

PROTEXPRESS USER'S GUIDE



NATIONAL[®]
CANCER
INSTITUTE

Center for Biomedical Informatics
and Information Technology

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ABOUT THIS GUIDE

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

- [Purpose](#) on this page
- [Audience](#) on this page
- *Topics Covered* on page 2
- *Additional References* on page 2
- *Text Conventions Used* on page 2
- *Credits and Resources* on page 3

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 35 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.
<i>Italics</i>	Highlights references to other documents, sections, figures, and tables.	See <i>Figure 4.5</i> .
<i>Italic boldface monospace type</i>	Represents text that you type.	In the New Subset text box, enter <i>Proprietary Proteins</i> .
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
Krishna Kanchinadam ²	Nonna Rabinovich ⁵	Carl Schaefer ¹	Carolyn Kelley Klinger ⁴
Scott Miller ²	Tom Boal ⁵	Anand Basu ¹	Krishna Kanchinadam ²
Steve Matyas ²		Xiaopeng Bian ¹	Mahidhar Narra ⁶
		Bill Mason ²	
		Brent Gendleman ²	
Systems and Application Support			
Bob Wysong ³	Andrea Johnson ³	Ralph Rutherford ³	Sriram Kalyansundaram ³
Nimish Shah ³			
¹ National Cancer Institute Center for Biomedical Informatics and Information Technology (NCI CBIIT)		² 5AM Solutions	³ Terrapin Systems
⁴ Lockheed Martin Management System Designers	⁵ NARTech	⁶ Stelligent	

Contacts and Support	
NCICB Application Support	http://ncicbsupport.nci.nih.gov/sw/ Telephone: 301-451-4384 Toll free: 888-478-4423

CHAPTER 1

WORKING WITH PROTEXPRESS

This section includes the following topics:

- *Getting Started* on page 5
- *Searching protExpress* on page 9
- *Viewing Experiment Details* on page 11
- *Creating a New Experiment* on page 11
- *Editing an Experiment* on page 20

Getting Started

This section includes the following topics:

- *Registering Users* on page 5
- *Logging In* on page 7
- *Resetting Your Password* on page 7
- *Using the Home Page* on page 8

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.

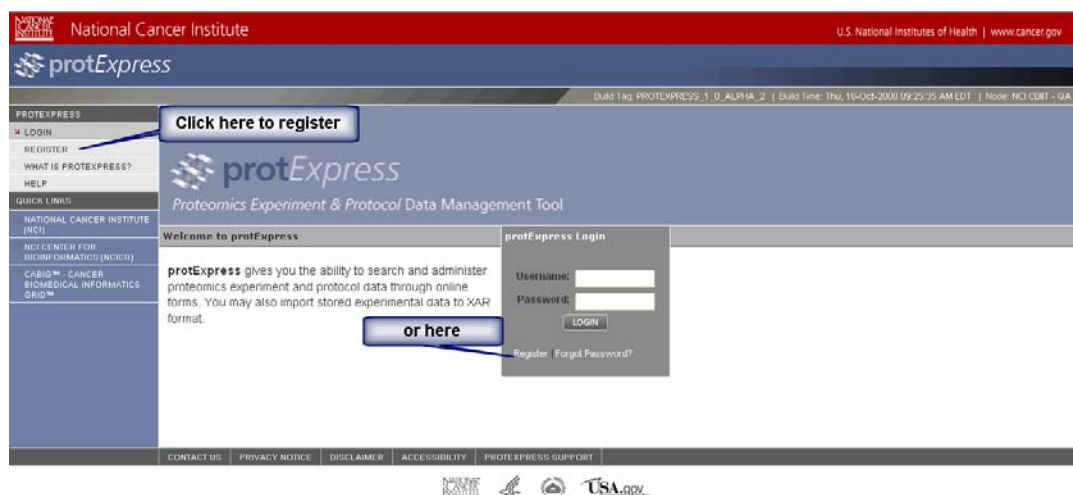


Figure 1.1 protExpress home page with registration links

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.

Register Help

Become a protExpress User

Welcome to protExpress. Submit the form below to request access to protExpress. Required fields are highlighted and have *asterisks*.

Security Information

Do you have an LDAP Account?: ☒ Yes ☐ No

Username:

Password:

Account Details

First Name:

Middle Initial:

Last Name:

E-Mail:

Organization:

Address Line 1:

Address Line 2:

City:

Country:

State:

Province:

Postal Code:

Phone:

Fax:

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.

Register

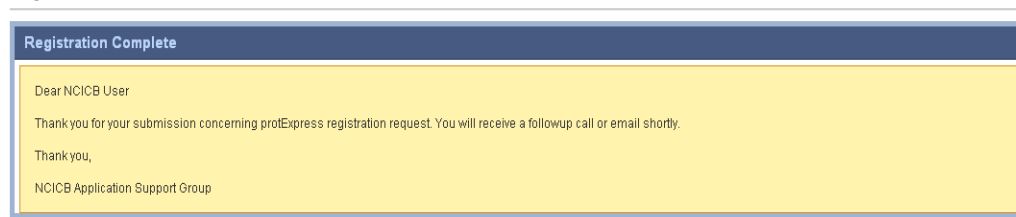
[Help](#)

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	<i>Searching protExpress</i> on page 9
Create a new experiment	<i>Creating a New Experiment</i> on page 11
Edit a recent experiment	<i>Editing an Experiment</i> on page 20
Download a recent experiment in XAR format	<i>Viewing Experiment Details</i> 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.

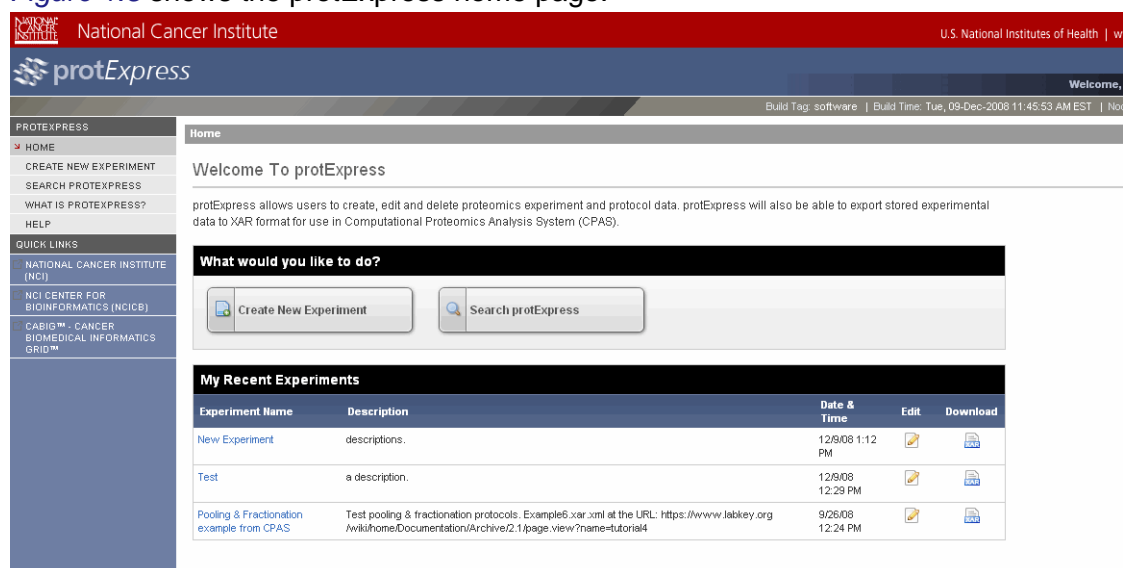


Figure 1.5 protExpress Home Page

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 <i>Viewing Experiment Details</i> on page 11.

Table 1.2 Explanation of Icons Used in protExpress

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

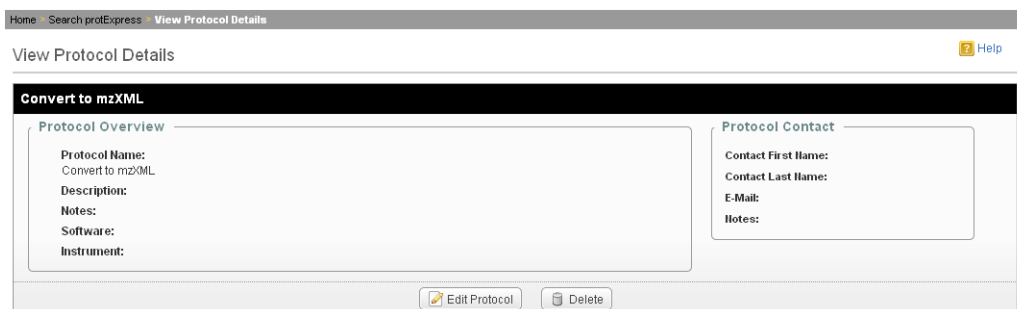


Figure 1.7 View Protocol Details page

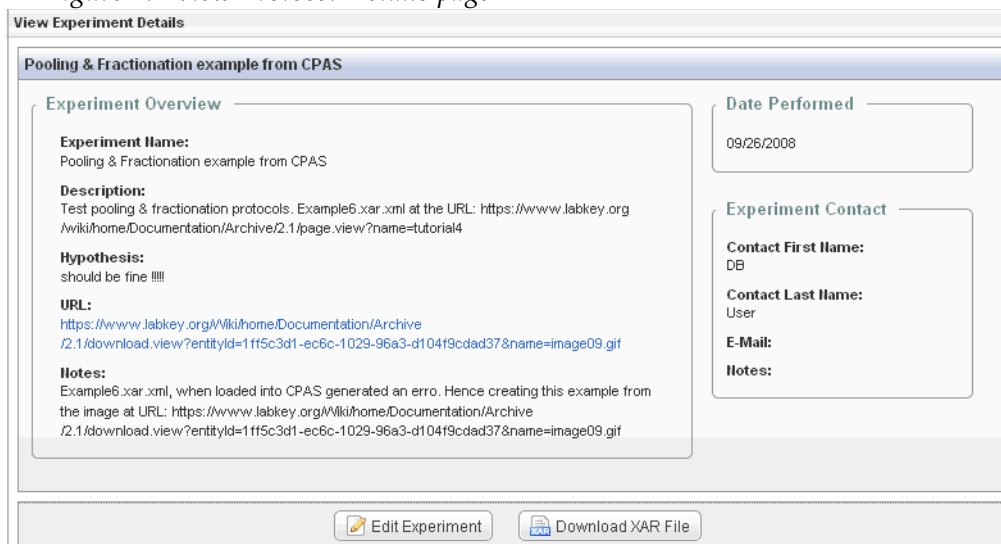


Figure 1.8 View Experiment Details page

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.
 Edit Experiment		Click to edit experiment details including the experiment as a whole, experiment runs, protocols, inputs, and outputs. For more information, see <i>Editing an Experiment</i> on page 20.
 Download XAR File		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

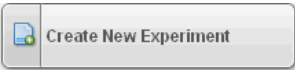
1. Identify the experiment. For more information, see *Identifying the Experiment* on page 12.
2. Add one or more protocols to the experiment. For more information, see *Adding Protocols to the Experiment* on page 14.
3. Add one or more inputs and outputs to the protocol. For more information, see *Adding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

- 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

- 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.

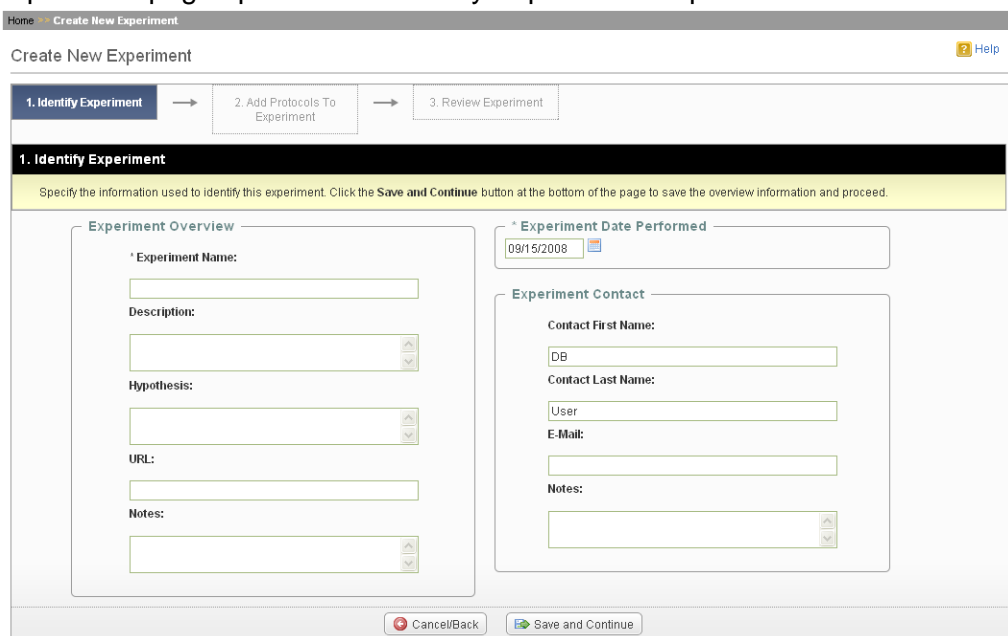


Figure 1.9 Identify experiment step in the create new experiment process

- 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 . The Add Protocols to Experiment page appears.

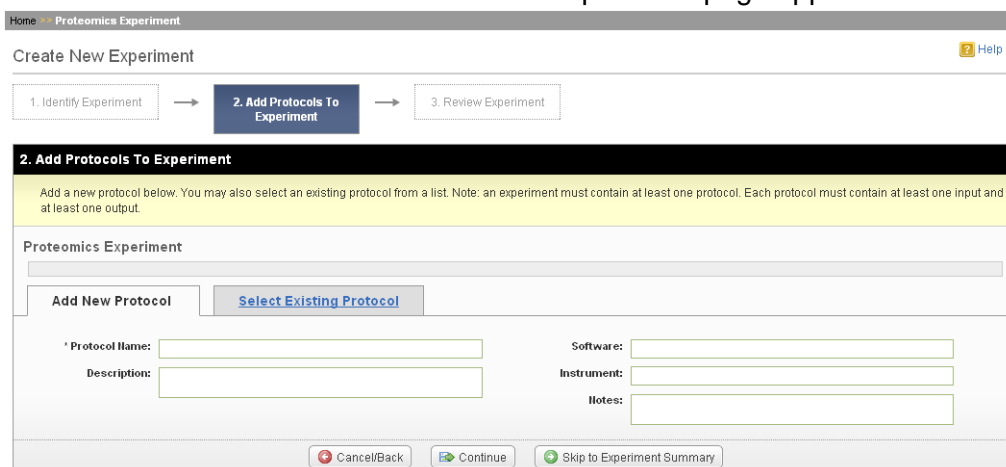




Figure 1.10 Add Protocols to Experiment step of the create new experiment process

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 . For more information, see *Adding Protocols to the Experiment* on page 14.

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

Adding Protocols to the Experiment

This section contains the following topics:

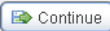
- *Adding a New Protocol to an Experiment* on page 14
- *Adding an Existing Protocol to an Experiment* on page 15
- *Reviewing and Saving the Protocol* on page 16

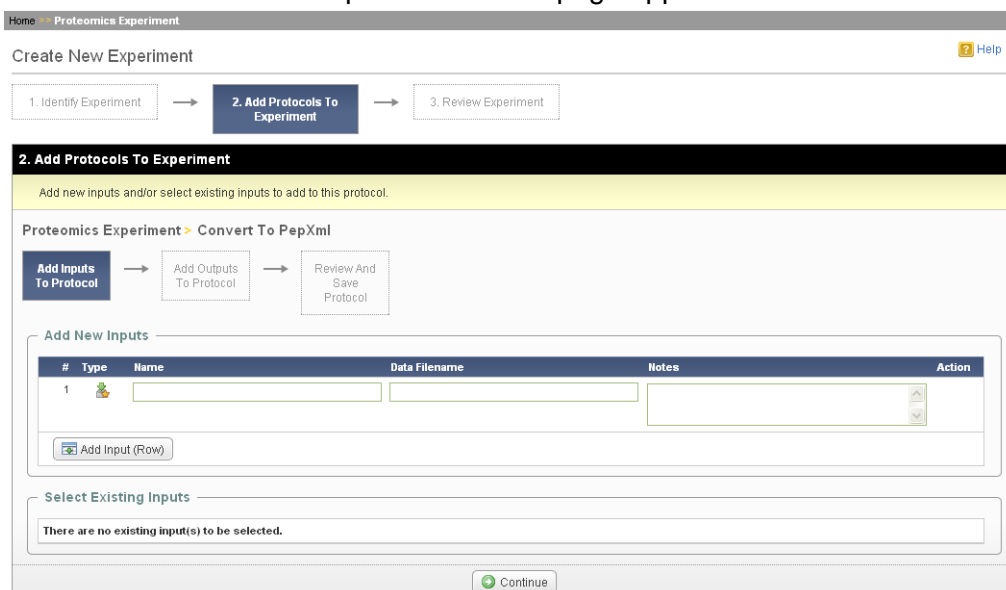
Adding a New Protocol to an Experiment

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 . The Add Inputs to Protocol page appears.



Home > Proteomics Experiment

Create New Experiment Help

1. Identify Experiment → **2. Add Protocols To Experiment** → 3. Review Experiment



2. Add Protocols To Experiment


Add new inputs and/or select existing inputs to add to this protocol.

Proteomics Experiment > Convert To PepXML

Add Inputs To Protocol → Add Outputs To Protocol → Review And Save Protocol


Add New Inputs



#	Type	Name	Data Filename	Notes	Action
1					



Select Existing Inputs

There are no existing input(s) to be selected.



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

- 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

- 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.

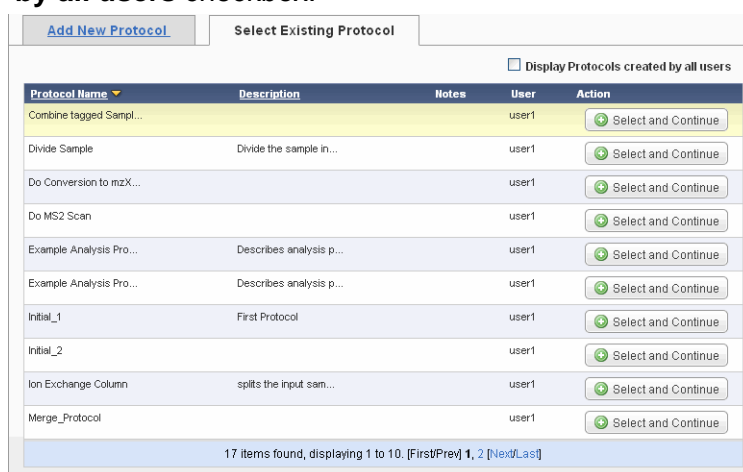
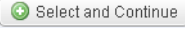




Figure 1.11 Select Existing Protocol tab

- Find the protocol you want to select and click . The protocol appears in the Experiment Navigation.
- Add inputs to the protocol or skip this step and click . For more information, see *Adding Inputs to the Protocol* on page 16.
- Add outputs to the protocol or skip this step and click . For more information, see *Adding Outputs to the Protocol* on page 17.
- 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

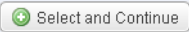
Examples of inputs include a tissue sample or a raw data file output from an LC/MS (Liquid Chromatography-Mass Spectrometry) machine.

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

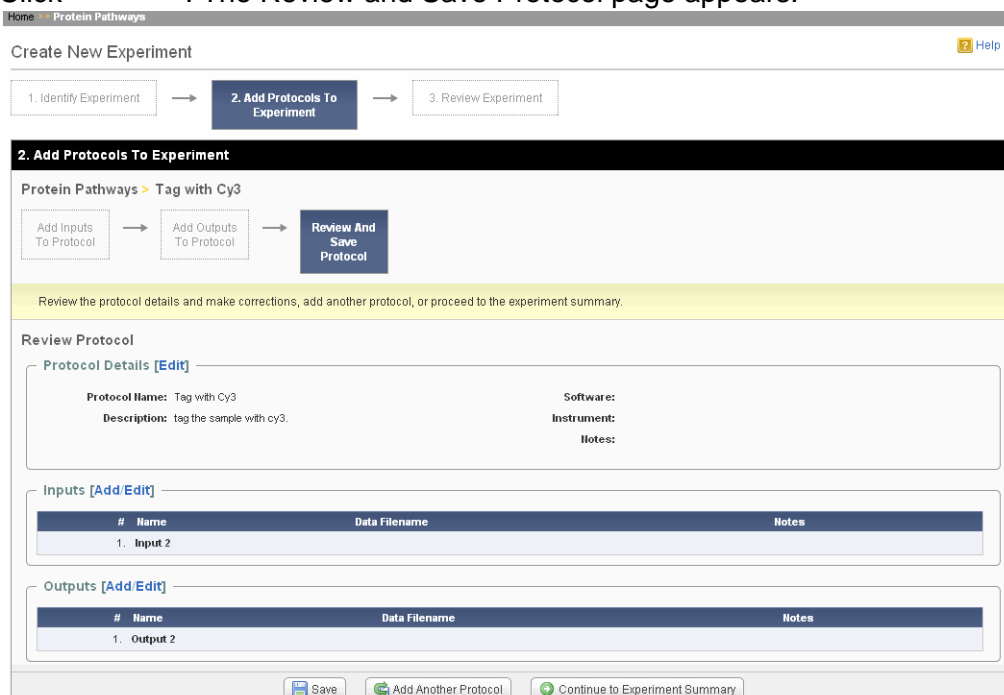
A *protocol* (called a *protocol application* in *CPAS*), produces *material* and/or *data* outputs. These outputs are usually inputs into the next protocol in the experiment run.

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.

- Click . The Review and Save Protocol page appears.



Home > Protein Pathways

Create New Experiment Help

1. Identify Experiment → **2. Add Protocols To Experiment** → 3. Review Experiment

2. Add Protocols To Experiment

Protein Pathways > Tag with Cy3

Add Inputs To Protocol → Add Outputs To Protocol → **Review And Save Protocol**

Review the protocol details and make corrections, add another protocol, or proceed to the experiment summary.

Review Protocol

Protocol Details [\[Edit\]](#)

Protocol Name: Tag with Cy3
Description: tag the sample with cy3.
Software:
Instrument:
Notes:

Inputs [\[Add Edit\]](#)

#	Name	Data Filename	Notes
1.	Input 2		

Outputs [\[Add Edit\]](#)

#	Name	Data Filename	Notes
1.	Output 2		

[Save](#) [Add Another Protocol](#) [Continue to Experiment Summary](#)

Figure 1.13 Review and Save Protocol page

- 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.

Home > Proteomics Experiment

Create New Experiment Help

1. Identify Experiment → 2. Add Protocols To Experiment → **3. Review Experiment**

3. Review Experiment

Review the experiment you created and make corrections, if necessary.

Proteomics Experiment

Experiment Identification [\[Edit\]](#)

Experiment Overview

Experiment Name:
Proteomics Experiment

Description:
Description

Hypothesis:

URL:

Notes:

Experiment Date Performed
2008-09-15

Experiment Contact

Contact First Name:
DB

Contact Last Name:
User

E-Mail:
klingerdc@nih.mail.gov

Notes:

Experiment Protocols [\[Add Edit\]](#)

#	Protocol Name	#Inputs	#Outputs	Edit
1.	Convert To PepXml	2	1	Edit

[Finished With Experiment](#) [Repeat Experiment](#)

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](#) on page 20
- [Editing an Experiment Run](#) on page 21
- [Editing Protocol Details](#) on page 29
- [Editing Input and Output Details](#) on page 30
- [Adding an Input to an Existing Experiment](#) on page 32

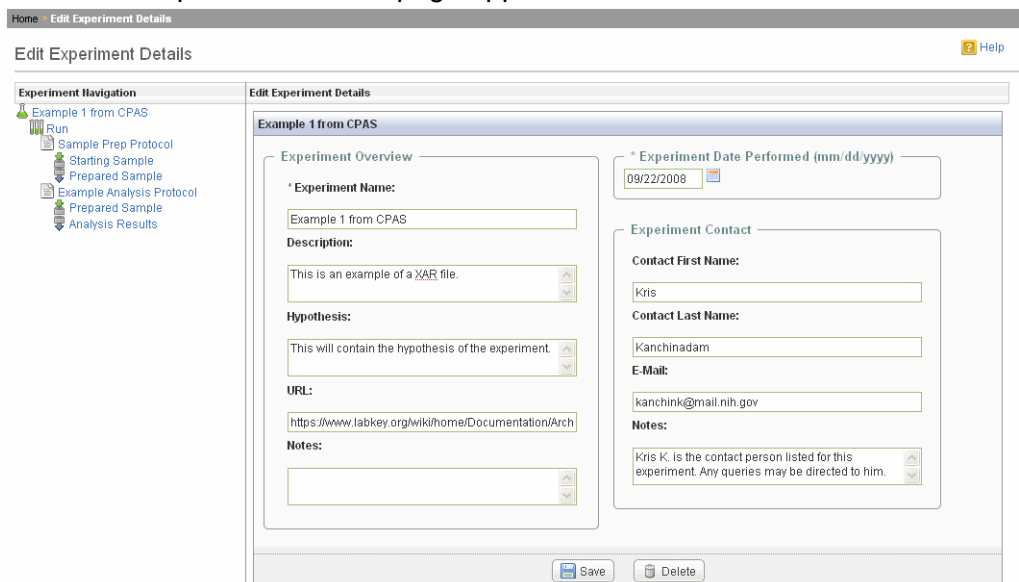
Editing Experiment Details

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 . For information on accessing this page, see [Viewing Experiment Details](#) on page 11.

The Edit Experiment Details page appears.




The screenshot shows the 'Edit Experiment Details' page. On the left is a sidebar titled 'Experiment Navigation' with a tree view containing: 'Example 1 from CPAS', 'Run', 'Sample Prep Protocol', 'Starting Sample', 'Prepared Sample', 'Example Analysis Protocol', 'Prepared Sample', and 'Analysis Results'. The main content area is titled 'Edit Experiment Details' and contains a form for 'Example 1 from CPAS'. The form is divided into two columns. The left column has sections for 'Experiment Overview' (with fields for Experiment Name, Description, Hypothesis, URL, and Notes) and 'Experiment Contact' (with fields for Contact First Name, Contact Last Name, E-Mail, and Notes). The right column has a field for 'Experiment Date Performed (mm/dd/yyyy)' set to '09/22/2008'. At the bottom of the form are 'Save' and 'Delete' buttons.


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* on page 22
- *Repeating an Experiment Run* on page 23
- *Deleting an Experiment Run* on page 24
- *Adding a Protocol to an Experiment Run* on page 26

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 . For information on accessing this page, see *Viewing Experiment Details* on page 11.
2. The Edit Experiment Details page appears.

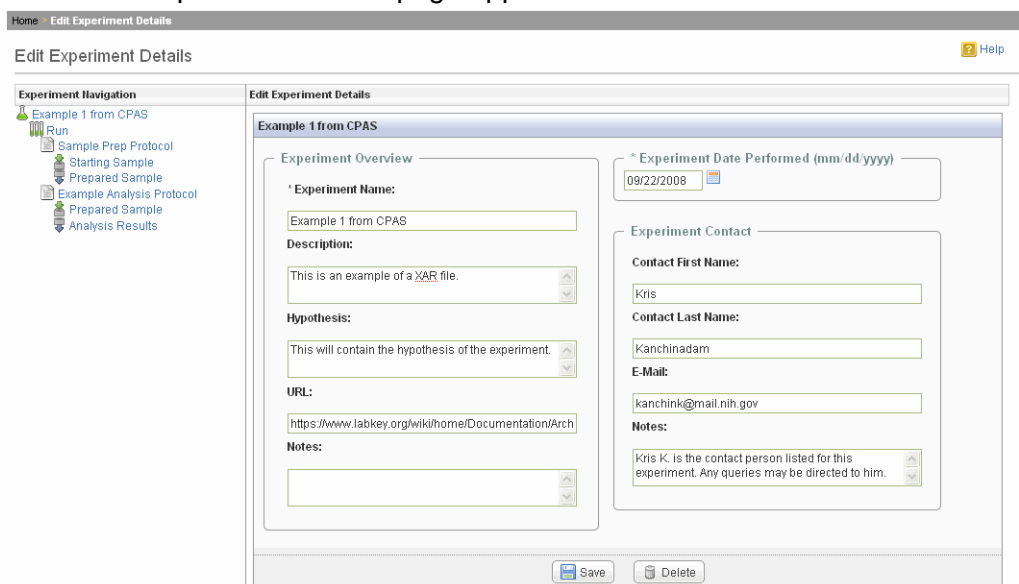



Figure 1.16 Edit Experiment Details page

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.

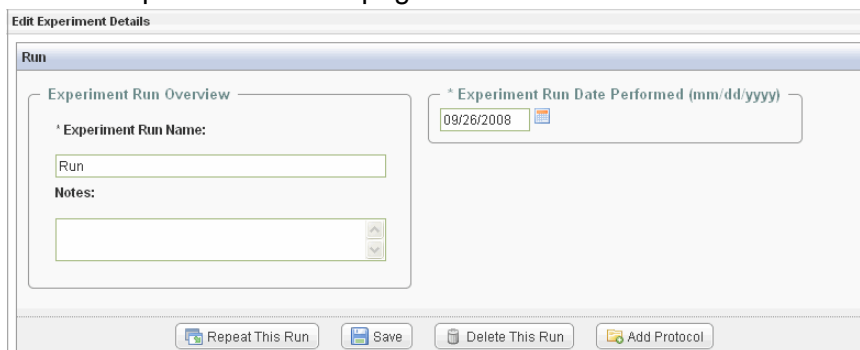



Figure 1.17 Experiment run details in the Edit Experiment Details page




4. Edit the experiment run's name, date performed, and notes as needed by entering new information in the respective fields.
5. Click . 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.

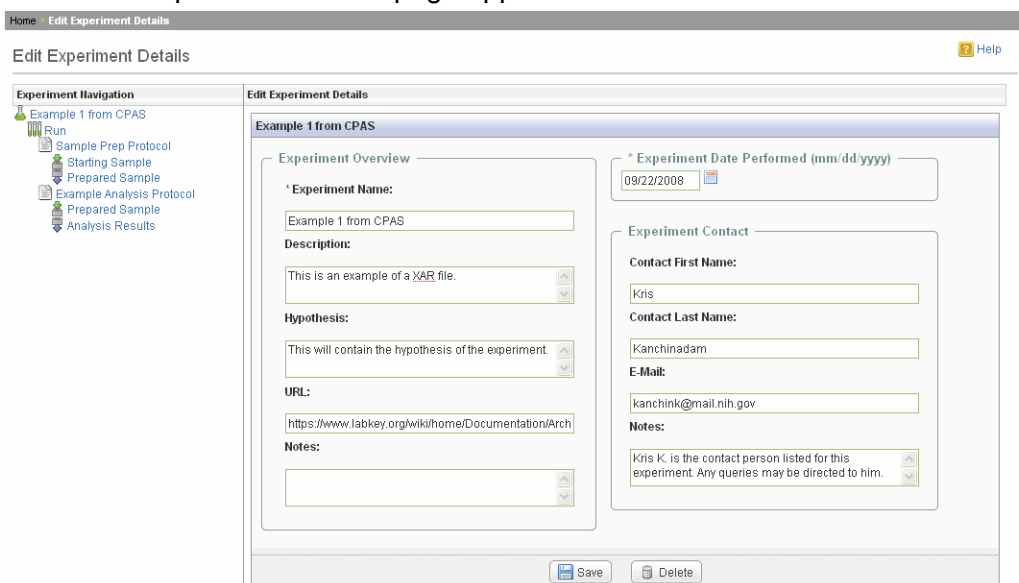
Note: Experiment runs are listed alphabetically in the Experiment Navigation.

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 . For information on accessing this page, see [Viewing Experiment Details](#) on page 11.
2. The Edit Experiment Details page appears.



The screenshot shows the 'Edit Experiment Details' page. On the left is the 'Experiment Navigation' sidebar with a tree view showing 'Example 1 from CPAS' and its sub-items: 'Run', 'Sample Prep Protocol', 'Starting Sample', 'Prepared Sample', 'Example Analysis Protocol', 'Prepared Sample', and 'Analysis Results'. The main area is titled 'Edit Experiment Details' and contains a form for 'Example 1 from CPAS'. The form has two main sections: 'Experiment Overview' and 'Experiment Contact'. The 'Experiment Overview' section includes fields for 'Experiment Name' (Example 1 from CPAS), 'Description' (This is an example of a XAR file.), 'Hypothesis' (This will contain the hypothesis of the experiment.), 'URL' (https://www.labkey.org/wiki/home/Documentation/Arch), and 'Notes'. The 'Experiment Contact' section includes a date field for 'Experiment Date Performed' (09/22/2008), and text input fields for 'Contact First Name' (Kris), 'Contact Last Name' (Kanchinadam), and 'E-Mail' (kanchink@mail.nih.gov). There is also a 'Notes' field for the contact. At the bottom of the form are 'Save' and 'Delete' buttons.

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.

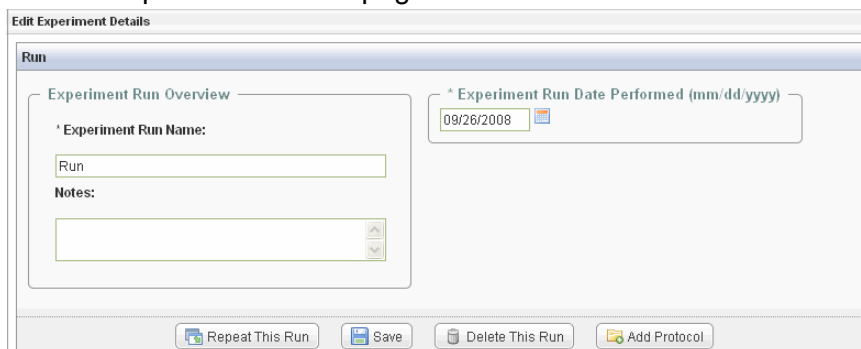
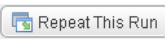





Figure 1.19 Experiment run details in the Edit Experiment Details page

4. Click . 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 . 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 Delete This Run. 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 . For information on accessing this page, see *Viewing Experiment Details* on page 11.
2. The Edit Experiment Details page appears.

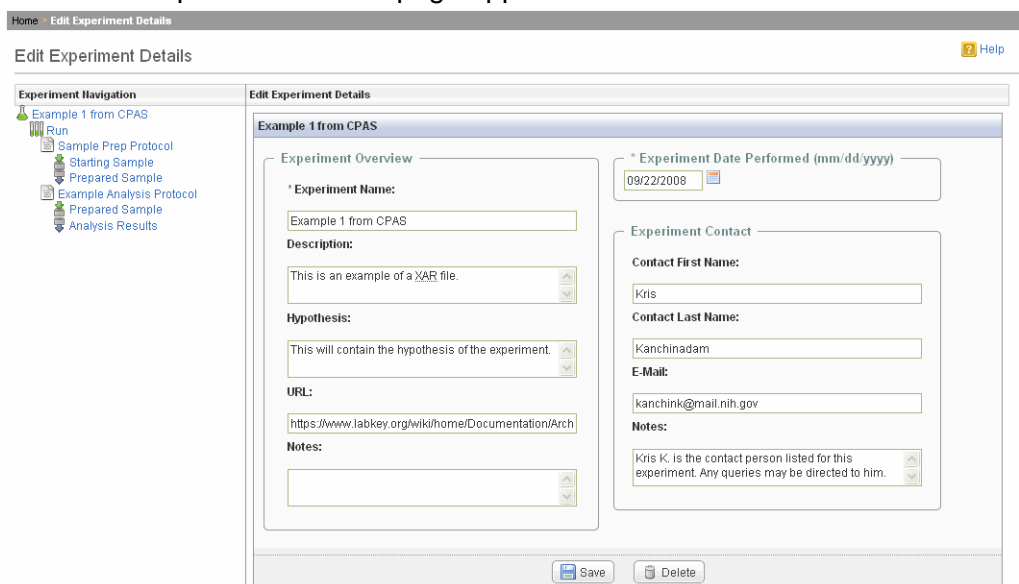



Figure 1.22 Edit Experiment Details page

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.

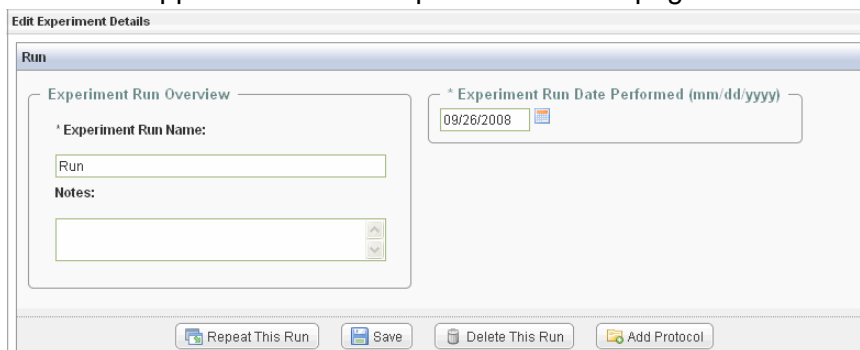


Figure 1.23 Experiment run details in the Edit Experiment Details page

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

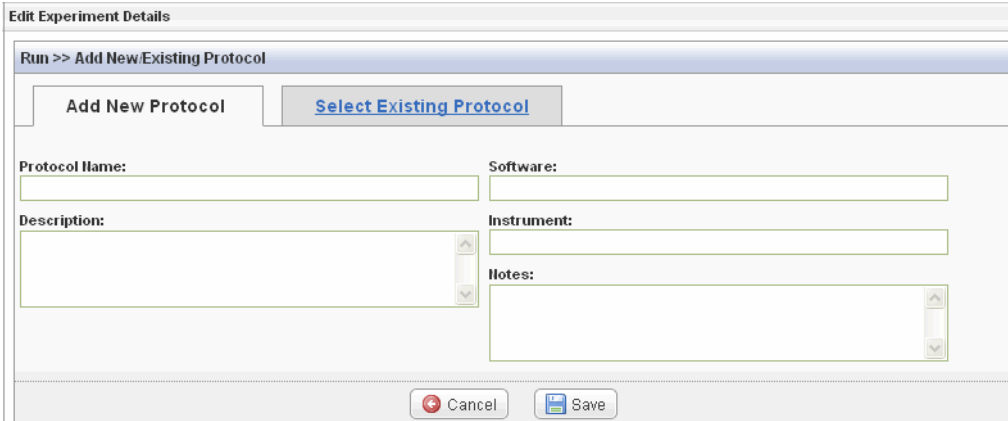



Figure 1.24 Add New/Existing Protocol page

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 . 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.

Run >> Add New/Existing Protocol

[Add New Protocol](#) **Select Existing Protocol**

☒ Display Protocols created by all users

Protocol Name	Description	Notes	User	Action
Combine tagged Sampl...			user1	Select and Continue
Divide Sample	Divide the sample in...		user1	Select and Continue
Do Conversion to mzX...			user1	Select and Continue
Do MS2 Scan			user1	Select and Continue
Example Analysis Pro...	Describes analysis p...		user1	Select and Continue
Example Analysis Pro...	Describes analysis p...		user1	Select and Continue
Ion Exchange Column	splits the input sam...		user1	Select and Continue
Sample Prep Protocol	Describes sample han...		user1	Select and Continue
Sample Prep Protocol	Describes sample han...		user1	Select and Continue
Tag with Cy3	tag the sample with ...		user1	Select and Continue

11 items found, displaying 1 to 10. [First/Prev] 1, 2 [Next/Last]

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.

Edit Protocol Details ? Help

Example Analysis Protocol

Protocol Overview

*** Protocol Name:**

Description:

Notes:

Software:

Instrument:

Protocol Contact




Contact First Name:

Contact Last Name:

E-Mail:

Notes:


Figure 1.26 Edit Protocol Details page

2. As needed, edit the protocol's properties.
3. Do one of the following:
 - Click  to save your changes. If you do not save your changes, you will lose them.
 - Click  to abandon your changes and return to the previous screen.
 - Click  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 . For information on accessing this page, see *Viewing Experiment Details* on page 11.

The Edit Experiment Details page appears.

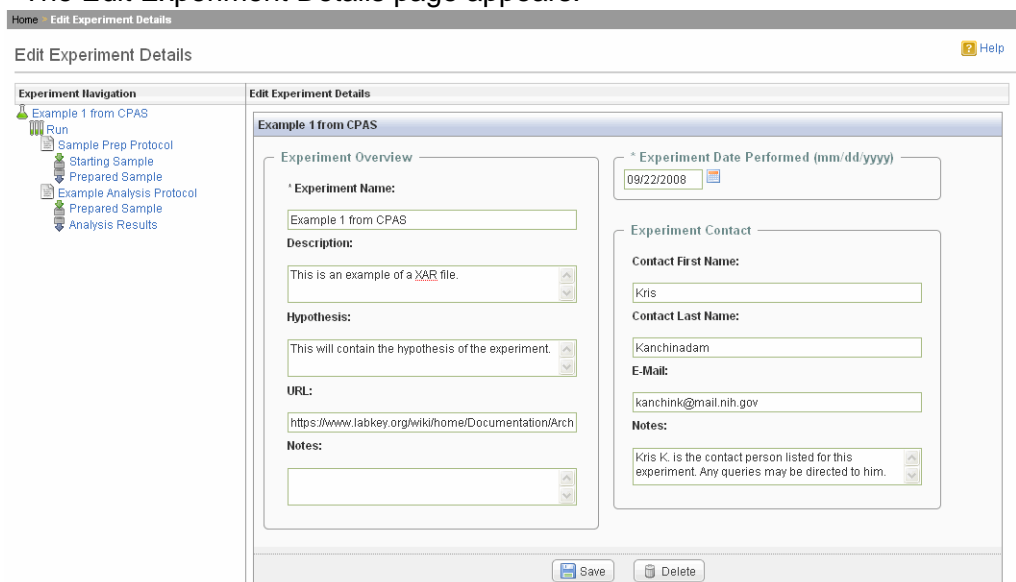




Figure 1.27 Edit Experiment Details page

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.

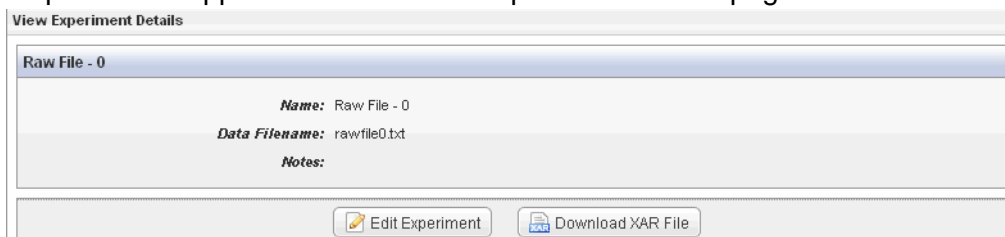


Figure 1.28 Input details within the Edit Experiment Details page

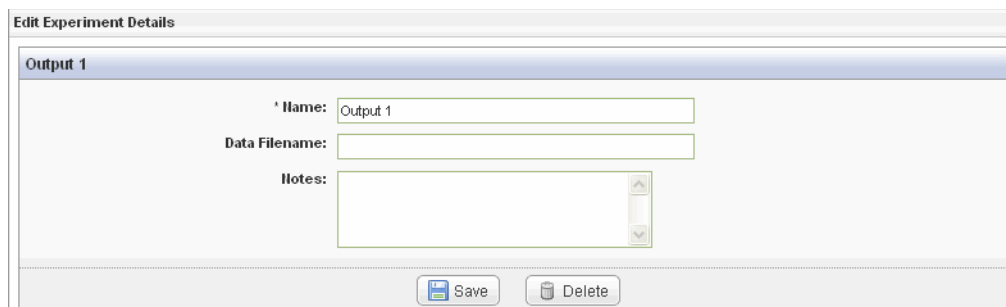




Figure 1.29 Output details within the Edit Experiment Details page

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.

The screenshot shows the 'Edit Experiment Details' page. On the left is the 'Experiment Navigation' sidebar with a tree view containing: 'Example 1 from CPAS', 'Run', 'Sample Prep Protocol', 'Starting Sample', 'Prepared Sample', 'Example Analysis Protocol', 'Prepared Sample', and 'Analysis Results'. The main area is titled 'Edit Experiment Details' and contains a form for 'Example 1 from CPAS'. The form is divided into two main sections: 'Experiment Overview' and 'Experiment Contact'. The 'Experiment Overview' section includes fields for 'Experiment Name' (Example 1 from CPAS), 'Description' (This is an example of a XAR file.), 'Hypothesis' (This will contain the hypothesis of the experiment.), 'URL' (https://www.labkey.org/wiki/home/Documentation/Arch), and 'Notes'. The 'Experiment Contact' section includes a date field 'Experiment Date Performed (mm/dd/yyyy)' (09/22/2008), 'Contact First Name' (Kris), 'Contact Last Name' (Kanchinadam), 'E-Mail' (kanchink@mail.nih.gov), and 'Notes' (Kris K. is the contact person listed for this experiment. Any queries may be directed to him.). At the bottom of the form are 'Save' and 'Delete' buttons.

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.

The screenshot shows the 'Edit Experiment Details' window. On the left is the 'Experiment Navigation' tree with a protocol selected. The main area is titled 'Ion Exchange Column' and contains a 'Protocol Overview' section with fields for 'Protocol Name' (Ion Exchange Column), 'Description' (splits the input sample), 'Notes', 'Software', and 'Instrument'. To the right is a 'Protocol Contact' section with fields for 'Protocol Date Performed' (09/26/2008), 'Contact First Name' (DB), 'Contact Last Name' (User), 'E-Mail', and 'Notes'. At the bottom are buttons for 'Save', 'Add Input', 'Add Output', and 'Delete This Protocol'.

Figure 1.31 Edit Experiment Details page with a protocol selected

- Click . Inputs appear in the Edit Experiment Details page.

The screenshot shows the 'Edit Experiment Details' window with the 'Run >> Do Conversion to mzXML >> Inputs' section selected. The 'Manage Inputs' section contains a table with columns: #, Type, Name, Data Filename, Notes, and Action. The table has two rows: Row 1 with 'Raw File - 0' and 'rawfile0.txt', and Row 2 with empty fields. Below the table is an 'Add Input (Row)' button. The 'Select Existing Inputs' section contains a table with columns: Name, Data Filename, Notes, and Action. It lists 'Chromatograph File' (chromatograph.txt) and 'mzXML File - 1' (mzxml_1.txt), each with a 'Select' button. At the bottom are 'Cancel' and 'Save' buttons.

#	Type	Name	Data Filename	Notes	Action
1		Raw File - 0	rawfile0.txt		
2					

Name	Data Filename	Notes	Action
Chromatograph File	chromatograph.txt		
mzXML File - 1	mzxml_1.txt		

Figure 1.32 Inputs on the Edit Experiment Details page

- If an empty row is not already in the Manage Inputs area, click . An empty row for a new input appears.
- In the **Name** field, enter a name for the input. This is a required field.
- 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.
- Click . 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

protExpress uses the emerging LSID standard (<http://www.omg.org/docs/dtc/04-05-01.pdf>) for identifying entities in its database, such as inputs, outputs, and experiment and protocol definitions. LSIDs are a specific form of URN (Universal Resource Name). Entities in the protExpress database will have an associated LSID field that contains a unique name to identify the entity.

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
<ObjectID>	An object identifier, unique within the namespace
<AuthorityID>	An Internet domain name
<NamespaceID>	A namespace identifier, unique within the authority
<RevisionID>	An optional version string

Table 1.6 Definitions of LSID variables

An example LSID might look like the following:

```
urn:lsid:genologics.com:Experiment.publ:Project.77.3
```

LSIDs are 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.

LSID Example

Here is an example of a valid LabKey LSID:

```
urn:lsid:labkey.org:Protocol.Folder-2994:SamplePrep.Biotinylation
```

This LSID identifies a specific protocol for a procedure called biotinylation. This LSID was created on a system with the LSID authority set to labkey.org. The namespace portion indicates that Protocol is the base type of the object, and the suffix value of Folder-2994 is added so that the same protocol can be loaded in multiple folders without a key conflict (see the discussion on substitution templates below). The ObjectID portion of the LSID can be named in whatever way the creator of the protocol chooses. In this example, the two-part ObjectID is based on a sample preparation stage (SamplePrep), of which one specific step is biotinylation (Biotinylation).

APPENDIX

A

PROTEXPRESS GLOSSARY

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

<i>Term</i>	<i>Definition</i>
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)	LDAP is 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)	<p>An emerging standard (http://www.omg.org/docs/dtc/04-05-01.pdf) by which biologically significant resources are uniquely named.</p> <p>LSIDs are multi-part strings with the parts separated by colons. They are of the form:</p> <pre>urn:lsid:<AuthorityID>:<NamespaceID>:<ObjectID>:<RevisionID></pre> <p>Each entity (input, output, protocol definition, experiment definition, etc.) in the protExpress database has an associated LSID field that contains a unique name to identify the entity.</p>
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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