PROTEXPRESS USER'S GUIDE

NATIONAL CANCER INSTITUTE®

Center for Biomedical Informatics
and Information Technology

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CONTENTS

About This Guide

This section introduces you to the *protExpress User's Guide*. It includes the following topics:

Purpose

This guide explains how to use protExpress, a proteomics experiment and protocol data management tool that you can use to search and manage proteomics experiment and protocol data. You can also use protExpress to export stored experimental data to XAR format.

Audience

Typical User

This guide is designed for bioinformaticians at the National Cancer Institute (NCI) and its affiliated institutions who need to annotate, store, and share proteomics experimental annotation and data as part of cancer research and clinical trials.

Prerequisites

To get the most out of this guide, you should be familiar with the following topics:

- Proteomics
- CPAS
- XAR

This documentation is not intended for programmers intending to install and deploy protExpress. For installation and deployment instructions, refer to the protExpress project in Gforge.

Topics Covered

The following brief overview explains what you will find in each chapter of this guide.

- *Working with protExpress* on page 5 explains how to use protExpress to manage protocol and experiment data.
- *protExpress Glossary* on page 37 is a glossary of terms related to protExpress.

Additional References

For more information about protExpress, see the following references:

- Analysis and Design Documents
- protExpress Object Model
- Requirements and Use Cases
- protExpress Installation and Deployment Instructions

Text Conventions Used

This section explains conventions used in this guide. The various typefaces represent interface components, keyboard shortcuts, toolbar buttons, dialog box options, and text that you type.

Convention	***Description***	***Example***
Bold	Highlights names of option buttons, check boxes, drop-down menus, menu commands, command buttons, or icons.	Click **Search**.
URL	Indicates a Web address.	http://domain.com
text in SMALL CAPS	Indicates a keyboard shortcut.	Press ENTER.
text in SMALL CAPS + text in SMALL CAPS	Indicates keys that are pressed simultaneously.	Press SHIFT + CTRL.
Italics	Highlights references to other documents, sections, figures, and tables.	See *Figure 4.5*.
Italic boldface monospace type	Represents text that you type.	In the **New Subset** text box, enter ***Proprietary Proteins.***
Note:	Highlights information of particular importance	**Note:** This concept is used throughout the document.
{ }	Surrounds replaceable items.	Replace {last name, first name} with the Principal Investigator's name.

Credits and Resources

The following people contributed to the development of protExpress.

protExpress Development and Management Teams			
Development	***Quality Assurance***	***Project and Product Management***	***Documentation***
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CHAPTER 1

WORKING WITH PROTEXPRESS

This section includes the following topics:

Getting Started

This section includes the following topics:

Registering Users

Your system administrator can manage user registration by validating against the database stored in protExpress or *LDAP*.

If the system administrator chooses to use the protExpress database, which is the default, the protExpress home page includes links to a registration page, as shown in *Figure 1.1* on page 6.

This topic explains how to add a user account to the protExpress database.

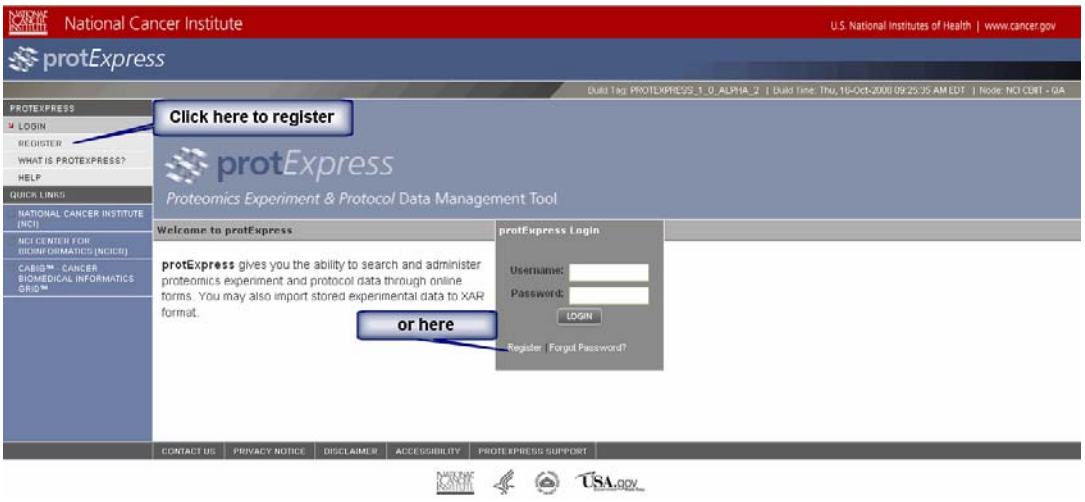


Figure 1.1 protExpress home page with registration links

To register to use protExpress

1. Click the **Register** menu in the upper left of the home page or the **Register** link in the protExpress Login area. The Register page appears.

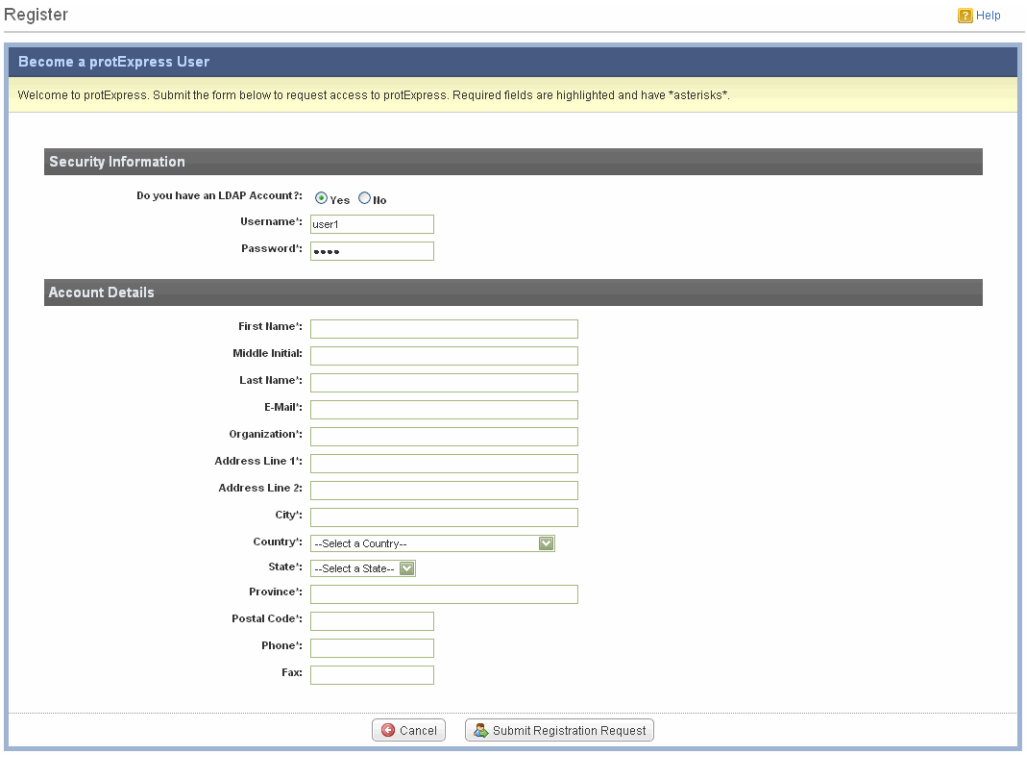


Figure 1.2 Registration page

2. Select the option corresponding to whether or not you have an LDAP account. If you do have an LDAP account, protExpress syncs up your registration with your LDAP account.

3. In the **Username** field, enter a name for the user that is unique within the local database and follows your standard naming conventions. This is a required field.
4. In the **First Name**, **Last Name**, **E-Mail Id**, **Password**, and **Password Confirmation** fields, enter the new user's information. All of these fields are required.
5. Click the **Submit Registration Request** button. If you entered all of the required information, the Registration Complete page appears.

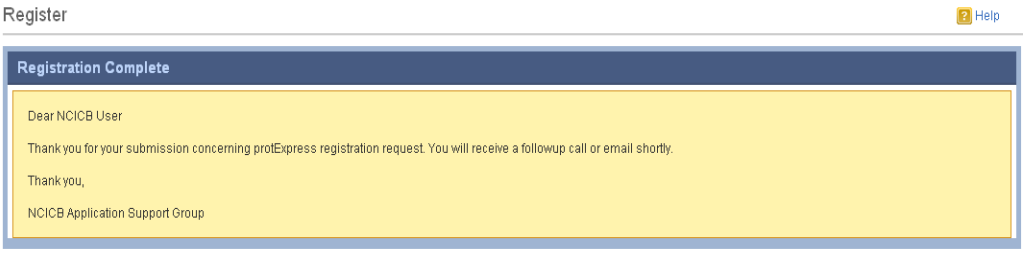


Figure 1.3 Registration Complete message

The NCICB Application Support group will contact you with your login information.

Logging In

To log in to protExpress, enter your username and password on the protExpress home page. If you do not yet have an account, see *Registering Users* on page 5.

Figure 1.4 Login area on the protExpress home page

If you have forgotten your password, click the **Forgot Password?** link. See *Resetting Your Password* for more information.

Resetting Your Password

If you forget your password, enter your username and e-mail address, and then click **Submit Request**. Both your username and e-mail address are required to reset your password.

Your username and e-mail address are the ones you specified when you registered with protExpress. If you don't remember your username, for example, contact your system administrator.

Using the Home Page

After logging in to protExpress, you arrive at its home page. You can do the following on this page:

Actions on the home page	***For more information, see...***
Search protExpress for any experiment or protocol	*Searching protExpress* on page 9
Create a new experiment	*Creating a New Experiment* on page 11
Edit a recent experiment	*Editing an Experiment* on page 20
Download a recent experiment in XAR format	*Viewing Experiment Details* on page 11

Table 1.1 Available actions on the protExpress home page and links to more information

To return to the home page after working in other areas of protExpress, click **HOME** in the main protExpress menu on the left.

Figure 1.5 shows the protExpress home page.

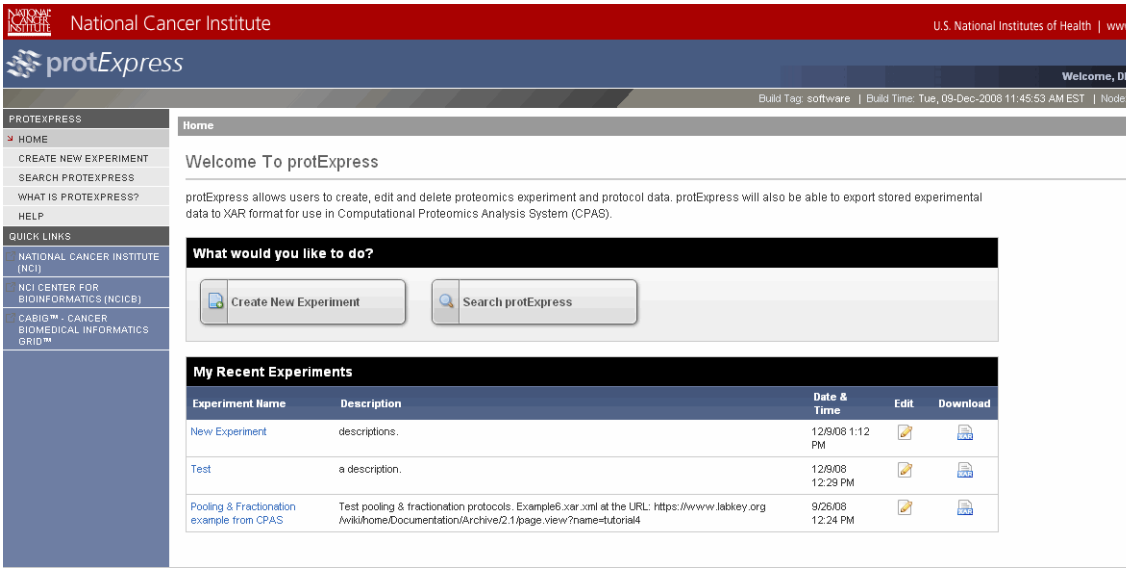


Figure 1.5 protExpress Home Page

Searching protExpress

The protExpress home page lists the *experiments* you most recently added. To find other data in protExpress, for example, *protocols* or experiments someone else created, you can search for them.

To search protExpress

1. On the home page, click the **Search protExpress** button or select the **Search protExpress** option in the menu on the left side of the page. The Search protExpress page appears.

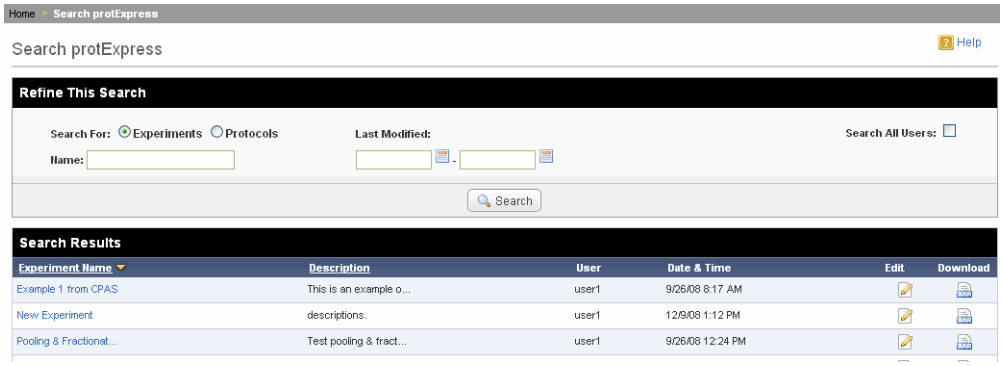


Figure 1.6 Search protExpress page

2. If you were to click **Search** using the default settings now, protExpress would return all of the *experiments* that *you* created. You may refine your search in any of the following ways:
   - Select either the **Experiments** or **Protocols** option in the Search For area.
   - In the Name field, enter one or more characters of the experiment or protocol name. The more characters you enter, the more precise your search and the fewer results you receive.
   - In the Last Modified fields, use the calendar to select or enter a date range during which the experiment or protocol was last modified.
   - Select the **Search All Users** option if you want to search all experiments or protocols in the protExpress database, not just those you created.
3. Click **Search**. Search results appear in a table below the search criteria.

   Note: You can sort the search results by clicking the name of the column you want to sort by. A yellow arrow ( ) indicates which column is currently sorting the list. Clicking that column's name again toggles the sort order between ascending and descending.

   Refer to the following table for an explanation of the symbols used in the search results.

Icon	*Explanation*
	You own this protocol or experiment and may edit it.

Table 1.2 Explanation of Icons Used in protExpress

Icon	Explanation
	Download this protocol or experiment in XAR XML format. When you view an experiment or a protocol in protExpress, at that time you can also download it in XAR XML format. For more information, see *Viewing Experiment Details* on page 11.

Table 1.2 Explanation of Icons Used in protExpress

4. Click a protocol or experiment name. The View Protocol Details or View Experiment Details page appears, respectively.

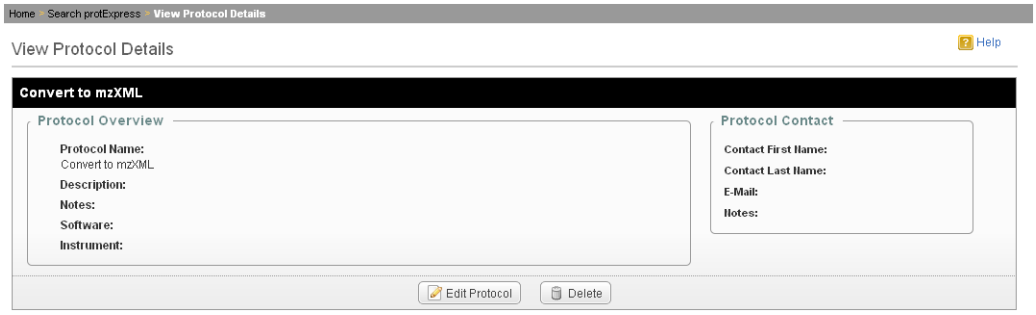


Figure 1.7 View Protocol Details page

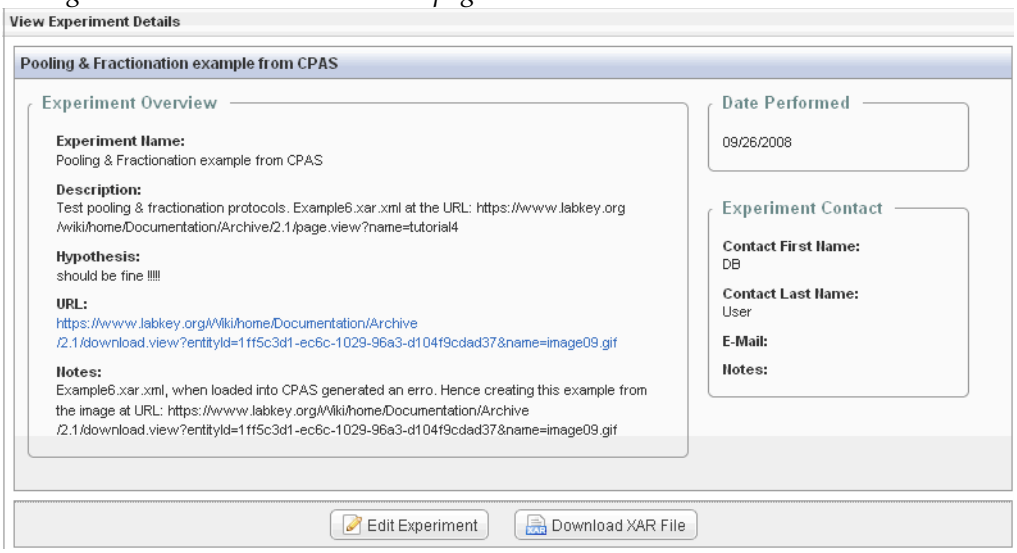


Figure 1.8 View Experiment Details page

Viewing Experiment Details

View an *experiment's* details by clicking the experiment's name link on either the protExpress home page or in search results. For more information, see *Using the Home Page* on page 8 and *Searching protExpress* on page 9.

When you open an experiment, the following information is available on the View Experiment Details page.

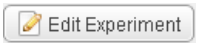
Feature	*Icon*	*Description*
Experiment Navigation > Experiment		Click the name next to this icon to view the following information about the experiment: Experiment Overview, Date Performed, and Experiment Contact.
Experiment Navigation > Experiment Run		Click the name next to this icon to view information about the parent experiment's experiment run. Information includes the experiment run's name, date performed, and notes. An experiment may have multiple runs, all of which appear in the experiment navigation above their associated protocols.
Experiment Navigation > Protocol		Click the name next to this icon to view the protocol overview, date performed, and contact for this experiment run.
Experiment Navigation > Input		Click the name next to this icon to view information about the parent protocol's input.
Experiment Navigation > Output		Click the name next to this icon to view information about the parent protocol's output.
		Click to edit experiment details including the experiment as a whole, experiment runs, protocols, inputs, and outputs. For more information, see *Editing an Experiment* on page 20.
		Click to download the experiment in XAR format. Your browser opens a window that prompts you to open or save the XAR file.

Table 1.3 Features of the View Experiment Details Page

Creating a New Experiment

Each step in the process of creating a new *experiment* has its own procedure in this documentation. This topic summarizes those procedures.

To create a new experiment

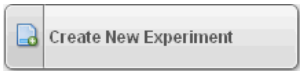
1. Identify the experiment. For more information, see *Identifying the Experiment* on page 12.
2. Add one or more protocols to the experiment. For more information, see *Adding Protocols to the Experiment* on page 14.
3. Add one or more inputs and outputs to the protocol. For more information, see *Adding Inputs to the Protocol* on page 16 and *Adding Outputs to the Protocol* on page 17.

4. Review and save the experiment. For more information, see *Reviewing the Experiment* on page 19.

Identifying the Experiment

You begin creating a new *experiment* by identifying it so that you and others can find it easily later. You must specify the experiment name and the date it was performed. All other identifying information is optional.

To identify the experiment

1. On the protExpress home page, click 

or click **Create New Experiment** in the menu on the left side of the page. The Create New Experiment page opens to the Identify Experiment step.

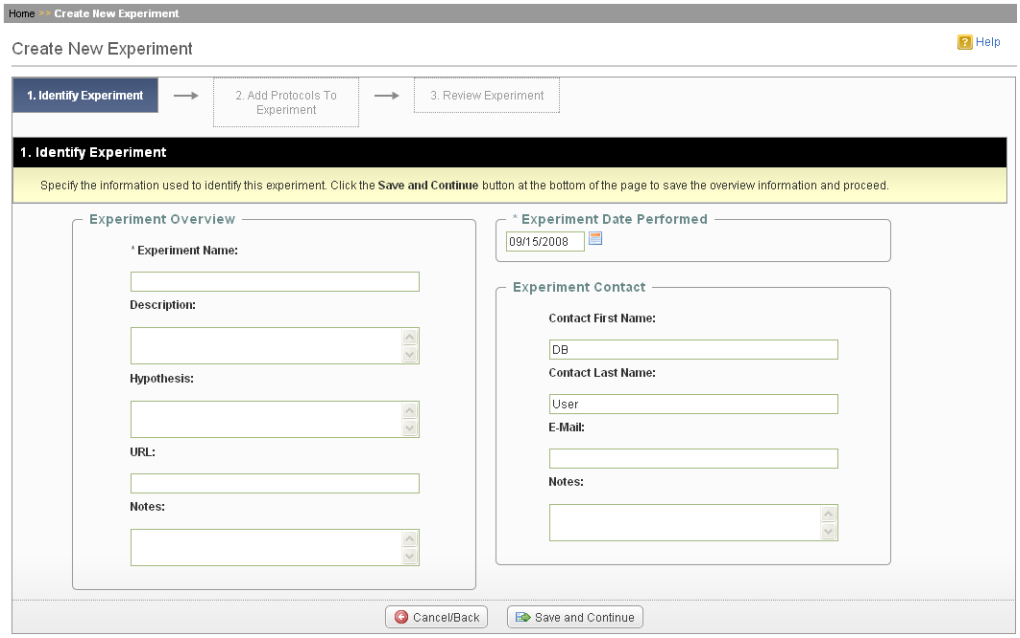


Figure 1.9 Identify experiment step in the create new experiment process

2. Enter information about the experiment. Field explanations are in the following table.

Field	***Description***
Experiment Name	Required field. Enter a name for the experiment using up to 200 characters.
Description	Enter a description of the experiment using up to 2000 characters.
Hypothesis	Enter the experiment's hypothesis using up to 500 characters.
URL	Enter the URL where more information about the experiment can be found. Use up to 200 characters.
Notes	Enter additional notes about the experiment using up to 2000 characters.

Table 1.4 Definitions of fields on the Identify Experiment page

Field	Description
Experiment Date Performed	Required field. Click the calendar icon and then click a date to select it. The date you select appears in the field.
Contact First Name	Enter the first name of a person who can be contacted about this experiment. Use up to 100 characters.
Contact Last Name	Enter the last name of a person who can be contacted about this experiment. Use up to 100 characters.
E-mail	Enter the e-mail address of the experiment's contact person. Use up to 100 characters.
Notes	Enter additional notes about the experiment's contact person. Use up to 1000 characters.

Table 1.4 Definitions of fields on the Identify Experiment page

3. Click Save and Continue. The Add Protocols to Experiment page appears.

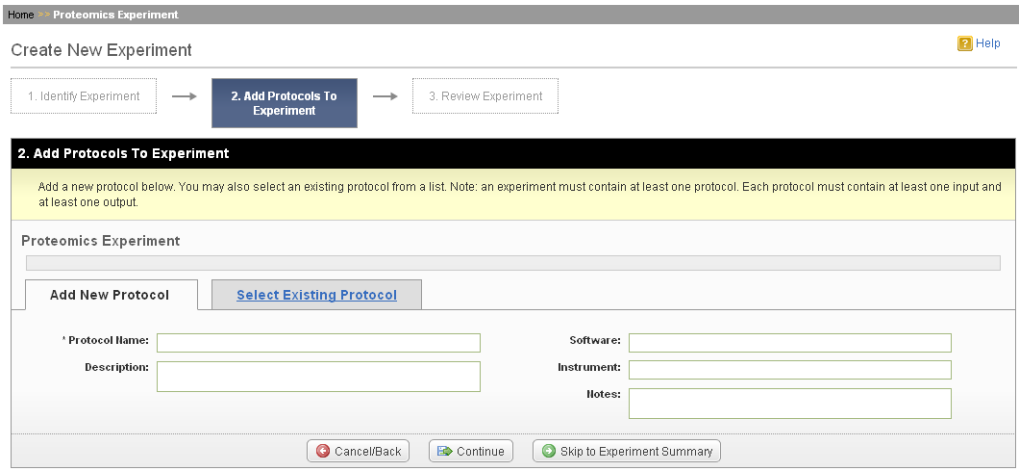


Figure 1.10 Add Protocols to Experiment step of the create new experiment process

protExpress has now created both the experiment and the first experiment run. You can add a protocol to that first experiment run now, as part of the create experiment process, or later, as you edit the experiment.

4. To add a protocol to the experiment now, click Continue. For more information, see *Adding Protocols to the Experiment* on page 14.

   To add a protocol to the experiment later, click Skip to Experiment Summary. For more information, see *Reviewing the Experiment* on page 19.

Adding Protocols to the Experiment

This section contains the following topics:

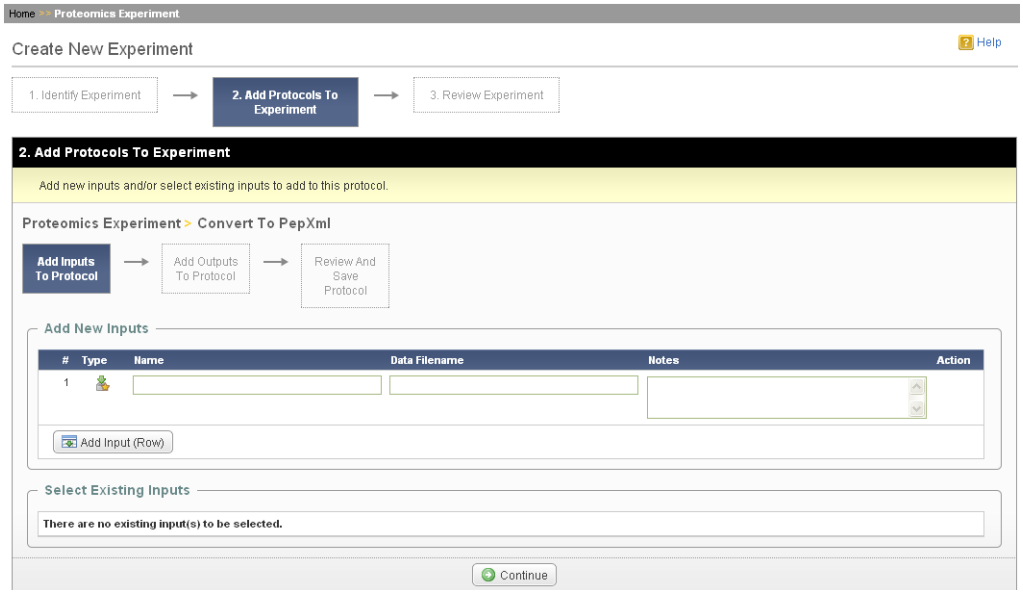
Adding a New Protocol to an Experiment

A protocol is a reusable entity that you can use across multiple *experiments*. However, an *instance* of a protocol applied to an *experiment run* is unique and you cannot apply it to other runs or experiments. In *CPAS*, each instance of a protocol in an experiment run is known as a *protocol application*.

Note: When you first create an experiment and add a protocol to it, you are simultaneously adding it to the experiment's first experiment run.

To add a new protocol to an experiment

1. On the Add Protocols to Experiment, Add New Protocol tab, in the Protocol Name field, enter a name for the new protocol. This is a required field.
2. Enter the protocol's description, associated software, and associated instrument, as well as the contact information for the protocol owner in the respective fields. Entering information in these fields is optional. Note that you can use the content of the Protocol Name and Description fields in a search for this protocol later.
3. Click Continue. The Add Inputs to Protocol page appears.



4. Add inputs to the protocol or skip this step and click Continue. For more information, see *Adding Inputs to the Protocol* on page 16.
5. Add outputs to the protocol or skip this step and click Continue. For more information, see *Adding Outputs to the Protocol* on page 17.

6. Review and save the protocol. For more information, see *Reviewing and Saving the Protocol* on page 16.

Adding an Existing Protocol to an Experiment

A protocol is a reusable entity that you can use across multiple *experiments*. However, an *instance* of a protocol applied to an *experiment run* is unique and you cannot apply it to other runs or experiments. In *CPAS*, each instance of a protocol in an experiment run is known as a *protocol application*.

Since a *protocol* is a reusable entity in protExpress, you can add an existing protocol to any *experiment* you created.

To add an existing protocol to an experiment

1. Click the **Select Existing Protocol** tab. All of the protocols you created appear in the list. To see all available protocols, click the **Display Protocols created by all users** checkbox.

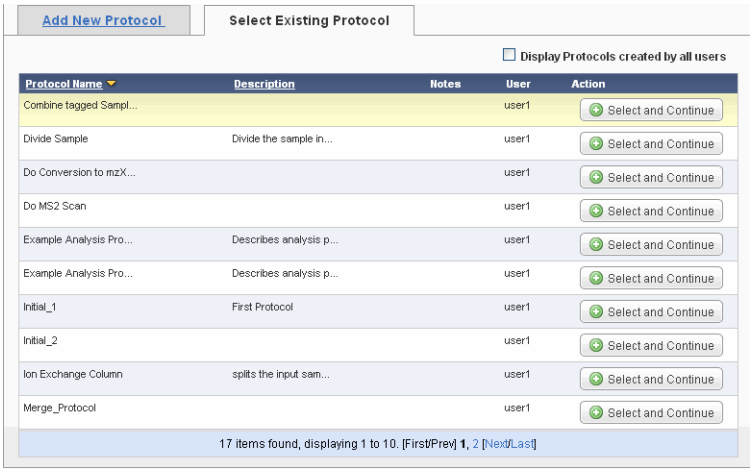


Figure 1.11 Select Existing Protocol tab

2. Find the protocol you want to select and click Select and Continue. The protocol appears in the Experiment Navigation.
3. Add inputs to the protocol or skip this step and click Continue. For more information, see *Adding Inputs to the Protocol* on page 16.
4. Add outputs to the protocol or skip this step and click Continue. For more information, see *Adding Outputs to the Protocol* on page 17.
5. Review and save the protocol. For more information, see *Reviewing and Saving the Protocol* on page 16.

Reviewing and Saving the Protocol

The final step when adding a *protocol* to an *experiment* is reviewing it for completeness and then saving it.

To review and save the protocol

1. Arrive at the Review and Save Protocol page. For more information, see *Adding Protocols to the Experiment* on page 14.

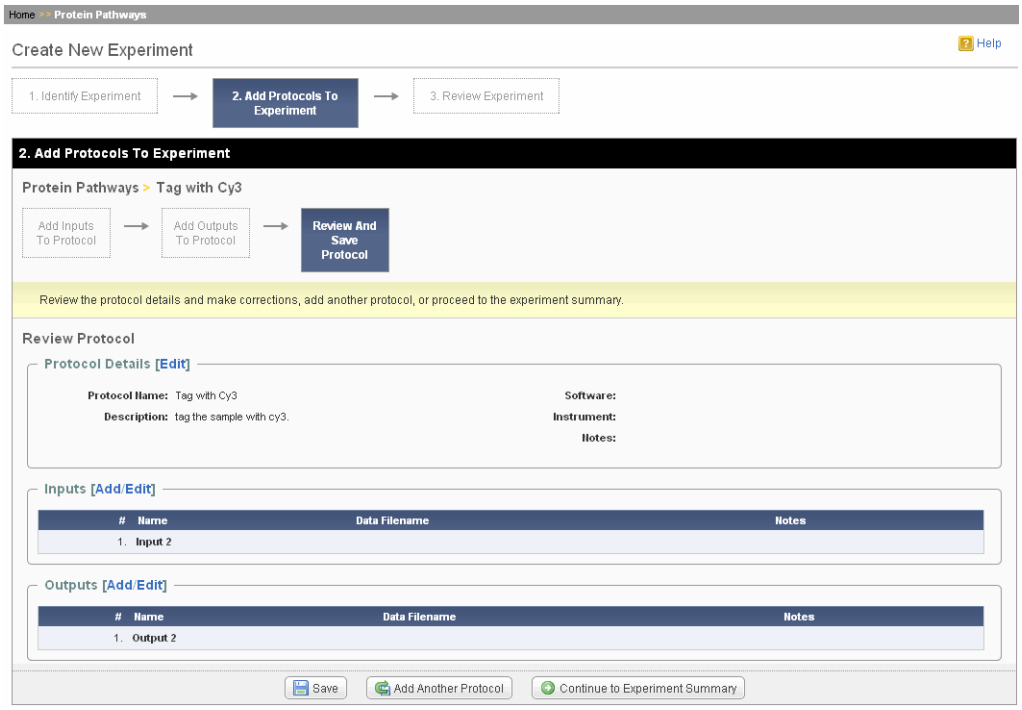


Figure 1.12 Review and Save Protocol page

2. Review the protocol details. Click **Edit** to change them.
3. Review the inputs and outputs. Click **Add** to add one to this protocol or **Edit** to change the data file name and/or notes.
4. Do one of the following:
   - To save your work, click Save.
   - To add another protocol to the experiment, click Add Another Protocol. For more information, see *Adding Protocols to the Experiment* on page 14.
   - To proceed to reviewing and finalizing the experiment, click Continue to Experiment Summary. For more information, see *Reviewing the Experiment* on page 19.

Adding Inputs to the Protocol

Examples of inputs include a tissue sample or a raw data file output from an LC/MS (Liquid Chromatography-Mass Spectrometry) machine.

Once you add an input to a protocol, you cannot add it as an input to any other protocol in the experiment run. You can select the output of a previous protocol as an input to a subsequent protocol in the experiment run. You can only do this once for each output.

To add a new input to the protocol

1. In the **Name** field, enter a name for the input. This is a required field.
2. In the **Data Filename** field, enter the file name of a data file associated with the input. This is an optional field. If the input is a material, leave this field blank.
3. In the **Notes** field, enter any other information pertinent to this input.
4. To add another input row, click 

and begin at step 1a of this procedure.
5. Click 

. The Add Outputs to Protocol page appears. For more information, see *Adding Outputs to the Protocol* on page 17.

To select an existing input

- In the Select Existing Inputs area, click 

in the row corresponding to the input you want to add. The only inputs that are available for you to select are outputs from previous protocols in the experiment run.

  The Add Outputs to Protocol page appears. For more information, see *Adding Outputs to the Protocol* on page 17.

Adding Outputs to the Protocol

A *protocol* (called a *protocol application* in *CPAS*), produces *material* and/or *data* outputs. These outputs are usually inputs into the next protocol in the experiment run.

You do not have to add an output now. To skip this step and add an output later, click 

without entering any other information.

To add a new output to the protocol

1. In the **Name** field, enter a name for the output. This is a required field.
2. In the **Data Filename** field, enter the file name of a data file associated with the output. This is an optional field. If the output is a material, leave this field blank.
3. In the **Notes** field, enter any other information pertinent to this output.
4. To add another input row, click 

and begin at step 1a of this procedure.

5. Click Continue. The Review and Save Protocol page appears.

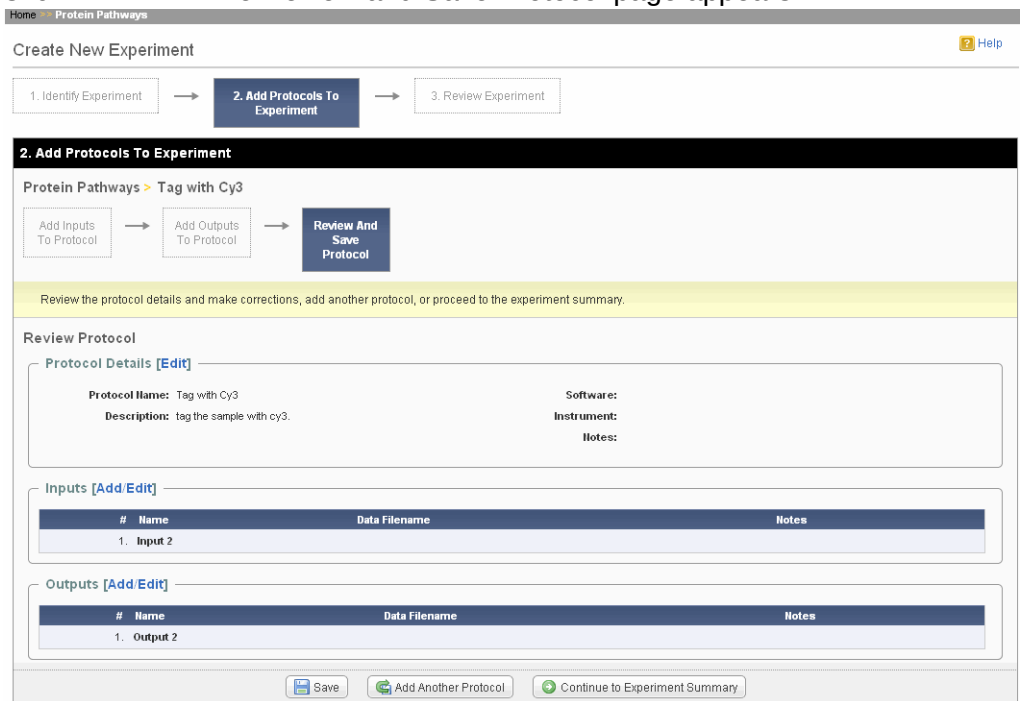


Figure 1.13 Review and Save Protocol page

6. Review and save the protocol. For more information, see *Reviewing and Saving the Protocol* on page 16.

Reviewing the Experiment

The last step in creating a new *experiment* is reviewing a summary of the experiment before finalizing it. While reviewing the experiment you have the opportunity to edit the experiment's identifying information and its protocol details.

To review and finalize the experiment

1. Arrive at the Review Experiment page. For more information, see *Creating a New Experiment* on page 11.

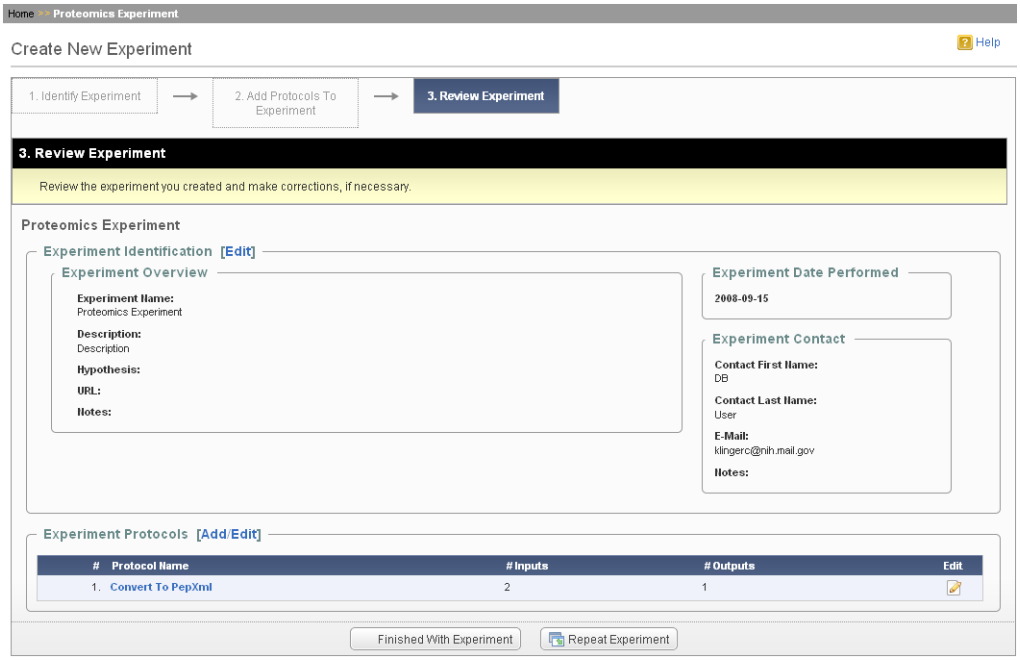


Figure 1.14 Review Experiment page

2. Do one of the following:
   - If no edits are required, click Finished With Experiment. The protExpress home page appears.
   - To repeat the experiment, click Repeat Experiment. You can modify any of the details of this repeated experiment. For more information, see *Editing Experiment Details* on page 20.

Editing an Experiment

As an experiment owner, you can edit any of the *experiment's* properties. Experiment properties in protExpress mirror those specified in the *XAR* format used by *CPAS*.

This section contains the following topics:

Editing Experiment Details

You can edit the experiment's name, description, hypothesis, URL, notes, date performed, and contact information.

To edit an experiment's details

1. Open the experiment you want to edit using one of the following methods:
   - In the My Recent Experiments area on the home page, click the **Edit** ( ) button in the row corresponding with the experiment you want to edit.
   - In search results, click the **Edit** ( ) button in the row corresponding with the experiment you want to edit. For more information on searching, see *Searching protExpress* on page 9.
   - On the View Experiment Details page, click Edit Experiment. For information on accessing this page, see *Viewing Experiment Details* on page 11.

   The Edit Experiment Details page appears.

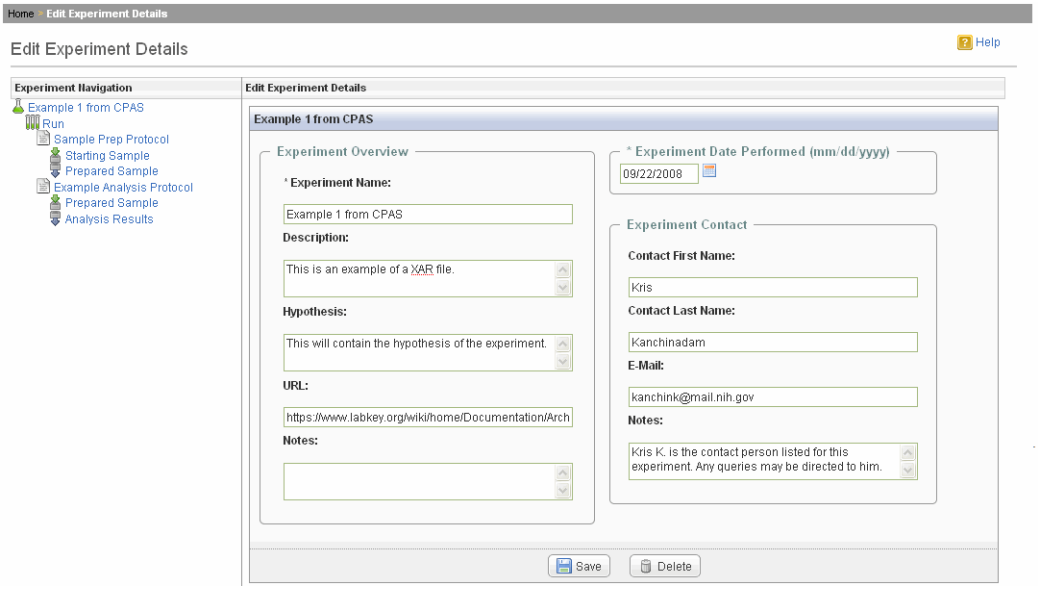


Figure 1.15 Edit Experiment Details page

2. As needed, edit the experiment's details in the text boxes on this page. Refer to the following table for more information about these details.

Field	***Expected Value***
Experiment Name (required field)	Experiment name
Description	Text comments about the experiment
Hypothesis	Hypothesis related to the experiment
URL	Web site with more information about the experiment
Notes	Additional information about the experiment
Experiment Date Performed (mm/dd/yyyy) (required field)	Enter the date the experiment was performed in mm/dd/yyyy format or click the calendar icon to select a date.
Contact First Name	Experiment owner's first name
Contact Last Name	Experiment owner's last name
Contact Email Address	Experiment owner's first name email address
Notes	Any other information that may help reach the experiment contact

Table 1.5 Properties of each experiment

3. When you have finished editing the experiment's details, click 

. A message indicating that the experiment has been successfully updated appears at the top of the page.

Note: Clicking 

removes the experiment from the database. Use with caution.

Editing an Experiment Run

You can edit the *experiment run's* name, date performed, and notes. You can also repeat the run, delete the run, and add more protocols to the run.

This section includes the following topics.

Editing Experiment Run Details

You can edit the experiment run's name, date performed, and notes.

To edit an experiment run's details

1. Open the experiment containing the experiment run you want to edit using one of the following methods:
   - In the My Recent Experiments area on the home page, click the **Edit** ( ) button in the row corresponding with the experiment you want to edit.
   - In search results, click the **Edit** ( ) button in the row corresponding with the experiment you want to edit. For more information on searching, see *Searching protExpress* on page 9.
   - On the View Experiment Details page, click Edit Experiment. For information on accessing this page, see *Viewing Experiment Details* on page 11.
2. The Edit Experiment Details page appears.

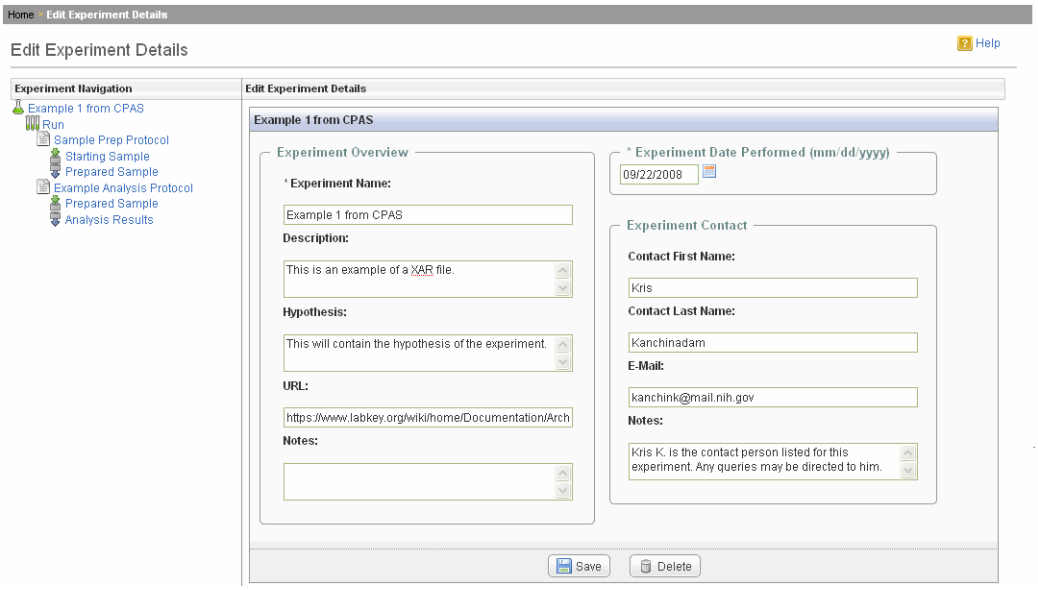


Figure 1.16 Edit Experiment Details page

3. In the Experiment Navigation on the left, click the experiment run you want to edit. Experiment runs are preceded by . The experiment run details appear in the Edit Experiment Details page.

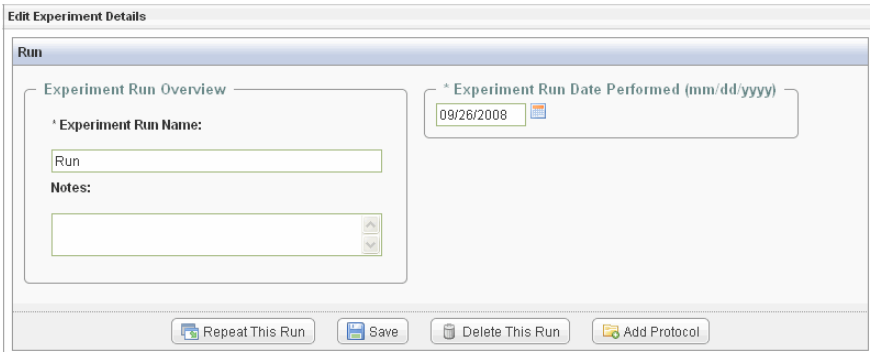


Figure 1.17 Experiment run details in the Edit Experiment Details page

4. Edit the experiment run's name, date performed, and notes as needed by entering new information in the respective fields.
5. Click Save. A message appears at the top of the page to note that the experiment run has been successfully updated. If you edited the experiment run's name, the new name appears in the Experiment Navigation.

   Note: Experiment runs are listed alphabetically in the Experiment Navigation.

Repeating an Experiment Run

You may want to base a new *experiment run* on an existing one. When you repeat an experiment you duplicate the experiment run's name, date performed, notes, and included *protocol applications*. You must add new inputs and outputs to those protocol applications.

To repeat an experiment run

1. Open the experiment containing the experiment run you want to edit using one of the following methods:
   - In the My Recent Experiments area on the home page, click the **Edit** ( ) button in the row corresponding with the experiment you want to edit.
   - In search results, click the **Edit** ( ) button in the row corresponding with the experiment you want to edit. For more information on searching, see *Searching protExpress* on page 9.
   - On the View Experiment Details page, click Edit Experiment. For information on accessing this page, see *Viewing Experiment Details* on page 11.
2. The Edit Experiment Details page appears.

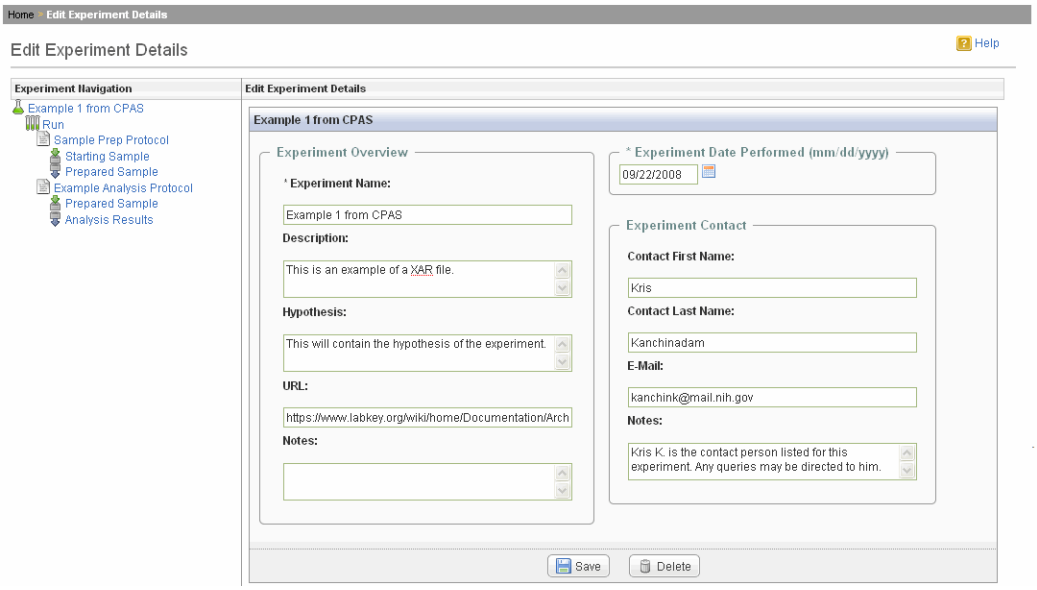


Figure 1.18 Edit Experiment Details page

3. In the Experiment Navigation on the left, click the experiment run you want to edit. Experiment runs are preceded by . The experiment run details appear in the Edit Experiment Details page.

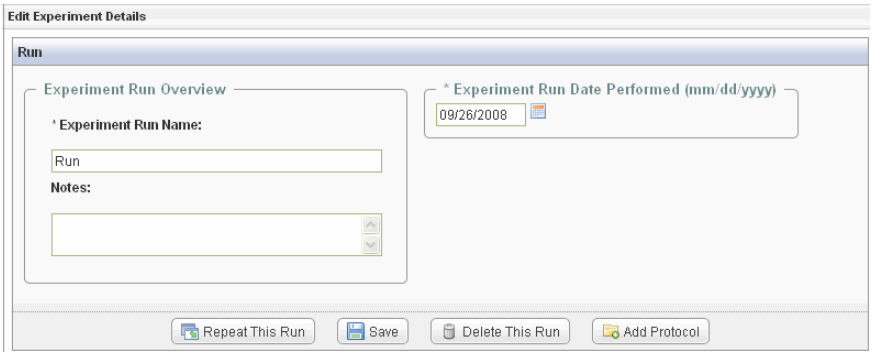


Figure 1.19 Experiment run details in the Edit Experiment Details page

4. Click Repeat This Run. The run's details and its protocols are copied and appear in the Experiment Navigation.

Deleting an Experiment Run

Deleting an *experiment run* does not delete any *protocols* applied to it, though it does permanently delete any of the run's inputs and outputs.

To delete an experiment run

1. Open the experiment containing the experiment run you want to delete using one of the following methods:
   - In the My Recent Experiments area on the home page, click the **Edit** () button in the row corresponding with the experiment you want to edit.
   - In search results, click the **Edit** () button in the row corresponding with the experiment you want to edit. For more information on searching, see *Searching protExpress* on page 9.
   - On the View Experiment Details page, click Edit Experiment. For information on accessing this page, see *Viewing Experiment Details* on page 11.

2. The Edit Experiment Details page appears.

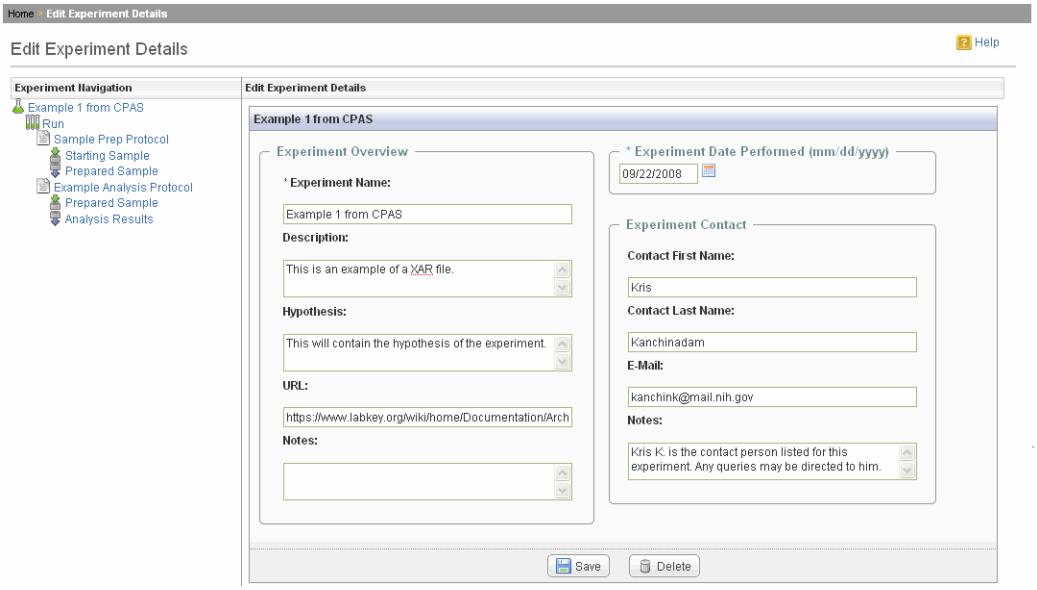


Figure 1.20 Edit Experiment Details page

3. In the Experiment Navigation on the left, click the experiment run you want to delete. Experiment runs are preceded by  . The experiment run details appear in the Edit Experiment Details page.

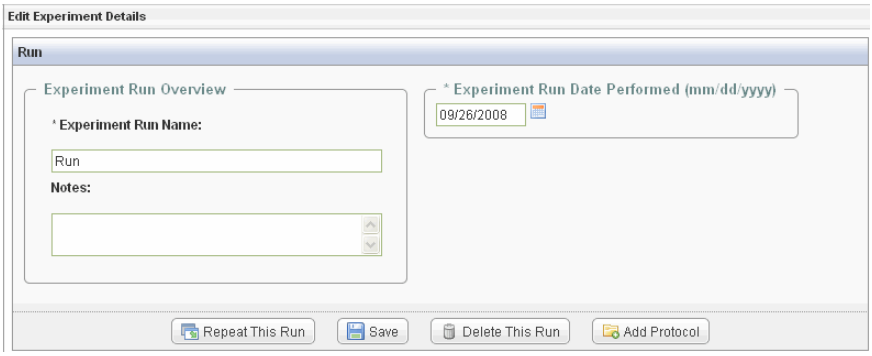


Figure 1.21 Experiment run details in the Edit Experiment Details page

4. Click 

. The experiment run is deleted and no longer appears in the Experiment Navigation.

Adding a Protocol to an Experiment Run

You can add a new or existing *protocol* to an *experiment run* by editing the *experiment*.

To add a protocol to the experiment run

1. Open the experiment containing the experiment run you want to add a new protocol to using one of the following methods:
   - In the My Recent Experiments area on the home page, click the **Edit** (✎) button in the row corresponding with the experiment you want to edit.
   - In search results, click the **Edit** (✎) button in the row corresponding with the experiment you want to edit. For more information on searching, see *Searching protExpress* on page 9.
   - On the View Experiment Details page, click Edit Experiment. For information on accessing this page, see *Viewing Experiment Details* on page 11.
2. The Edit Experiment Details page appears.

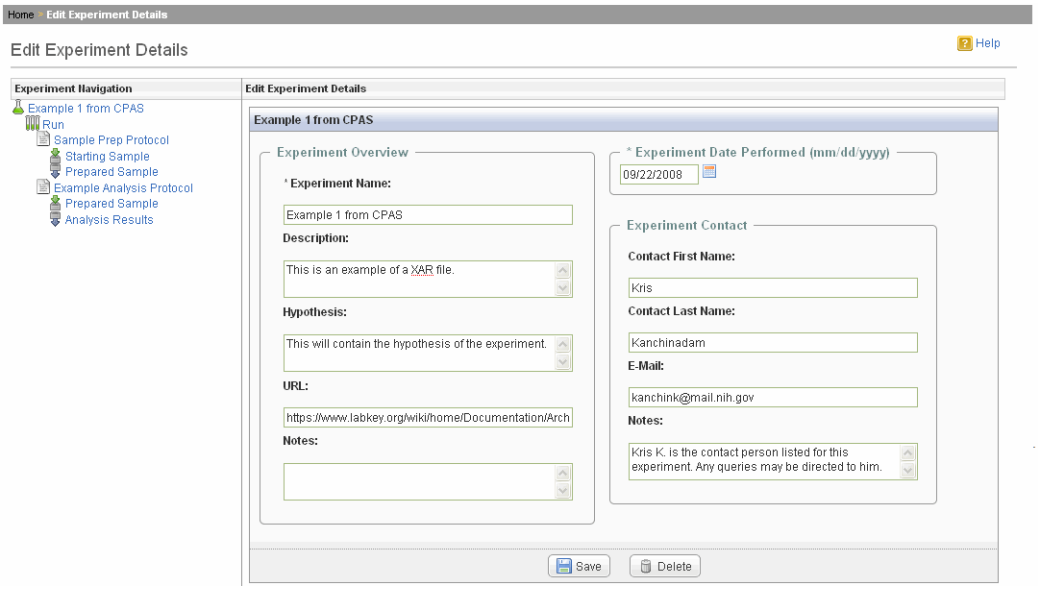


Figure 1.22 Edit Experiment Details page

3. In the Experiment Navigation on the left, click the experiment run you want to add a new protocol to. Experiment runs are preceded by . The experiment run details appear in the Edit Experiment Details page.

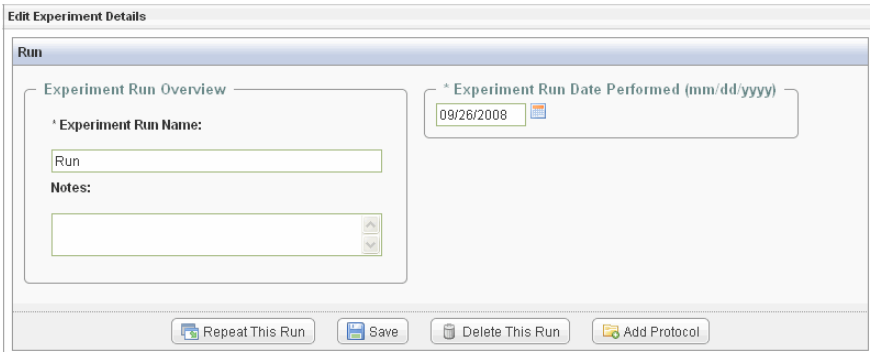


Figure 1.23 Experiment run details in the Edit Experiment Details page

4. Click Add Protocol. The Add New/Existing Protocol page appears.

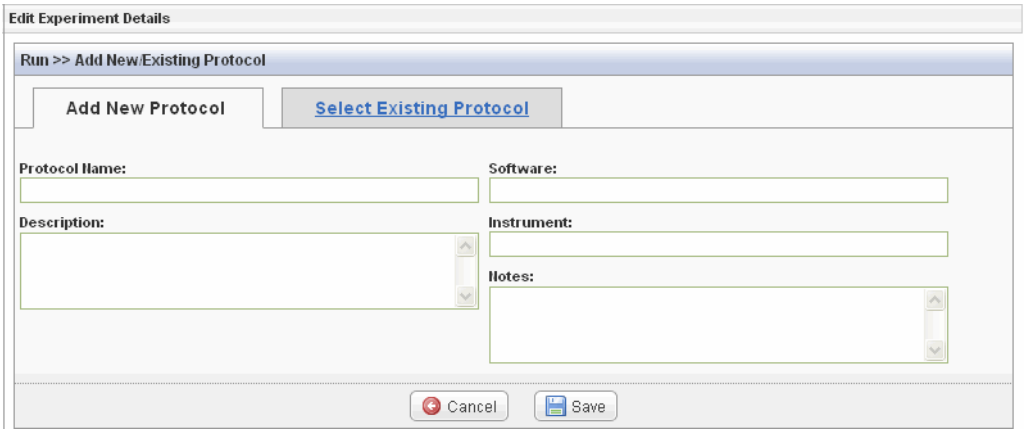


Figure 1.24 Add New/Existing Protocol page

5. Add a new protocol or select an existing protocol to add to the experiment run.

   To create a new protocol to add to the experiment run, do the following:

   a. In the Protocol Name field, enter a name for the new protocol. This is a required field.

   b. In the respective fields, enter the protocol's description, associated software, and associated instrument, as well as the contact information for the protocol owner. Entering information in these fields is optional.

   Note: You can use the content of the Protocol Name and Description fields in a search for this protocol later.

   c. Click Save. The protocol appears in the Experiment Navigation, under its experiment run.

To add an existing experiment to the experiment run

a. Select the **Select Existing Protocol** tab. All of the protocols you created appear. To see more protocols, select the **Display Protocols created by all users** checkbox.

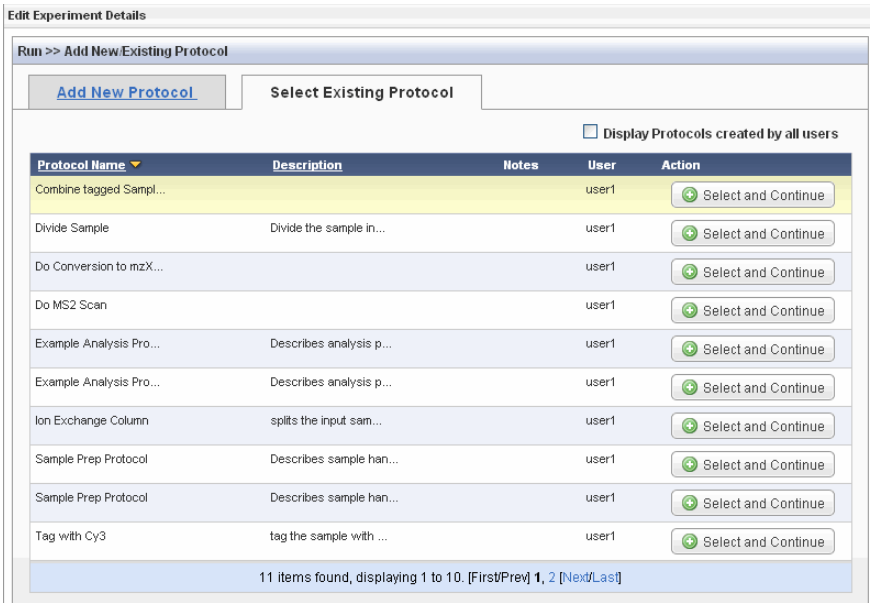


Figure 1.25 Add New/Existing Protocol page, Select Existing Protocol tab

b. In the row corresponding with the protocol you want to add to this experiment run, click Select and Continue. The protocol appears in the Experiment Navigation, under its experiment run.

For more information on adding new or existing protocols to the experiment run, see *Adding a New Protocol to an Experiment* on page 14 and *Adding an Existing Protocol to an Experiment* on page 15.

The new protocols appear in the Experiment Navigation.

Editing Protocol Details

As a *protocol* owner, you can edit any of the protocol's properties. Protocol properties in protExpress mirror those specified in the *XAR* format used by *CPAS*.

To edit protocol details

1. Find the protocol you want to edit on either the protExpress home page or by conducting a protocol search (see *Searching protExpress* on page 9 for more information on searching for a protocol), and click in the corresponding row. The Edit Protocol Details page appears.

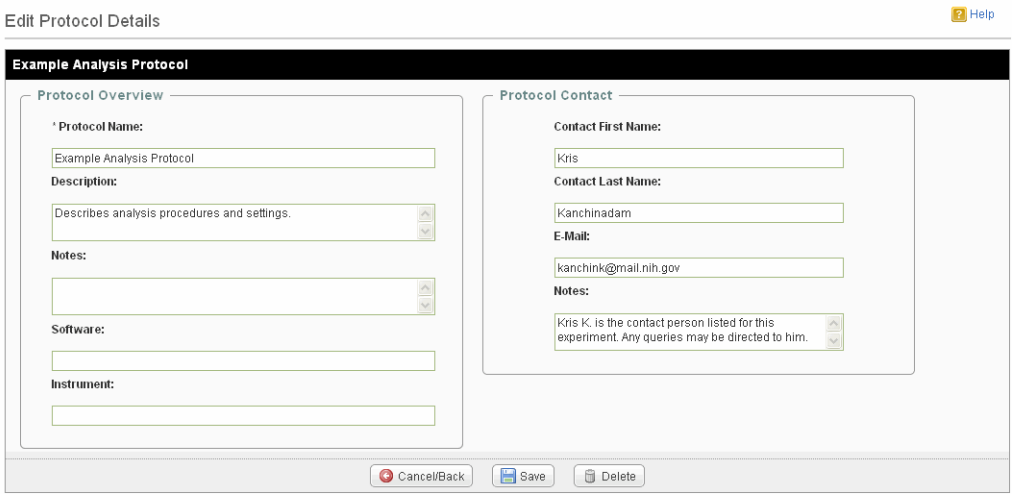


Figure 1.26 Edit Protocol Details page

2. As needed, edit the protocol's properties.
3. Do one of the following:
   - Click Save to save your changes. If you do not save your changes, you will lose them.
   - Click Cancel/Back to abandon your changes and return to the previous screen.
   - Click Delete to delete the protocol. Be cautious when doing this! Deleting a protocol also deletes its inputs and outputs.

Editing Input and Output Details

You can edit an input's name and data file name.

To edit input and output details

1. Open the experiment that contains the input or output you want to edit using one of the following methods:
   - In the My Recent Experiments area on the home page, click the **Edit** ( ) button in the row corresponding with the experiment you want to edit.
   - In search results, click the **Edit** ( ) button in the row corresponding with the experiment you want to edit. For more information on searching, see *Searching protExpress* on page 9.
   - On the View Experiment Details page, click Edit Experiment. For information on accessing this page, see *Viewing Experiment Details* on page 11.

   The Edit Experiment Details page appears.

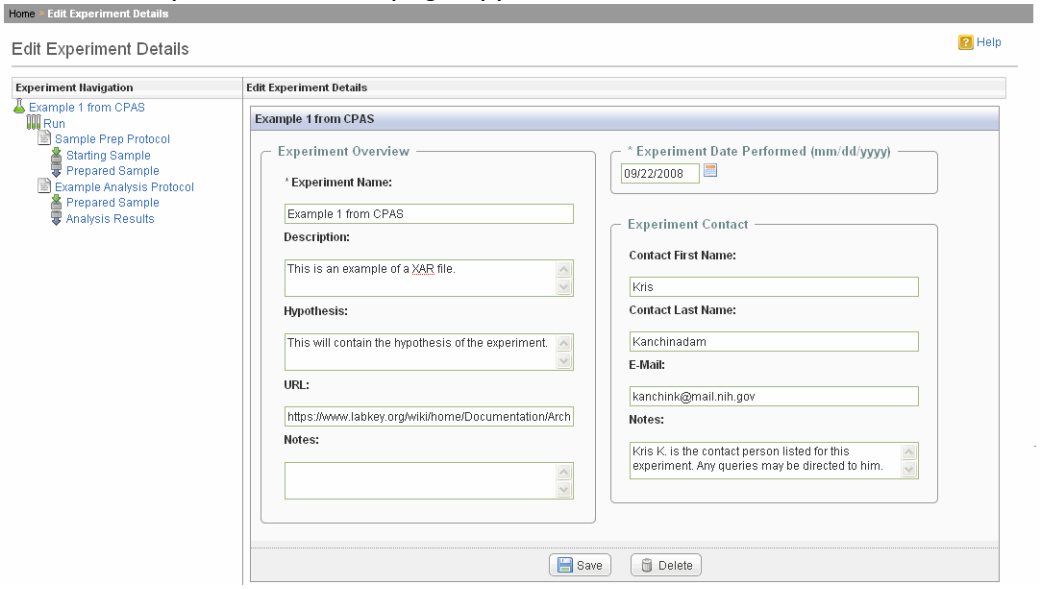


Figure 1.27 Edit Experiment Details page

2. In the Experiment Navigation on the left, click the input or output you want to edit. Inputs are preceded by and outputs are preceded by . The input or output details appear within the Edit Experiment Details page.

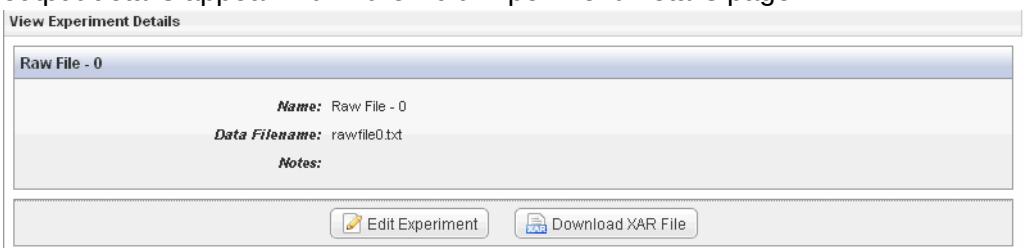


Figure 1.28 Input details within the Edit Experiment Details page

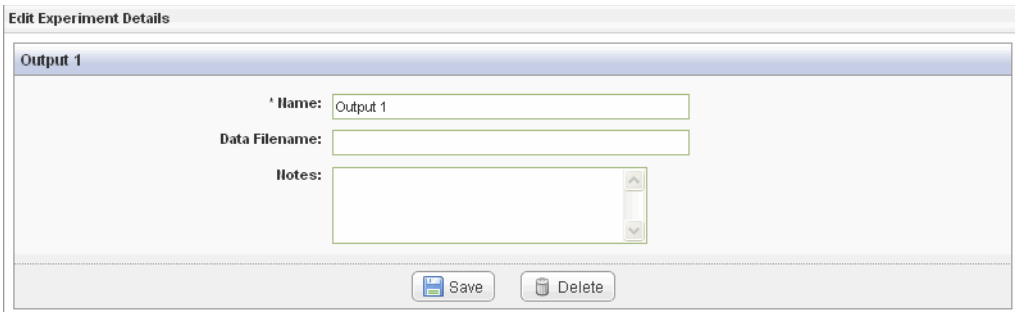


Figure 1.29 Output details within the Edit Experiment Details page

3. Edit the input or output's name, data file name, and notes as needed by overwriting information that may already be in those fields.
4. When you have finished editing the input or output's details, click Save. A message indicating that the input or output has been successfully updated appears at the top of the page.

   Note: To delete the input or output, click Delete. This removes the input or output from all protocols to which it has already been added.

Adding an Input to an Existing Experiment

Inputs are reusable entities within protExpress that you can apply to multiple *protocols*. You can either create a new input or add an existing input to an *experiment*.

To add an input to a protocol in an existing experiment

1. In the list of recent experiments on the protExpress home page or in the results of a search for experiments, open an experiment you created by clicking its Edit icon ( ). This should be the experiment that contains the protocol to which you want to add an input. For more information, see *Using the Home Page* on page 8 and *Searching protExpress* on page 9. The Edit Experiment Details page appears, displaying information about the experiment.

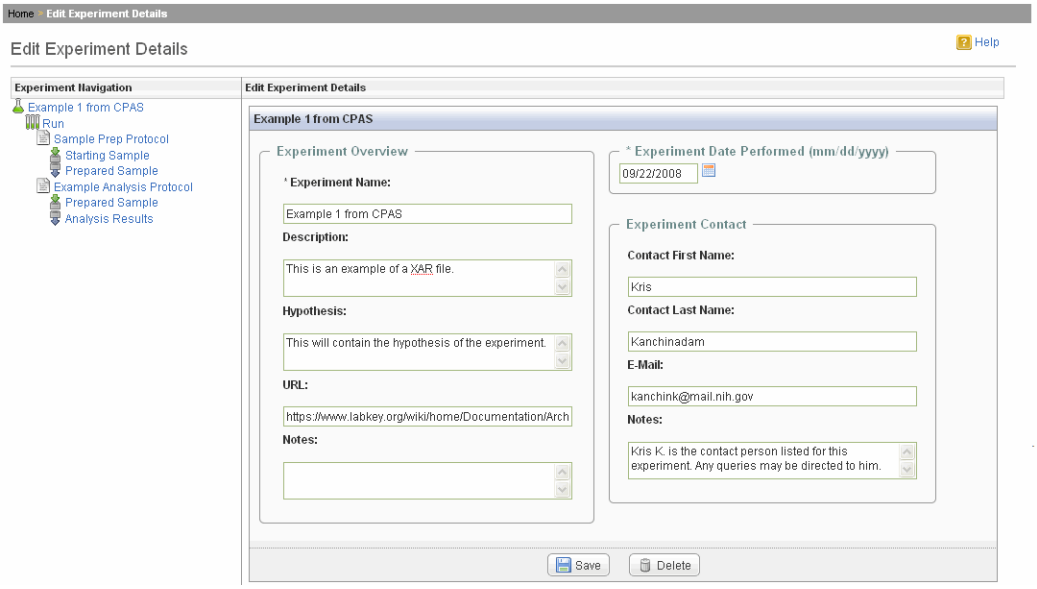


Figure 1.30 Edit Experiment Details page

2. In the Experiment Navigation on the left, select the protocol to which you want to add the input by clicking its name.

   Note: In the Experiment Navigation, protocols are preceded by .

The protocol details appear in the Edit Experiment Details page.

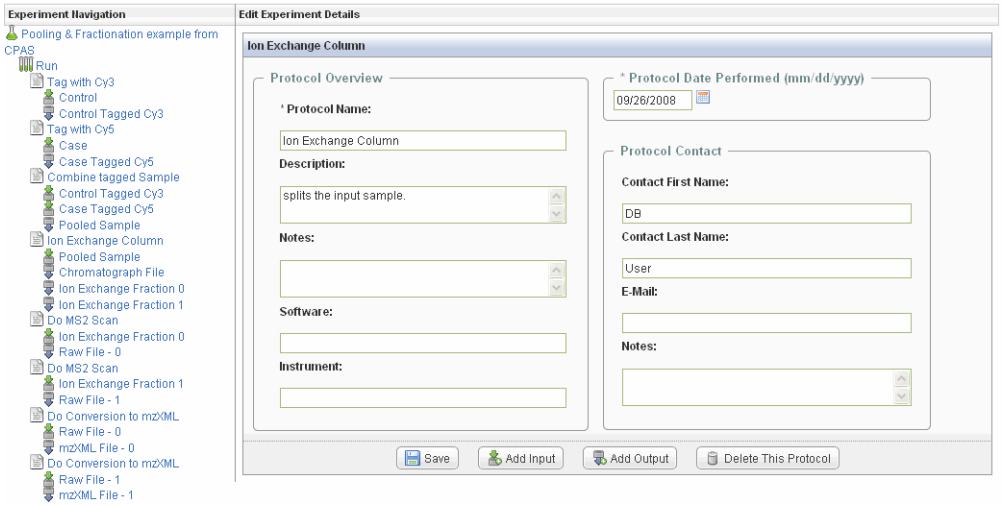


Figure 1.31 Edit Experiment Details page with a protocol selected

3. Click Add Input. Inputs appear in the Edit Experiment Details page.

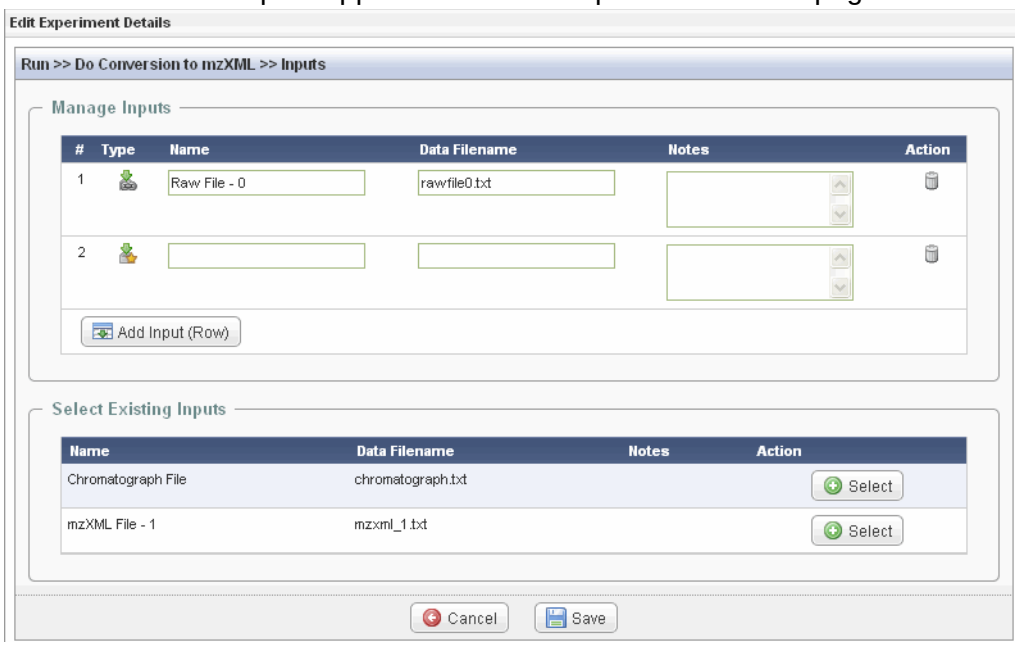


Figure 1.32 Inputs on the Edit Experiment Details page

4. If an empty row is not already in the Manage Inputs area, click Add Input (Row). An empty row for a new input appears.
5. In the **Name** field, enter a name for the input. This is a required field.
6. In the **Data Filename** field, enter the file name of a data file associated with the input. This is an optional field. If the input is a material, leave this field blank.
7. Click Save. The protocol details appear on the Edit Experiment page. You can see the input you added in the Experiment Navigation, under its protocol.

Constructing LSIDs

LSID is an emerging standard (http://www.omg.org/docs/dtc/04-05-01.pdf). They are a specific form of URN (Universal Resource Name) and a solution to a difficult problem: how to identify entities unambiguously across multiple systems. While LSIDs tend to be long strings, they are generally easier to use than other approaches to the identifier problem, such as large random numbers or Globally Unique IDs (GUIDs). LSIDs are easier to use because they are readable by humans, and because the LSID parts can be used to encode information about the object being identified.

LSIDs are multi-part strings with the parts separated by colons. They are of the form:

```
urn:lsid:<AuthorityID>:<NamespaceID>:<ObjectID>:<RevisionID>
```

The variable portions of the LSID are set as follows:

Variable	***Definition***
`<AuthorityID>`	Identifies the issuer of the LSID. Usually, an Internet domain name. Example, nci.nih.gov
`<NamespaceID>`	Identifies the context in which a particular object id is unique. Example – Experiment, or Protocol.
`<ObjectID>`	Identifies the object within a particular namespace. For example, This could be the Id used to identify an object in a database.
`<RevisionID>`	An optional version string

Table 1.6 Definitions of LSID variables

LSID Example

Here is an example of a valid LSID:

```
urn:lsid:nci.nih.gov:Protocol:SamplePrep.Analysis
```

This LSID could be used to identify a specific protocol for a procedure called `Analysis`. In this example, the authority is set to `nci.nih.gov`. The namespace indicates that the LSID identifies a Protocol, and the object ID is `SamplePrep.Biotinylation` (which should uniquely identify the protocol in the system).

protExpress and LSIDs

The XAR format, supported by protExpress, uses LSIDs to identify entities such as inputs, outputs, and experiment and protocol definitions. However, protExpress does not use LSIDs to identify these entities in its database. protExpress generates LSIDs on the fly when exporting an experiment into the XAR format.

A valid LSID generated by protExpress could be:

```
urn:lsid:nci.nih.gov:Protocol:8:1.0
```

Here, the LSID identifies a protocol in the system with and ID of 8 (this ID uniquely identifies the protocol in the system).

Note: The different parts of an LSID (Authority ID, Namespace ID, and Revision ID) are configurable in protExpress. For more information on how to configure the LSIDs, refer to the section "Update Configuration Parameters in the Database" in the *protExpress Local Installation Guide*.

APPENDIX A

PROTEXPRESS GLOSSARY

This glossary defines acronyms, abbreviations, and terminology used in protExpress.

Term	*Definition*
CPAS (Computational Proteomics Analysis System)	A web-based system built on the LabKey Server for managing, analyzing, and sharing high volumes of tandem mass spectrometry data. CPAS employs open-source tools provided by the Trans Proteomic Pipeline, developed by the Institute for Systems Biology.
Data	A data object refers to a measurement value or control value, or a set of such values. Data objects can be references to data stored in files or in database tables, or they can be complete in themselves. Data objects can be copied and reused a limitless number of times. Data objects are often generated by instruments or computers, which may make it important to keep track of machine models and software versions in the applications that create data objects.
Experiment	A grouping of experiment runs for the purpose of comparison or export. Currently an experiment run belongs to one and only one experiment, which must live in the same folder in CPAS.
Experiment Run	A series of experimental steps performed on specific inputs, producing specific outputs.
LDAP (Lightweight Directory Access Protocol)	An application protocol for querying and modifying directory services running over TCP/IP.

Table A.1 Glossary of terms used in protExpress

Term	Definition
LSID (Life Science Identifier)	An emerging standard (http://www.omg.org/docs/dtc/04-05-01.pdf) by which biologically significant resources are uniquely named. LSIDs are multi-part strings with the parts separated by colons. They are of the form: `urn:lsid:<AuthorityID>:<NamespaceID>:<ObjectID>:<RevisionID>` The XAR format, supported by protExpress, uses LSIDs to identify entities such as inputs, outputs, and experiment and protocol definitions. However, protExpress does not use LSIDs to identify these entities in its database. protExpress generates LSIDs on the fly when exporting an experiment into the XAR format.
Material	A material object refers to some biological sample or processed derivative of a sample. Examples of material objects include blood, tissue, protein solutions, dyed protein solutions, and the content of wells on a plate. Materials have a finite amount and usually a finite life span, which often makes it important to track measurement amounts and storage conditions for these objects.
protExpress	A proteomics experiment and protocol data management tool that you can use to search and administer proteomics experiment and protocol data through online forms
Proteomics	Large-scale study of proteins, particularly their structures and functions
Protocol	A description of how an experimental step is performed. A Protocol object describes an operation that takes as input some Material and/or Data objects, and produces as output some Material and/or Data objects. In protExpress, a protocol is a reusable entity that can be associated with any experiment.
Protocol Application	The application of a protocol to some specific set of inputs, producing some outputs. A protocol application belongs to an experiment run, whereas protocol objects themselves are often shared across runs. When the same protocol is applied to multiple inputs in parallel, the experiment run will contain multiple protocol applications object for that protocol object. Protocol applications have associated parameter values for the parameters declared by the protocol.
XAR File	A compressed, single-file package of experimental data and descriptions. A XAR file expands into a single root folder with any combination of subfolders containing experimental data and settings files. At the root of a XAR file is a xar.xml file that serves as a manifest for the contents of the XAR as well as a structured description of the experiment that produced the data.

Table A.1 Glossary of terms used in protExpress

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