PROT*EXPRESS*

User's Guide

National Cancer Institute

Center for Bioinformatics

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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
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- *Additional References* on page 2
- *Text Conventions Used* on page 2
- *Credits and Resources* on page 3

Purpose

This guide provides an overview of protExpress. It explains how to use ...

Audience

Typical User

This guide is designed for ... who want to ...

Prerequisites

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

- <topic>
- <topic>
- <topic>

This documentation is not intended for ...

Topics Covered

If you have worked with previous versions of protExpress, see *Additional References* on page 2.

If you are new to protExpress, read this brief overview, which explains what you will find in each chapter and appendix.

- <Chapter Number & Name> introduces ...
- <Chapter Number & Name> describes ...
- <Chapter 3> ...
- <Appendix Number & Name> provides general information about ...
- <Appendix Number & Name> is a glossary of terms related to protExpress.

Additional References

For more information about protExpress, see the following references:

- <Reference>
- <Reference>

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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WORKING WITH PROTEXPRESS

This section includes the following topics:

- *Using the Dashboard* on page 5
- *Managing Protocols* on page 6
- *Managing Experiments* on page 9
- *Working with Inputs* on page 10
- *Working with Outputs* on page 11
- *Importing Data* on page 11
- *Exporting Data* on page 11

Using the Dashboard

After logging in to protExpress, you arrive at the Dashboard. To return to the Dashboard after working in other areas of protExpress, click **Dashboard** in the protExpress menu.

The protExpress Dashboard lists the three protocols and three experiments that you must recently added to protExpress, along with the dates when you added them. Only protocols and experiments that you own appear in these lists.

You can start the following tasks from the Dashboard:

- View a protocol or an experiment
- Search for a protocol or an experiment to view
- Add a new protocol or an experiment
- Edit a protocol or an experiment
- Import experiment data

For more information, see:

Managing Protocols

This section includes the following tasks:

Searching for a Protocol

The protocol you want to work with may not appear in the Dashboard, which lists only the three protocols you most recently added to protExpress. To find other protocols, you can search for them.

To search for a protocol

1. On the Dashboard, click [Search] in the Protocols area or select the **Protocols** menu. The Search Protocols page appears.

Figure 3.1 Search Protocols page

2. Optionally, enter or select one or more search criteria. The more search criteria you specify, the fewer results you receive. Search criteria are all optional and include:

   ○ **Name**: enter any character in the protocol name

   ○ **Description**: enter any character in the protocol description

   ○ **Type**: select Protocol Application, Experiment Run, or Experiment Run Output

   Note: If you do not enter or select any search criteria, all protocols in protExpress appear in the search results.

3. Click **Search**. Search results appear in a table below the search criteria. You can now edit any protocol in the list.

For more information, see:

- *Editing a Protocol* on page 7

●   *Deleting a Protocol* on page 9

Adding a Protocol

When you add a *protocol*, protExpress considers you the protocol's owner and you are the only one who can edit it.

To add a protocol

1. On the Dashboard or Search Protocols page, click [Add New Protocol]. The Add New Protocol page appears.
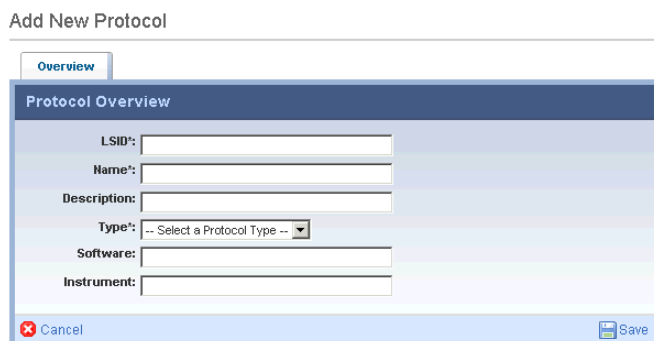

Figure 3.2 Add New Protocol page

2. In the **LSID** box, enter the *Life Science Identifier* for the protocol. This is a required field.

3. In the **Name** box, enter a name for the new protocol. This is a required field.

4. From the **Type** list, select a protocol type. Options include *Protocol Application*, *Experiment Run*, and Experiment Run Output.

5. Optionally, enter the protocol's description and its associated software and instrument in the boxes with those names.

6. Click [Save]. The Edit Protocol: *Protocol Name* page appears.

    The Overview tab contains the values you entered in steps *2.* - *5.* You can now optionally provide additional information about the protocol in the Input/Output, Contact, and Parameters tabs. For more information about these tabs, see *Editing a Protocol* on page 7.

Editing a Protocol

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 a protocol

1. On the Dashboard, click [edit icon] or in the Actions column on the Search Results page, click **Edit**. The Edit Protocol: *Protocol Name* page appears.

2. As needed, edit the protocol's properties that are listed in the Overview, Input/ Output, Contact, and Parameters tabs. Refer to *Table 3.1* below for more information about these properties.

3. Before moving to another tab, click 🖫 Save to save your changes or click ❌ Cancel to delete them. If you do not click 🖫 Save before moving to another tab, you will lose your changes.

Note: Hover your mouse over the maroon, dotted text below to see a popup window with more information about the word.

Options Available on Each Tab	Expected Value
Overview Tab	
LSID (required)	Life Science Identifier
Name (required)	Protocol name
Description	Protocol description
Type	Select Protocol Application, Experiment Run, or Experiment Run Output
Software	Software associated with protocol
Instrument	Instrument associated with protocol
Input/Output Tab	
Max Input Material	Maximum number of material input objects generated for this protocol application
Max Input Data	Maximum number of data input objects generated for this protocol application
Output Material	Description of output material
Output Data	Description of output data
Output Material Type	Base type of output material (default type is `Material`)
Output Data Type	Base type of output data (default type is `Data`)
Contact Tab	
First Name	Protocol owner's first name
Last Name	Protocol owner's last name
Email Address	Protocol owner's first name email address
Contact Id	Any other unique identifier for the protocol owner
Parameters Tab	
Application LSID Template	Information about the application LSID template, which directs how application LSIDs are formed at load time
Application Name Template	Information about the application name template, which directs how application names are formed at load time
Output Material LSID Template	Information about the output material LSID template,which directs how output material LSIDs are formed at load time
Output Material Name Template	Information about the output material name template, which directs how output material names are formed at load time

Table 3.1 Properties of each protocol

Options Available on Each Tab	Expected Value
Output Data LSID Template	Information about the output data LSID template, which directs how output data LSIDs are formed at load time
Output Data Name Template	Information about the output data name template, which directs how output data names are formed at load time
Output Data File Template	Information about the output data file template,which directs how output data files are formed at load time
Output Data Directory Template	Information about the output data directory template, which directs how output data directories are formed at load time

Table 3.1 Properties of each protocol

Deleting a Protocol

Documentation to come.

Managing Experiments

This section includes the following procedures:

- *Searching for an Experiment* on page 9
- *Adding an Experiment* on page 10
- *Adding an Experiment Run* on page 10
- *Editing an Experiment Run* on page 10
- *Adding a Protocol Application* on page 10
- *Editing a Protocol Application* on page 10
- *Editing an Experiment* on page 10
- *Deleting an Experiment* on page 10

Searching for an Experiment

The Dashboard lists the three experiments you most recently added to protExpress. To find other experiments, you can search for them.

To search for an experiment

1. On the Dashboard, click **Search** in the Experiments area or select the **Experiments** menu. The Search Experiments page appears.

2. Optionally, enter or select one or more search criteria. The more search criteria you specify, the fewer results you receive. Search criteria are all optional and include:

    ○ **Name**: enter any character in the experiment name

    ○ **Description**: enter any character in the experiment description

    ○ **Type**: select Protocol Application, Experiment Run, or Experiment Run Output

> **Note:** If you do not enter or select any search criteria, all experiments in protExpress appear in the search results.

3. Click **Search**. Search results appear in a table below the search criteria. You can now edit any experiment in the list.

For more information, see:

- *Editing an Experiment* on page 10
- *Deleting an Experiment* on page 10

Adding an Experiment

Documentation to come.

Adding an Experiment Run

Documentation to come.

Editing an Experiment Run

Documentation to come.

Adding a Protocol Application

Documentation to come.

Editing a Protocol Application

Documentation to come.

Editing an Experiment

Documentation to come.

Deleting an Experiment

Documentation to come.

Working with Inputs

Documentation to come.

Working with Outputs

Documentation to come.

Importing Data

Documentation to come.

Exporting Data

Documentation to come.

PROTEXPRESS GLOSSARY

This glossary definies 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.
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 A.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.
Protocol Application	The application of a protocol to some specific set of inputs, producing some outputs. A protocol application is like an instance of the protocol. 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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