PROTEXPRESS USER'S GUIDE



This is a U.S. Government work.

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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 3 explains how to use protExpress to manage protocol and experiment data.
- protExpress Glossary on page 25 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 this document.

protExpress Development and Management Teams		
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CHAPTER

2

WORKING WITH PROTEXPRESS

This section includes the following topics:

- Getting Started on page 3
- Searching protExpress on page 7
- Viewing Experiment Details on page 9
- Creating a New Experiment on page 10
- Editing Protocol Details on page 19
- Editing Experiment Details on page 20
- Working with Experiment Runs on page 21

Getting Started

This section includes the following topics:

- Registering Users on page 3
- Logging In on page 5
- Resetting Your Password on page 5
- Using the Home Page on page 6

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 2.1* on page 4.

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

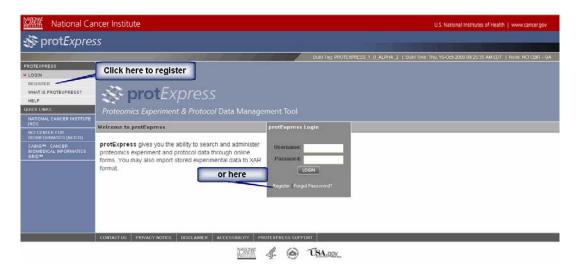


Figure 2.1 protExpress home page with registration links

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.

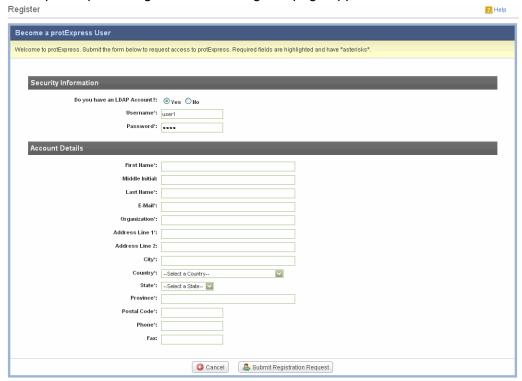


Figure 2.2 Registration page

Select the option corresponding to whether or not you have an LDAP account. If you do have an LDAP account, protExpress synchs 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.
- 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 2.3 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 3.



Figure 2.4 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 7
Check the status of a recent experiment	Viewing Experiment Details on page 9
Create a new experiment	Creating a New Experiment on page 10
Edit a recent experiment	Editing Experiment Details on page 20
Download a recent experiment in XAR format	Viewing Experiment Details on page 9

Table 2.1 Available actions on the protExpress home page and where to find more information about them

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

Figure 2.5 shows the protExpress home page.

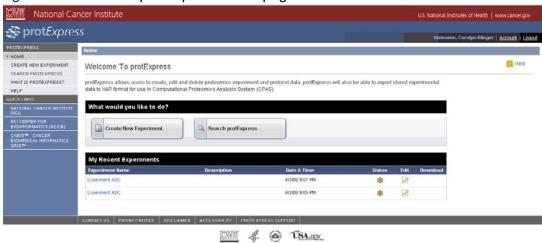


Figure 2.5 protExpress Home Page

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

 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.

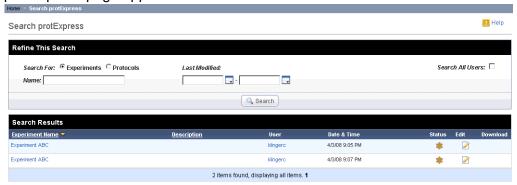


Figure 2.6 Search protExpress page

- 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.
 - o 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
4	The protocol or experiment is complete.
	A protocol is complete when it includes at least one input and one output.
	An experiment is complete when it contains at least one complete protocol.
*	The protocol or experiment is incomplete.
	To complete a protocol, add at least one input and at least one output.
	To complete an experiment, add at least one complete protocol.

Table 2.2 Explanation of Icons Used in protExpress

Icon	Explanation
	You own this protocol or experiment and may edit it.
	Download this protocol or experiment in XAR XML format. This icon only appears next to complete protocols and experiments. See above in this table for an explanation of what makes a protocol or experiment complete.
	When you view a complete experiment or 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 9.

Table 2.2 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 2.7 View Protocol Details page



Figure 2.8 View Experiment Details page

For more information, see:

- Editing Protocol Details on page 19
- Editing Experiment Details on page 20

Viewing Experiment Details

When you open an experiment, the following information is available in the View Experiment Details page (see *Figure 2.8* on page 9).

Feature		Description
Experiment Navigation		Displays the structure of an experiment in the following way:
	Ī	Click the name next to this icon to view the following information about the experiment: Experiment Overview, Date Performed, and Experiment Contact.
		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.
	1111	Click the name next to this icon to view the protocol overview, date performed, and contact for this experiment run.
	*	Click the name next to this icon to view information about the parent protocol's input.
	-	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 Experiment Details</i> on page 20.
Downloax 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 2.3 Features of the View Experiment Details Page

Creating a New Experiment

To create a new experiment you must identify the experiment, add one or more new or existing protocols to it (during the create process or later), review the experiment, and then save it. For more information, see:

- Identifying the Experiment on page 10
- Adding a Protocol to an Experiment on page 12
- Working with Inputs on page 14
- Working with Outputs on page 17
- Reviewing the Experiment on page 17

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 the Create New Experiment button 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.

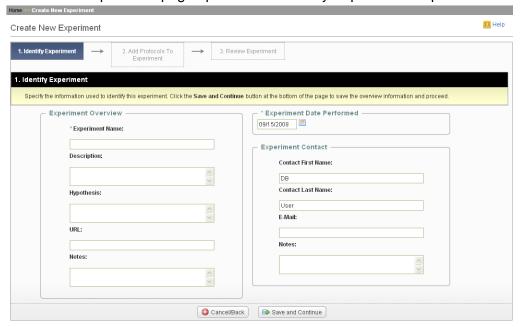


Figure 2.9 Identify experiment step in the create new experiment process

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.
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.

Table 2.4 Definitions of fields on the Identify Experiment page

Field	Description
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 2.4 Definitions of fields on the Identify Experiment page

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

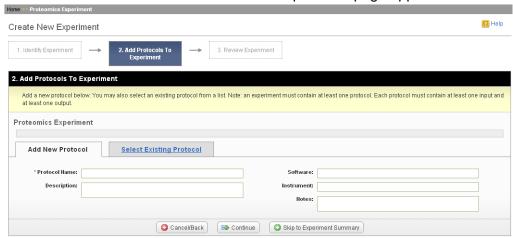


Figure 2.10 Add Protocols to Experiment step of the create new experiment process

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.

Note: A complete experiment includes at least one complete protocol. A complete protocol includes at least one input and one output.

4. To add a protocol to the experiment now, click ——Continue . To proceed, see Adding a Protocol to an Experiment on page 12.

To add a protocol to the experiment later, click Skip to Experiment Summary. To proceed, see *Reviewing the Experiment* on page 17.

Adding a Protocol to an Experiment

A protocol is a reusable entity that you can use across mutliple experiments. However, an *instance* of a protocol applied to an experiment run is unique and you cannot apply it to other runs or experiments.

You can add a protocol to an experiment by creating a new one or by selecting an existing protocol. You can add a protocol to an experiment while creating a new experiment or later, while editing an experiment.

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

Note: A complete experiment includes at least one complete protocol. A complete protocol includes at least one input and one output.

When you add a protocol to a new experiment, you begin from the Add Protocols to Experiment page, Add New Protocol tab.

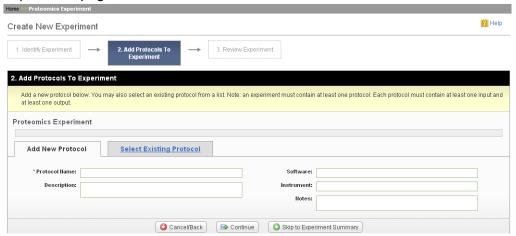


Figure 2.11 Add Protocols to Experiment page, Add New Protocol tab

When you add a protocol to an existing experiment run, you begin from the Add New/ Existing Protocol page.

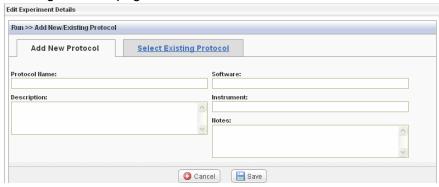


Figure 2.12 Edit Experiment Details page, Add New Protocol tab

To add a new protocol to an experiment

- 1. Click the **Add New Protocol** tab if it is not already selected.
- In the Name field, enter a name for the new protocol. This is a required field.
- Enter the protocol's description and its associated software, associated instrument, and 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 Name and Description fields in a search for this protocol later.
- Click size. The protocol is 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 2.13 Select Existing Protocol tab

2. Find the protocol you want to select and click Select and Continue appears in the Experiment Navigation.

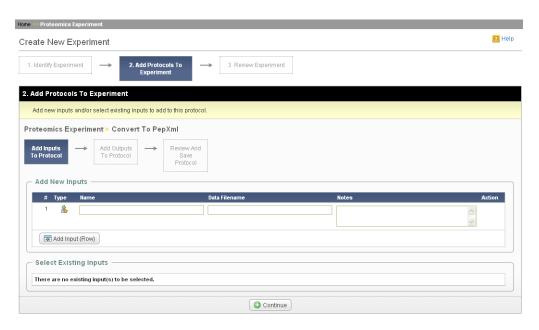
Working with Inputs

[NOTE: ALL OF THIS INFO WILL CHANGE]

You can specify data and material inputs available to all protocols in protExpress.

This section contains the following topics:

- Adding an Input on page 15
- Editing an Input on page 16
- Deleting an Input on page 16



Adding an Input

[NOTE: ALL OF THIS INFO WILL CHANGE]

Once you add an input to an experiment, it serves as input to each of the associated experiment runs. You can add as many inputs as necessary for the experiment.

To add an input

- 1. Open the experiment to which you want to add one or more inputs using either of the following methods:
 - In the My Experiments area on the Dashboard, click in the row corresponding with the experiment you want to edit.
 - After searching for an experiment (see Searching protExpress on page 7), click in the row of the search results that corresponds with the experiment you want to edit.

The Edit Experiment page appears.

2. Select the Input(s) tab.

Figure 2.14 Input(s) tab on the Edit Experiment page

Figure 2.15 Add New Input page

- In the Name field, enter a name for the global input. This is a required field.
- In the **Data File Name** field, enter the file name of a data file associated with the global inpu. This is an optional field. If the global input is a material, leave this field blank.

Note: protExpress uses standard naming conventions to automatically generate an *LSID* for the global input.

6. Click Save. The Edit Input page appears.

Editing an Input

[NOTE: ALL OF THIS INFO WILL CHANGE]

You can edit an input's name and data file name. You cannot edit the LSID.

To edit an input

- 1. Open the experiment that contains the input you want to edit using either of the following methods:
 - o In the My Experiments area on the Dashboard, click in the row corresponding with the experiment.
 - After searching for an experiment (see Searching protExpress on page 7), click in the row corresponding with the experiment.

The Edit Experiment page appears.

Select the Input(s) tab.

Figure 2.16 Input(s) tab on the Edit Experiment page

3. In the Actions column, click on the row corresponding with the input you want to edit. The Edit Input page appears.

Figure 2.17 Edit Input page

- 4. Modify the input's name and/or data file name.
- 5. Click Save.

Deleting an Input

[NOTE: ALL OF THIS INFO WILL CHANGE]

You can delete inputs that you have not applied to any active protocols. Before you can delete a input that is an input to an active protocol, you must first delete it from that protocol.

To delete an input

- 1. Open the experiment that contains the input you want to delete using either of the following methods:
 - o In the My Experiments area on the Dashboard, click in the row corresponding with the experiment.
 - After searching for an experiment (see Searching protExpress on page 7), click in the row corresponding with the experiment.

The Edit Experiment page appears.

Note: Several tabs on the Edit Experiment page present experiment data in a list. You can sort any of the columns in these lists by clicking the column name. Clicking the column name twice toggles the sort order between ascending and descending. The column currently responsible for sorting

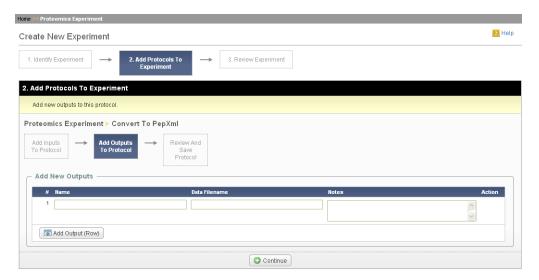
the list has a double arrow (\square) beside the column name. The highlighted arrow represents the sort order.

2. Select the Input(s) tab.

Figure 2.18 Input(s) tab on the Edit Experiment page

3. In the Actions column, click Delete in the row corresponding with the input you want to delete. A message appears confirming that you have deleted the input.

Working with Outputs

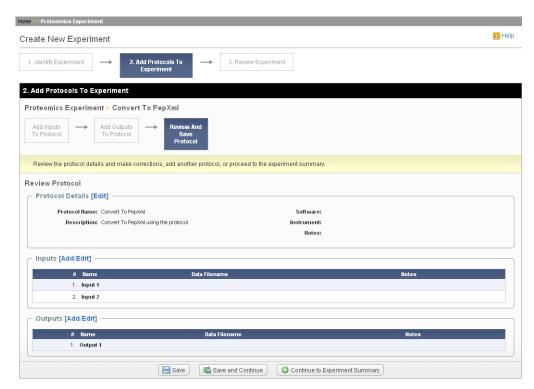


Next step:

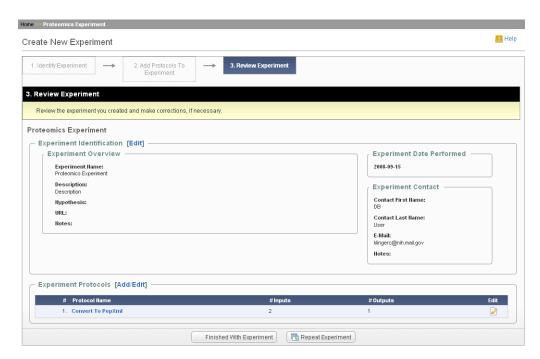
Reviewing the Experiment on page 17

Reviewing the Experiment

[This topic contains some information.]



After clicking Continue to Experiment Summary, you see the following:



If you click Finished With Experiment, you return to the Welcome to protExpress page.

Adding a Protocol to an Experiment Reviewing the Experiment

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 Home page or Search Results page, and click . The Edit Protocol Details page appears.

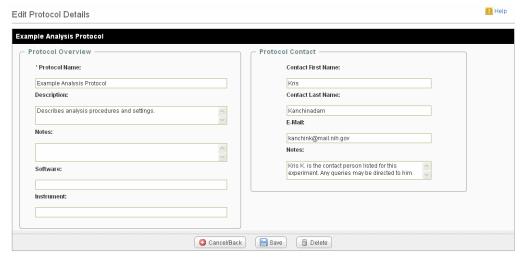


Figure 2.19 Edit Protocol Details page

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

Editing Experiment Details

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*.

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.
 - o In the 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 7.
 - On the View Experiment Details page, click <u>Fedit Experiment</u>. For more information on accessing this page, see *Viewing Experiment Details* on page 9.
- 2. The Edit Experiment Details page appears.

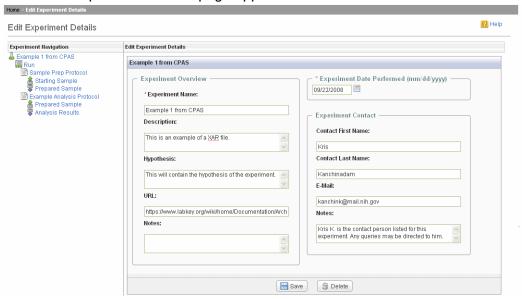


Figure 2.20 Edit Experiment Details page

3. 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

Table 2.5 Properties of each experiment

Field	Expected Value
Experiment Date Peformed (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 2.5 Properties of each experiment

4. When you have finished editing the experiment's details, click save. A message indicating that the experiment has been successfully updated appears at the top of the page.

Note: Clicking Delete removes the experiment from the database. Use with caution.

Working with Experiment Runs

[NOTE: ALL OF THIS INFO WILL CHANGE]

An experiment run is an instance of an experiment.

This section contains the following topics:

- Adding an Experiment Run on page 21
- Editing an Experiment Run on page 22
- Deleting an Experiment Run on page 22

Adding an Experiment Run

[NOTE: ALL OF THIS INFO WILL CHANGE]

To add an experiment run

- 1. Open the experiment to which you want to add an experiment run using either of the following methods:
 - o In the My Experiments area on the Dashboard, click in the row corresponding with the experiment you want to edit.
 - After searching for an experiment (see Searching protExpress on page 7), click in the row of the search results that corresponds with the experiment you want to edit.

The Edit Experiment page appears.

Select the Experiment Runs tab.

Figure 2.21 Experiment Runs tab on the Edit Experiment page

3. Click Add New Experiment Run. The Add New Experiment Run page appears.

Figure 2.22 Add New Experiment Run page

- 4. In the **Name** field, enter a name for the experiment run. This is a required field.
- 5. In the **Comments** field, enter any comments relevant to this experiment run. This is an optional field.

Note: protExpress uses standard naming conventions to automatically generate an *LSID* for the experiment run.

6. Click Save.

Editing an Experiment Run

[NOTE: ALL OF THIS INFO WILL CHANGE]

To edit an experiment run

- Open the experiment that contains the experiment run you want to edit using either of the following methods:
 - In the My Experiments area on the Dashboard, click in the row corresponding with the experiment.
 - After searching for an experiment (see Searching protExpress on page 7), click in the row corresponding with the experiment.

The Edit Experiment page appears.

2. Select the **Experiment Runs** tab.

Figure 2.23 Experiment Runs tab on the Edit Experiment page

- 3. Click in the row corresponding with the experiment run you want to edit. The Edit Experiment Run page appears.
- 4. Edit the experiment run fields as necessary.
- 5. Click Save.

Deleting an Experiment Run

[NOTE: ALL OF THIS INFO WILL CHANGE]

To delete an experiment run

- 1. Open the experiment that contains the experiment run you want to delete using either of the following methods:
 - o In the My Experiments area on the Dashboard, click in the row corresponding with the experiment.
 - After searching for an experiment (see Searching protExpress on page 7), click in the row corresponding with the experiment.
- 2. The Edit Experiment page appears.

3. Select the **Experiment Runs** tab.

Figure 2.24 Experiment Runs tab on the Edit Experiment page

4. In the Actions column, click Delete in the row corresponding with the experiment run you want to delete. A message appears confirming that you have deleted the experiment run.

APPENDIX 3

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)	LAn application protocol for querying and modifying directory services running over TCP/IP.
LSID (Life Science Identifier)	Persistent, location-independent, resource identifiers for uniquely naming biologically significant resources including species names, concepts, occurrences, genes or proteins, or data objects that encode information about them.

Table 3.1 Glossary of terms used in protExpress

Term	Definition
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 3.1 Glossary of terms used in protExpress

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