tables will be checked for the presence of the identified abbreviations. If present, the footnote text will be added below the table. If the abbreviation is not present, the footnote will not be added.

To edit a contextual footnote

- In the Contextual Footnotes list, select the footnote to edit.
- Click (**Edit Footnote** icon).
- Make the desired changes in the *Contextual Footnotes* dialog and click **Save**.

To delete a contextual footnote

- In the Contextual Footnotes list, select the footnote to delete.
- Click X.

Report document setup

Select the document format

Reporter generates Word and PDF files as output.

To specify which format to generate, in the **Options** tab, check the boxes for the desired format: **Word Document**, **PDF**, or both.

Use a Word template

To select a predefined Word template file (`.dotx` or `.dotm`) to apply when generating the report:

- Select the **Report Setup** tab.
- Enter the path to the template file or click **Browse** to navigate and select the file from file system or click **Project Documents** to select the template from the Documents folder for an open project.

Specify page settings

Note: Page settings are not available if a template is specified.

To define size, margins, and orientation of the report pages:

- Select the **Report Setup** tab.
- Select a size from the **Page Size** dropdown menu.
- Enter or use the arrows to set each of the margins for the report pages.
- Click the desired orientation of the pages (**Portrait** or **Landscape**). This can be changed with Section Page Break.

Include captions in document contents lists

The table and figure captions can be added to either the Table of Contents or in separate lists of tables and/or figures.

- Select the **Report Setup** tab.
- Check the **Table and Figure Captions Listings** box to include captions in the report.
- Click the desired radio button to indicate where to add the captions.
- If the option to **Include Table and Figure Captions in Separate List(s)** is selected, use the checkboxes to select the lists to create: **Include List of Tables**, **Include List of Figures**, or both.

Handling lost connections

Connection between an input source and the Reporter object can occasionally be lost.

- The result that is mapped as the input source is no longer available.
  For example, a Reporter object has an AutoPilot Toolkit table as its input source. The AutoPilot Toolkit settings are then modified to not include that particular table in the output and the AutoPilot Toolkit object is re-executed.
- The object generating the input source is no longer available.
  For example, a Reporter object has an AutoPilot Toolkit table as its input source. The AutoPilot Toolkit object is then removed from the Workflow.
- The connector to the input is deleted in the Workflow Diagram.

When a lost connection occurs, an icon will appear next to the associated Input item in the Reporter object.

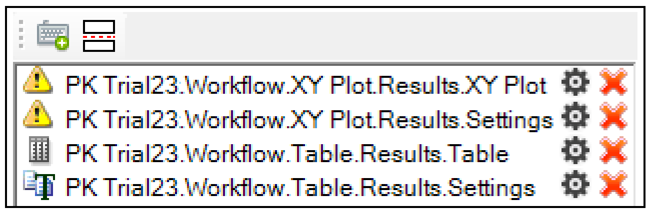


Figure 58-3. Setup tab showing a lost connection of a Reporter item

To re-establish the connection, recheck the Input Object or remove it and then add a new Input Object.

Object output

The Reporter object shown in the following image was executed to produce the example output for this section.

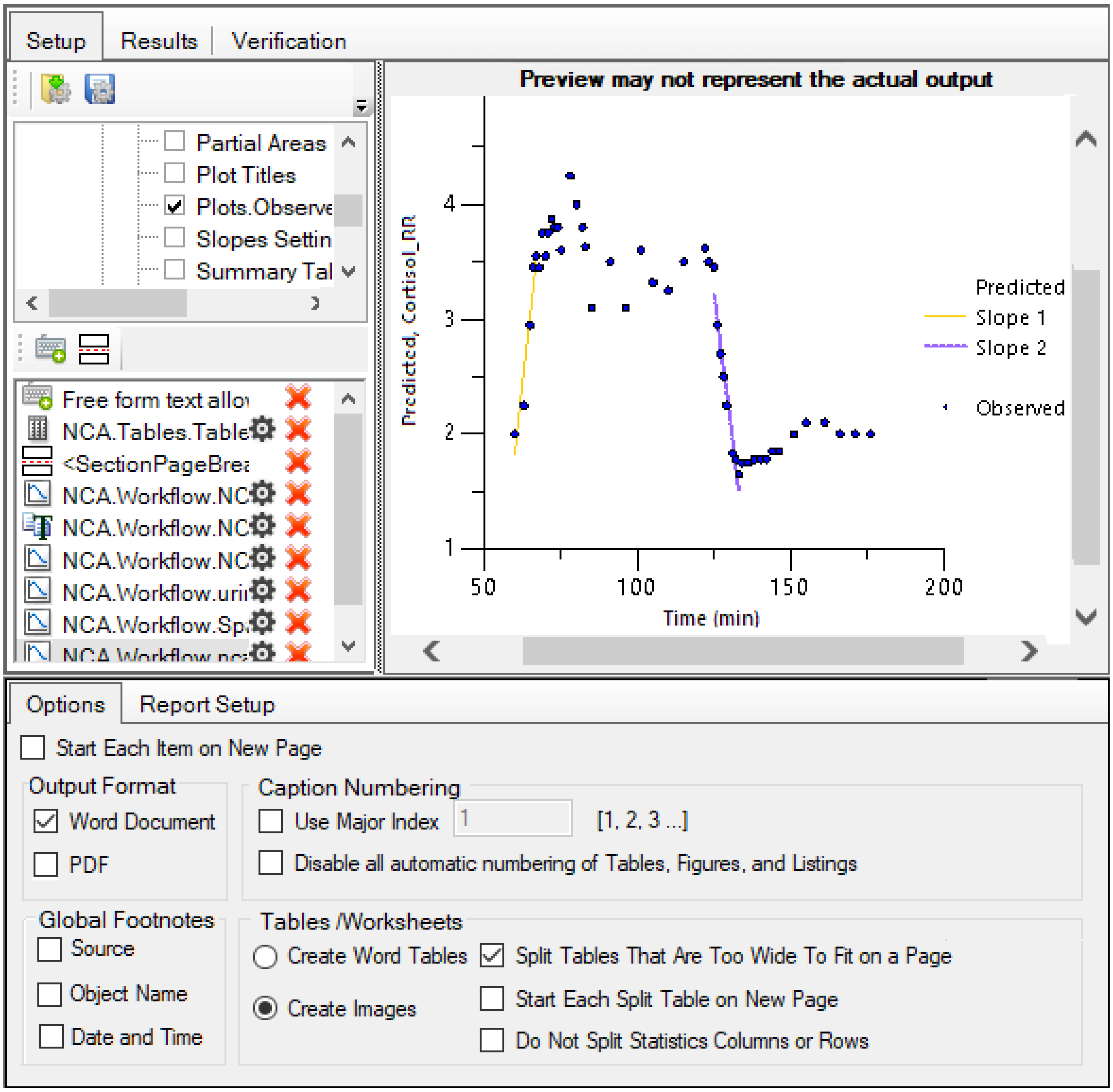


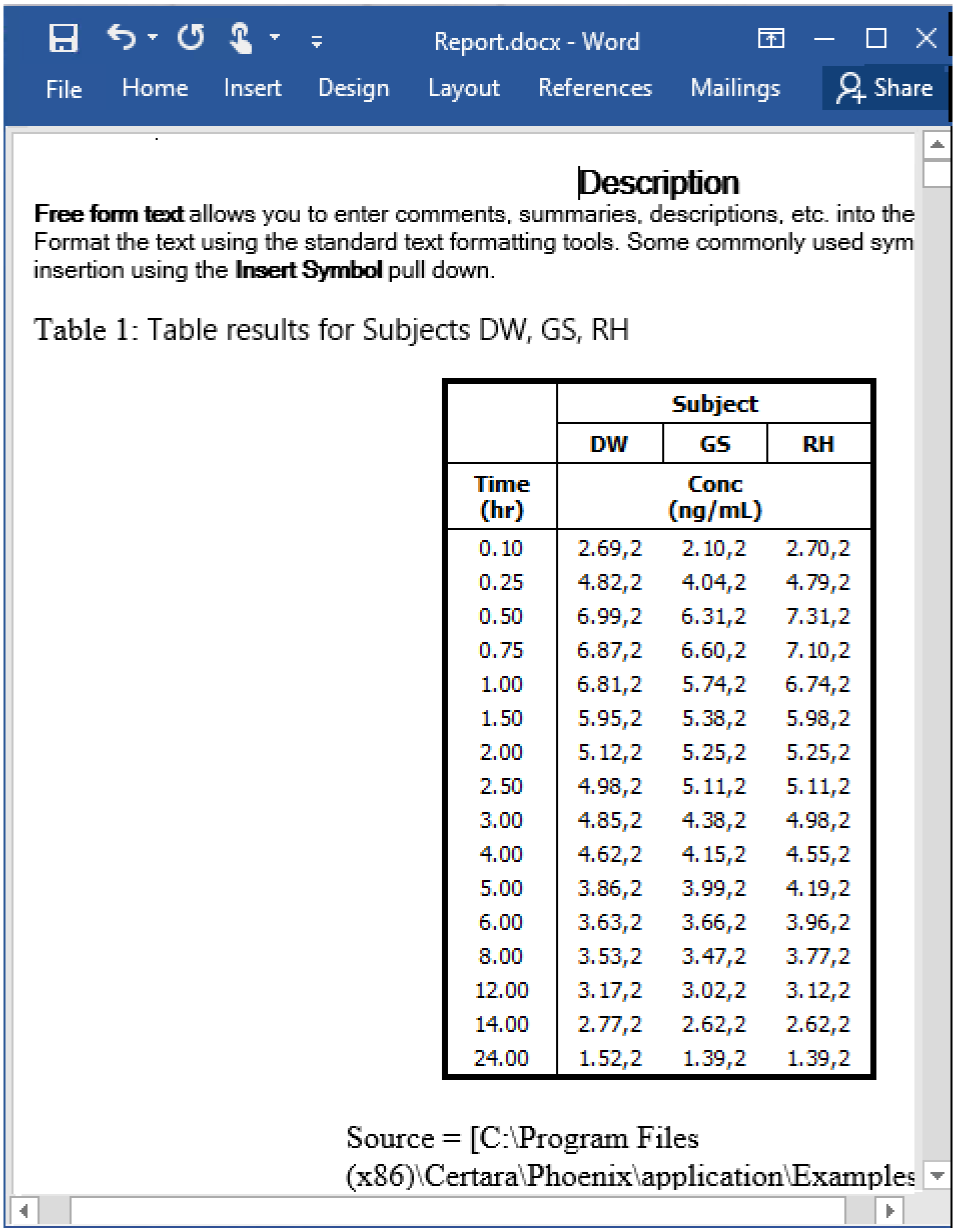
Figure 58-4. Reporter object setup used to generate example output

To open the Reporter output document

- Click the **Results** tab.
- Click **Report** under Results.

The following are pictures of the Word document containing the Reporter output.

The Description is an example of the Free Form Text item. This is followed by a results table from a Table object. The table has a caption and a footnote shows the table's source.



Description

Free form text allows you to enter comments, summaries, descriptions, etc. into the
Format the text using the standard text formatting tools. Some commonly used sym
insertion using the **Insert Symbol** pull down.

Table 1: Table results for Subjects DW, GS, RH

	Subject		
	DW	GS	RH
Time (hr)	Conc (ng/mL)		
0.10	2.69,2	2.10,2	2.70,2
0.25	4.82,2	4.04,2	4.79,2
0.50	6.99,2	6.31,2	7.31,2
0.75	6.87,2	6.60,2	7.10,2
1.00	6.81,2	5.74,2	6.74,2
1.50	5.95,2	5.38,2	5.98,2
2.00	5.12,2	5.25,2	5.25,2
2.50	4.98,2	5.11,2	5.11,2
3.00	4.85,2	4.38,2	4.98,2
4.00	4.62,2	4.15,2	4.55,2
5.00	3.86,2	3.99,2	4.19,2
6.00	3.63,2	3.66,2	3.96,2
8.00	3.53,2	3.47,2	3.77,2
12.00	3.17,2	3.02,2	3.12,2
14.00	2.77,2	2.62,2	2.62,2
24.00	1.52,2	1.39,2	1.39,2

Source = [C:\Program Files (x86)\Certara\Phoenix\application\Examples

Figure 58-5. Example output showing free form text and tables with captions and/or footnotes

The next image shows one of the NCA results plot for which a footnote has been defined.

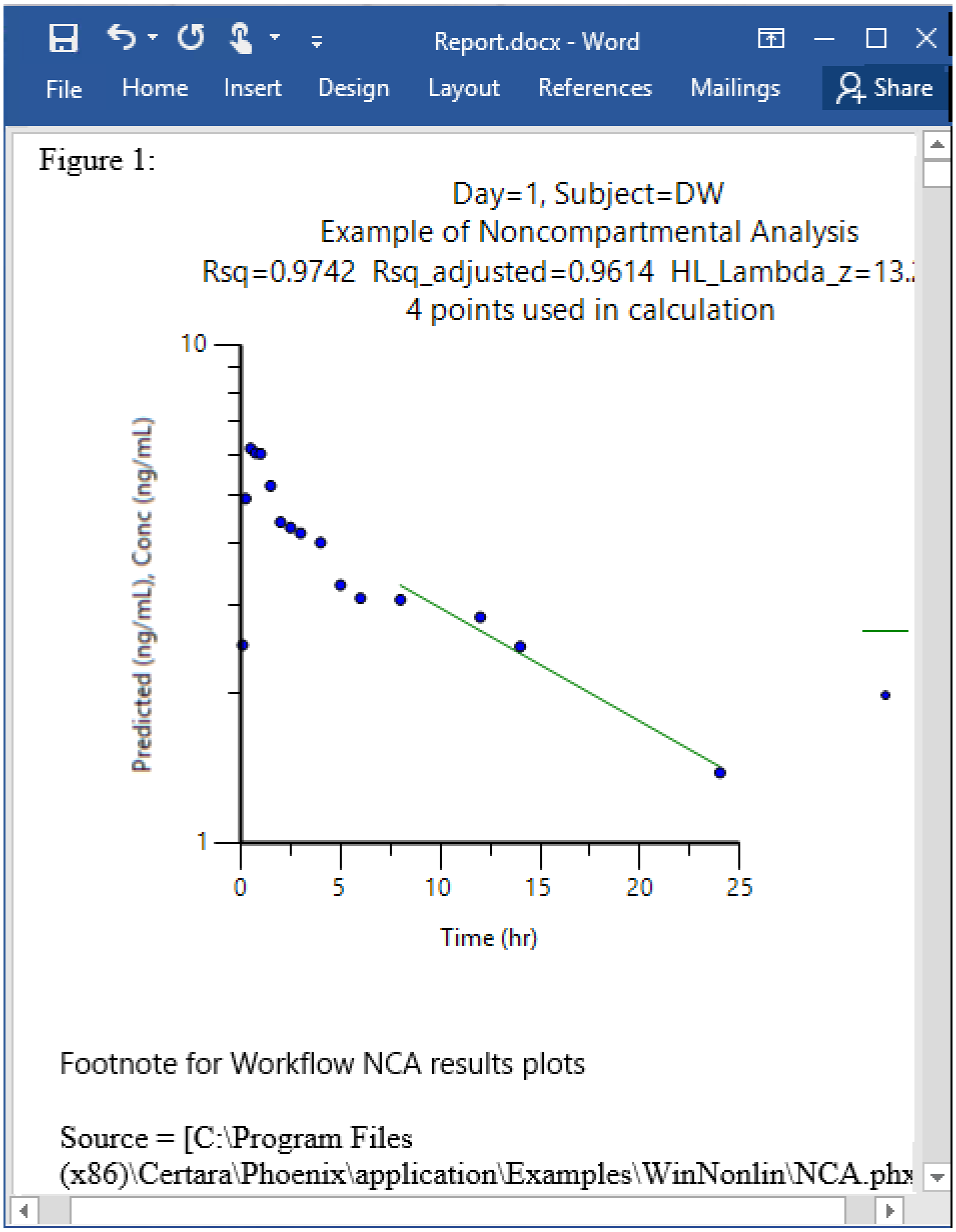


Figure 58-6. Example output showing a graph, caption, and footnotes

Several pages follow, each with an additional NCA results plot. Then several pages of text show the contents of the Core Output file for the NCA analysis.

The following image shows a two-column lattice of graphs. The latticed figure has it's own number and each cell within the lattice is numbered as well. Note that the footnote that was added appears below each latticed figure.

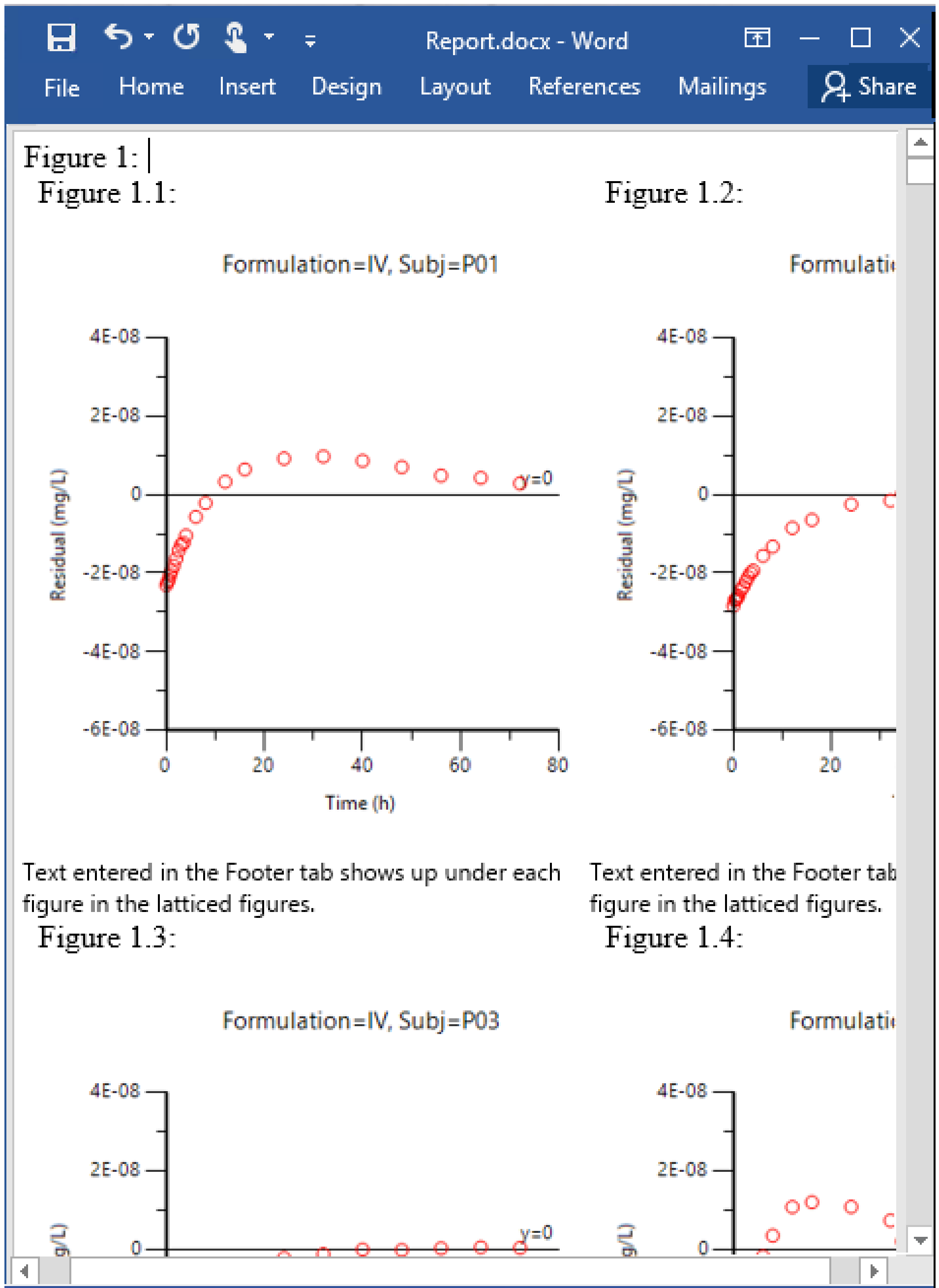
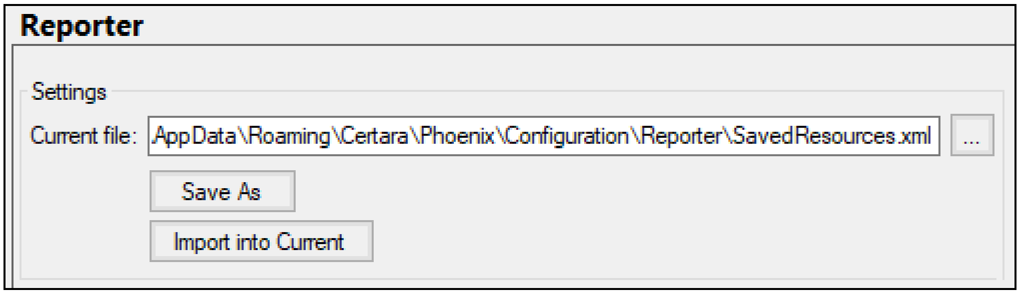


Figure 58-7. Example output showing a lattice of graphs and footnote

Setting up preferences

By default, saved captions and footnotes are added to the file. The Reporter panel of the *Preferences* dialog is where the XML file to use for populating the Caption and Footnote panels' pulldown menus is specified. This file also contains contextual footnote information. The default file is: C:\Users\<user>\AppData\Roaming\Certara\Phoenix\Configuration\Reporter\SavedResources.xml.

- Select **Edit > Preferences**.
- In the *Preferences* dialog, select the **Reporter** item in the menu tree.



Captions and footnotes can be shared between users. This can be done by users loading an XML file with a set of pre-defined captions and footnotes (click **[…]**) or by merging captions and footnotes from a different file into the one currently in use (**Import into Current**).

To save the contents of the currently selected XML file to a file with a different name, click **Save As** and specify the new file's name and location.

R Shell

The R Shell object imports R scripts and datasets for use in Phoenix.

Note: Phoenix program plugins, such as the R Shell object, assume that the corresponding third party software is installed and running properly.

Note: S-PLUS code must be converted to R for use within Phoenix.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > External Software > R Shell**.
Main menu: **Insert > External Software > R Shell**.
Right-click menu for a worksheet: **Send To > External Software > R Shell**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Additional information is available on the following topics:

Setting up preferences
User interface description
Importing/Writing the code to access the external program
Executing a third party tool object
Results

Setting up preferences

Global preferences are available to the user. Some third party tool objects require certain global settings to be specified prior to use. There are optional settings to enable editing of scripts in external programs from within Phoenix. Some optional preferences can streamline the workflow by automatically filling in or setting options in the object's UI with information entered by the user in the *Preferences* dialog.

Setup access to the external program
Specify a development environment
Define a default output location

Setup access to the external program

- Select **Edit > Preferences**.
- In the *Preferences* dialog, select the object in the menu tree.
- Enter the directory path to the executable in the first field or click **Browse** to locate and select the directory.

Specify a development environment

There is a Development Environment section available on the preference pages. When the development environment is defined in this section, users can access that environment from the third party tool object's Options tab with the **Start** button. This allows users to edit scripts in other specified environments, and then pull the updated scripts back into Phoenix, at which time, the script can be executed from Phoenix and the output processed through the normal Phoenix workflow.

- In the **Command** field, enter the directory path to the executable or click **Browse** to locate and select the file.
- In the **Arguments** field, enter any arguments/keywords to use when starting up the environment.

Note: Proper development environment setup for Tinn-R requires that `$WorkDir\$File` be entered in the **Arguments** field.

Define a default output location

Setting the output folder in the *Preferences* dialog eliminates the need to enter the information in the Options tab for each run. The fields will automatically be filled with the paths entered here.

- Enter the directory path in the **Default Output Folder** field or use the **Browse** button.

Note: If the user specifies a default output location, the user must ensure that they have write access.

- Turn on the **Create a unique subfolder for each run** checkbox to generate and then store the output from each run in a new subfolder of the output folder.

User interface description

Setup tab
Options tab
Result Filters tab

Setup tab

The **Setup** tab allows mapping of scripts to the object. The Mappings panel(s) of the Setup tab displays the column headers specified in the script file. The Text panel allows users to map a script file to the object and view the contents.

Note: Any apostrophe marks in the input data (e.g., 5'-deoxy-) should be removed or substituted, as they can prevent Phoenix from reading the data. Apostrophes are interpreted as quotation marks, so data between two apostrophes is considered to be a single cell value. This can result in the number of columns not being the same for all rows,

Context associations for R Shell objects change depending on the column headers, or input, defined in the script file. Not all R scripts define or use mapping contexts. If the `#WNL_IN #` statement does not define any mapping contexts, then there are no mapping options available in the Mappings panel.

How dataset Mappings panels are defined in R scripts

Before the script is mapped, there are no data inputs into the R Shell object. The data inputs are defined in the `attach()` statement in the script. When using an imported dataset or a results worksheet as input for an R script, one or more `attach()` statements must be in the script in order to map an input dataset or sets.

The `attach()` statement in the script requires the following format:

```
attach(dataname) #WNL_IN context1 context2 context3 etc#
```

Each `attach()` statement creates a data mappings panel that allow users to map a dataset as input for the script, and users can map study data to the contexts defined in the `attach()` statement. If the study variable names are the same as the context names, the study variables are automatically mapped to the appropriate contexts. For example,

```
attach(Eta) #WNL_IN Id nV nCl#
```

A data input called Eta is created in the object and is listed in the Setup and Diagram tabs. Also, the data mapping contexts Id, nV, and nCl are created in the Eta Mappings panel.

Note: Using the `#WNL_IN #` comment to create mapping contexts is optional. If it is used, the column names in the comment must be space-delimited.

If the `attach()` statement does not have `#WNL_IN … #`, then Phoenix treats the data as an external source specified in the script and not as an imported dataset. Scripts written in this manner would be difficult to share as the sources might not be able to be located on a different computer.

The example R script (`plotpredtable.r`), available in …`\Examples\R`, has these lines:

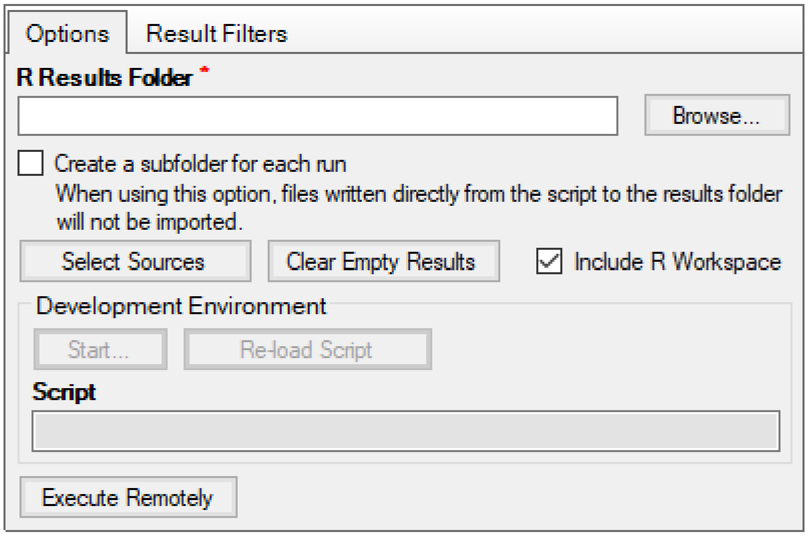
```
attach(Residuals) #WNL_IN ID IVAR TAD POPPRED INDPRED
      OBS IRES WTIRES WRES CWRES PCWRES CdfPCWRES CdfDV#

attach(Eta) #WNL_IN Id nV nCl#
```

When using the R object for accessing the Model Comparer results for NLME or NONMEM, the default csv file generated for importing into R will not work. The columns beginning with “#” prevent the file from loading into R. To avoid this problem, set up Model Comparer so it will not generate these particular output columns, or explicitly state the columns to import by using the commenting mechanism for mapping in the R tool. For example, use a script similar to the following to list the columns to import and then map the columns:

```
attach(compare.df) #WNL_IN Hide Compare Name Sort
      Method Description Lineage LogLik -2(LL) AIC
      BIC -2(LL)Delta AICDelta BICDelta NumParms
      NumObs NumSubj pvalue
```

Options tab

The Options tab is used to define a location for the output, access development environment, and start a remove execution.



Entering an output location is optional. If a directory is not specified then Phoenix places output in a temporary folder that is deleted after Phoenix is closed. This may be preferred when sharing third party tool projects with other users, as the output folder is machine specific and may not exist on other machines. If users want to save the results from a third party tool object run to a disk, then they must either specify an output folder or manually export each result to disk.

The results folder set in the Options tab must match the export folder location set in the script. For example, if the export path in an R script is `c:\\local\\`, then the R Shell results folder must also be `C:\Local`. To make sharing projects involving R Shell objects easier, set the results folder in the Options tab to the `getwd` value and refer to `getwd` in the code. Files written to the path returned from `getwd` end up in the output folder and in the results.

- Enter the output folder path in the field or click **Browse** to specify the output folder location.
- Turn on the **Create a subfolder for each run** checkbox to add a new results folder in the specified output location each time the object is executed.

  This option prevents the output from being overwritten with each run, especially if the default output folder option, under **Edit > Preferences**, is being used.
- Click **Select Sources** to include additional files along with the mapped input.
- Click the **Clear Empty Results** to remove any results published by the object that are empty.
- Turn on the **Include R Workspace** checkbox to have Phoenix store the R Workspace with the results.

  The R Workspace, called RData in the results, can then be re-used in other R objects by using the **Select Sources** button to select it as a source for that object.
- To start the development environment, click **Start** in the Development Environment section of the Options tab.

  The development environment as configured in the *Preferences* dialog is started. (See "Specify a development environment".)

- When script work is completed, click **Reload Script** to bring the modified script into Phoenix for use in the next execution of the object.

Result Filters tab

See the “Result Filters tab” description for the PsN object.

Importing/Writing the code to access the external program

The R Shell object must have code that will allow it to initiate the external program and submit jobs. The code can be stored as a script file, imported into the project, and mapped to the object, or the code can be directly entered into the object.

Import and map file containing code

The process is the same as for many other Phoenix objects. Refer to “Importing datasets” common task description.

Write code in the Text panel

Instead of importing and mapping a script file, users can write their own code or copy and paste code from another source. (For more information, see the “Write code in the Text panel” section for the PsN object.)

Adding shortcuts in scripts

The input can be defined within the script as a shortcut by adding the following at the beginning of the script.

```
#PHX_SHORTCUT(Data)
```

The text entered between the parentheses is used as the variable’s name (e.g., `Data`).

Phoenix will parse the script and prepend the variable to the script, with the shortcut path being stored assigned as the value.

```
Data <-”C:\\Path\\To\\File”
```

In the script, the user can use the variable assigned the path to read or manipulate the file.

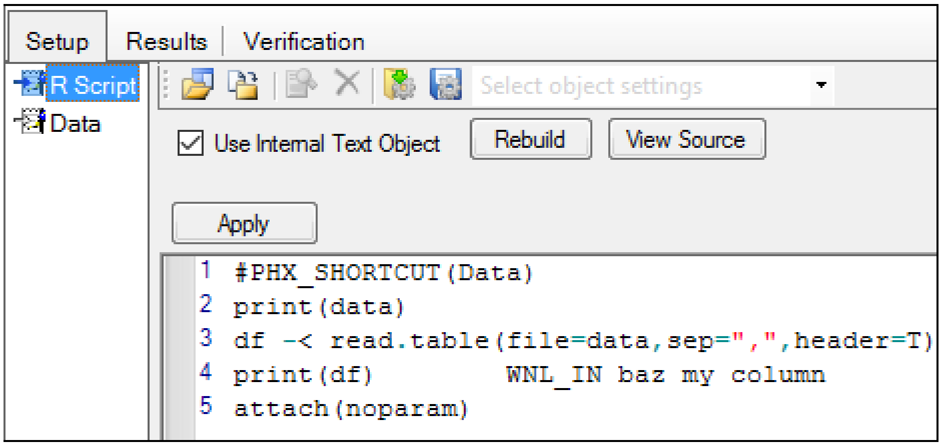
To add a shortcut to a script

- With the object inserted in the project, click **R Shell** in the Setup list.
- Either type the script directly in the field or click  (**Select Source** icon) and select the script (which has already been imported into the **Code** folder).
- Type the following as the first line in the script:

```
#PHX_SHORTCUT(Data)
```

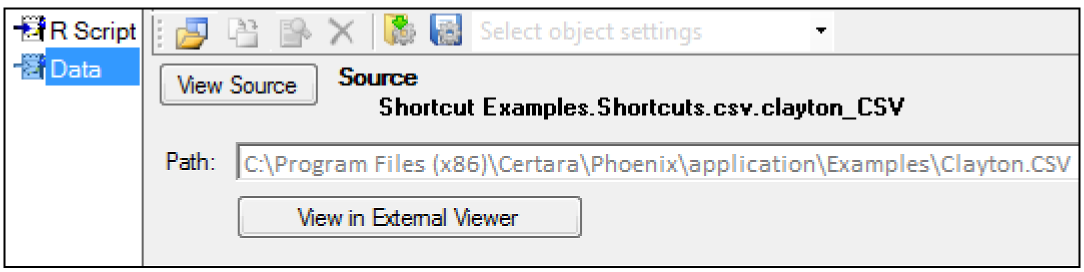
- Click **Apply**.

The following image is the R Shell Setup panel showing the contents of the script. Notice the first line, indicating that a shortcut will be the source of the input data.

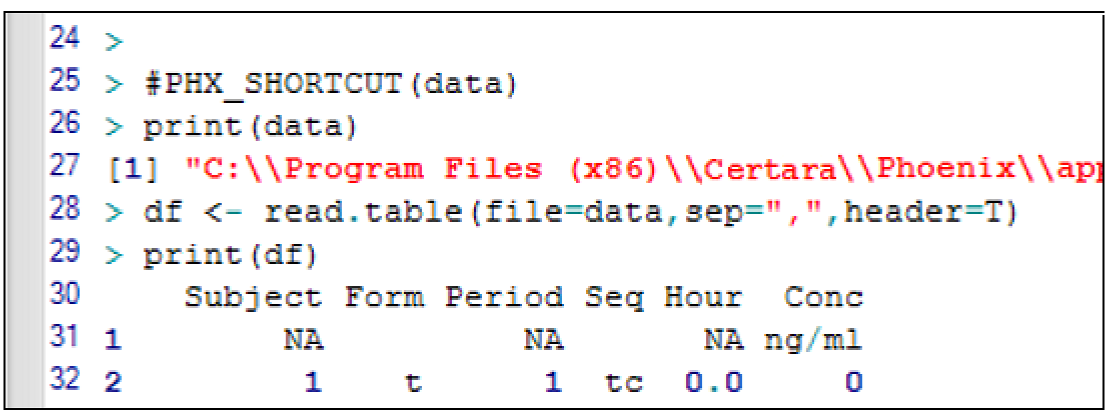


- Select the new **Data** item in the list.

The Data panel shows the full path behind the shortcut.



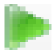
The log file produced from executing the object contains the definition used for the shortcut. Below is an image of the **R Log** file.



Filtering results by size

See the “Filtering results by size” section for the PsN object.

Executing a third party tool object

Click  (**Execute** icon) or to run the job remotely, click **Execute Remotely** in the Options tab.

Executing a third party tool object remotely sends the job to the server that is defined in the *Preferences* dialog (**Edit > Preferences > Remote Execution**). See “Phoenix Configuration” for instructions. The project is saved automatically.

The project must have been saved at least once prior to executing on RPS, otherwise execution will not pass validation and a validation message will be generated.

At this point, the step being executed on RPS, along with any dependent objects, has been locked. It is now safe to close the project or to continue working in Phoenix.

In Phoenix, some objects in a workflow allow the user to click and execute the last object in a chain and it will re-run any necessary objects earlier in the workflow. This is not true for the R object. Either the workflow or the individual objects must be executed to obtain the current source data for the R object.

Results

The results are displayed on the Results tab. The output falls into the following categories:

Output Data: Datasets in tabular form

Text Output: Settings files, log files, and other text output

Other: Other kinds of files, for example: documents, export files, binary files, etc.

Images: Graphs or other images in recognized image formats (jpg, tiff, emf, etc.)

SAS Shell

The SAS Shell object imports SAS scripts and datasets for use in Phoenix.

Note: Phoenix program plugins, such as the SAS Shell object, assume that the corresponding third party software is installed and running properly.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > External Software > SAS Shell**.
Main menu: **Insert > External Software > SAS Shell**.
Right-click menu for a worksheet: **Send To > External Software > SAS Shell**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

For a SAS script to work in the SAS Shell object, a "`/*WNL_IN*/`" comment must be added. When the script is parsed, the SAS Shell object will recognize this line in the script as defining the data input. For example:

```
libname indata XPORT "input.xpt"; /*WNL_IN Subject Time Concen*/
proc copy in=indata out=work;
run;
```

The `indata` library reference name is used by the SAS Shell object for mapping the input dataset.

Notice that this example code has column names listed in the comment: Subject, Time, and Concen. The SAS object will use these as context headings in the Mappings panel of the Setup tab. Not all SAS scripts define or use mapping contexts. If the `/*WNL_IN*/` comment does not define any mapping contexts, then there are no mapping options available in the Mappings panel.

When the script containing the example lines of code shown above is submitted to SAS during execution of the object, the dataset mapped to `indata` will be converted to a SAS transport file named `input.xpt` and copied to the temporary `work` directory where SAS will perform any other processing steps outlined in the script file.

Additional information is available on the following topics:

Setting up preferences
User interface description
Importing/Writing the code to access the external program
Executing a third party tool object
Results

See also SAS example.

Setting up preferences

Global preferences are available to the user. Some third party tool objects require certain global settings to be specified prior to use. There are optional settings to enable editing of scripts in external programs from within Phoenix. Some optional preferences can streamline the workflow by automatically filling in or setting options in the object's UI with information entered by the user in the *Preferences* dialog.

Set up access to the external program
Specify a development environment
Define a default working directory and output location

Set up access to the external program

- Select **Edit > Preferences**.
- In the *Preferences* dialog, select the object in the menu tree.
- Enter the directory path to the executable in the first field or click **Browse** to locate and select the directory.
- Click **Test** to make sure the correct file is selected.

Note: If JPS is run as a Windows Service, installation of SAS must be local to the JPS.

Note: If JPS is run as a Console application, the path to the SAS executable may be a Networked location not local to the JPS.

Specify a development environment

There is a Development Environment section available on the preference pages. When the development environment is defined in this section, users can access that environment from the third party tool object's Options tab with the **Start** button. This allows users to edit scripts in other specified environments, and then pull the updated scripts back into Phoenix, at which time, the script can be executed from Phoenix and the output processed through the normal Phoenix workflow.

- In the **Command** field, enter the directory path to the executable or click **Browse** to locate and select the file.
- In the **Arguments** field, enter any arguments/keywords to use when starting up the environment.

Note: Proper development environment setup for Tinn-R requires that `$WorkDir\$File` be entered in the **Arguments** field.

Define a default working directory and output location

Setting the output folder in the *Preferences* dialog eliminates the need to enter the information in the Options tab for each run. The fields will automatically be filled with the paths entered here.

- Enter the directory path in the **Default Output Folder** field or use the **Browse** button.
- Turn on the **Create a unique subfolder for each run** checkbox to generate and then store the output from each run in a new subfolder of the output folder.

Note: If the user specifies a default output location, the user must ensure that they have write access.

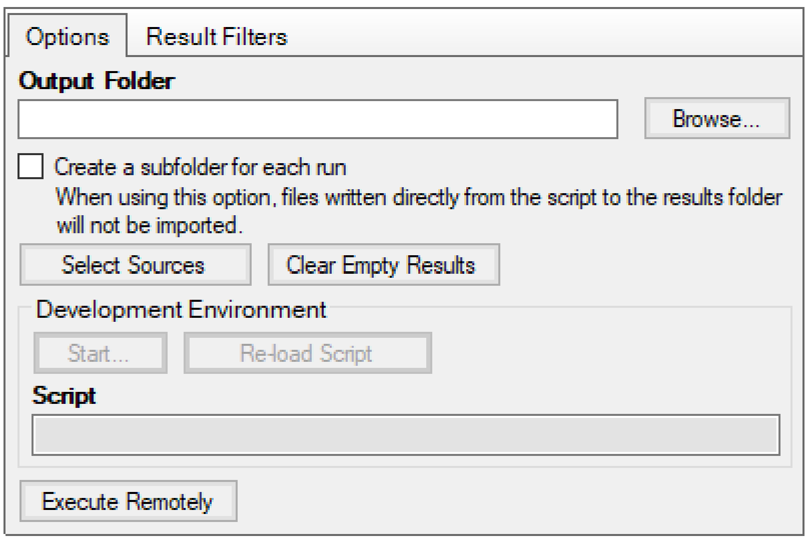
User interface description

Setup tab

The **Setup** tab allows mapping of datasets and script files to the object. The Mappings panel(s) of the Setup tab displays the column headers specified in the script file. The Text panel allows users to map a script or control/model file to the object and view the contents.

Options tab

The Options tab is used to define a location for the output, access development environment, and start a remove execution.



Entering an output location is optional. If a directory is not specified then Phoenix places output in a temporary folder that is deleted after Phoenix is closed. This may be preferred when sharing third party tool projects with other users, as the output folder is machine specific and may not exist on other machines. If users want to save the results from a third party tool object run to a disk, then they must either specify an output folder or manually export each result to disk.

The results folder set in the Options tab must match the export folder location set in the script. To make sharing projects involving SAS Shell objects easier, set the results folder in the Options tab to the `getwd` value and refer to `getwd` in the code. Files written to the path returned from `getwd` end up in the output folder and in the results.

- Enter the output folder path in the field or click **Browse** to specify the output folder location.
- Turn on the **Create a subfolder for each run** checkbox to add a new results folder in the specified output location each time the object is executed.

This option prevents the output from being overwritten with each run, especially if the default output folder option, under **Edit > Preferences**, is being used.

- Click **Select Sources** to include additional files along with the mapped input.
- Click the **Clear Empty Results** to remove any results published by the object that are empty.
- To start the development environment, click **Start** in the Development Environment section of the Options tab.

  The development environment as configured in the *Preferences* dialog is started. (See "Specify a development environment".)
- When script work is completed, click **Reload Script** to bring the modified script into Phoenix for use in the next execution of the object.

Result Filters tab

See the "Result Filters tab" description for the PsN object.

Importing/Writing the code to access the external program

The SAS Shell object must have code that will allow it to initiate the external program and submit jobs. The code can be stored as a script file, imported into the project, and mapped to the object, or the code can be directly entered into the object.

Import and map file containing code
Write code in the Text panel
Adding shortcuts in scripts
Filtering results by size

Import and map file containing code

The process is the same as for many other Phoenix objects. Refer to "Importing datasets" common task description.

Write code in the Text panel

Instead of importing and mapping a script/control file to use the third party tool object, users can write their own code or copy and paste code from another source. (For more information, see "Write code in the Text panel" section for the PsN object.

Changes made to the special comment (`/*WNL_IN */`) statement are reflected in the data Mappings panel. Changes made to a mapped script do not change the script in the Code folder.

Adding shortcuts in scripts

The input can be defined within the script as a shortcut by adding the following to the script.

```
*PHX_SHORTCUT(Data);
```

The text entered between the parentheses is used as the variable's name (e.g., `Data`).

```
&let Data="C:\\Path\\To\\File";
```

In the script, the user can use the variable assigned the path to read or manipulate the file.

To add a shortcut to a script

- With the object inserted in the project, click the **SAS Script** in the Setup list.
- Either type the script directly in the field or click (**Select Source** icon) and select the script from the **Code** folder.
- Type the following as the first line in the script:

```
*PHX_SHORTCUT(Data);
```

- Click **Apply**.
- Select the new **Data** item in the list.

The Data panel shows the full path behind the shortcut.

```
&let Data="C:\\Path\\To\\File";
```

The log file produced from executing the object contains the definition used for the shortcut.

Filtering results by size

See the "Filtering results by size" section for the PsN object.

Executing a third party tool object

Click (**Execute** icon) or to run the job remotely, click **Execute Remotely** in the Options tab.

Executing a third party tool object remotely sends the job to the server that is defined in the *Preferences* dialog (**Edit > Preferences > Remote Execution**). See "Phoenix Configuration" for instructions. The project is saved automatically.

The project must have been saved at least once prior to executing on RPS, otherwise execution will not pass validation and a validation message will be generated.

At this point, the step being executed on RPS, along with any dependent objects, has been locked. It is now safe to close the project or to continue working in Phoenix.

In Phoenix, some objects in a workflow allow the user to click and execute the last object in a chain and it will re-run any necessary objects earlier in the workflow. This is not true for the R object. Either the workflow or the individual objects must be executed to obtain the current source data for the R object.

Results

Phoenix only supports using SAS Transport Format (XPORT) Version 5 files (*.xpt) in order to export datasets from Phoenix to SAS. The SAS transport file names must be specified in the SAS script.

The output files are also defined in the SAS script, so only common output files that Phoenix always generates are listed here.

All output files defined in the script are placed in the output folder specified in the Options tab. If an output folder is not specified, the file are placed in a temporary directory in C:\Users\<user name>\AppData\Local\Temp, depending on the operating system. The directory is deleted when Phoenix is closed.

Log File: Text file that contains a list of the functions SAS performs based on the script.

Settings: Text file that contains third party tool object settings internal to Phoenix.

SAS example

Note: This example assumes that the path to the SAS executable has already been specified in Phoenix. (Select **Edit > Preferences > SAS**.)

This example generates a PROC mean and a graph from NCA data. Let's take a closer look at one of the lines in the SAS script file we will be using (`proc_mean_plus_grf.sas`).

```
libname indata XPORT "Final_Pa.xpt"; /*WNL_IN auclast tmax cmax aucinfob
lambda_z hl_lz*/
```

The WNL_IN comment has been added to the SAS script to tell the Phoenix SAS Shell object that this line specifies the input information. The `indata` library reference name is used by the SAS object for mapping the input dataset. The column names that follow `WNL_IN` (auclast, tmax, cmax, aucinfob, lambda_z, and hl_lz) will be used by the SAS object as the context headings in the Mappings panel.

When the script is submitted to SAS during execution of the object, the dataset mapped to `indata` is converted to a SAS transport file named `Final_PA.xpt` and copied to the temporary `work` directory where SAS performs any other processing steps outlined in the script file.

Let's continue with the example steps:

1. Create a new project named `SAS_Example`.
2. Import the SAS script file `proc_mean_plus_grf.sas` from …`\Examples\SAS\Example2`.

   The script is added to the project's Code folder and is parsed for comments indicating the data input "`/*WNL_IN*/`" as well any column names listed in the comment.
3. Import `Final_Parameters.csv` from …`\Examples\SAS\Example2`. (Be sure to check the **Has units row** option.)
4. Select workflow in the Object Browser and then select **Insert > External Software > SAS Shell**.
5. With **SAS Script** selected in the Setup list, expand the Code folder and drag **proc_mean_plus_grf.sas** to the Mappings panel.
6. Select **indata** in the Setup list and drag **Final Parameters** from the Data folder to the Mappings panel. (Notice that the context headings are the same as the names specified in the script file.)
7. Map the study variable **AUCINF_D_obs** to the **aucinfob** context.
8. Map the study variable **HL_Lambda_z** to the **hl_lz** context.
9. Specify an output location in the SAS object's Options tab by typing the path directly in the **Output Folder** field or by using the **Browse** button.
10. Click (**Execute** icon) to execute the SAS object.

In addition to the `aucdescrp.xpt` output file, the example script also calls for some additional xpt files to be created (`finpar2.xpt`, which contains only datasets where Lz is defined, and `finpar.xpt`). The `finpar2.xpt` file is then used to generate a graph (`cmax_log.gif`). All output files defined in the script are placed in the output folder specified in the Options tab (step 9).

This concludes the SAS example.

SigmaPlot Shell

The SigmaPlot Shell object imports SigmaPlot scripts and datasets for use in Phoenix.

Note: Phoenix program plugins, such as the SigmaPlot Shell object, assume that the corresponding third party software is installed and running properly.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > External Software > SigmaPlot Shell**.
Main menu: **Insert > External Software > SigmaPlot Shell**.
Right-click menu for a worksheet: **Send To > External Software > SigmaPlot Shell**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Additional information is available on the following topics:

User interface description
Importing/Writing the code to access the external program
Executing a third party tool object
Results

User interface description

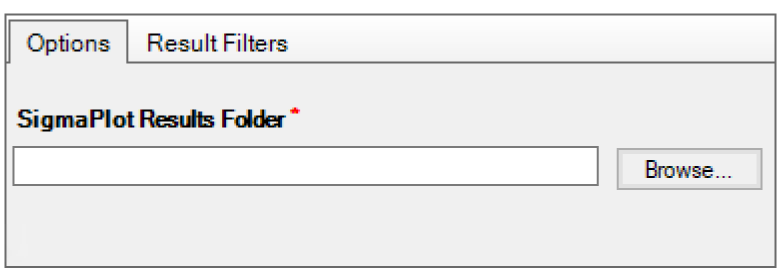
Setup tab
Options tab
Result Filters tab

Setup tab

The **Setup** tab allows mapping of datasets and script files to the object. The Mappings panel simply lists the columns found in the dataset. The Text panel allows users to map a script or control/model file to the object and view the contents.

Options tab

The Options tab is used to define a location for the output.



The results folder set in the Options tab must match the export folder location set in the script. To make sharing projects involving SigmaPlot Shell objects easier, set the results folder in the Options tab to the `getwd` value and refer to `getwd` in the code. Files written to the path returned from `getwd` end up in the output folder and in the results.

Enter the output folder path in the field or click **Browse** to specify the output folder location.

Result Filters tab

See the "Result Filters tab" description for the PsN object.

Importing/Writing the code to access the external program

The SigmaPlot Shell object must have code that will allow it to initiate the external program and submit jobs. The code can be stored as a script or control/model file. These code sources can be imported into the project and mapped to the object, or the code can be directly entered into the object.

Import and map file containing code
Write code in the Text panel
Filtering results by size

Import and map file containing code

The process is the same as for many other Phoenix objects. Refer to "Importing datasets" common task description.

Write code in the Text panel

Instead of importing and mapping a script/control file to use the third party tool object, users can write their own code or copy and paste code from another source. (For more information, see the "Write code in the Text panel" section for the PsN object.

Changes to column headers in the `.NamedRanges.Add` statement are reflected in the Dataset Mappings panel. Changes made to a mapped script do not change the script in the Code folder.

Filtering results by size

See the "Filtering results by size" section for the PsN object.

Executing a third party tool object

Click (**Execute** icon).

In Phoenix, some objects in a workflow allow the user to click and execute the last object in a chain and it will re-run any necessary objects earlier in the workflow. This is not true for the R object. Either the workflow or the individual objects must be executed to obtain the current source data for the R object.

Note: Executing a Sigma Plot script that attempts to write results to a non-existent folder can result in Sigma Plot getting 'stuck' in a state where the only way to close the application is to kill it with Window's task manager. Check the output folder names in the export statements of the scripts to confirm you are writing to an existing directory.

Results

The results are displayed on the Results tab. The output for SigmaPlot Shell objects falls into the following categories:

Output Data: Datasets in tabular form

Text Output: Settings files, log files, and other text output

Other: Other kinds of files, for example: documents, export files, binary files, etc.

Images: Graphs or other images in recognized image formats (jpg, tiff, emf, etc.)

Table

The Table object generates a report- and analysis-ready HTML table containing worksheet data and optional summary statistics. Eight table types provide a choice of layouts and summary statistics, with flexible formatting options.

Note: The Table object does not use case-sensitive comparisons when sorting and grouping data.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Reporting > Table**.
Main menu: **Insert > Reporting > Table**.
Right-click menu for a worksheet: **Send To > Reporting > Table**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Additional information is available for the following topics:

User interface description
Results
Table template for merged worksheet data
Create report-ready table from NCA results example
Using custom tables example

User interface description

Main Mappings panel
Table Preview panel
Options tab
Statistics tab
Style tab
Column/Sort Order tab
Custom Tables tab

Main Mappings panel

Use the Main Mappings panel to identify how input variables are used in a Table object. Required input is highlighted orange in the interface.

Click the option buttons in the Main Mappings panels to map the data types in the dataset to the appropriate context associations. Context associations for a Table object change depending on which table type is selected in the Options tab. Required input is highlighted orange in the interface.

None: Data types mapped to this context are not included in any analysis or output.

Row ID: Data types mapped to this context are used to create the rows in the output table.

Data: The observation data used to create the table. Multiple variables in a dataset can be mapped to this context.

Dependency: Dependent values require variables to be mapped to the Row ID and Row Stratification contexts. Dependent values are matched to values mapped to Row ID and Row Stratification and are displayed separately in the output table.

Row Stratification: Data types mapped to this context are used to create row breaks based on individual values in the data type.

Column Stratification: Data types mapped to this context are used to create column breaks based on individual values in the data type.

Table Preview panel

The Table Preview panel allows users to see a preview of the table output. The Preview Panel is updated any time a new table type is selected in the **Table Type** menu.

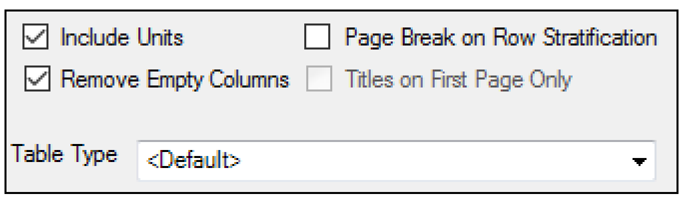
Options tab

The Options tab list contains several items that allow users to select and format a table.

Table options
Precision/Alignment options
Title options
Column Titles options
Table Body options
Statistics options
Footers options

Table options

The Table options are used to format the output table.



- Use the **Include Units** checkbox to toggle between including/excluding units in the input dataset in the output table. (The default is checked, include units.)
- Use the **Remove Empty Columns** checkbox to toggle between removing/including empty columns in the output table. (The default is checked, remove empty columns.)
- Check the **Page Break on Row Stratification** checkbox to create a printing page break in the output table for every new value of the variable mapped to the **Stratification Row** context. Use this option to decrease the uploading time for extremely large tables.
  If **Page Break on Row Stratification** is checked, the **Titles on First Page Only** checkbox becomes available.
- Check the **Titles on First Page Only** checkbox to only display the table title on the first page. If unchecked, the title will be repeated on all subsequent pages containing the table.
- In the **Table Type** menu, select the table type to use to create the output table:

Default: Computes and displays summary statistics for each column included under Data. Statistics are computed separately for each unique combination of values for the group variable(s), if any. Users can also map variables to the Dependency context.

Table 1: Column Summary by Row Stratification. Computes summary statistics for each column included under Data. Statistics are computed separately for each unique combination of values for the group variable(s), if any.

Table 2: Column Detail by Row Stratification. Raw data for each column selected under Data. It does not generate summary statistics. Data are sorted alphanumerically by group variable values, then by Row ID variable values, in the order listed.

Table 3: Column Detail and Summary by Row Stratification. Adds summary statistics to Table 2. It lists the raw data for each variable at each value of the Row ID variable(s), and summarizes it for each unique combination of group variable values, if any.

Table 4: Column Summary by Row and Column Stratification. Like Table 1, this type generates summary statistics and displays them without the raw data. Separate statistics are computed for each unique combination of Row and Column Stratification values.

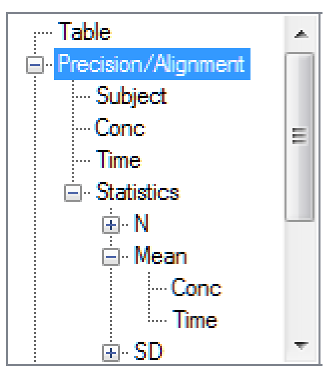
Table 5: Column Detail by Row and Column Stratification. Reports raw data for each column mapped to the Data context, for each variable mapped to Row ID. A separate listing is included for each unique combination of values for the Row and Column Stratification variables, with Column Stratification variable values in adjacent columns.

Table 6–7: Column Detail and Summary by Row and Column Stratification. Adds computation of summary statistics to the listing of raw data as presented in Table 5. Statistics are computed separately for each unique combination of Row and Column Stratification variable values. Columns ordered by cross variable within variable (all Column Stratification variable values are grouped together, with one set for each regular variable).

Table 8: Row Detail by Row and Column Stratification. Same as Table 6, with summary statistics in columns instead of rows. Statistics are calculated for each Row ID variable value, within Row and Column Stratification variable values.

Precision/Alignment options

Any study variables mapped to a context other than **None** and any statistics selected in the Statistics tab are listed under **Precision/Alignment**.



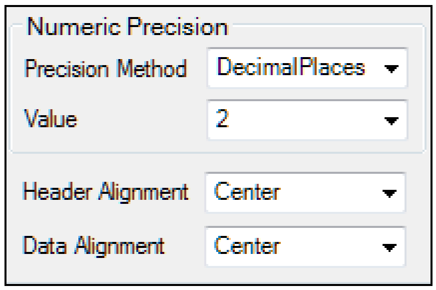
For each table type, the following contexts cause variables to be listed under **Precision/Alignment**.

Default: Row ID, Data, Dependency, Row Stratification, or Column Stratification contexts
Table 1: Data, Stratification Row
Table 2: Row ID, Data, and Stratification Row
Table 3: Row ID, Data, and Stratification Row
Table 4: Data, Stratification Row, and Stratification Column

Table 5: Row ID, Data, Stratification Row, and Stratification Column
Table 6 and 7: Row ID, Data, Stratification Row, and Stratification Column
Table 8: Row ID, Data, Stratification Row, and Stratification Column

Except for Table 2 and Table 5, the contexts listed above will display variables for each summary statistic.

- Select the **Precision/Alignment** node.
  Setting the numeric precision and output value alignment here will affect all variable columns in the table.
- Select a variable underneath **Precision/Alignment**.
  The options are the same as those available when the **Precision/Alignment** node is selected. However, setting the numeric precision and output value alignment here will only affect the selected variable's column.



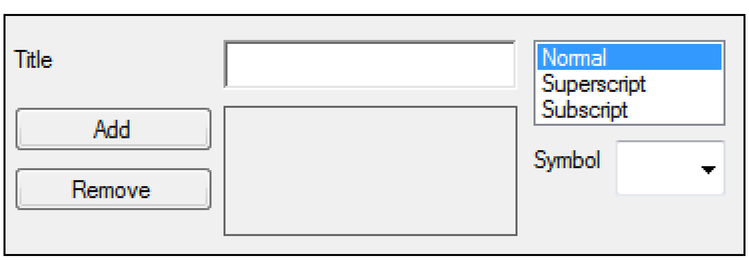
- In the **Precision Method** menu, select **Decimal Places** or **Significant Digits** to set the number of digits used to display the values.
- In the **Value** menu, select the number of significant digits or decimal places used to display the values.
- In the **Header Alignment** menu, select the alignment of the header in the output table.
- In the **Data Alignment** menu, select the alignment of the values in the output table.
- Select a statistic underneath **Precision/Alignment** in the Options tab list.

  Make the same precision and alignment selections for the statistics that were made for the variables.

  As with the variables, when the Statistics node is selected, adjustments to the precision and alignment options will affect all of the statistics rows.
- Select a variable underneath a statistic to set the precision and the data alignment. The header alignment option is not available at this level.

Title options

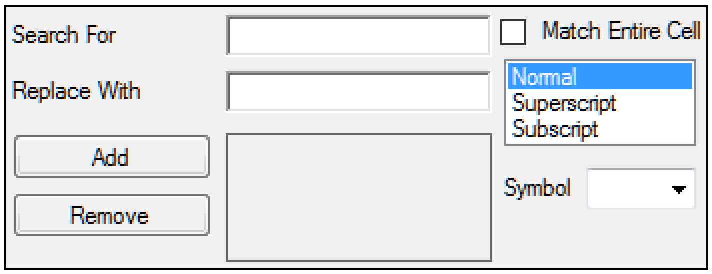
The Title options are used to add titles to the output table.



- In the **Title** field, type a title for the table.
- Select **Superscript** or **Subscript** to change the positioning of the text being entered, then select **Normal** to return to the default positioning.
- In the **Symbol** menu, select one of supported symbols to add to the title.
- Click the **Add** button to add the title.
- To remove a title, select the title with the pointer and click the **Remove** button.

Column Titles options

The Column Titles options are used to replace column headers in the input dataset with new headers.



- In the **Search For** field, type the column header to be replaced.
- In the **Replace With** field, type the column title used to replace the column header in the dataset.
- Check the **Match Entire Cell** checkbox to match on the contents of the entire cell during a search/replace (e.g., `Subject` will match `Subject` but not `Subject 1` or `Subject 2`). If unchecked, search and replace will match any part of the cell value (e.g., `max` will find a match in both `Tmax` and `Cmax`).

The rest of the options are the same as described in “Title options”.

Table Body options

The Table Body options are used to replace text or numerical values in the input dataset with new values. The options are the same as described in “Column Titles options”.

Statistics options

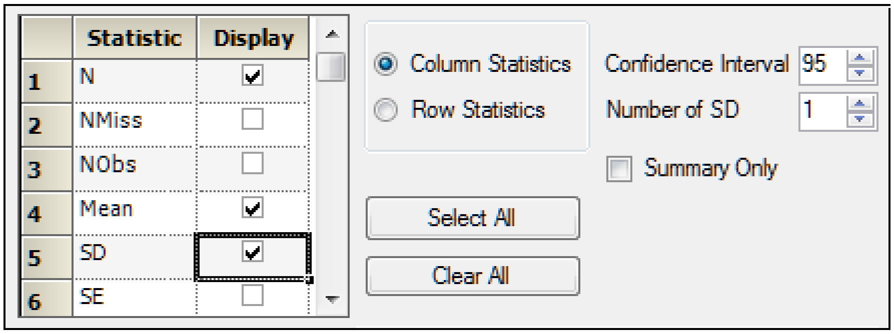
The Statistics options are used to replace statistic names in the output table. The options are the same as described in “Column Titles options”.

Footers options

The Footer options are used to add footers to the output table. Simply type the footer in the **Footer** field. The rest of the options are the same as described in “Title options”.

Statistics tab

The Statistics tab is used to add summary statistics to a table. Table types 2 and 5 do not allow users to add summary statistics.



For a complete list of available summary statistics and descriptions of each one, see "Statistical results and computational formulas".

- Check the **Display** checkbox beside each summary statistic to include it in the output table.
- Click the **Select All** button to select all summary statistics.
- Click the **Clear All** button to clear all selected summary statistics.

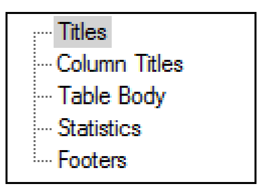
  The **Column Statistics** and **Row Statistics** option buttons are automatically selected for table types 1, 3, 4, and 6-8.

  The **Summary Only** checkbox is unavailable for table types 1, 3, 4, and 6-8.

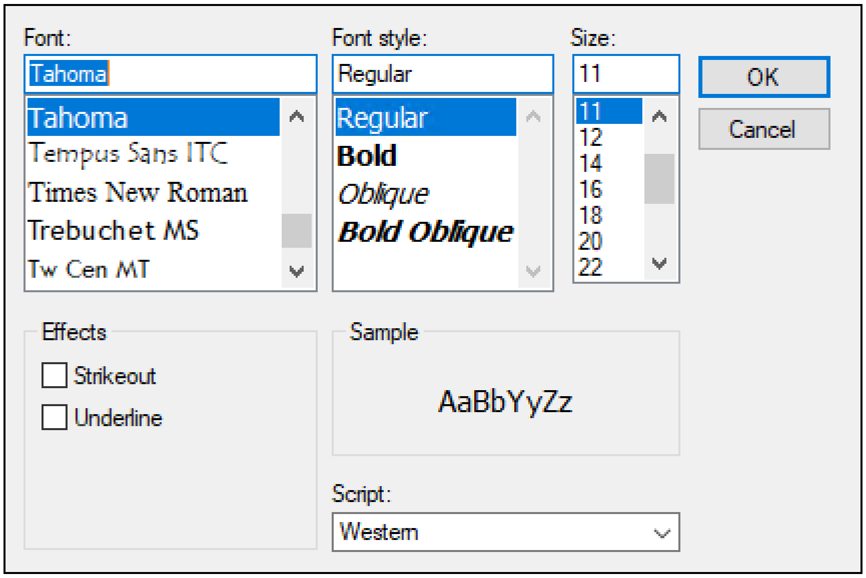
  If the Default table type is selected, then users can select the **Column Statistics** and **Row Statistics** option buttons and the **Summary Only** checkbox.
- In the **Confidence Interval** box, type or select the confidence interval to apply to the summary statistics.
- In the **Number of SD** box, type or select the number of standard deviations to apply to the summary statistics.

Style tab

The Style tab list contains several items that allow users to format parts of a table.



- Select **Titles** in the Style tab list.
- Click the **Select Font** button to open the *Font* dialog and change the titles font.

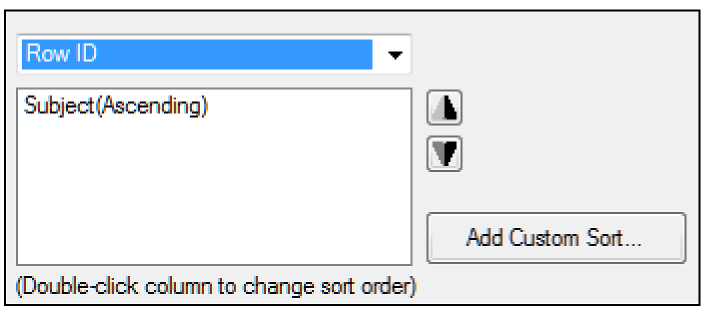


- Select the font type, style, size, effect, and script.
- Click **OK** to accept the changes or **Cancel** to leave the font the same.

- Repeat for **Column Titles**, **Table Body**, **Statistics**, and **Footers** to make changes to their fonts.
- To reset all font changes, click the **Reset All To Default** button.

Column/Sort Order tab

The Column/Sort Order tab allows users to change the arrangement and sort order of data types used to create a table.



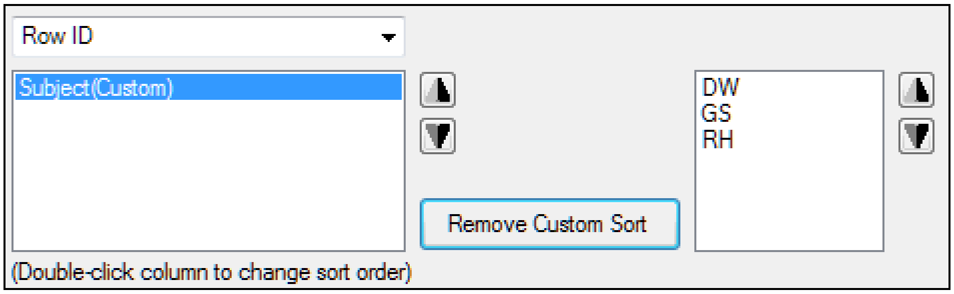
- Select an item from the menu. The items available in the menu change depending on the selected table type and the variables mapped to each context.

  Row ID, **Row Stratification**, or **Column Stratification** requires at least one variable be mapped to the corresponding context.

  Data and **Dependency** requires two or more variables be mapped the corresponding context.

  Statistics requires two or more statistics be selected for display in the Statistics tab.
- To change the sort order of **Row ID**, **Row Stratification**, or **Column Stratification** variables from ascending to descending and back again, double-click the variable.
- To change the display order of variables or statistics listed, select an item in the list and click the up or down arrow buttons to reorder the list.

- To sort rows based on a list of row IDs:
  - Select the column in the **Row ID** list.
  - Click the **Add Custom Sort** button to display a second list of all values in that column. (The word Custom is added to the column's name in the first list.)



  - Select an ID in the second list and use the arrow buttons to change the display order.
  - To remove a custom sort order, select the column in the first list and click **Remove Custom Sort**.

Custom Tables tab

The Custom Tables tab is used to select custom tables. Each custom table has its own set of context mappings and are designed to use with specific datasets.

Custom tables are defined using XSLT files. Each XSLT file must be added to the `CustomTables.xml` file. By default, all files needed to create custom tables are located in `C:\Program Files (x86)\Certara\Phoenix\application\Plugins\Table\Custom`.

See an example in "Using custom tables example".

- In the **Select Custom Table** menu, select a custom table.

  Phoenix comes with two custom tables:

  Bioavailability Statistical Summary: A statistical summary of the comparative bioavailability data.

  Bioequivalence Demographics: A demographic profile of subjects completing a bioequivalence study. One table is created per study.

  When a custom table is selected, only the Custom Tables tab remains available.
- In the **Select Custom Table** menu, select **None** to return to the normal Table object user interface.

Results

Table: Worksheet containing the output HTML table.

Settings: Text file containing the input worksheet used and the options selected.

Note: Extra-wide tables can become truncated when printed directly from Phoenix. This is due to a print limitation in Internet Explorer. If this occurs, copy the table from the Results tab to the Tables folder and use the **Edit in Excel** functionality to format as desired.

Table template for merged worksheet data

In WinNonlin 5.2.1, there was a table template 9 that used data from two merged worksheets. For example, merged PK data from an input worksheet and PK parameter estimates from a modeling output worksheet.

This table type presents raw data at different sample times and PK parameters in columns, with a row for each subject or ID variable. It generates summary statistics for each unique combination of group and ID variable values. The two datasets must be merged using these group and ID variable values.

Although no longer available in the Phoenix interface, template 9 can be recreated by selecting the **Default** table type and using the Merge Worksheets object.

- Import the source data into a project.
- Add a **Merge Worksheets** object to the workflow.
- Drag the dataset from the Data folder to the Merge Worksheets' Mappings panel.
- Merge the worksheets using common sort keys. The variables mapped to the **Sort** context must match in both worksheets.

  The variables do not need to have identical names, but they must be the same type of variable with overlapping sets of values. The variable values are used to merge values from both datasets.

  One set of summary statistics are computed for each unique combination of Sort variable values.
- Map other variables to be included in the table to the **Included Column** context.
- Check the **Carry Along Data For Like Sort Levels** checkbox.
- Execute the Merge Worksheets object.
- Add a Table object to the workflow.
- Map the Merge Worksheets object's **Result** worksheet to the Table object.
- In the Table object's Options tab, select **Default** in the **Table Type** menu.
- Map the variables in the merged dataset to the appropriate contexts.
- Specify any other table options and execute the Table object.

Create report-ready table from NCA results example

PK parameters for six subjects for both Tablet and Capsule formulations were computed.

The input data for this example are located in the Phoenix examples directory. This example will create a table using the parameters Cmax, Tmax, AUCall, and AUClast.

Most Phoenix objects require the same basic steps for their use. However, there may be multiple paths to accomplishing a step (e.g., main menu, right-click menu, drag-and-drop, etc.). For simplicity, only one is listed here.

Note: Any object added to a project can be viewed in its own window by selecting the object in the Object Browser and double-clicking it or pressing **ENTER**. All instructions for setting up and executing an object are the same whether the object is viewed in its own window or in Phoenix's viewing.

The completed project (`Tables.phxproj`) is available for reference in …`\Examples\Data and Plots`.

Import the final parameter estimates data

1. Create a new project with the name `Tables`.
2. Import the file …`\Examples\WinNonlin\Supporting files\Profiles Output.xls`.
   In the *File Import Wizard* dialog, select the **Has units row** option for the **Final Parameters Pivoted**, **Dosing Used**, and **Summary Table** worksheets, using the **Next Arrow** button to move through the worksheets being imported.
   Click **Finish**.

Set up the Table object

1. Right-click **Final Parameters Pivoted** in the Data folder and select **Send To > Reporting > Table**.
2. In the Options tab below the Setup panel, select **Table 3 - Column Detail and Summary by Row Stratification** from the **Table Type** menu.
3. Map **Subject** to the **Row ID** context.
   Map **Form** to the **Stratification Row** context.
   Map **Tmax**, **Cmax**, **AUClast**, and **AUCall** to the **Data** context.
   Leave the rest mapped to **None**.

Table type 3 sorts by the row variable within values of the stratification row variable. It does not compute summary statistics for each level of the row variable. Table type 3 also sorts the data by stratification row variable value and computes summary statistics for each value.

These variables provide data for the body of the table. (Select the Table Preview panel in the Setup list to view an example of the final table output.)

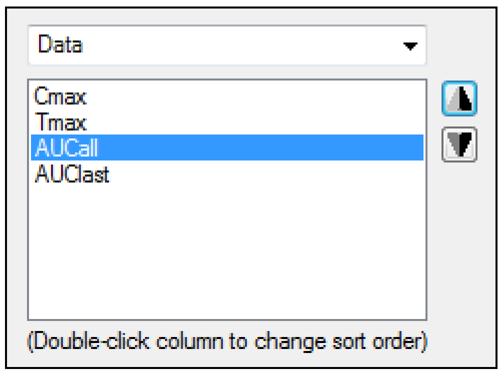
Select and format summary statistics

1. Select the **Statistics** tab below the Setup panel.
2. Check the checkboxes in the **Display** column to select the following summary statistics: **N**, **Mean**, **SE**, **Min**, **Median**, **Max**.
3. Go to the **Options** tab, expand the **Precision/Alignment** node in the menu tree, and select **Subject**.

4. Select **0** in the **Value** menu.
5. Enter a title for the table by selecting **Titles** in the Options menu tree.
   – In the **Title** field type `Table 1` and click **Add**.
   – Continue by typing `Pharmacokinetic Parameters` in the **Title** field and click **Add**.
6. Select the **Column/Sort Order** tab.

   The columns in the final table are displayed in the order set here. Use the up arrow and down arrow buttons to change the order in which the Data columns are displayed.

   The pull-down menu offers the following options:
   Row Stratification to view study parameter(s) mapped to Row Stratification.
   Row ID to view study parameter(s) mapped to Row ID.
   Data to view study parameter(s) mapped to Data.
   Statistics to view the items selected on the Statistics tab.
7. Select **Data** from the menu.
8. Select **Cmax** in the Column Order list and click the **Up Arrow** button.
9. Select **AUCall** in the Column Order list and click **Up Arrow** button.



The Table object's Style tab can be used to change the table display options, such as font, font size, font color, and alignment. Style selections are not necessary for this example.

Execute and view the Table object results

1. Click (**Execute** icon) to execute the object.

Table 1
Pharmacokinetic Parameters

Form	Subject	Cmax (ng/mL)	Tmax (min)	AUCall (min*ng/mL)	AUClast (min*ng/mL)
Capsule	1	2069.17	15.00	72987.92	72987.92
	2	3420.67	15.00	126155.16	126155.16
	3	2741.25	10.00	82521.25	82521.25
	4	2185.66	15.00	76222.58	76222.58
	5	1543.46	10.00	36783.97	36783.97
	6	1502.93	10.00	51971.92	51971.92
	N	**6**	**6**	**6**	**6**
	Mean	**2243.856**	**12.500**	**74440.469**	**74440.469**
	SE	**300.317**	**1.118**	**12473.762**	**12473.762**
	Min	**1502.93**	**10.00**	**36783.97**	**36783.97**
	Median	**2127.41**	**12.50**	**74605.25**	**74605.25**
	Max	**3420.67**	**15.00**	**126155.16**	**126155.16**
Tablet	1	2475.00	10.00	58519.25	58519.25
	2	3770.00	10.00	109772.01	109772.01
	3	4058.75	15.00	141616.94	141616.94
	4	2051.60	10.00	60794.00	60794.00
	5	1546.90	10.00	33960.21	33960.21
	6	1815.80	5.00	51782.00	51782.00
	N	**6**	**6**	**6**	**6**
	Mean	**2619.676**	**10.000**	**76074.068**	**76074.068**
	SE	**429.530**	**1.291**	**16670.086**	**16670.086**
	Min	**1546.90**	**5.00**	**33960.21**	**33960.21**
	Median	**2263.30**	**10.00**	**59656.63**	**59656.63**
	Max	**4058.75**	**15.00**	**141616.94**	**141616.94**

Figure 64-1. Table type 3 results

This concludes the Create Report-Ready Table example.

Using custom tables example

The custom table types are included to provide additional reporting options. In custom table types, all output formatting, statistics, styles, sorting, and other options are predefined through an XML file and style sheets.

Once a custom table is defined, users do not need to make any further option selections. The only possible selections users can make are mapping the input data types to the mapping contexts in the custom table.

Most Phoenix objects require the same basic steps for their use. However, there may be multiple paths to accomplishing a step (e.g., main menu, right-click menu, drag-and-drop, etc.). For simplicity, only one is listed here.

Note: Any object added to a project can be viewed in its own window by selecting the object in the Object Browser and double-clicking it or pressing **ENTER**. All instructions for setting up and executing an object are the same whether the object is viewed in its own window or in Phoenix's viewing.

The completed project (`Tables.phxproj`) is available for reference in …`\Examples\Data and Plots`.

Add a table object using the Send To menu

This example uses a dataset that contains demographic data for a population used in a bioequivalence study.

1. From within an open project, import the file …`\Examples\WinNonlin\Supporting files\Bioequivalence Demographics.dat`.
2. Right-click **Bioequivalence Demographics** in the Data folder and select **Send To > Reporting > Table**.
3. Select the **Custom Tables** tab below the Setup panel.
4. In the **Select Custom Table** menu, select **Bioequivalence Demographics.**

All other tabs are removed from the Table object user interface when a custom table is selected. This is because the custom table type contains preconfigured table options.

The study data types are automatically mapped to the appropriate mapping contexts.

Execute and view the results

1. Execute the object.

Study No. NaN			
		Treatment Groups	
		Test Product N = 12	Reference Product N = 9
Age (Years)	Mean ± SD Range	30±10.331 19.00 - 52.00	30±9.8967 19.00 - 49.00
Age Groups	< 18 18 - 39 40 - 64 65 - 75 > 75	0(0.0%) 9(75.0%) 3(25.0%) 0(0.0%) 0(0.0%)	0(0.0%) 7(77.8%) 2(22.2%) 0(0.0%) 0(0.0%)
Sex	Male Female	8(66.7%) 4(33.3%)	6(66.7%) 3(33.3%)
Race	Asian Black Caucasian Hispanic Other	2(16.7%) 4(33.3%) 2(16.7%) 3(25.0%) 1(8.3%)	2(22.2%) 4(44.4%) 0(0.0%) 2(22.2%) 1(11.1%)
BMI	Mean ± SD Range	20±4.1587 19.50 - 34.20	20±4.7673 19.50 - 34.20

Study No. NaN			
		Treatment Groups	
		Test Product N = 8	Reference Product N = 6
Age (Years)	Mean ± SD Range	30±10.331 19.00 - 52.00	30±10.342 25.00 - 51.00
Age Groups	< 18 18 - 39 40 - 64 65 - 75 > 75	1(12.5%) 5(62.5%) 2(25.0%) 0(0.0%) 0(0.0%)	0(0.0%) 4(66.7%) 2(33.3%) 0(0.0%) 0(0.0%)
Sex	Male Female	4(50.0%) 4(50.0%)	4(66.7%) 2(33.3%)
Race	Asian Black Caucasian Hispanic Other	3(37.5%) 0(0.0%) 2(25.0%) 2(25.0%) 1(12.5%)	3(50.0%) 0(0.0%) 2(33.3%) 1(16.7%) 0(0.0%)
BMI	Mean ± SD Range	20±4.1587 19.50 - 34.20	20±4.9203 20.50 - 33.30

Figure 64-2. Bioequivalence Demographics table results

2. Close this project by right-clicking the project and selecting **Close Project**.

This concludes the Using Custom Tables example.

Watson Import Object

The Watson Import object uses the Watson LIMS plug-in to access active studies in Watson LIMS. Data from Watson LIMS are imported into a Phoenix project as either a study Workbook or as a study in Integral.

The Watson LIMS plug-in assumes that the Watson LIMS software is installed and running properly.

This section includes the following topics:

Setting up preferences

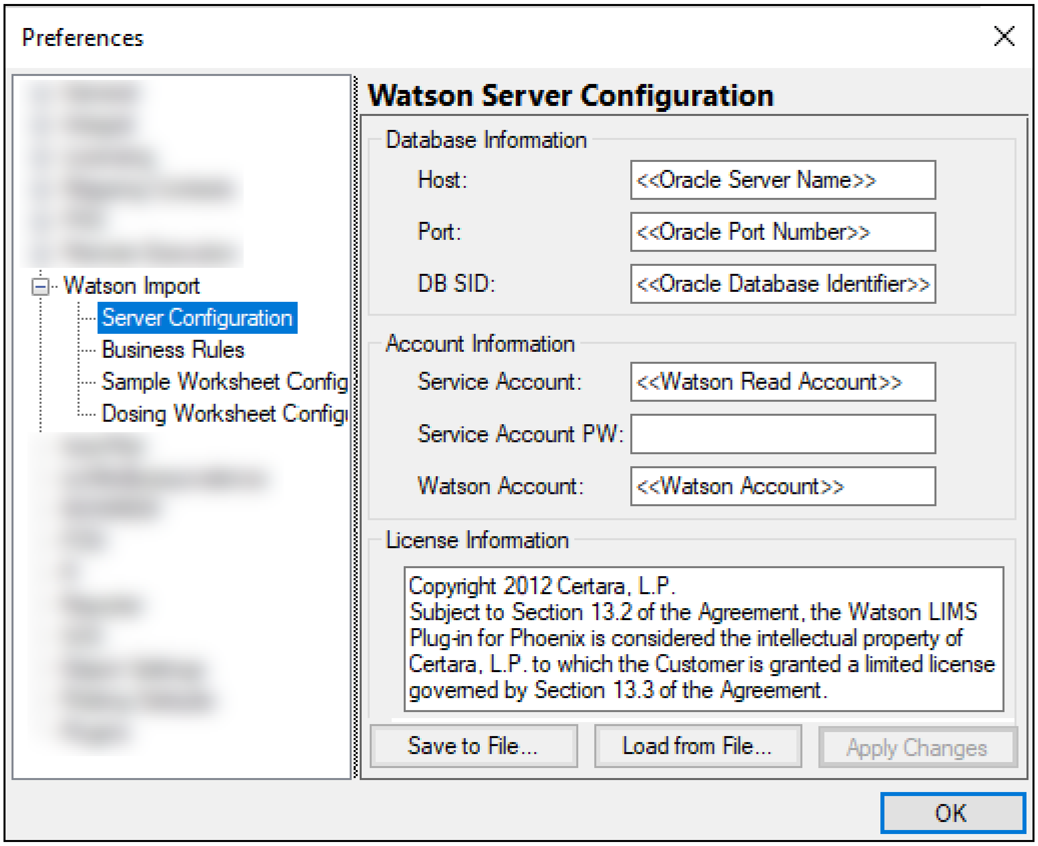
A number of preferences for the Watson Import object are available to the user via the *Preferences* dialog (**Edit > Preferences**).

Each tab of preferences has the following buttons available:

Save to File stores the configuration selections to a specified file.
Load from File loads configuration selections from a specified file.
Apply Changes saves the configuration settings as the active configuration.

Server configuration

In the *Preferences* dialog, select **Watson Import > Server Configuration**.



Host: Enter the name or IP address of the Oracle Server where the Watson schema is located.

Port: Enter the port of the Oracle Server where the Watson database is located (Oracle's default port number is 1521).

DB SID: Enter the name of the Oracle database where the Watson schema is located.

Service Account: Enter the name of the Oracle database account used to select data from the Watson schema. This account needs to be located in the same Oracle database as the Watson schema and must have select privileges on all tables in the Watson Account schema.

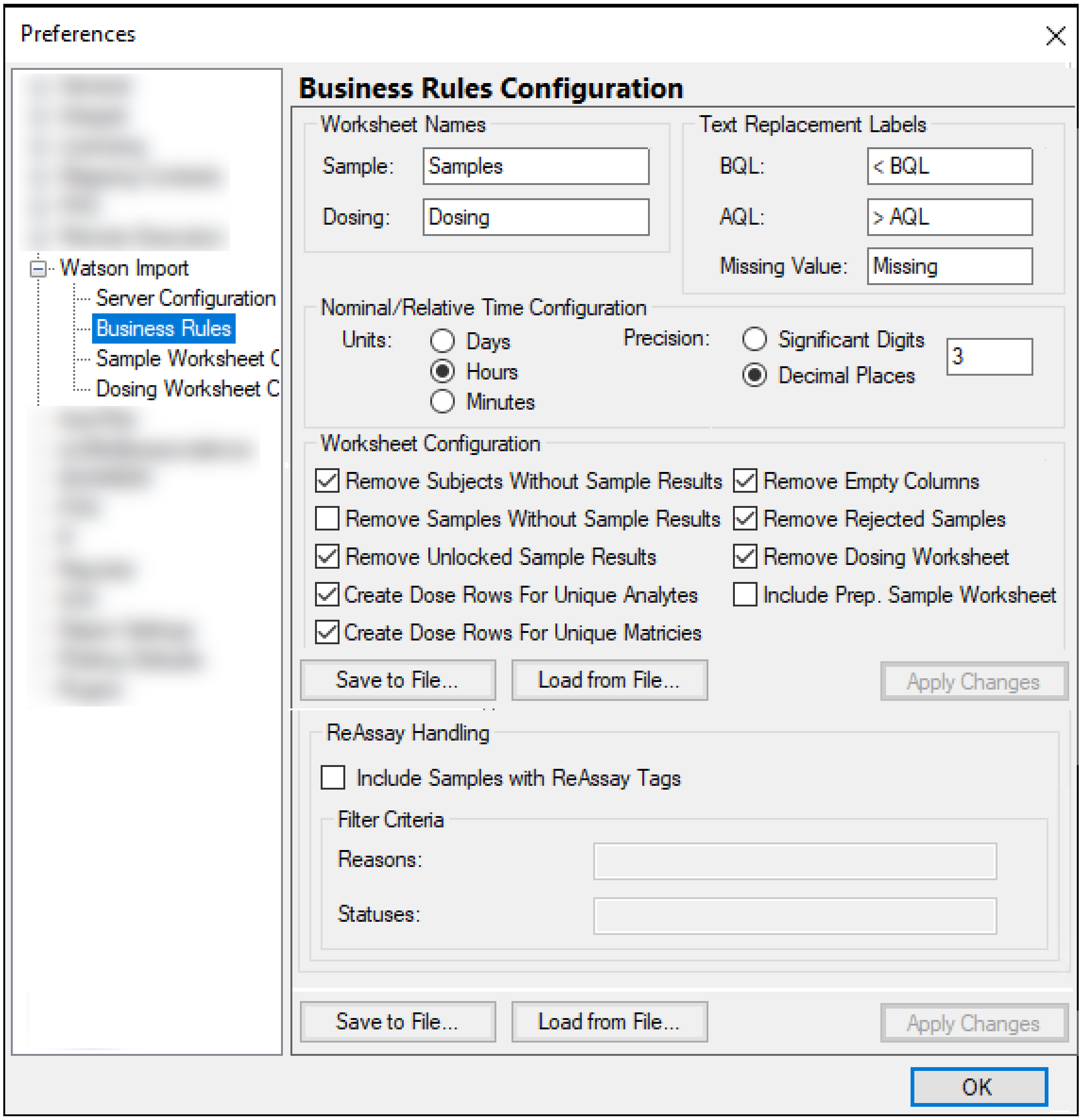
Service Account PW: Enter the password for the Service Account.

Watson Account: Enter the name of the Watson schema. The Watson LIMS plug-in uses this to select data from the Watson schema (e.g., `select * from watson.study`). This is usually set to `watson`.

Info field: Lists copyright and specific licensing information.

Business rules configuration

In the *Preferences* dialog, select **Watson Import > Business Rules**.



Sample: Enter the name of the Sample Worksheet that is created in the Phoenix project.

Dosing: Enter the name of the Phoenix Dosing Worksheet that is created in the Phoenix project.

BQL: Enter the text used to represent values from Watson that are below the limit of quantification.

AQL: Enter the text used to represent values from Watson that are above the limit of quantification.

Missing Value: Enter the text to display in cells that are missing data.

Units: Specify the unit of the transferred columns (**Days**, **Hours**, **Minutes**).

Precision: Specify the precision of the time columns transferred from Watson by selecting either **Significant Digits** or **Decimal Places** and entering the numeric value for the precision in the adjacent field.

Remove Subjects Without Sample Results: Only import subjects with at least one concentration value in Watson. Default is checked.

Remove Samples Without Sample Results: Only import designed samples that have a corresponding sample result in Watson. Default is unchecked.

Remove Unlocked Sample Results: Only import samples from Watson where the sample result is locked. This option is grayed out by default.

Create Dose Rows For Unique Analytes: Create additional dosing rows for each unique analyte in the study. Default is checked.

Create Dose Rows For Unique Matrices: Create additional dosing rows for each unique matrix in the study. Default is checked.

Remove Empty Columns: Only import a column of data from Watson when at least one value exists in the column. This rule is applied before the **Missing Text Value** is applied. Default is checked.

Remove Rejected Samples: Remove samples that have been rejected from the sample dataset.

Remove Dosing Worksheet: Do not create a dosing worksheet on a transfer from Watson. Default is checked.

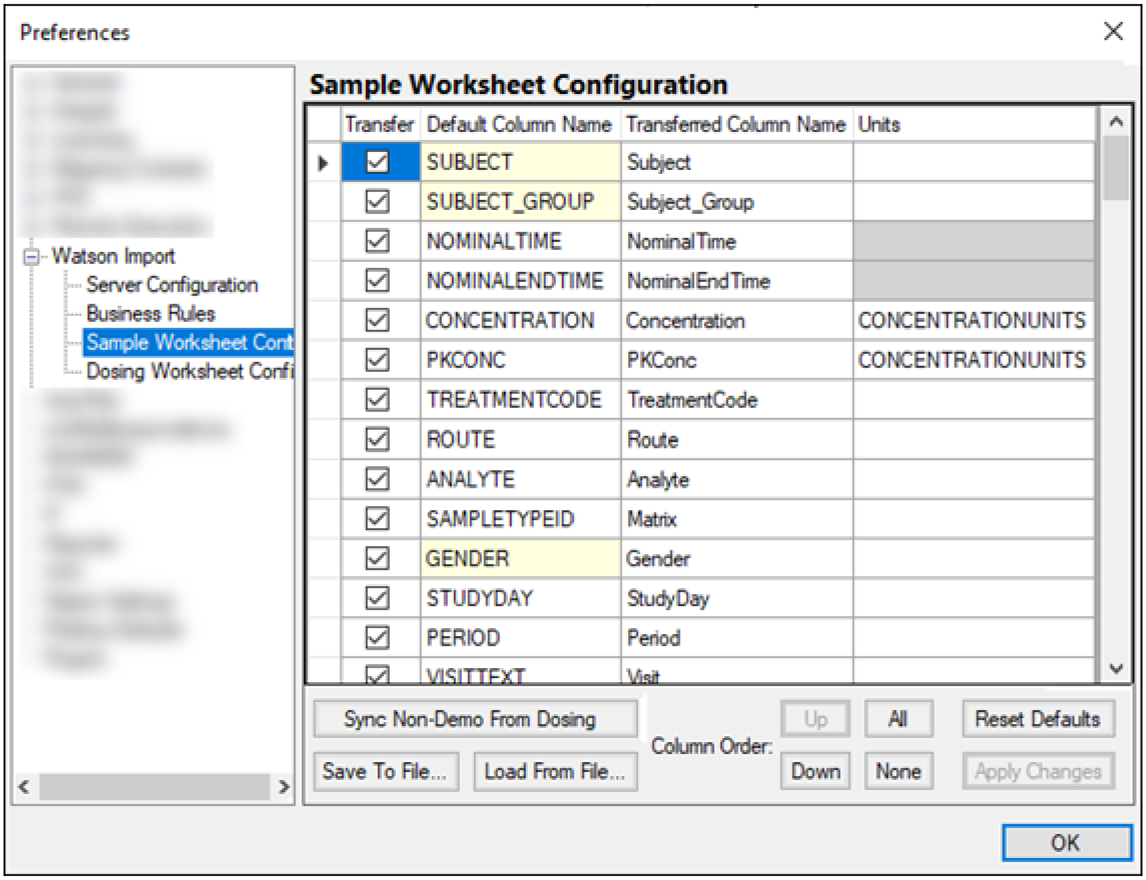
Include Prep. Sample Worksheet: Create a prepared sample worksheet

Include Samples with ReAssay Tags: Include reassayed data in the worksheets returned to Phoenix. When checked, the **Filter Criteria** options become available: **Reasons**: Enter the reason for the reassay (e.g., `Mandatory Repeats` or `Incurred Sample Repeats`). Reassayed samples that match the reason will be included during import. If not, the sample is removed. **Statuses**: Enter the status of the reassay (e.g., `acc`). Reassayed samples that match the status will be included. If not, the sample is removed.
If there is no entry for **Reasons** and **Statuses**, but the **Include Samples with ReAssay Tags** option is checked, then all of the reassayed data is imported.

Sample and Dosing worksheet configuration

The layout and options available in the Sample Worksheet Configuration are identical to those available in the Dosing Worksheet Configuration are discussed in this single section.

In the *Preferences* dialog, select **Watson Import > Sample Worksheet Configuration** or **Dosing Worksheet Configuration**.



Columns

Transfer: Check the checkbox to transfer the column during the Watson import.
Uncheck the checkbox for columns that are not to be transferred.

Default Column Name: Displays the Watson column name and is not editable.
Cells in this table column that are in yellow are time independent (demographics) and are shared across the Dosing and Sample Worksheet configurations.
Configurations applied to these columns will be replicated to both the Dosing and Sample Worksheets.

Transferred Column Name: Enter the name of the column as it will appear in the Phoenix Worksheet after the Watson import is completed.

Units: Define the unit for the transferred column.
Set the units of a column to a fixed value by entering a text entry surrounded by single quotes (e.g., 'year', 'min'). Or set the units of a column to a transferred column from Watson (e.g., CONCENTRATIONUNITS or DOSEUNITS). Cells in this column that are highlighted in gray cannot be set because these fields are not applicable or are populated based on a business rule.

Other Settings

Sync Non-Demo From Samples: Synchronize configuration settings from the columns that are shared across the Dosing and Sample Worksheet configurations (e.g., Treatment, Period).

Column Order: Click the **Up** or **Down** to move the selected row up or down the list, respectively. This will impact the order that the columns appear from left to right in the Phoenix Worksheet.

All/None: Click **All** to check all of the **Transfer** checkboxes. Click **None** to uncheck all of the **Transfer** checkboxes.

Reset Defaults: Restore the Worksheet configuration options to the original default selections.

Importing the Watson Study as a study worksheet

Select **Watson > Create Study Workbook**.

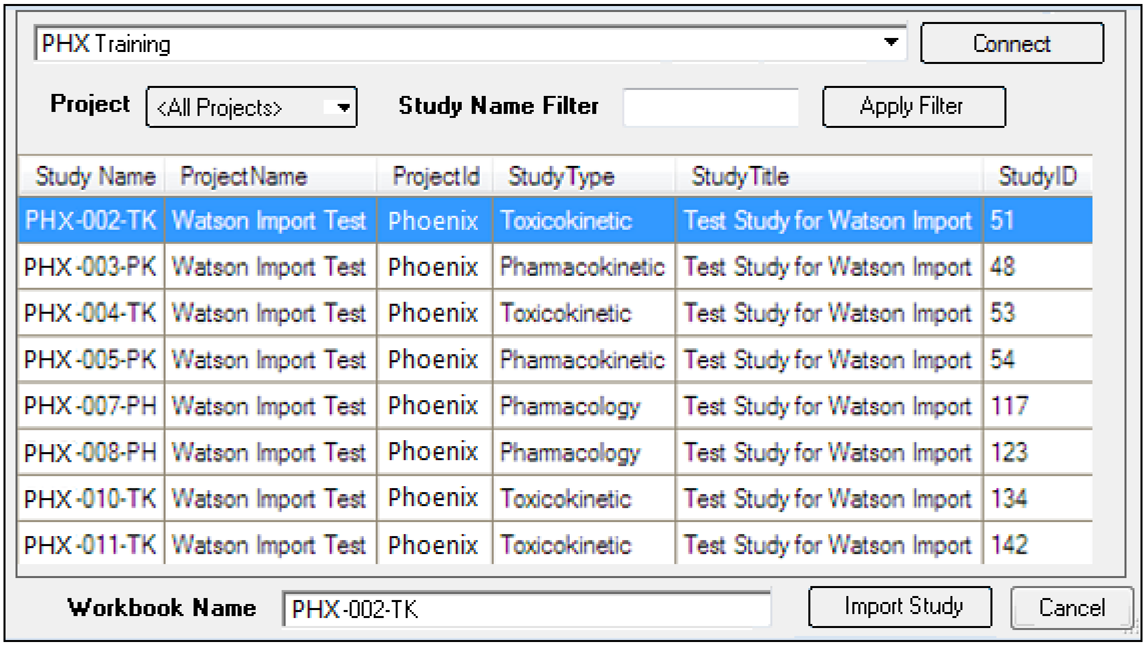


Figure 65-1. Select Watson Study to Import dialog

In the dialog, click a row to select the study to import and then click **Import Study**.

Once the import is complete, the name of the study is add under the Data section of the Phoenix Object Browser.

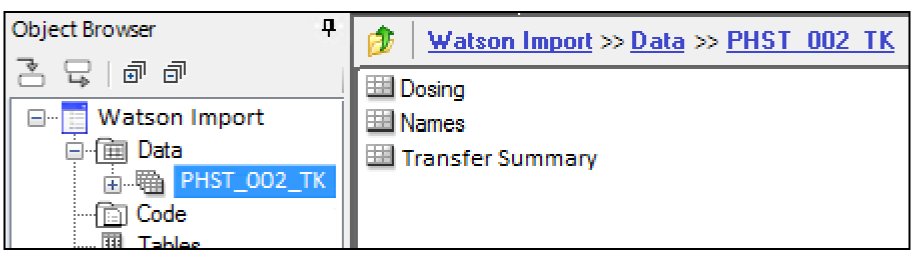


Figure 65-2. Imported Watson study is added to the Data folder

Note that the Dosing and Samples Worksheets may or may not be created depending on the Business Rules that were set up in the *Preferences* dialog. The Transfer Summary Worksheet provides information about the importing process.

Use the **Watson > Refresh Study Workbook** menu option to update the data with any changes that have been made to the study data.

Importing the Watson Study in Integral

Select **Watson > Create Study Workbook**.

Click **Connect** and log in to Integral.

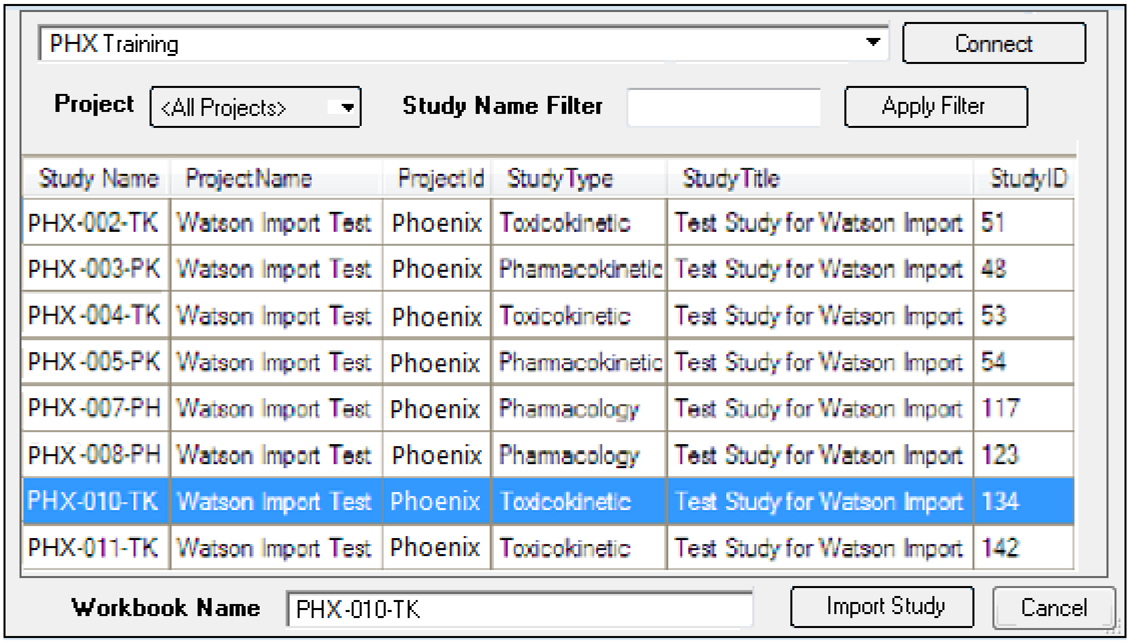


Figure 65-3. Select Watson Study to Import dialog

In the dialog, click a row to select the study to import and then click **Create Study**.

Once the import is complete, select **Integral > Browser**.

The study will be displayed in the Integral browser tree.

A right-click menu is available for the Watson study item containing the same options as other Integral studies. There is an additional item on the menu called **Update Watson Study**, which updates the data with any changes that have been made to the study data.

See “Integral” for details on the functionality available.

The Watson Import object creates the study in two steps: 1) create the study with subjects and samples; 2) append dosing.

Worksheet-Related Objects

The following operational objects can be used to modify worksheet content:

Append Worksheets
Crossproduct Worksheets
Enumerate Worksheets
Join Worksheets
Merge Worksheets
Pivot Worksheet
Rank Worksheet
Split Worksheet
Stacker

Append Worksheets

Append columns of two or more worksheets into one worksheet. The selected columns are appended side by side, unless they use the same column header name, in which case they are presented in a stacked format.

Worksheet columns are appended based on whether or not column headers match, and the order in which input worksheets are mapped to the object. For example, if the Time column in the first work-sheet is selected as the source column, and then Concentration in the second worksheet is selected as the source column, then the output worksheet places the Time column first and the Concentration col-umn second.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Data Management > Append Worksheets**.
Main menu: **Insert > Data Management > Append Worksheets**.
Right-click menu for a worksheet: **Send To > Data Management > Append Worksheets**.

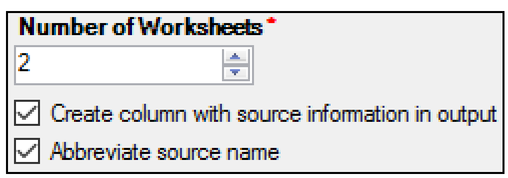
Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Mappings panel

The Mappings panel allows users to specify which columns in a worksheet are included in the new worksheet. Required input is highlighted orange in the interface.

None: Data types mapped to this context are not included in the result.
Source Column: The column or columns that are appended together in a new worksheet.

Options tab



- In the **Number of Worksheets** box, select or type the number of worksheets to use in the append operation.
  Each worksheet that is added creates another Worksheet Mappings panel in the Setup tab.
- Select the **Create column with source information in output** checkbox to include the names of the input worksheets used to create the output worksheet in a separate column.
- Select the **Abbreviate source name** checkbox to abbreviate the names of the input worksheets listed in the source column in the output worksheet.
  If this option is selected then only the name of the worksheet, and not the full name of the input source, is displayed in the Source column.

Results

The **Append Worksheets** object generates one worksheet and one text file.

Results: The appended worksheet.

Settings: Text file containing input worksheets used and the options selected.

Crossproduct Worksheets

Use common sort keys in two worksheets to create two new worksheets that are the result of a Cartesian cross product transformation. Users specify the common sort keys and the carry along parameters or variables used to create the output worksheets.

For example, assume the following two datasets are mapped to a **Crossproduct** object:

Dataset 1:

```
Period  Data
A       1
A       2
B       3
B       4
```

Dataset 2:

```
Phase  Color
X      R
X      B
Y      Y
Y      V
```

If **Period** and **Phase** are mapped to **Sort**, and **Data** and **Color** are mapped to **Carry Along**, then the output worksheets look like this:

Worksheet AB:

```
Period  Phase  Data
A       X      1
A       X      2
A       Y      1
A       Y      2
B       X      3
B       X      4
B       Y      2
B       Y      4
```

Worksheet BA:

```
Period  Phase  Color
A       X      R
A       X      B
A       Y      Y
A       Y      V
B       X      R
B       X      B
B       Y      Y
B       Y      V
```

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Data Management > Crossproduct Worksheets**.
Main menu: **Insert > Data Management > Crossproduct Worksheets.**
Right-click menu for a worksheet: **Send To > Data Management > Crossproduct Worksheets**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Mappings panel

The Mappings panel allows users to specify which columns in a worksheet are involved in the worksheet transformation. Required input is highlighted orange in the interface.

Sort: Categorical variable(s) identifying individual data profiles, such as subject ID.
Carry Along: Variables or parameters from each worksheet that are used to create the cross product output worksheets.

Users can specify multiple sort keys and carry along values. It is also possible to select a sort key from only one input worksheet. That sort key is then applied to both output worksheets. Users can also choose no sort keys, in which case Phoenix assumes that a single profile is the sort key for both input worksheets.

Results

The **Crossproduct Worksheets** object generates two worksheets and one text file.

Worksheet AB: Combination of worksheet 1 and 2 sort keys, and worksheet 2 carry along values.

Worksheet BA: Combination of worksheet 2 and 1 sort keys, and worksheet 1 carry along values.

Settings: Text file containing input worksheets used and the options selected.

Enumerate Worksheets

Assign ordinal values to the unique values in specified columns of a Phoenix worksheet. If more than one column is selected, there is an option to enumerate all unique combinations of all selected columns. The user can select to start the numeration at zero or one. One typical usage of this tool is to convert covariates to numerical values for modeling in Phoenix NLME.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Data Management > Enumerate Worksheets**.
Main menu: **Insert > Data Management > Enumerate Worksheets**.
Right-click menu for a worksheet: **Send To > Data Management > Enumerate Worksheets**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Additional information is available for the following topics:

Mappings panel
Output Column Names panel
User Supplied Values panel
Options tab
Results

Mappings panel

The Mappings panel allows users to specify which columns in a worksheet are involved in the worksheet transformation. Required input is highlighted orange in the interface.

Enumerate: Column(s) to enumerate.

Output Column Names panel

Column names can be assigned manually using the Output Column Names panel in the Setup tab.

Type the new name in the Output Column Name column of the table.

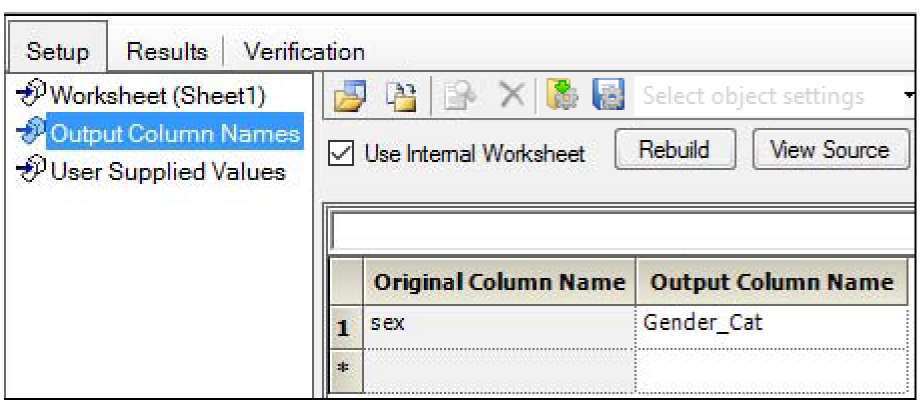
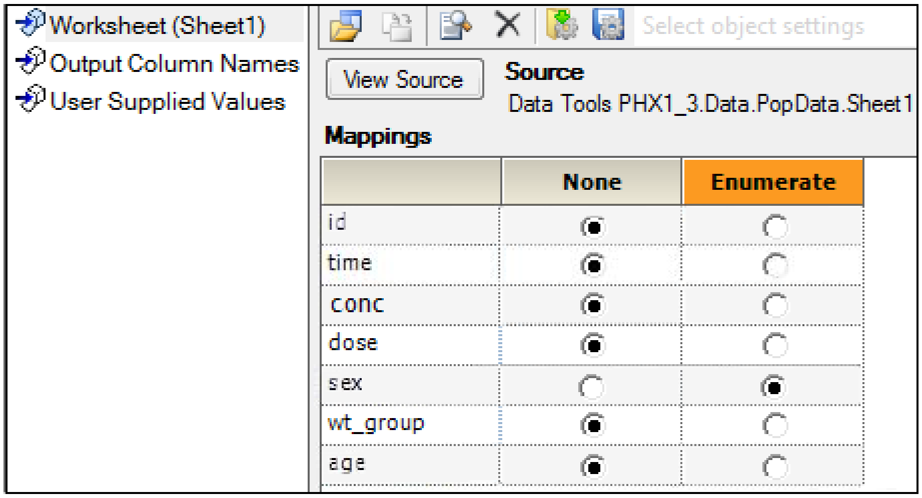


Figure 69-1. Enumerated worksheet with new column name

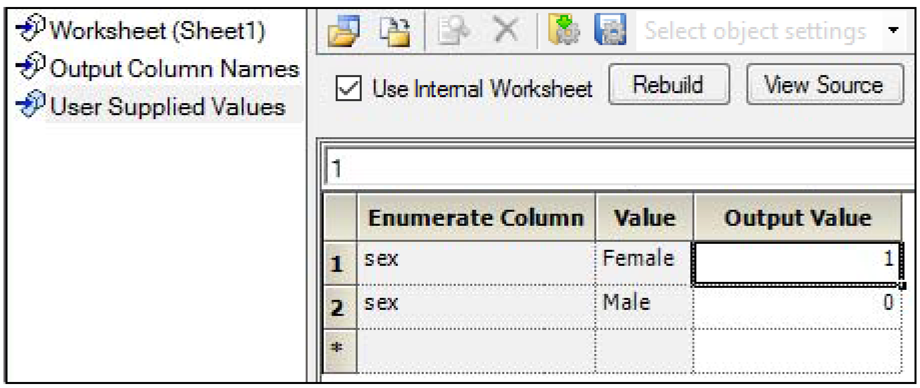
User Supplied Values panel

Output values can be assigned manually using the User Supplied Values panel in the Setup tab.



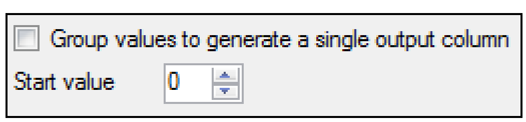
Because Female is alphabetically before Male, the values assigned by default will be **0** to Females and **1** to Males. To indicate other values to assign, use the Setup option **User Supplied Values**.

In this example, Female has been assigned **1** and **0** to Males.



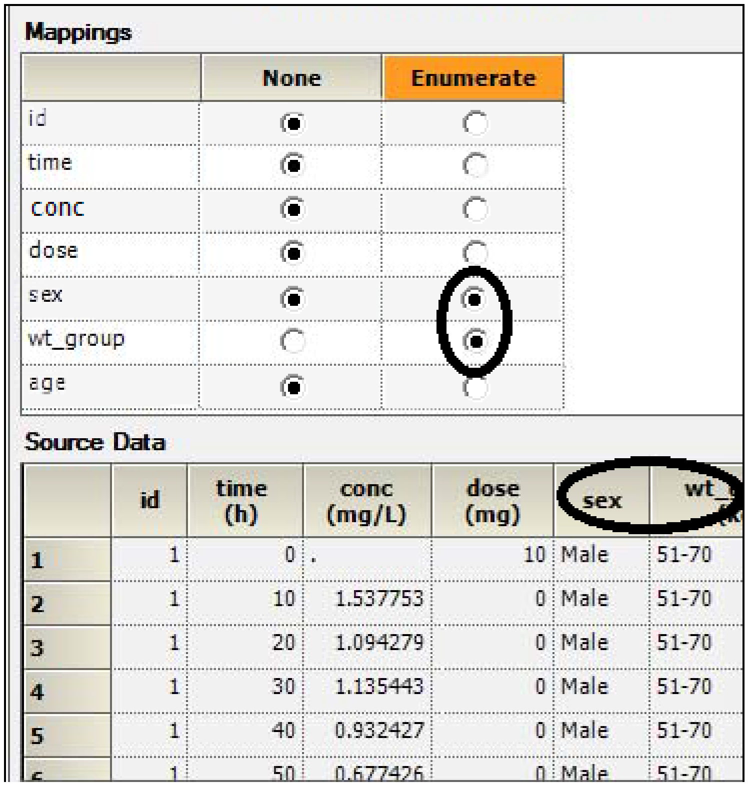
The default is for the output to concatenate the word **code** to the selected Enumerate column's original name to create the output column. In this case, the output column will be named **Sex_code**.

Options tab



- Check the **Group Values to Generate a Single Output Column** box group values in the output. This option can only be applied when more than one column is mapped to **Enumerate**.
- Set the **Start Value** to begin the enumeration at **0** or **1**. This option only works if there are no **User Supplied Values** worksheet defined.

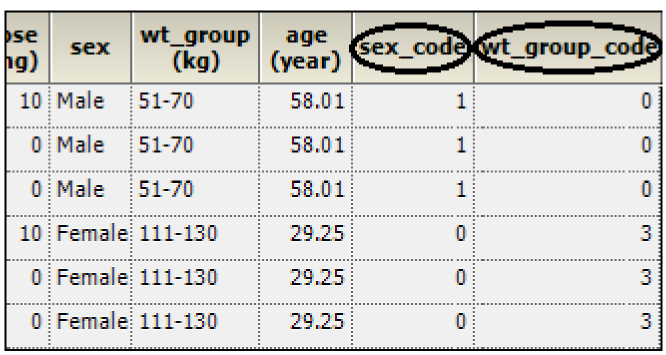
In the example below, the source data includes a column of sex and weights and both **sex** and **wt** are selected to enumerate.



	id	time (h)	conc (mg/L)	dose (mg)	sex	wt_
1	1	0	.	10	Male	51-70
2	1	10	1.537753	0	Male	51-70
3	1	20	1.094279	0	Male	51-70
4	1	30	1.135443	0	Male	51-70
5	1	40	0.932427	0	Male	51-70
6	1	50	0.677426	0	Male	51-70

Figure 69-2. Mappings set for enumerating two columns available in the source

If the **Group Values to Generate a Single Output Column** box is not checked, the output will show a column for each variable.



ose (mg)	sex	wt_group (kg)	age (year)	sex_code	wt_group_code
10	Male	51-70	58.01	1	0
0	Male	51-70	58.01	1	0
0	Male	51-70	58.01	1	0
10	Female	111-130	29.25	0	3
0	Female	111-130	29.25	0	3
0	Female	111-130	29.25	0	3

Figure 69-3. Output with Group Values option turned off

If the **Group Values to Generate a Single Output Column** box is checked, then the output generates a single column, by default called **Code**, that has levels for the mapped data. For this example, that will result in levels zero to six, all the combinations for the two variables are enumerated together.

ose	sex	wt	age	Code
10	0	53.81	43.74	0
0	0	53.81	43.74	0
0	0	53.81	43.74	0
0	0	53.81	43.74	0
10	0	61.98	47.29	1
0	0	61.98	47.29	1
0	0	61.98	47.29	1
0	0	61.98	47.29	1

Figure 69-4. Output with Group Values option turned on

Results

The **Enumerate Worksheet** object generates one worksheet and one text file.

Results: The enumerated worksheet.
Settings: Text file containing input worksheets used and the options selected.

Join Worksheets

Join two worksheets based on one or more sort keys. The object can perform two types of joins: inner and outer. Each one corresponds to inner and outer joins used in SQL (structured query language). The result of an SQL join will be sorted by the sort keys.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Data Management > Join Worksheets**.
Main menu: **Insert > Data Management > Join Worksheets**.
Right-click menu for a worksheet: **Send To > Data Management > Join Worksheets**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Additional information is available for the following topics:

Mappings panel
Sort Map panel
Options tab
Results

Mappings panel

The Mappings panel allows users to specify which columns in a worksheet are involved in the worksheet transformation. Required input is highlighted orange in the interface.

Sort: The variable(s) to match by when joining the worksheets.
Source Column: The additional column(s) to include in a new worksheet.

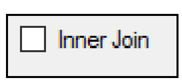
Sort Map panel

By default, the **Join Worksheets** object requires that columns mapped to the **Sort** context have the same name. The Sort Map panel allows users to mix and match or override column names. For example, if the two columns being merged have different names, such as Subject and ID, the Sort Map panel can be used to specify matching columns in the two worksheets.

	Worksheet 1 Sorts	Worksheet 2 Sorts
1	Subject	ID
2	Conc	YObs
*		

In this example, the Subject column in worksheet 1 is joined/merged to the ID column in worksheet 2, and the Conc column in worksheet 1 is joined/merged to the YObs column in worksheet 2.

Options tab



The default join for the **Join Worksheets** object is an outer join. Check the **Inner Join** box to use an inner join to combine the two worksheets. Both types of joins combine rows from the worksheets that have matching values for the sort keys, but an inner join does not retain any of the unmatched rows, whereas an outer join also retains the rows from both worksheets that do not have a matching value in the other worksheet.

Note that the Join Worksheet object uses a Cartesian join (also called cross join) in the many-to-many case for matched values, i.e., the case where, for a specific set of values to match on, both worksheets have multiple rows with those values.

Results

The **Join Worksheets** object generates one worksheet and one text file. The output worksheet is sorted alphabetically or numerically based on the sort keys and the order they were mapped.

Result: The joined worksheets.
Settings: Text file containing input worksheets used and the options selected.

Joining raw data and modeling output in tables example

This example shows how to reproduce table template 9 that was used in WinNonlin 5.3 and earlier. Phoenix does not have a specific table type for this template. The main difference between table template 9 and the other table templates in WinNonlin is that two datasets are joined to create the final output. The Phoenix Table object only works with one dataset at a time. To produce a table similar to table template 9 it is necessary to use Phoenix's Join Worksheets object prior to creating the table.

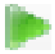
In this example, two datasets are joined by the Sort variables in both datasets. The Default table type in Phoenix is used to recreate table template 9 in WinNonlin. These steps include:

Recreating WinNonlin's table template 9 in Phoenix

This example uses two datasets, `clayton.CSV` and `clayton_pk.dat`. `clayton.CSV` contains time and concentration data for two formulations. `clayton_pk.dat` contains the Final Parameters output from a noncompartmental analysis.

1. Create a new project named `Join`.
2. Import the files …`\Examples\WinNonlin\Supporting files\clayton.CSV` and `clayton_pk.dat`.
   In the *File Import Wizard* dialog, select the **Has units row** option for `clayton.CSV` only.
3. Right-click **clayton** in the Data folder and select **Send To > Data Management > Join Worksheets**.
4. Map **Subject** to the **Sort** context.
   Map **Form** to the **Sort** context.
   Leave **Period** mapped to **None**.
   Leave **Seq** mapped to **None**.
   Map **Hour** to the **Source Column** context.
   Map **Conc** to the **Source Column** context.
5. Select Worksheet 2 from the Setup list.
6. Drag the **clayton_pk** worksheet from the Data folder to the Join Worksheets object's Worksheet 2 Mappings panel and map the input columns to the contexts as follows:
   Map **Subject** to the **Sort** context.
   Map **Form** to the **Sort** context.
   Map **Tmax** to the **Source Column** context.
   Map **Cmax** to the **Source Column** context.

Map **AUClast** to the **Source Column** context.
Leave the rest mapped to **None**.

7. Click  (**Execute** icon) to execute the object.
8. Right-click **Workflow** in the Object Browser and select **New > Reporting > Table**.
9. In the Table 1 object's Mappings panel click  (**Select Source** icon).
10. In the dialog, expand Join Worksheets, select **Result**, and click **OK**.
11. Map the input columns to the contexts as follows:
    Map **Subject** to the **Row ID** context.
    Map **Form** to the **Stratification Row** context.
    Map **Hour** to the **Stratification Column** context.
    Map **Conc** to the **Data** context.
    Map **Tmax**, **Cmax**, and **AUClast** to the Dependency context.

Setting up the summary statistics

1. Select the **Statistics** tab below the Setup panel.
2. Check the checkboxes in the **Display** column to select the following summary statistics: **N**, **Mean**, **SE**.
3. Select the **Options** tab.
4. With **Table** selected in the Options menu tree, check the **Page Break on Row Stratification** checkbox.
5. Expand **Precision/Alignment** in the Options menu tree, click **Hour** and select **1** in the **Value** menu.
6. Under **Precision/Alignment**, click **Subject** in the Options menu tree and select **0** in the **Value** menu.
7. Enter a title for the table by selecting **Titles** in the Options menu tree.
   – In the **Title** field type `Table 2` and click **Add**.
   – In the **Title** field type `Raw Data and Pharmacokinetic Parameters` and click **Add**.

Executing and viewing the results of the joining

1. Execute the object.

Table 2
Raw Data and Pharmacokinetic Parameters

		Hour											
		0.0	0.5	1.0	1.5	2.0	3.0	4.0	6.0	8.0			
Form	Subject	Conc (ng/mL)									Tmax	Cmax	AUClast
c	1	0.00	0.05	0.06	0.06	0.05	0.06	1.58	1.06	0.81	4.00	1.58	5.48
	2	0.00	0.06	0.06	0.06	0.06	0.22	0.89	1.35	0.46	6.00	1.35	4.85
	3	0.00	0.05	0.05	0.05	0.05	0.06	0.24	0.77	0.18	6.00	0.77	2.25
	4	0.00	0.08	0.06	0.10	0.06	0.08	0.10	0.10	1.23	8.00	1.23	1.83
	5	0.00	0.07	0.10	0.67	2.25	1.63	1.41	0.79	0.44	2.00	2.25	7.87
	6	0.00	0.05	0.05	0.08	0.07	0.08	0.63	0.85	0.39	6.00	0.85	3.26
	7	0.00	0.07	0.07	0.07	0.07	0.34	3.00	2.96	1.47	4.00	3.00	12.39
	8	0.00	0.07	0.07	0.08	0.07	0.31	2.05	0.52	0.19	4.00	2.05	4.78
	9	0.00	0.09	0.07	0.10	0.09	0.10	0.10	0.60	0.22	6.00	0.60	1.87
	10	0.00	0.10	0.08	0.11	1.61	1.36	0.97	0.31	0.18	2.00	1.61	4.97
	11	0.00	0.09	0.10	0.09	0.11	1.18	1.98	1.12	0.52	4.00	1.98	7.13
	12	0.00	0.08	0.08	0.09	0.08	0.09	0.09	0.56	0.27	6.00	0.56	1.80
	13	0.00	0.08	0.08	0.10	0.08	0.30	2.40	1.43	0.39	4.00	2.40	7.34
	14	0.00	0.10	0.11	0.07	0.10	0.65	0.27	1.04	0.92	6.00	1.04	4.27
	15	0.00	0.09	0.09	0.10	0.09	0.08	0.11	2.67	0.86	6.00	2.67	6.65
	16	0.00	0.06	0.05	0.06	0.05	0.34	0.36	1.47	0.82	6.00	1.47	4.76
	17	0.00	0.05	0.06	0.06	0.06	0.07	1.90	1.76	0.59	4.00	1.90	7.16
	18	0.00	0.07	0.07	0.07	0.07	0.07	2.47	0.61	0.36	4.00	2.47	5.51
	N	**18**	**18**	**18**	**18**	**18**	**18**	**18**	**18**	**18**	**18**	**18**	**18**
	Mean	**0.000**	**0.073**	**0.073**	**0.112**	**0.279**	**0.390**	**1.142**	**1.109**	**0.572**	**4.889**	**1.654**	**5.232**
	SE	**0.000**	**0.004**	**0.004**	**0.033**	**0.144**	**0.116**	**0.229**	**0.178**	**0.088**	**0.369**	**0.173**	**0.629**

Figure 70-1. Default table type Formulation c results

Table 2
Raw Data and Pharmacokinetic Parameters

		Hour											
		0.0	0.5	1.0	1.5	2.0	3.0	4.0	6.0	8.0			
Form	Subject	Conc (ng/mL)									Tmax	Cmax	AUClast
t	1	0.00	0.10	0.10	0.86	1.04	0.51	0.24	0.12	0.10	2.00	1.04	2.52
	2	0.00	0.15	3.30	3.80	2.43	1.29	0.84	0.38	0.12	1.50	3.80	8.88
	3	0.00	0.09	0.09	0.10	0.11	0.10	0.11	0.09	0.12	8.00	0.12	0.79
	4	0.00	0.12	0.47	0.62	0.37	0.20	0.15	0.13	0.11	1.50	0.62	1.68
	5	0.00	0.12	1.85	2.92	1.85	0.99	0.73	0.42	0.19	1.50	2.92	6.95
	6	0.00	0.08	0.14	0.12	0.14	0.16	0.15	0.11	0.16	3.00	0.16	1.04
	7	0.00	0.09	0.10	0.13	0.18	0.28	0.11	0.09	0.07	3.00	0.28	0.99
	8	0.00	0.72	2.62	1.86	1.33	0.82	0.45	0.17	0.17	1.00	2.62	5.60
	9	0.00	0.07	0.22	0.27	1.51	0.68	0.41	0.16	0.13	2.00	1.51	3.16
	10	0.00	0.08	0.09	0.34	1.37	0.68	0.56	0.15	0.10	2.00	1.37	3.20
	11	0.00	2.15	3.74	3.20	2.40	1.45	0.65	0.41	0.23	1.00	3.74	9.82
	12	0.00	0.06	0.21	0.73	1.16	0.68	0.35	0.12	0.09	2.00	1.16	2.91
	13	0.00	0.06	1.79	1.76	1.20	0.82	0.41	0.18	0.09	1.00	1.79	4.59
	14	0.00	0.09	2.51	2.27	1.59	1.15	0.87	0.40	0.16	1.00	2.51	7.04
	15	0.00	0.30	1.55	1.37	1.00	0.37	0.23	0.13	0.10	1.00	1.55	3.44
	16	0.00	0.08	0.09	0.39	0.52	0.82	0.45	0.11	0.10	3.00	0.82	2.49
	17	0.00	0.07	1.63	2.57	1.94	1.22	0.60	0.19	0.10	1.50	2.57	6.19
	18	0.00	0.07	0.72	1.07	0.89	0.46	0.28	0.14	0.09	1.50	1.07	2.85
	N	**18**	**18**	**18**	**18**	**18**	**18**	**18**	**18**	**18**	**18**	**18**	**18**
	Mean	**0.000**	**0.250**	**1.179**	**1.354**	**1.168**	**0.704**	**0.422**	**0.194**	**0.124**	**2.083**	**1.647**	**4.118**
	SE	**0.000**	**0.118**	**0.289**	**0.277**	**0.170**	**0.096**	**0.058**	**0.028**	**0.010**	**0.384**	**0.271**	**0.640**

Figure 70-2. Default table type Formulation t results

This concludes the Joining Raw Data and Model Output in Tables example.

Merge Worksheets

Merges selected data from any two worksheets into a new worksheet, following the order of the data in the first worksheet and combining rows with matched values, followed by the data from the second worksheet that has not already been merged in. Note that, because Merge retains the unmatched data, Merge is similar to an Outer Join, with the main difference being the order of the output.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Data Management > Merge Worksheets**.
Main menu: **Insert > Data Management > Merge Worksheets**.
Right-click menu for a worksheet: **Send To > Data Management > Merge Worksheets**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Mappings panel

The Mappings panel allows users to specify which columns in a worksheet are involved in the worksheet transformation. Required input is highlighted orange in the interface.

Sort: The variable(s) to match by when merging the worksheets.
Included Column: Variables mapped to this context are included in the output worksheet.

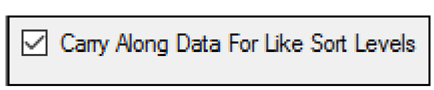
Sort Map panel

By default, the **Merge Worksheets** object requires that columns mapped to the **Sort** context have the same name. The Sort Map panel allows users to mix and match or override column names. For example, if the two columns being merged have different names, such as Subject and ID, the Sort Map panel can be used to specify matching columns in the two worksheets.

	Worksheet 1 Sorts	Worksheet 2 Sorts
1	Subject	ID
2	Conc	YObs
*		

In this example, the Subject column in worksheet 1 is joined/merged to the ID column in worksheet 2, and the Conc column in worksheet 1 is joined/merged to the YObs column in worksheet 2.

Options tab



Check the **Carry Along Data For Like Sort Levels** box to replicate data when the number of matched rows are not equal in the two worksheets. The Merge tool will combine the rows sequentially until it runs out of matched data in one of the worksheets (unlike the Cartesian join in the Join worksheets object). Then it will either carry down the last available value from that worksheet, if the option is checked, or leave a blank cell for the worksheet that has run out of matched data, if the option is not checked.

Results

The **Merge Worksheets** object generates one worksheet and one text file.

Result: The merged worksheets.
Settings: Text file containing input worksheets used and the options selected.

Pivot Worksheet

Pivot worksheets based on switching the columns and rows in a worksheet. For example, if a worksheet had Subject, Parameter, and Parameter Value columns, and a user wanted to place each parameter in its own column, this object can transpose the worksheet based on selections made in the Worksheet Mappings panel.

The Pivot Worksheet object is primarily used to unstack, or pivot, stacked datasets like the Final Parameters output worksheet from a PK or NCA model.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Data Management > Pivot Worksheet**.
Main menu: **Insert > Data Management > Pivot Worksheet**.
Right-click menu for a worksheet: **Send To > Data Management > Pivot Worksheet**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Mappings panel

The Mappings panel allows users to specify which columns in a worksheet are involved in the worksheet transformation. Required input is highlighted orange in the interface.

Column Header: Data type to use for creating the column headers in the output worksheet. Only one data type can be mapped to this context.

Values: Data type to fill the columns for each column header. Only one data type can be mapped to this context.

Row Header: Data types to use for defining the rows in the pivoted worksheet. Multiple data types can be mapped to this context. Each combination creates a unique set of profiles that are used to order the output worksheet rows.

Unit: Source data column containing unit information. When checked, the units become part of the column header upon pivoting. If incompatible units (including blank units) are found in the unit column, then the pivot will not be able to be performed until these inconsistencies are resolved or units are unmapped.

Carry: Data types to carry over unchanged in the output worksheet.

Attribute: Data types to combine with the data type mapped to **Values** to create additional column headers.

Results

The **Pivot Worksheet** object generates one worksheet.

Result: The pivoted output worksheet.

Rank Worksheet

Create a new column in an output worksheet by ranking columns in the source worksheet in ascending or descending order and sorting them based on the **Group By** selections.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Data Management > Rank Worksheet**.
Main menu: **Insert > Data Management > Rank Worksheet**.
Right-click menu for a worksheet: **Send To > Data Management > Rank Worksheet**.

Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Mappings panel

The Mappings panel allows users to specify which columns in a worksheet are involved in the worksheet transformation. Required input is highlighted orange in the interface.

Group By: Phoenix generates a separate set of ranking values for each unique value or group of values in columns mapped to the **Group By** context.

Rank: Parameters or variables mapped to **Rank** are ranked in ascending or descending order.

Any study variable or parameter mapped to the **Group By** context acts as a sort key in the output worksheet. If enough data types are mapped to **Group By** to create individual profiles for each rank, then the ranking column values never go above one.

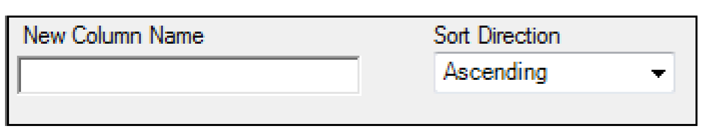
Data types mapped to **Rank** are ranked either numerically or alphabetically, depending on the data contained in the column.

If there are no matching values in a column mapped to the **Rank** context, and one or no columns are mapped to **Group By**, then the ranking count is incremented by one.

For every matching value in any column mapped to the **Rank** context, the ranking count is incremented by 0.5 for every N+1 matching values. For example, if the ranked column starts with two matching values, then the ranking for the first two values is 1.5 and 1.5. If the ranked column starts with three matching values the ranking is 2, 2, and 2. If there are four the ranking is 2.5, 2.5, 2.5, and 2.5.

When matching values are encountered, the normal incrementation by one is stopped, the matching values are given equal ranking numbers, and the incrementation resumes normally with the next non-matching value.

Options tab



- In the **New Column Name** field, type a name for the ranking column.

  The ranking column ranks the data types mapped to **Rank** in incremental order based on how many unique values are in the ranked data.

- In the **Sort Direction** menu, select an ascending or descending sort direction for the rank column.

Results

The **Rank Worksheet** object generates one worksheet and one text file. The output worksheet is arranged alphabetically or numerically based on the first selected sort key.

Ranked: The ranked values, in ascending or descending order.

Settings: Text file containing input worksheet used and the options selected.

Split Worksheet

Split a worksheet based on the data types that are mapped to the **Sort** context. The worksheet is divided into separate worksheets based on the sort key. For example, if a column named **Subject ID** is mapped to **Sort**, then a worksheet for each subject ID is created in the output.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Data Management > Split Worksheet**.
Main menu: **Insert > Data Management > Split Worksheet**.
Right-click menu for a worksheet: **Send To > Data Management > Split Worksheet**.

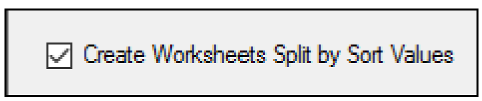
Note: To view the object in its own window, select it in the Object Browser and double-click it or press **ENTER**. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Mappings panel

The Mappings panel allows users to specify which columns in a worksheet are involved in the worksheet transformation. Required input is highlighted orange in the interface.

Sort: Data types to use for creating the separate output worksheets.
Ignore: Data types to exclude from any output worksheets.

Options tab



Check the **Create Worksheets Split by Sort Values** box (the default) to create a separate worksheet for each data type mapped to **Sort**, along with the Unique Values worksheet (which lists the number of occurrences of each Sort).

If this box is unchecked, then only the Unique Values worksheet is created in the output.

Results

The number of worksheets the **Split Worksheet** object creates is based on the number of unique values in the data types mapped to the **Sort** context. The worksheet names are derived from the values in the data types mapped to **Sort**.

The Unique Values worksheet is always created. The Unique Values worksheet lists the number of times a sort key or keys are present in the input worksheet. For example, if **Time** is mapped to **Sort**, and there are 10 time values per profile, then each time value is listed in one column, and the total instances of each time value is listed in the **Count** column.

The **Split Worksheet** object also creates one text file.

Separate worksheets: The values of each data type mapped to Sort, along with the associated values in the worksheet for each unique sort profile.

Unique Values: Lists the number of times a sort key(s) are present in the input worksheet.

Settings: Text file containing input worksheet used and the options selected.

Stacker

Primarily used to convert unstacked datasets, like the Final Parameters Pivoted worksheet output from a PK or NCA model. The **Stacker** object moves values stored in column headings into rows. When data is stacked by parameter, the separate parameter columns are "stacked" in one column and the parameter values are arranged beside each parameter in the stacked column.

Use one of the following to add the object to a Workflow:

Right-click menu for a Workflow object: **New > Data Management > Stacker**.
Main menu: **Insert > Data Management > Stacker**.
Right-click menu for a worksheet: **Send To > Data Management > Stacker**.

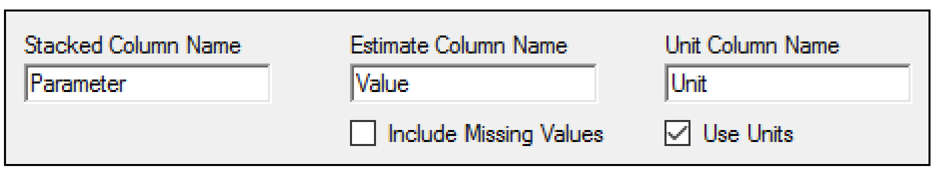
Note: To view the object in its own window, select it in the Object Browser and double-click it or press ENTER. All instructions for setting up and execution are the same whether the object is viewed in its own window or in Phoenix view.

Mappings panel

The Mappings panel allows users to specify which columns in a worksheet are involved in the worksheet transformation. Required input is highlighted orange in the interface.

Carry: Data types mapped to carry over into the stacked output worksheet. Note that the order in which the Carry columns are selected is the order they will appear in the output worksheet.
Stack: Data types to stack in a single column. The values in each stacked column are then placed beside each column header in a separate column.

Options tab



- In the **Stacked Column Name** field, type a name for the output column that contains the stacked data.
- In the **Estimate Column Name** field, type a name for the output column that contains the values that are matched with the stacked data.
- Check the **Include Missing Values** box to carry empty rows through to the results worksheet. This allows the user to keep track of records for which a parameter (e.g., a PK parameter) could not be calculated for some reason.
- In the **Unit Column Name** field, type a name for the output column that contains the units that are matched with the stacked data.
- Clear the **Use Units** checkbox if the input worksheet does not use units or units are not needed in the output.

Results

The **Stacker** object generates one worksheet and one text file.

Stacked: The stacked data types and their associated values and units, if any.
Settings: Text file containing input worksheet used and the options selected.

Phoenix Configuration

Phoenix provides many configurable settings for the user to manage via the *Preferences* dialog. There is also a configuration file containing options that can be adjusted as necessary for local environments (see “Phoenix Config file”).

Select **Edit > Preferences** to set Phoenix defaults using the *Preferences* dialog.

General options

Set location of saved Phoenix projects and copy `Examples` directory.

Licensing options

Activate and retrieve a license, and add a licensing server. See “Licensing of Phoenix software”.

Mapping contexts

Set up **Global Contexts** and identify column names to associate with specific variables. Set up **Context Associations** to automatically map variable names with specific data inputs in Phoenix operational objects.

PKS

Default Save Options: See the PKS “Configuring default save options” section.
Instances: See the PKS “Setting up a PKS connection” section.

Remote Execution

JMS: Enable the Phoenix Job Management Service (JMS).
RPS: Enable many third party objects to be executed remotely.
Compute Grid: Add, modify settings, delete grids. The grids listed are the ones presented on the **Execute on** menu in the Run Options tab.

Watson Import

Configure the server, set up business rules for the import and specify the content for the resulting sample and dosing worksheets. See “Setting up preferences” for details.

AutoPilot

Open the AutoPilot Toolkit Administrator Module to configure business rules, system settings, and output, including formatting. See the “Administration Module”.

LinMixBioequivalence

Control the default model for a 2x2 average bioequivalence crossover design involving nonreplicated data. When **Default for 2x2 crossover set to all fixed effects** is unchecked, the default fixed effects model is Sequence+Formulation+Period and random model is Subject(Sequence). When the option is checked, the fixed effect model becomes Sequence+Formulation+Period+Subject(Sequence) and the random effects model becomes unspecified. See “Nonreplicated crossover designs”.

NONMEM, PsN, R, Reporter, SAS

Set the paths to access the external programs, define output directories, and set up development environments for modifying scripts for the third party programs from within Phoenix. See NONMEM’s “Setting up preferences”, PsN’s “Setting up preferences”, R’s “Setting up preferences”, Reporter’s “Setting up preferences”, and SAS’ “Setting up preferences” for more details.

NLME

In the **NLME root run folder** field, type a path to the default temporary folder for NLME runs or click **Browse** to use the *Browse For Folder* dialog to select a new folder. The default is `C:\Users\<username>\AppData\Local\Temp\Phoenix`.

Object Settings

Manage saved object settings files. The list is grouped by operational object. Set the default file to use for object settings, delete saved files, import/export settings files to and from Phoenix. See "To set object settings preferences for operational objects" in the Operational Objects section.

Plotting defaults

Manage the default display settings for plots.

Plugins menu

Select the top-level **Plug-ins** item to view and control the status for installed Phoenix plug-in modules. Select a specific plug-in page to view the plug-in version and description.

General options

In the *Preferences* dialog, click the (+) sign beside **General** to expand the menu tree.

Select **General > Projects** to display the Project Settings page.

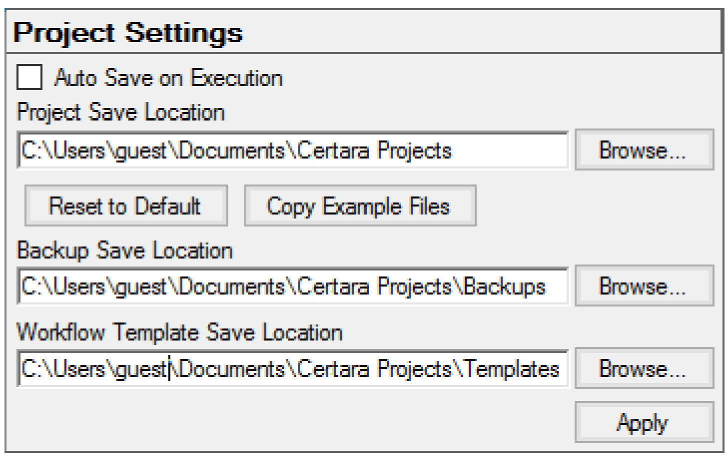


Figure 76-1. Project Settings preferences

Check the **Auto Save on Execution** box to have Phoenix save a back up copy of the project every time a workflow or operational object is executed.

In the **Project Save Location** field, type a path to the directory in which to save Phoenix project files (the use of environment variables when defining the path is supported) or click **Browse** to use the *Browse For Folder* dialog to select a new directory. The default is `C:\Users\<username>\My Documents\Certara\Phoenix Projects`.

Click **Reset to Default** to change the project save location back to its default location.

Click **Copy Example Files** to create a copy of the `Examples` directory installed with Phoenix in your project save location.

In the **Backup Save Location** field, type a path to the directory in which to place automatically saved projects or click **Browse** to use the *Browse For Folder* dialog to select a new directory. The default is `C:\Users\<username>\My Documents\Certara\Phoenix Projects\Backups`.

In the **Workflow Template Save Location** field, type a path to the directory in which to place saved templates or click **Browse** to use the *Browse For Folder* dialog to select a new directory. The default is `C:\Users\<username>\My Documents\Certara\Phoenix Templates`.

Click **Apply** to apply the changes.

Note: For large projects, the autosave option can decrease performance as the benefits of saving automatically after every object execution may be far outweighed by the time it takes. In those cases, this option is not recommended and users should manually save their projects.

Mapping contexts

Mapping contexts are used to associate inputs into operational objects with columns in a dataset. There are two mapping context pages: the *Global Contexts* page and the *Context Associations* page.

The *Global Contexts* page is used to specify potential columns in a dataset that belong to a particular data input. Potential column names are columns in a worksheet that are typically associated with a mapping context. For example, ID is a potential column name for Subject, and Hour is a potential column name for Time.

The global contexts are then used to map the columns to operational object inputs in the *Context Associations* page.

Global contexts

To identify column names typically used for a particular data input

Click the (+) sign beside Mapping Contexts.

Select **Global Contexts** in the menu tree.

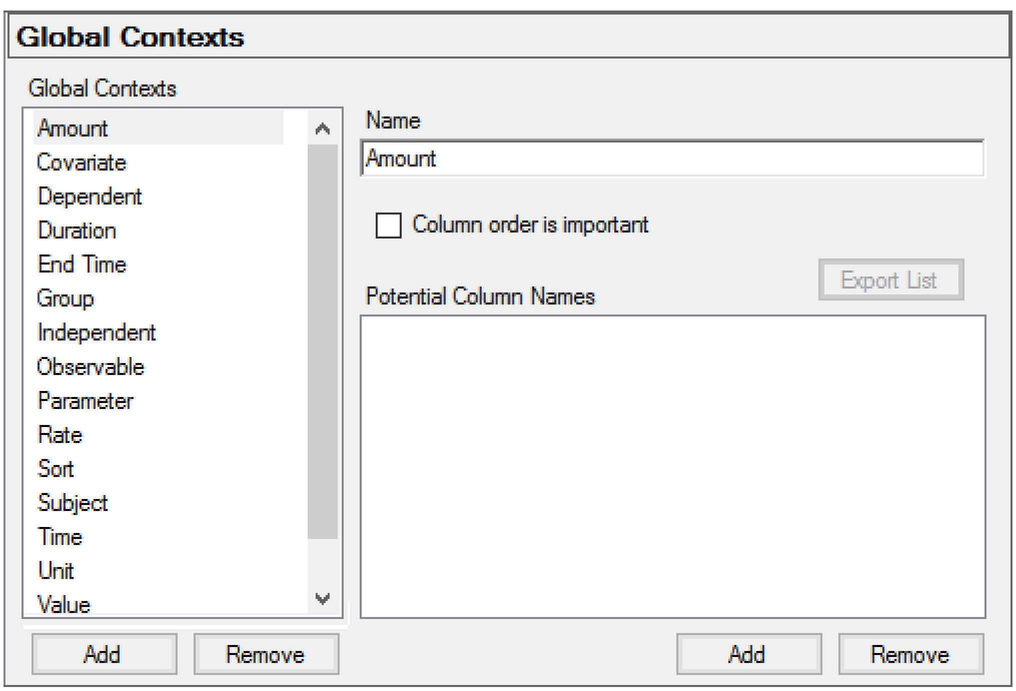


Figure 76-2. Global Contexts preferences

Check the **Column order is important** box to maintain order of columns.

Select a context in the list.

To add/remove a global context

To ***add*** to the list of global contexts, click **Add** underneath the **Global Contexts** list and type the global context name in the list.

To ***remove*** a global context, select the context in the **Global Contexts** list and click **Remove** below the list.

To add/remove a column name

To ***add*** to the list of potential column names, click **Add** underneath the **Potential Column Names** field and type the name of the column in the **Potential Column Names** field.

To ***remove*** a potential column name, select the name in the **Potential Column Name** field and click **Remove** below the field.

Context Associations

To map columns to specific inputs in each operational object

Select **Context Associations** in the menu tree.

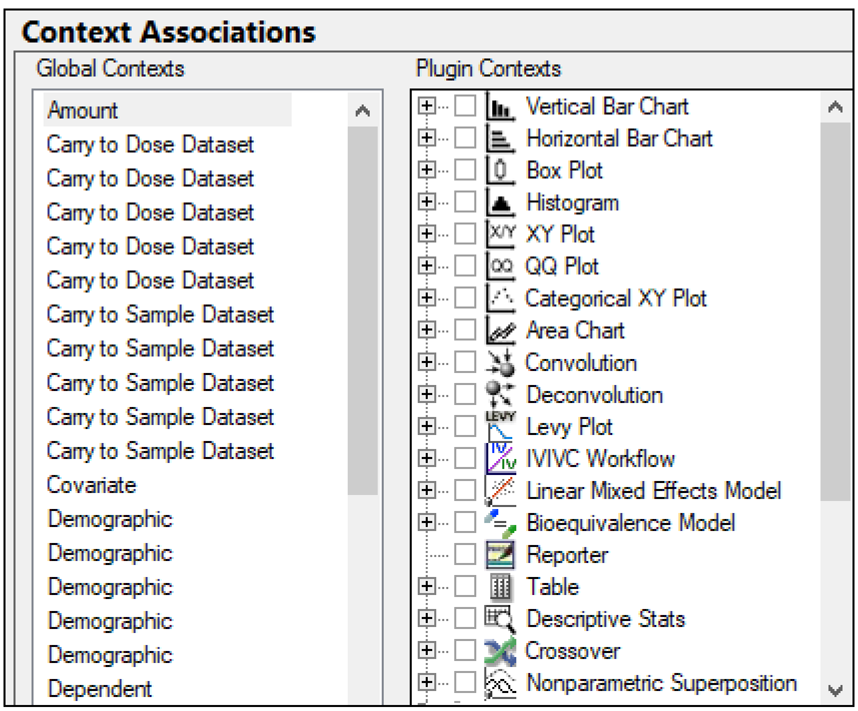


Figure 76-3. Context Associations preferences

Select a context in the **Global Contexts** list.

In the **Plugin Contexts** list, click the (+) sign beside an operational object to view a list of its data inputs.

Check the box(es) to associate that operational object's input with the dataset column(s) specified in the **Global Contexts** list.

When a dataset with a column that matches the global context is mapped to that operational object, the column is automatically mapped to that input.

Example usage

Suppose a user always wants the subject identifier column in a dataset to map to the Sort context in the NCA object. The user would do the following:

1. Select **Global Contexts**.
2. Select **Subject** in the **Global Contexts** list.
3. In the **Potential Column Names** box, add any column names used to contain subject identifiers, such as ID or Subject.
4. Select **Context Associations**.
5. Select **Subject** in the **Global Contexts** list.
6. Click the (+) sign beside **NCA** to view all NCA data inputs.
7. Check the box beside **Sort**.
   The subject identifier column is now associated with the Sort context in the NCA object.
8. Click **OK** to close the *Preferences* dialog.
9. Import a dataset that contains subject identifiers. (The subject identifier column must have a name specified in the *Global Contexts* dialog.)
10. Insert an NCA object and map the dataset to the object.

The subject identifier column is automatically mapped to the Sort context in the NCA object's Main Mappings panel.

JMS

The *Job Management* dialog allows users to specify the address and protocol used by the Phoenix Job Management System™ (JMS™), how often to send data packets to the JMS, and setting the address for viewing remote jobs via the RPS web UI.

To set preference options for JMS

In the *Preferences* dialog, expand **Remote Execution** and select **JMS**.

Check the **Remote Submit Enabled** box to use the JMS.

In the **Job Queue Server** (JQS) field, enter the JQS network address.

In the **Port** field, enter the JQS port number.

In the **Protocol** menu, select TCP or HTTP.

In the **Polling Interval** box, type or select the number of times per second that Phoenix sends data packets to the JMS.

In the **RPS Queue Address** field, enter the fully qualified address of the RPS queue (e.g., `http://myserver:8080/PhoenixServer`).

RPS

To use RPS from Phoenix, users must have an RPS license, and they must enable RPS in the Phoenix configuration. (Refer to "Remote Processing Server".)

To set preference options for RPS

In the *Preferences* dialog, expand **Remote Execution** and select **RPS**.

Check the **Enable Remote Execution** box.

Click **Define** to specify the location of the RPS queue.

In the server definition dialog enter the server name, the root context, and the port.

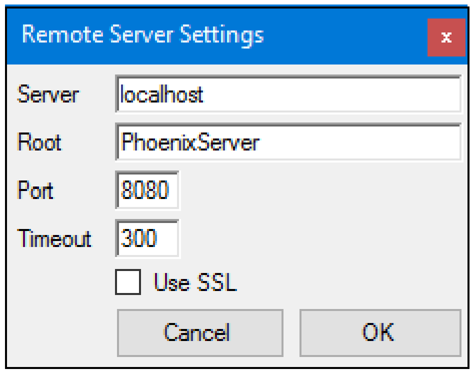


Figure 76-4. Server definition dialog

Click **OK**.

At this point the information provided will be validated by attempting to communicate with the server.

Select the object types for which remote execution is to be enabled by checking the box in the **Execute Remotely** column next to the object type.

Compute Grid

Phoenix is capable of implementing parallel computing in two distinct ways to optimize the use of computational grids and multicore computers. A description of these two methods and the advantages and challenges will help the user select the optimal method for each project.

The first is called parallelizing by model (PBM), in which individual NLME models are sent to individual computation cores for execution. One example of PBM would be a 200 replicate bootstrap, which requires 200 independent NLME models to be run. Using PBM, each of the 200 models would be sent to 200 separate compute nodes, with each model running on a single compute node from initial estimates to final parameters. PBM is extremely useful to simultaneously execute many NLME models.

The second method is called parallelizing within model (PWM), in which an individual NLME model is spread across multiple computation cores for execution. One example of PWM would be a simple estimation of a single PK/PD model. Using PWM, the one model would be spread across 50 computation cores, allowing successful minimization to be done more quickly than if the local computer was used. PWM is extremely useful with models that have long run times to achieve convergence.

Phoenix supports both PBM and PWM and even supports a combination of the two. An example of combining PBM and PWM can be seen in a stepwise covariate search. During the first step, let's assume there are 8 models to be run (base + 7 possible covariates). Phoenix will run all 8 models simultaneously (PBM) with each model using 20 computation cores (PWM). Combining PBM and PWM can be extremely powerful to reduce overall run times with complex PK/PD model development activities.

The following outlines the parallelization method implemented for each run mode and each computation platform supported in Phoenix NLME 8.1:

Simple: Run None PBM PWM None PWM PBM PWM None PWM

Windows: MultiCore (PBM), MPI (PWM)
Linux: MultiCore (PBM), MPI (PWM), SGE_MPI/LSF_MPI/TORQUE_MPI (PWM)

Scenarios Run:

Windows: MultiCore (PBM), MPI (PWM and PBM)
Linux: MultiCore (PBM), MPI (PWM and PBM), SGE_MPI/LSF_MPI/TORQUE_MPI (PWM and PBM)

Stepwise Cov Search Run:

Windows: MultiCore (PBM), MPI (PWM and PBM)
Linux: MultiCore (PBM), MPI (PWM and PBM), SGE_MPI/LSF_MPI/TORQUE_MPI (PWM and PBM)

Shotgun Cov Search Run:

Windows: MultiCore (PBM), MPI (PWM and PBM)
Linux: MultiCore (PBM), MPI (PWM and PBM), SGE_MPI/LSF_MPI/TORQUE_MPI (PWM and PBM)

Profile Run:

Windows: MultiCore (PBM), MPI (PWM and PBM)
Linux: MultiCore (PBM), MPI (PWM and PBM), SGE_MPI/LSF_MPI/TORQUE_MPI (PWM and PBM)

Predictive Check Run: No parallelization method implemented.

Simulation Run: No parallelization method implemented.

Selection of the desired grid mode in the Phoenix *Preferences* dialog is critical to achieving the desired type of parallelization for the submitted run mode. For example, a user who submits an NLME model in Simple run mode to a compute grid set to Linux/SGE will result in the model running on a single core of the grid. However, that same model submitted to a compute grid set to Linux/SGE_MPI will be parallelized using PWM.

Setting up grids

There are two methods for setting up grids to run parallel executions in Phoenix. The Compute Grid page of the *Preferences* dialog, see “Compute Grid preferences” is one method. The other is editing the configuration files directly (either as an administrator or a user), see “Configuration files”.

Phoenix supports the following modes of parallelization:

- **MultiCore** (Windows, Linux): Parallelize (single models) across multiple cores on a single machine (i.e., 32-core Linux or Windows computer).
- **MPI** (Windows, Linux): Parallelize (single models and/or single model parallelized by subject) across multiple cores on an MPI Cluster.
- **LSF** (Linux): Parallel execution of single model runs (e.g., bootstrap and shotgun covariate search) on an LSF grid. Individual models are not parallelized across multiple cores.

- **LSF_MPI** (Linux): Parallel execution and parallelization across multiple cores of all model runs on a LSF grid. All models are run simultaneous and are parallelized across multiple cores. Phoenix determines the optimal parallelization strategy for each model run. Supports all Phoenix run modes.
- **SGE** (Linux): Parallel execution of single model runs (e.g., bootstrap and shotgun covariate search) on an SGE grid. Individual models are not parallelized across multiple cores.
- **SGE_MPI** (Linux): Parallel execution and parallelization across multiple cores of all model runs on a SGE grid. All models are run simultaneous and are parallelized across multiple cores. Phoenix determines the optimal parallelization strategy for each model run. Supports all Phoenix run modes.
- **TORQUE** (Linux): Parallel execution of single model runs (e.g., bootstrap and shotgun covariate search) on a TORQUE grid.
- **TORQUE_MPI** (Linux): Parallel execution and parallelization across multiple cores of all model runs on a TORQUE grid. All models are run simultaneous and are parallelized across multiple cores. Phoenix determines the optimal parallelization strategy for each model run. Supports all Phoenix run modes.

Example grid definitions for different parallel modes can be found in the `PhoenixParallelExecutionSettings.txt` file and modified with company-specific settings. (See "Configuration files" for details on modifying this file.)

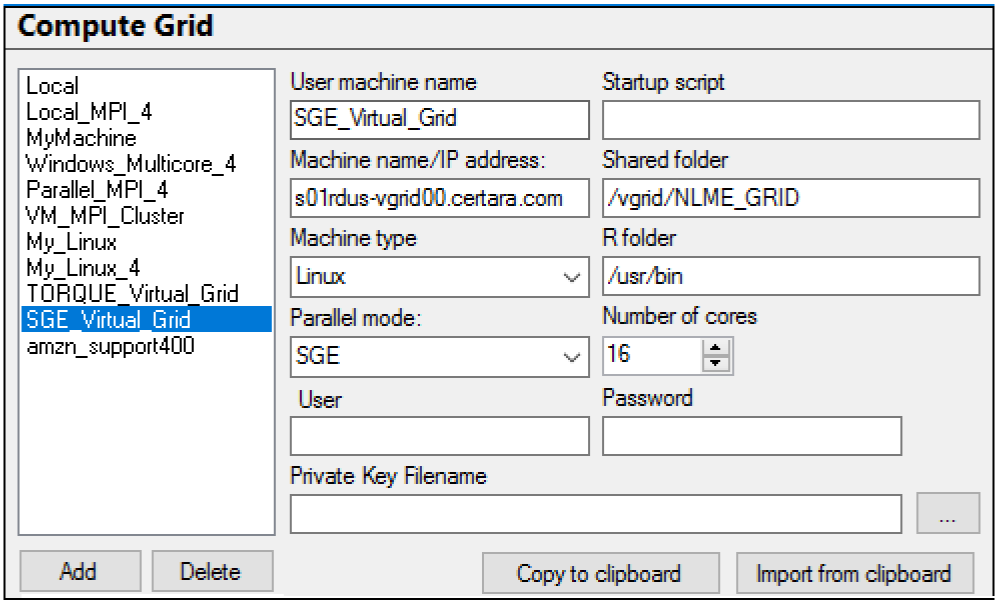
Note: When a grid is selected for executing an NLME object, loading the grid can take some time and it may seem that the application has stopped working.

Make sure that there is adequate disk space on the grid for execution of all jobs. A job will fail on the grid if it runs out of disk space.

Compute Grid preferences

In the *Preferences* dialog, expand **Remote Execution** and select **Compute Grid**.

The Compute Grid page allows users to add, modify, or delete the setup for a grid. The list of grids on the left of the page is the list you will see in the **Execute on** pull-down menu in the Run Options tab for an NLME object.



To set up a new grid

Click **Add** and enter all of the following information for the new grid:

User machine name: Name to appear in the selection box on the Run Options tab of Phoenix models.

Startup script: Script to execute on the remote host to setup the run environment.

Machine name/IP address: Actual machine name or its IP address.

Shared folder: Location where the application can write results/temporary files on the remote machine.

Machine type: Choose from **Windows** or **Linux**.

R folder: Path to R on the remote machine.

Parallel mode: If the machine type is **Windows**, choose from **None**, **MultiCore**, **MPI**, **LSF**. If the machine type is **Linux**, choose from **None**, **MultiCore**, **MPI**, **TORQUE**, **SGE**, **SGE_MPI**, **TORQUE_MPI**, **LSF**, **LSF_MPI**.

Number of cores: Number of computational cores available on this grid.

User: Username for logging into the host. This is required to use the grid, unless using a private key file.

Password: Password for logging into the host. This is required to use the grid unless using a private key file.

Private Key Filename: As an alternative to entering a username and password, enter the name of the private key file to use for ssh private keyfile authentication or use the ellipsis button to display a file browser for selecting the file. See “Setting up an ssh private key file”.

To modify grid settings

Select the grid from the list.

Adjust the settings in the page as described.

Press the **Enter** key.

Changes are automatically updated in the user's custom `PhoenixParallelExecution-Settings.txt` file.

To delete a grid platform:

Select the grid from the list.

Click **Delete**.

The grid is automatically removed from the user's custom `PhoenixParallelExecution-Settings.txt` file.

Configuration files

There are two system-wide files that are used in the configuration of grids: `PhoenixParallelExecutionSettings.txt` and `PhoenixParallelExecutionSettings.xml`, located in `<Phoenix_install>/application`. The list of grids shown in the "Compute Grid preferences" figure above comes from the `PhoenixParallelExecutionSettings.txt` file that is installed with Phoenix, after removing the comment syntax from all of the definitions in the file. (Initially, all but the first two platforms are commented out.)

Administrators can modify the `PhoenixParallelExecutionSettings.txt` and `PhoenixParallelExecutionSettings.xml` files to be site-specific. Each user can also customize the grids by placing copies of these files in: `C:\Users\<username>\AppData\Roaming\Certara\Phoenix\` and customizing them.

Setting up an ssh private key file

On the server Linux system, generate keys.

```
mkdir ~/.ssh /* if you do not have this directory already */
chmod 700 ~/.ssh
ssh-keygen -t rsa
```

Take default location and press **Return** key for passphrase

```
Generating public/private rsa key pair.
Enter file in which to save the key (~/.ssh/id_rsa):
Enter passphrase (empty for no passphrase):
Enter same passphrase again:
Your identification has been saved in ~/.ssh/id_rsa.
Your public key has been saved in ~/.ssh/id_rsa.pub.
```

Transfer key to remote system.

Simply copy ~/.ssh/id_rsa to a secure location on windows. You will specify this file in the **Remote Execution > Compute Grid** settings page in the *Preferences* dialog.

Add public key to server list.

```
cp ~/.ssh/authorized_keys ~/.ssh/authorized_keys_Backup
cat ~/.ssh/id_rsa.pub >> ~/.ssh/authorized_keys
```

Make keys secure.

```
chmod 600 ~/.ssh/authorized_keys
```

Test that you can connect to remote Linux system without a password.

– Open PuTTY.
– Enter the hostname in the *PuTTY Configuration* dialog.
– Go to the **SSH > Auth** category.
– Enter the keyfilename (that was transferred) in the **Private key file for authentication** field.
– Click **Open**.

Plotting defaults

The Plotting Defaults page of the *Preferences* dialog allows users to adjust a number of display settings that will be used as the defaults for plots. The settings in this dialog apply to the output of Plotting objects, as well as to any plots created from other operational objects, such as NCA. They do not override any user-specified settings in projects.

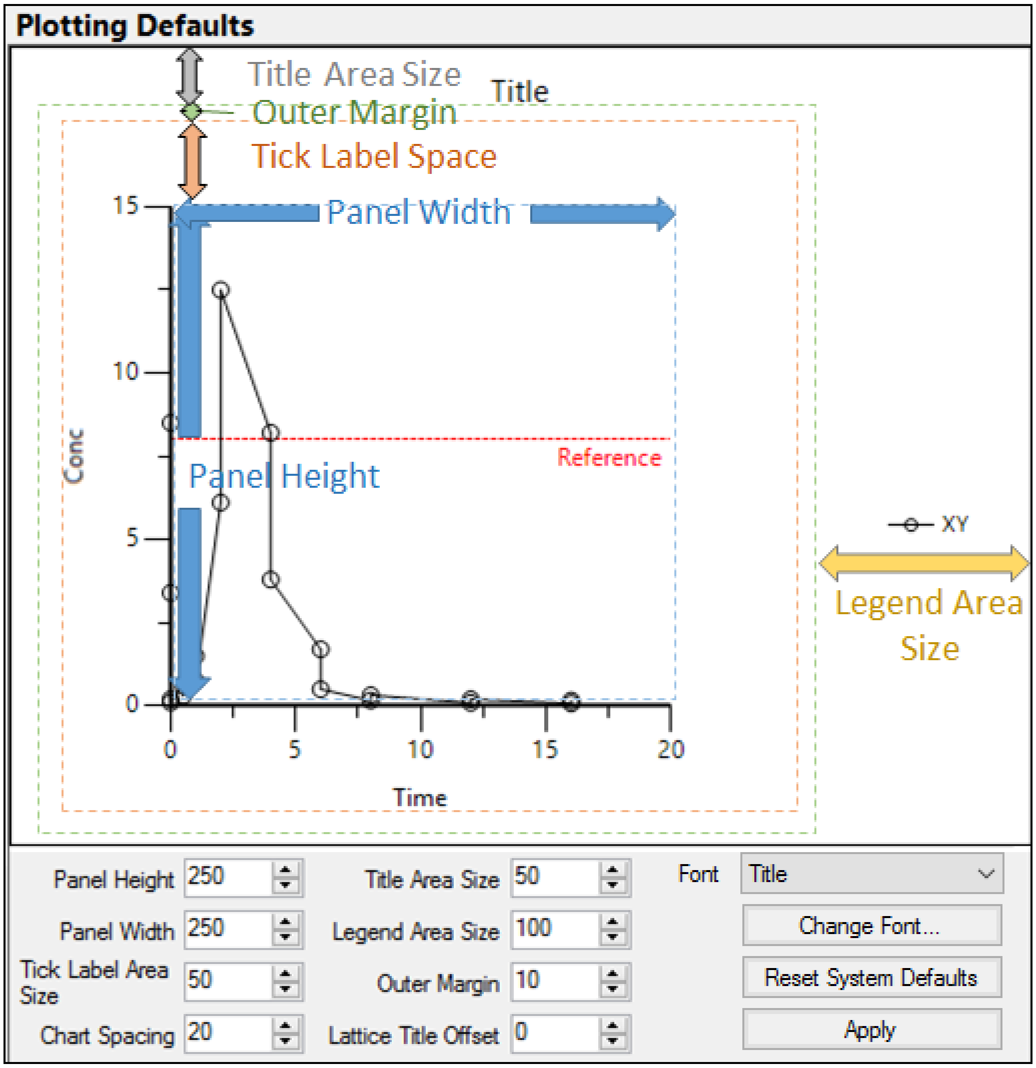


Figure 76-5. Plotting Defaults preferences

Panel Height and Panel Width: The size of the plot drawing area.

Tick Label Area Size: How wide the tick label area is from the axes.

Chart Spacing: The distance between multiple graphs.

Title Area Size: How wide the area is where the title is displayed.

Legend Area Size: How wide the area is for the legend.

Outer Margin: The size of the space between the graph title and the tick label area.

Lattice Title Offset: Distance to shift the Lattice Title from the graphs in the lattice.

Font: Select the item whose font is to be changed.

Change Font: Display the Font dialog for modifying the selected item's font, size, style, etc.

Reset System Defaults: Resets all of the values in the Plotting Defaults page to the Phoenix system defaults.

Apply: Click to save the settings as the plot defaults.

Note: When saving a project, only those plot settings that have been changed in the user interface will be saved with the project. Any settings that have not been modified in the interface will not be saved with project, as the default plot settings will be applied when the project is reopened.

Plugins menu

The **Plugins** menu is used to view the status of Phoenix plug-ins and add new plug-ins. Phoenix plug-ins are listed in three groups: General, System, and Non-Loaded. Each group has its own tab in the Plugins menu. Plug-ins can be viewed individually by expanding the **Plugins** menu.

The **Plugins** menu provides the following information on Phoenix plug-ins: the name, version number, and state, either started or not started.

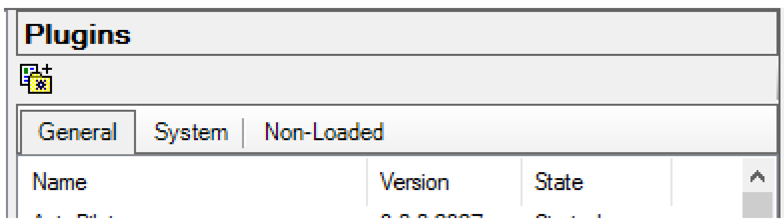


Figure 76-6. Plugins preferences

Plug-ins in the General tab are operational objects. These plug-ins are responsible for providing Phoenix functions such as drug modeling, charting, and dataset manipulation. The General tab displays the name, version number, and state of each operational object plug-in.

Plug-ins in the System tab are used to provide Phoenix framework functions. The name, version, and state of each framework plug-in is listed.

The Non-Loaded tab displays information on why a plug-in failed to load. If a plug-in fails to load its state is listed as “FailedToStart.” If it has not yet been loaded, the state is listed as “Not Loaded.” Select the failed plug-in to display any details on the failure in the **Reason** field.

To add a new plug-in

Select **Plugins** in the *Preferences* dialog and click (**Load Plugin** icon) .

In the *Load Plugin* dialog, select a plug-in manifest or plug-in assembly.

A plug-in manifest is a file that describes the plug-in.
A plug-in assembly is the plug-in DLL.

The plug-in is added to the General or System tab, depending on the type of plug-in selected.

Phoenix Config file

In the file `Phoenix.exe.config` (or `Phoenix32.exe.config`) there are two path properties that can be configured, if necessary, for your local environment.

- `tempDirectoryRoot`: Users can use this property to specify where Phoenix writes temporary files. The path must be fully qualified, and it does ***not*** support the use of environment variables. For example, to have Phoenix use the Phoenix application data folder for the temporary storage, you might specify a path like this:

  ```
  tempDirectoryRoot="C:\Users\UserName\AppData\Roaming\Certara\Phoenix\Temp"
  ```

  The default value is <blank> which will cause Phoenix to use the default system temporary directory.

- `repositoryDirectory`: This property is used to specify the location that Phoenix uses as a working folder for open projects. Use a fully qualified path name to enter an alternate path. This property supports the use of environment variables. For example, to use the system temporary file location, you could specify a path like this:

  ```
  repositoryDirectory="%TEMP%\ScratchRepository"
  ```

  The default value is "`%APPDATA%\Certara\Phoenix\ScratchRepository`".

Index