

# caBench-to-Bedside 1.0

## User's Manual

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**caBIG™** *cancer Biomedical Informatics Grid™*

an initiative of the National Cancer Institute

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# Table of Contents

Chapter 1	Introduction.....	6
	In this chapter .....	6
	Introduction to caB2B .....	6
	Getting started with caB2B .....	7
	Overview of the Manual .....	7
	Organization of the User Manual.....	8
	Document Text Conventions .....	8
Chapter 2	Overview of the caB2B.....	9
	In this chapter .....	9
	Introduction to Category and Limits.....	9
	The Home page.....	11
	Search data – The Query Wizard.....	12
	Choose Search Category .....	13
	Define Limit.....	16
	Limit Set – Diagrammatic View .....	17
	Define Search Results View.....	23
	View Search Results .....	25
	Viewing and Saving Data List.....	30
Chapter 3	Experiments.....	33
	In this Chapter .....	33
	What are Experiments and Projects?.....	33
	Creating an Experiment.....	34
	Viewing the Existing Experiments .....	36
	Opening an Experiment.....	36
	Working with an Experiment.....	37

Analyzing Data .....	41
Visualizing Data.....	44
Chapter 4    Appendix 1 .....	48
Examples of category search .....	48
Define Limit: Operators and Values .....	52
Record Details View .....	54
Administrator defined categories.....	54
BioDataCube .....	55
Types of Filters .....	56
Chapter 5        Troubleshooting	

# Chapter 1 Introduction

## In this chapter

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This chapter explains the scope and function of the caB2B application. It helps you understand how to use caB2B to satisfy diverse biomedical research needs. It contains the following sections:

- Introduction to caB2B
- Getting started with caB2B
- Overview of the manual
- Organization of the manual
- Document text conventions

## Introduction to caB2B

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The NCI caBIG™ project creates a common, extensible informatics platform that integrates diverse data types and supports interoperable analytic tools. caBIG™ is developing separate applications that will facilitate individual steps involved in micro-array analysis. These applications are also useful to bio-informaticians.

caGrid is the infrastructure for caBIG that helps integrate these applications. caGrid can be used to perform investigations involving data integration and analytical services from diverse research communities.

caBench-to-Bedside (caB2B) is an application that leverages these tools in a user-friendly graphical user interface (GUI). caB2B can be used by the physician scientist to perform operations such as:

- **Query any caGrid data service to obtain data.**  
The data service can be a single data service, multiple data services, or a combination of the two services using semantically interoperable Common Data Elements (CDEs).  
  
For example, caB2B allows investigators to query tissue banks at multiple cancer centers, design studies that focus on very specific tumor subtypes and to target less common tumors by pooling bio-specimen resources. This alleviates the problem of small sample size in a study.
- **Collect data and create experiments.**  
caB2B also enables investigators to perform novel in silico experiments using micro-array data that have been archived. These capabilities facilitate the process of identifying genes that are up-regulated or down-regulated in specific cancers and enable investigators to view data in the context of biological pathways. Investigators gain further understanding of the complex system of cancer biology by identifying genes important to the development and treatment of cancer. These capabilities could lead to more effective identification of novel drug targets, and improved treatment strategies.
- **Perform various analyses** by using various grid-enabled analytical services.

caB2B enables individual users to work on common platforms to access caGrid resources in real time from common data and analytical services.

- **Visualize analysis results** using charts and dendrograms.

## Getting started with caB2B

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- To start caB2B client, refer to the Installation Guide.
- To search for data sets refer to “Search data – The Query Wizard”.
- To design experiments, refer to “Experiments”.

## Overview of the Manual

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This manual provides the details of how to use caB2B application to

- Search data sets of interests
- Create an experiment from data sets
- Analyze data
- Visualize data

All the chapters in this user’s manual begin with an introductory statement and is followed by a list of topics included in that chapter.





## Organization of the User Manual

Following table summarizes the chapters in this manual.

Chapter in caB2B	Chapter Contents
2. Overview of caB2B	General overview Searching categories Adding limits Defining output Viewing the results Saving data
3. Experiments	Creating Experiments Analyzing data Visualizing data
6. Appendix 1	Examples of category search Operators in Defining limit Details of the various records Various filters

## Document Text Conventions

Following table illustrates documentation conventions represented in this manual.

Convention	Description	Example		
	Indicates information of particular interest	<table><tr><td></td><td>Administrator can create a new category.</td></tr></table>		Administrator can create a new category.
	Administrator can create a new category.			
<div>CAUTION</div>	Indicates that you should be particularly aware of the information provided.	<table><tr><td>CAUTION</td><td>It deletes permanently.</td></tr></table>	CAUTION	It deletes permanently.
CAUTION	It deletes permanently.			



# Chapter 2 Overview of caB2B

## In this chapter

---

This chapter describes details of how to search data using caB2B in the following sections:

- Introduction to some concepts
- Overview of Home Page
- Search data
- Choose Search Category
- Define Limit
- Define Search Results View
- View Search Results
- Viewing and Saving Data List

## Introduction to Category and Limits

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### What is a Category?

A category is a collection of *searchable* attributes. You can use a category to search, view, and add data to experiments. Every UML class in an application is, trivially, a category. For example, Participant is a UML class from *caTissue Core* application.

Examples:

Participant is a category consisting of attributes like

- Identifier
- First Name
- Last Name
- Gender
- Race


Gene Annotation is a category consisting of attributes like

- Entrez Gene ID
- Gene Symbol
- Gene Name
- GenBank Accession Number
- Taxonomy ID

- Chromosome

## Why do we need categories?

Categories are designed to help you to easily locate all the data elements needed for your search.


	<p>Categories are created by the administrator.</p> <p>Your administrator can create new categories based on your requirements. If there are queries that you perform regularly, discuss them with your administrator.</p>
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## What is a Limit?

A limit is a condition (or criterion or predicate or condition) on a category. It is the smallest unit of a query. For example, *female participants*

## What is a query?

The collection of limits is a query. For example, *female participants who have DNA specimens collected from their breast*. This query has two limits: *female participants*, *DNA specimens from breast*. There are two categories involved in this query: *Participant* and *Specimen*.

	<p>Your administrator can create a new category that contains relevant data elements from Specimens and Participants. That way you can enter all the limits in a single category.</p>
---	---

# The Home page

For details on installing and starting the caB2B client, refer to the *Client Installation* chapter of the Installation Manual.

When the caB2B application is launched, you see the caB2B Home page as shown below.

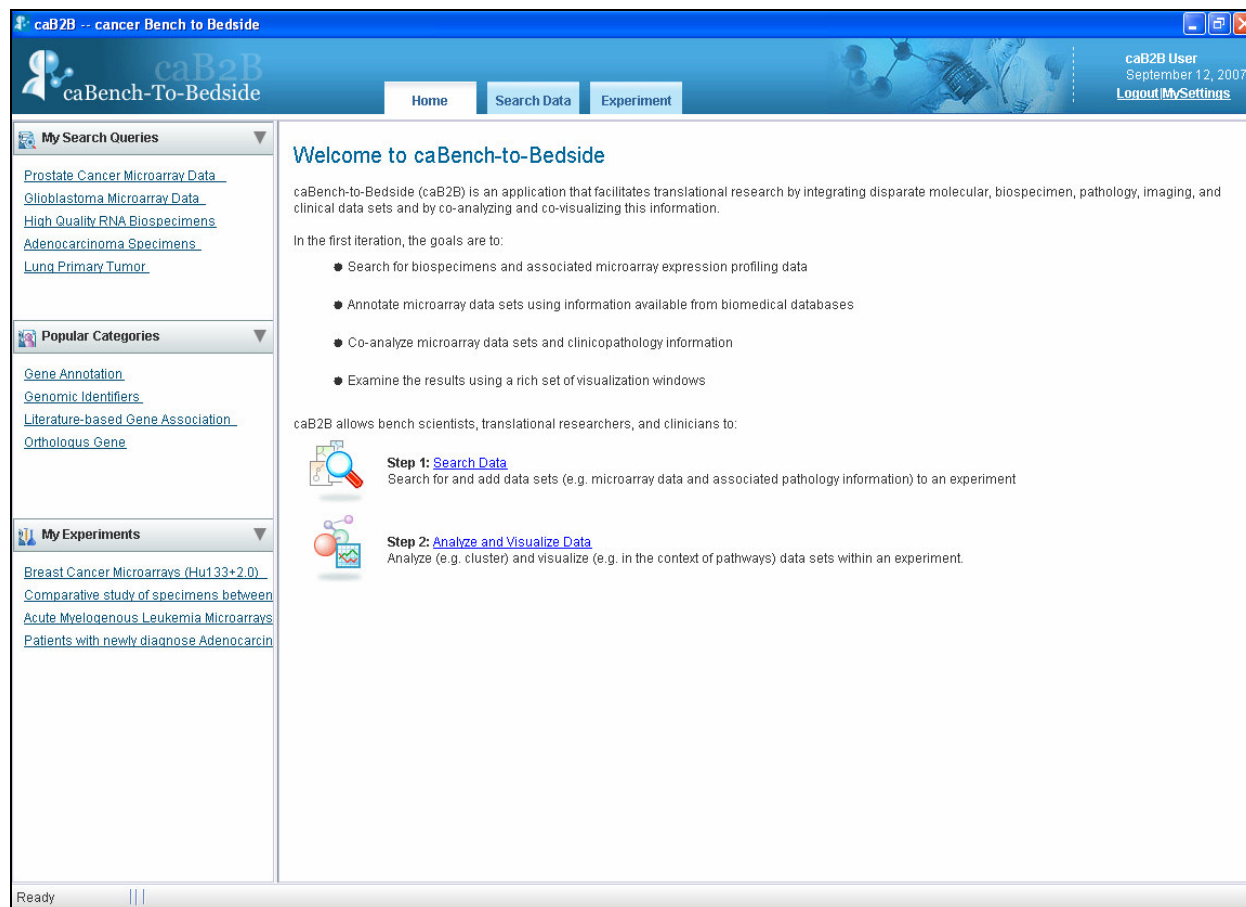


Figure 1: caB2B Home page

As mentioned in the Introduction section, a caB2B end user would typically perform the following steps:

1. Perform queries to obtain the data set of interest. Details of this step are provided in the chapter, [Searching Data](#).
2. Analyze and visualize data. Details of this step are provided in the [Experiment](#) chapter.

## Search data – The Query Wizard

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This section provides details of the steps that required to obtain data. Click the **Search Data** link on the **Home** page to open the **Search data for Experiment** wizard (Figure 2: Choose Search Category Tab).

The wizard guides you through the following steps:

STEP ONE	STEP TWO	STEP THREE	STEP FOUR	STEP FIVE
Choose Search Category	Add Limits	Choose Output Category	View Search Results	View Data List

The steps used to search data are:

1. Choose Search Category: Search for Category to apply limits.
2. Add Limits: Add limits on the selected Category
3. Choose Output Category (Optional): Select the output format (i.e. define the results view)
4. View Search Results: View the results view in a Google-like search results page and add data to the data list (or shopping cart).
5. View Data List: View the data you have added in the data list and create Experiment.

## Choose Search Category

This step helps you search for the category on which you have limits.. For example, if you have a query with limits on participants, you can use this feature to first find the *Participant* category.

Click the category of interest and open a page to enter the limits on that category.

To find the categories, do the following:

Type the search string in the text box. *Gene, gender, rna, experiment* are examples of search strings.

Click the **Search** button or press ENTER.

Categories that match the string you entered are displayed as hyperlinks along with a short description.

Once you find a Category of your choice, click the **Category** to proceed to the next step.

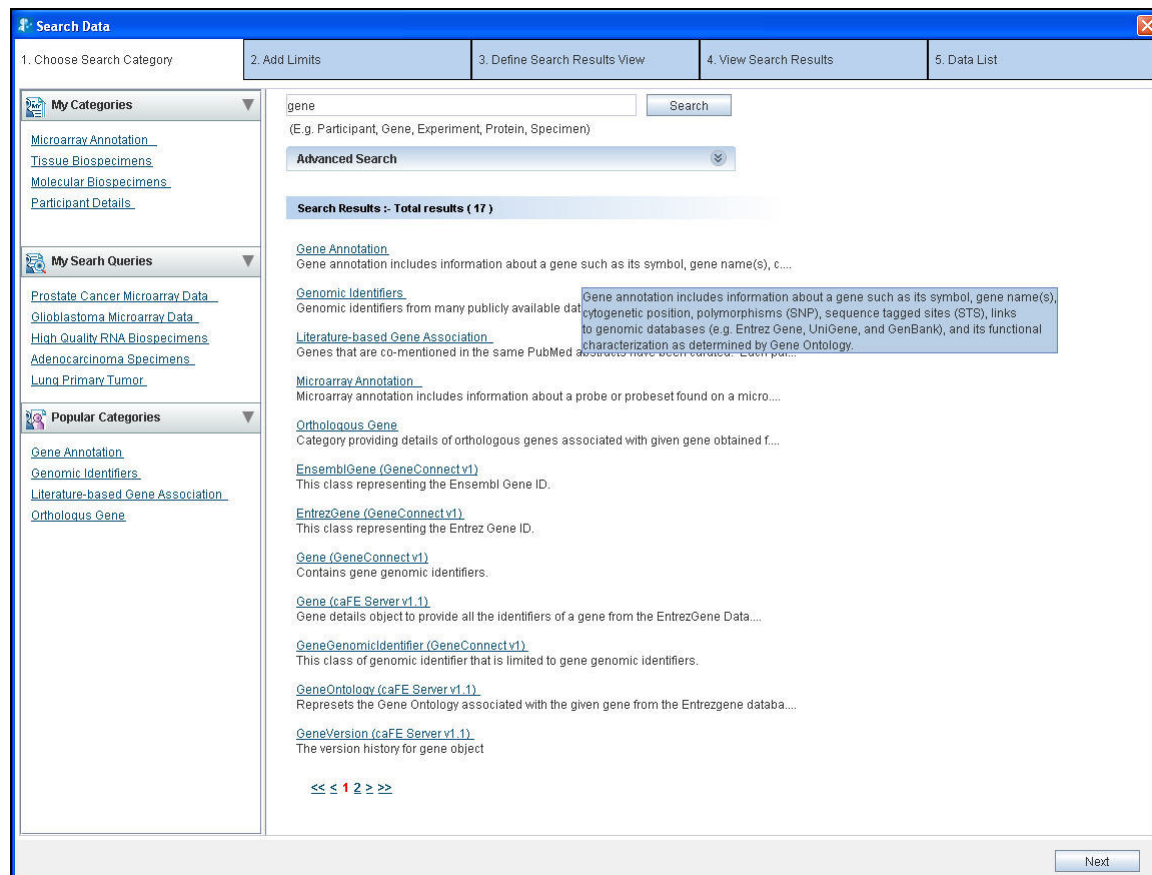


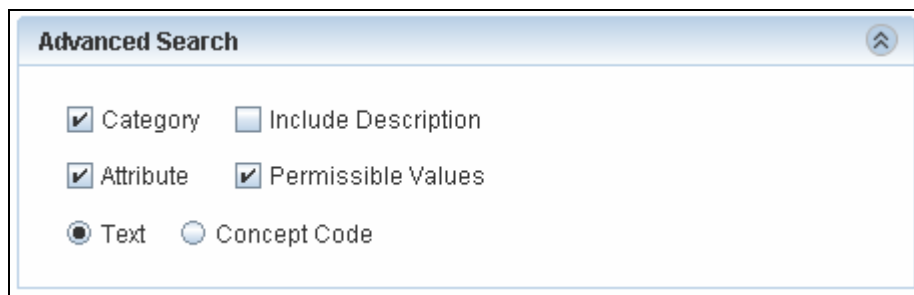
Figure 2: Choose Search Category Tab

More on searching:

- The search performed is partial and is not case-sensitive. Hence the search for terms such as *Gene*, *gen* or *GENE* returns the same results.
- If a category's description is long, you can view the complete description as a tool-tip by positioning the mouse over that description.
- If the number of matching categories is large, the system displays the results in multiple pages. Click the page numbers at the bottom to navigate to different pages.
- You can separate the multiple search terms using spaces or tabs. The system searches for each term individually and displays a collective set of matching categories. For example, if you enter the search string *Participant Gene*, you will find the categories that match either *Participant*, *Gene*, or both.

## Advanced Search (\*)

Expanding the **Advanced Search** box displays the advanced options that help you refine the category search. The following is the default selection of the various options:



The screenshot shows a window titled "Advanced Search" with a close button in the top right corner. Inside the window, there are four checked checkboxes: "Category", "Attribute", "Permissible Values", and "Text". There are also two unchecked checkboxes: "Include Description" and "Concept Code".

Figure 3: Advanced search

If the system returns too many results for your Category search, you can use the **Advanced Search** to narrow your search.

Table 3

Option	Description
<i>Check Boxes</i>	
<i>Category</i>	Includes the category names in the search.
<i>Attribute</i>	Attribute (also known as data element) is the lowest unit of the searchable items. A category contains many attributes.  Select this check box to include the individual attribute names in the search.  For example: select <i>attribute</i> and search for <i>gender</i> . You will find the category Participant since it contains an attribute by name <i>Gender</i> .
<i>Permissible value</i>	<i>Some attributes contain a fixed set of values. For example, Gender can be Male, Female or Unspecified. Organ can be heart, lung, breast, and so on.</i>

<i>Option</i>	<i>Description</i>
	<p>This fixed set is known as <b>Permissible Values</b>.</p> <p>Select this check-box to include the permissible values in the search. So if you select the permissible value as <i>Male</i> the system displays the Participant category since it contains an attribute <i>Gender</i> which contains a permissible value <i>Male gender</i>.</p>
<i>Include Description</i>	Includes the description text in the search.
Option Buttons	
<i>Text</i>	<p>The system matches the search string that you type with the name of the category, its attributes, or the permissible values based on the text.</p> <p>This is the simple, most commonly used and the default way of searching a category.</p>
<i>Concept Code</i>	<p>The system treats the search string that you type as an EVS concept code. The system matches this concept code with the concept code of the category, its attributes, or the permissible values. The results contain matching categories .</p> <p><b>Note: Include Description</b> check-box will be enabled only for a <b>text based search</b> when you select the <b>Category</b> check box, the <b>Attribute</b> check box, or both.</p>

Additional refinements that you can make with these options are illustrated in the **Appendix 1 Examples** of category search.

## Define Limit

A limit is a condition (or criterion or predicate) on a category and Multiple limits together form a query. The following table outlines two example queries and the limits added to them.


Table 4

Example	Category	Limits
Get the details about all the African male participants	Participant	Gender equals Male Race equals African
Biospecimens from prostate adenocarcinoma	Specimen Characteristics	Tissue Site equals prostate
	Specimen Collection Group	Clinical diagnosis equals adenocarcinoma

### Steps for defining a limit

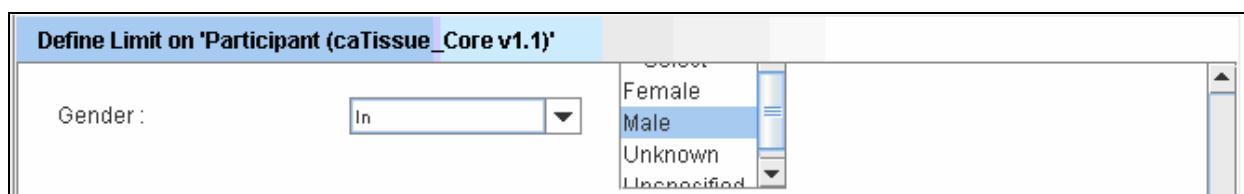
Perform the following steps to define a limit:

1. Choose an operator from the list of operators adjacent to the attribute you wish to constrain.
2. Specify the constraining values.

	For a detailed explanation of the various operators and how to specify values, refer to <b>Define Limit: Operators and Values</b> .
---	---

Example:

Single constraint – Show all male participants



Define Limit on 'Participant (caTissue\_Core v1.1)'

Gender : In

Female  
Male  
Unknown  
Unspecified

Figure 4: Male participants



Example:

Multiple constraints within one limit: male participants who are alive

Define Limit on 'Participant (caTissue\_Core v1.1)'

Gender : In   
 Female   
 Male   
 Unknown   
 Unspecified

Identifier : Between

Last Name : Contains

Middle Name : Contains

Sex Genotype : In   
 -- Select --   
 Klinefelter's Syndrome   
 Mosaic including XXXXY   
 Not Specified   
 Renta Y Syndrome

Social Security Number : Contains

Vital Status : In   
 -- Select --   
 Alive   
 Dead

Figure 5: Male participants who are alive

#### CAUTION

Do not forget to click the **Add Limit** button at the bottom of the **Define Limits** screen before proceeding. If you forget to click this button, the constraints that you specify will not be saved.

## Limit Set – Diagrammatic View

The **Limit Set** panel displays all the limits that were added in the **DiAGrammatic** view (DAG view). Whenever you add a new limit, the system adds a yellow rectangle to the DAG view. This rectangle represents the limit you added. As you continue to add limits, the system adds corresponding rectangles to the DAG view.

These rectangles in the DAG view give you a graphical view of all the limits that have been added.

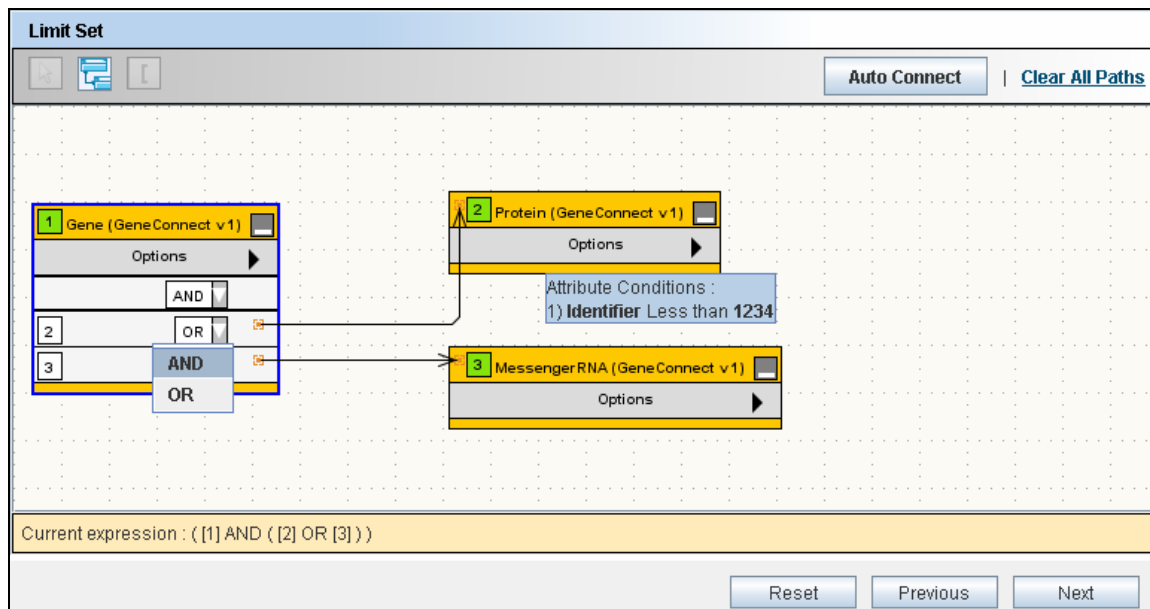
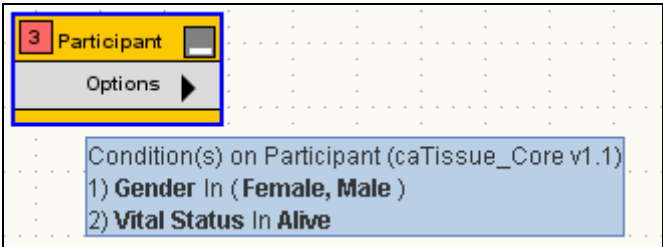
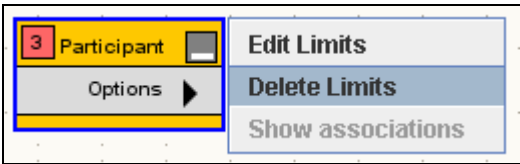


Figure 6 : Limit Set Pane

## DAG Operations

You can perform the following operations within the DAG view:

Table 5

View details of the limit	<p>Position your mouse over a node to view the details of that limit.</p> 
Edit the limit	<p>Click <b>Edit Limits</b> from the <b>Options</b> menu of the node whose limits you wish to edit. Alternatively, double click the title of the node.</p>  <p>This opens the limit in the <b>Define Limit</b> Error! Reference source not found.panel in the edit mode. Edit the constraints in the <b>Define Limit</b> panel, and click the <b>Edit Limit</b> button.</p>
Delete the limit	<p>Select the nodes that you wish to delete and press DELETE.</p> <p>Alternatively, you can delete a single node by selecting <b>Delete Limits</b> from the <b>Options</b> menu of the node as shown above.</p>

## Connecting the Limits

You must connect all the limits before proceeding to the next step.

When you specify multiple limits, you need to connect these limits to form an expression. You can connect two limits using either the **AND** or the **OR** operator. The following is an example of how the DAG looks when the limits are connected.

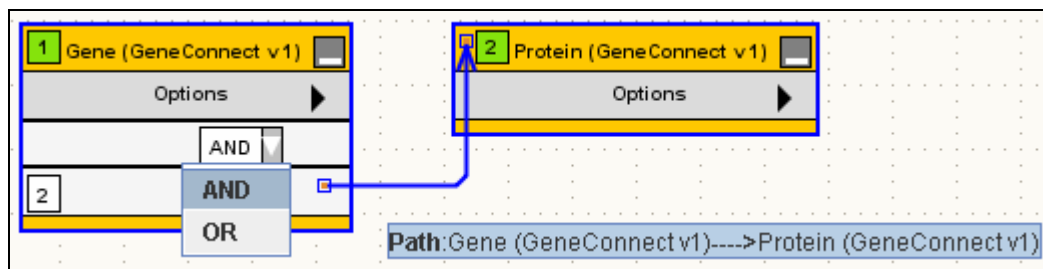


Figure 7: Connected Nodes

If there are only two limits in the query, you have to connect only those two rectangles

To connect the limits, you need to specify the following:

- The **path** to be taken in connecting the nodes
- The logical operator (**AND**, **OR**) in the dropdown box in a node

The rest of this section focuses on various ways in which you can specify the path(s).

### What is a Path?

A path tells the system **how** two categories are to be connected. A path is a way to travel from one category to another. There could be multiple ways to connect two categories and the results of the query will differ based on the path you choose.

For example, consider the two categories *Specimen* and *Site* (from the caTissue Core application). A *Specimen* is associated with the *Site* category in two ways: 1) Site where the specimen was *collected* 2) Site where the specimen is *stored*.

That means there are two paths between *Specimen* and *Site*: 1) through Storage Container 2) through Specimen Collection Group for the collection site.

Query example 1: Show all the available specimens collected in Barnes Jewish Hospital. In this query, as you are specifically interested in a particular collection site, you should choose the path through Specimen Collection Group.

Query example 2: Show all the available specimens stored in Barnes Jewish Hospital. In this query, as you are specifically interested in a particular storage site, you must choose the path through Storage Container.

Therefore it is important to choose the right path for your query.

## Connecting Limits

Click the **Auto Connect** button. The system will automatically connect all the boxes based on the settings done by your administrator.

However, the administrator might not have configured the path between all the categories. In such cases, you can manually connect the limits as described below.

Example query: For all the male participants, show all the available specimens collected in Barnes Jewish Hospital.

1. After adding the three limits on *Participant*, *Specimen* and *Site* the DAG view will look like the figure below.

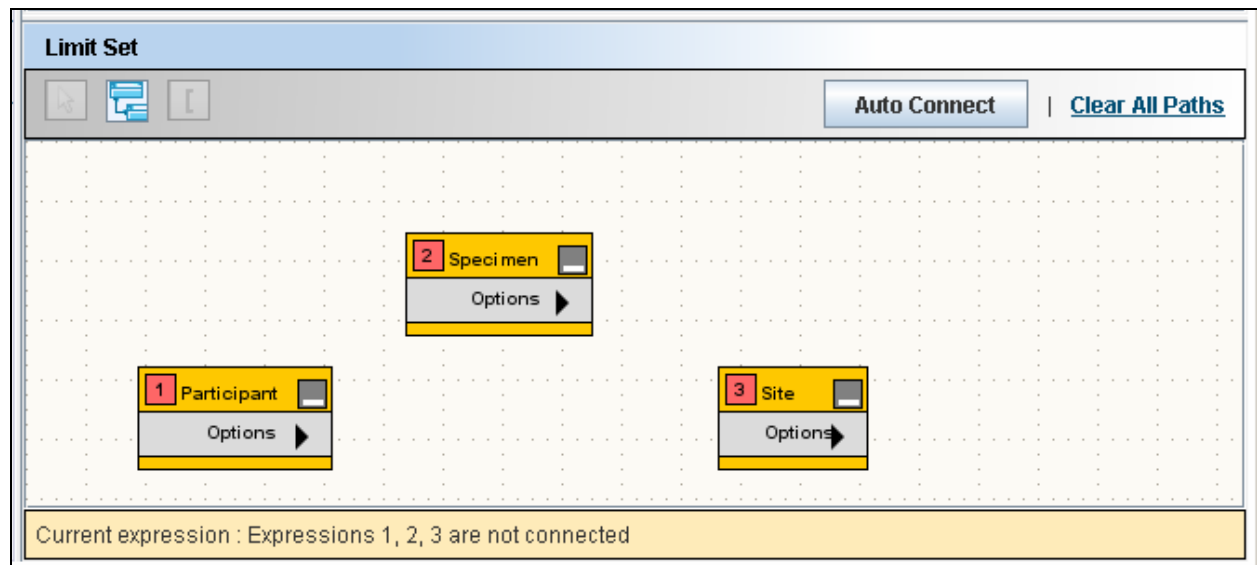



Figure 8: Limit Set

2. Click the *Participant* and the *Specimen* rectangles to select them.
3. Click the **Connect Limits**  icon to connect the two nodes. The resulting DAG view is shown in Fig.9 below.

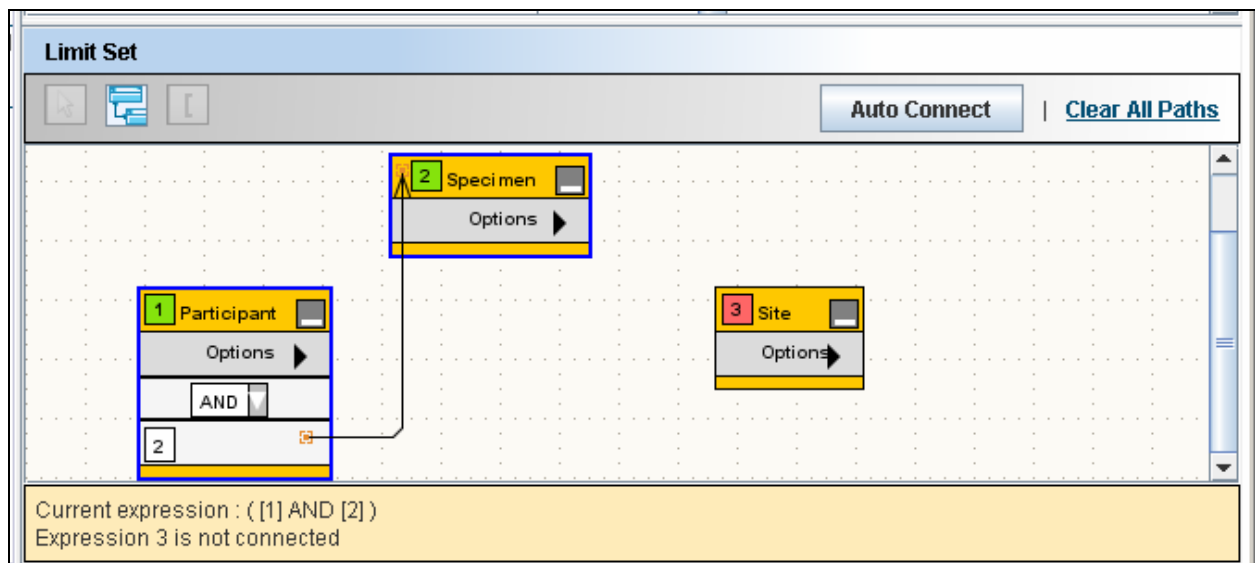



Figure 9: Limit Set with Two Connected Limits

**Note:** There is only one path between *Participant* and *Specimen*, therefore the system automatically connects it.

4. Select the *Specimen* and *Site* rectangles and click the **Connect Limits**  icon.
5. Since there are more than one paths between *Specimen* and *Site*, the system cannot connect the limits on its own. So it displays the **Ambiguity Resolver** window. The **Ambiguity Resolver** window is shown in Fig.10 below:

Path Ambiguity Resolver		
General Path Curated Path		
Select	Paths	PathPopularity
<input type="checkbox"/>	Specimen >> (specimenCollectionGroup) >> SpecimenCollectionGroup >> (site) >> Site	50 %
<input type="checkbox"/>	Specimen >> (storageContainer) >> StorageContainer >> (site) >> Site	50 %

Figure 10: Path Ambiguity Resolver

The **Ambiguity Resolver** now shows two paths between *Specimen* and *Site*: 1) through Specimen Collection Group for the collection site 2) through Storage Container.

6. Select the first path to find out the collection site.
7. Once the path(s) are determined, the system creates a connection between the two nodes (see figure below). You can position the mouse over the connection to view the path(s) that you chose.

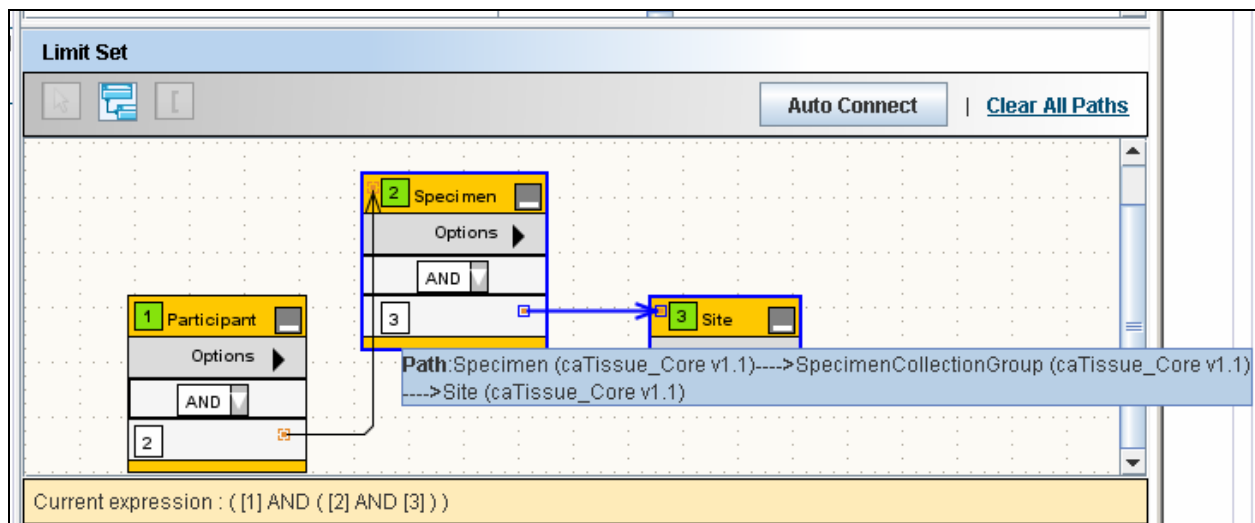


Figure 11: Limit Set with Three Connected Limits

8. Specify the operator (**AND** or **OR**) using the dropdown box in the node.
9. Click the **Next** button to go to the next step.

### Deleting a Connection

You can delete a connection by clicking the connection and pressing the DELETE key.

## The Information Panel

The **Information** panel is located at the bottom of the **Limit Set** panel.

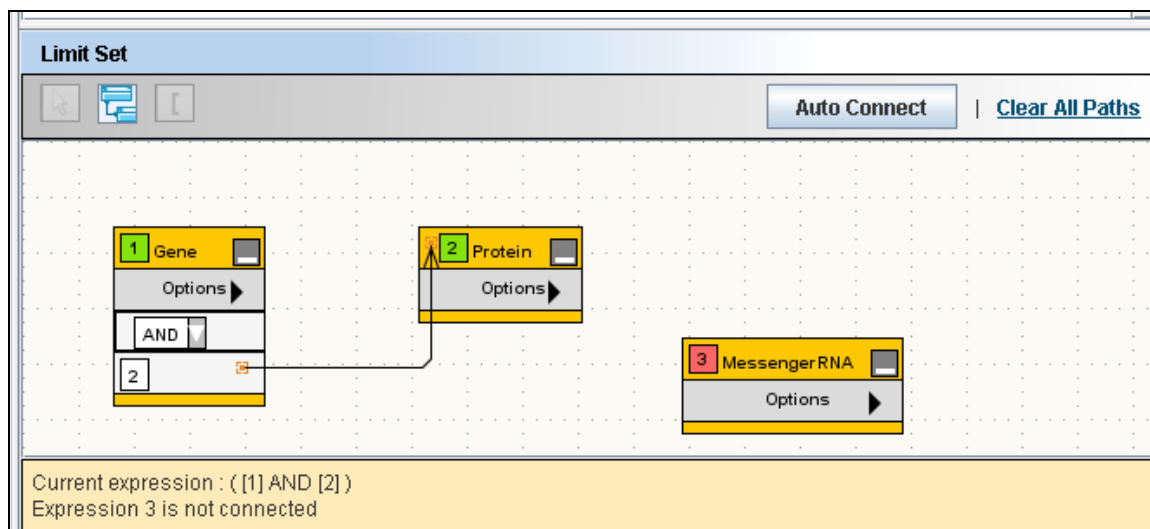


Figure 12: The Information Panel

The **Information** panel provides the following information:

- The expression formed as a result of the way you have connected the limits
- Limits that not yet connected to any other limit
- To execute the query, there should not be any unconnected rectangles.

## Reset, Previous and Next Buttons

These buttons are located at the right hand bottom of the screen.

- The **Reset** button clears all the limits that you have specified.
- The **Previous** button takes you to **Choose Search Category** step of the wizard.
- The **Next** button takes you to the **Choose Output Category** step of the wizard. A valid query allows you to proceed to the next step. If the query is invalid, an appropriate error message is displayed.

## Define Search Results View

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After specifying the limits, user proceeds to choose the category for the data. For example, “show all the participants who had biospecimens collected from their breast”. *Participant* is the category that you want to view, based on a limit on the specimens.

The **Define Search Results View** tab enables you to select the output category for the query.

Figure 13: Define Search Result View.

All the categories with specified limits are shown in the **Select Default View** dropdown box at the bottom of the screen. From the **Select Default View** dropdown box, select the category whose data you wish to obtain.

	<p>Ignore the other contents of this screen such as the check boxes and hyperlinked categories. Those are intended to allow you to fetch data for multiple related categories in one go. However, this feature is not supported in this release of caB2B.</p>
--	---

## The Next and Previous Buttons

- To edit the limits, click the **Previous** button and go to the **Define Limit** step.
- Click the **Next** button to execute the query that you have created.

<p><b>CAUTION</b></p>	<p>On clicking the <b>Next</b> button, the system will execute the query and fetch the data from appropriate data services over the caGrid.</p> <p>This step could be time-consuming based on the network speed and the complexity of the query.</p>
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## View Search Results

The **View Search Results** tab displays the results obtained by executing the query you had defined in the previous steps. The concept of viewing results in caB2B is similar to viewing results after a Google search. The similarities are as follows:

- caB2B returns a set of records that match your limits.
- Some details of the record is displayed along with the record.
- You can click on one of the records to view more details.
- There you can view additional associated information for the record you are viewing. For example, from Participants you can see the Collection Protocol in which they registered. This is similar to Google where, after you click one of the hyperlinks, you can traverse into the other web pages by clicking the hyperlinks within that page.
- As in Google, the results are divided into multiple pages for easy navigation.
- If you find any data of your interest, you can add it to a shopping cart known as **Data List**.

The following image displays a typical results view. The **View Search Results** tab displays the records that match the limits and also the data that you have already added to the data list.

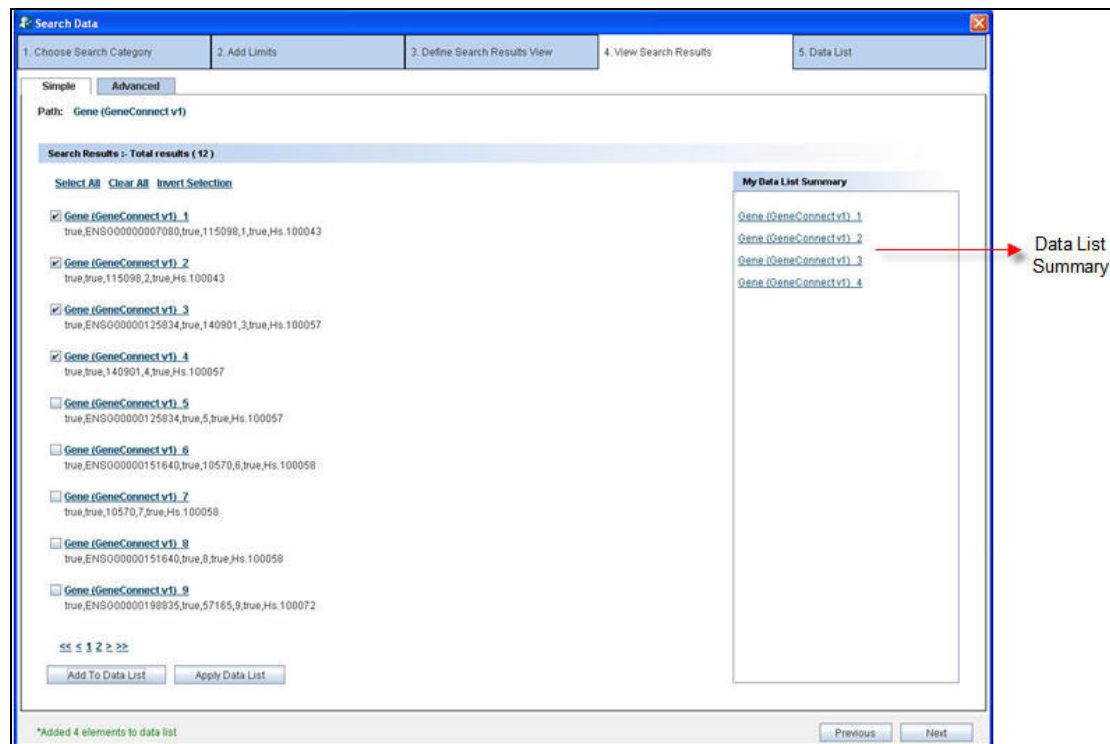


Figure 14: View Search Results

## Record Details

Click on the hyperlink of a record on the **View Search Results** to take you to the **Record Details** page.

Here you can view the values of all the attributes of the category.

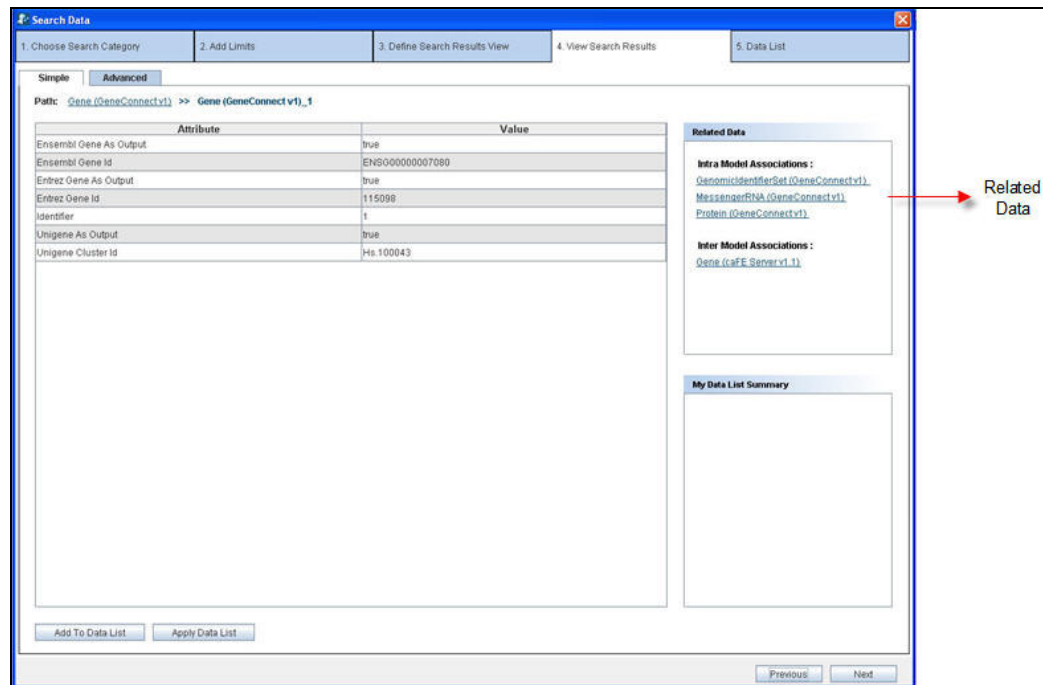


Figure 15: Results' Details

A view of the Results Details page is shown in Figure 15 (above) and shows the following sections:

- Value of all the data elements in the record
- Links to related data
- Summary of the records that you have already added to the data list

### Related Data

In Figure 15 above, the **Related Data** box on the right displays the categories that are related to the current category. Click on any of the categories to display records for that category. For example, if you are currently viewing records of Gene(GeneConnect), the following categories are shown in the related data box:

- GenomicIdentifierSet (GeneConnect)
- Protein (GeneConnect)
- MessengerRNA (GeneConnect)
- Gene (caFE Server)

If you now click *Protein*, you would see the Proteins related to the Gene you are currently viewing.

### Breadcrumbs

#### Definition of Breadcrumbs – Wikipedia

**Breadcrumbs** or **breadcrumb trails** are a navigation technique used in user interfaces. Its purpose is to give users a way to keep track of their location within programs or documents.

As you traverse the results view, breadcrumbs are displayed at the top of the page. For example, if you are viewing a Protein record related to a Gene, you would see the path as

Gene >> Gene \_1 >> Protein >> Protein\_5

This means that you originally queried for Gene. Then you fetched related proteins for Gene\_1. From the proteins obtained, you are currently viewing details of Protein\_5.


Click any of the links in the breadcrumbs to navigate back to the corresponding page. For example, you can click *Gene* in the above path to go back to the page where you were shown the list of Genes.

### ***Adding data to the Data List***

A data list is like a shopping cart. As you traverse through the results and find some interesting data you can add it to the shopping cart.

You can add data to the data list in two ways:

- Click the **Add to Data** List button
- Click the **Apply to Data** List button

	As you add the data to the data list, they are reflected in the <b>My Data List Summary</b> box on the right hand side.
---	---

### **Add to Data List**

Select the record that you want to add to the data list and click the **Add to Data List** button. You can either add one record at a time or add multiple records by selecting the checkboxes placed along with the record summary.

### **Using Apply Data List**

#### **Why use Apply Data List**

Going back to the Results Details page in Figure 15: Results' Details the following sections are shown:

- Value of all the data elements in the record
- Links to related data: you can obtain data for categories related to a particular category.
- Summary of the records that you have already added to the data list

A typical user query might do the following:

1. Fetch the data for the *Gene* category.
2. Fetch the related data from the category *Chromosome* for a record of *Gene*, for example, *Gene\_1*.

3. Add the *Chromosome* record to the data list.

The resulting data list is shown in Fig. 16 (below).

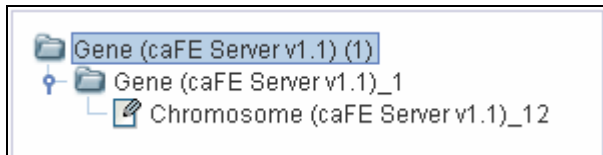


Figure 16: Data List

If you wish to obtain the *Chromosome* data for some more *Gene* records you have to fetch the related *Chromosome* for each *Gene* record one at a time. The **Apply Data List** functionality allows you to fetch the *Chromosome* for several *Gene* records in a single operation. To do this perform the following steps:

1. Fetch the data for the *Gene* category.
2. Fetch the related data from the category *Chromosome* for a record of *Gene*, for example, *Gene\_1*.
3. Add the *Chromosome* record to the data list.
4. From the **View Results** screen for the *Gene* records, (see Figure 14: View Search Results) select *Gene* records for which you want the related *Chromosome* records.
5. Click the **Apply Data List** button.
6. A message is displayed in the status bar when the operation is complete. Click **Next** to see the data list. . Fig. 17 shows the resulting data list.

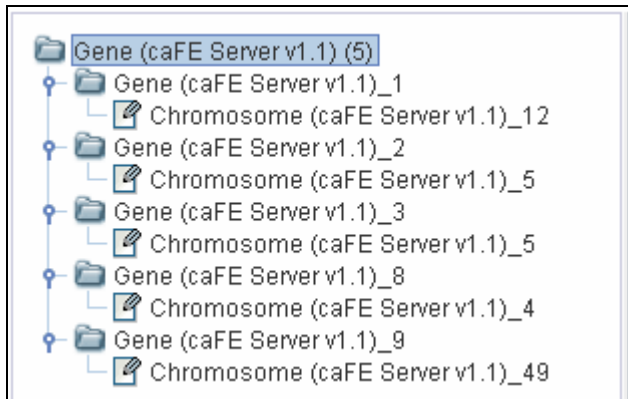


Figure 17: Result of Apply Data List to genes with id 2, 3, 8, 9

Thus, once you obtain the related data for a particular record, **Apply Data List** allows you to fetch similar related data for several other records easily.

### How the Apply Data List functionality works

To understand this functionality better, consider a slightly more complicated data list below:

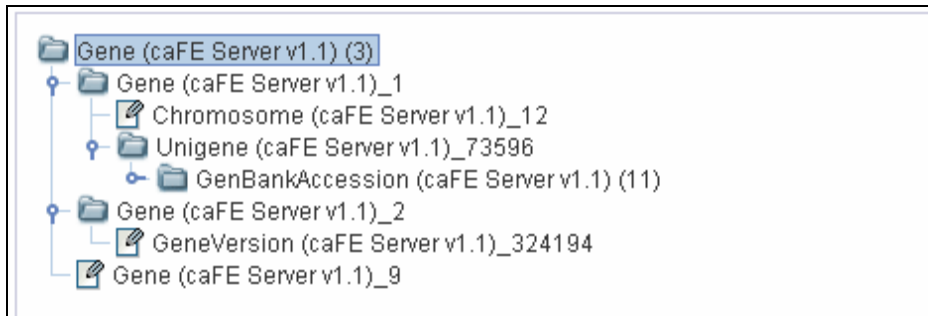


Figure 18: Example 3- Data List

#### Example 3

The following records have been added to the data list

- For *Gene\_1*, related *Chromosome*, *Unigene*, and *GenBankAccession* records are present.
- For *Gene\_2*, related *GeneVersion* is present.
- For *Gene\_9*, there is no other related data.

Now, **Apply Data List** to the genes *Gene\_1*, *Gene\_2* and *Gene\_9*. The resulting data list is shown below:

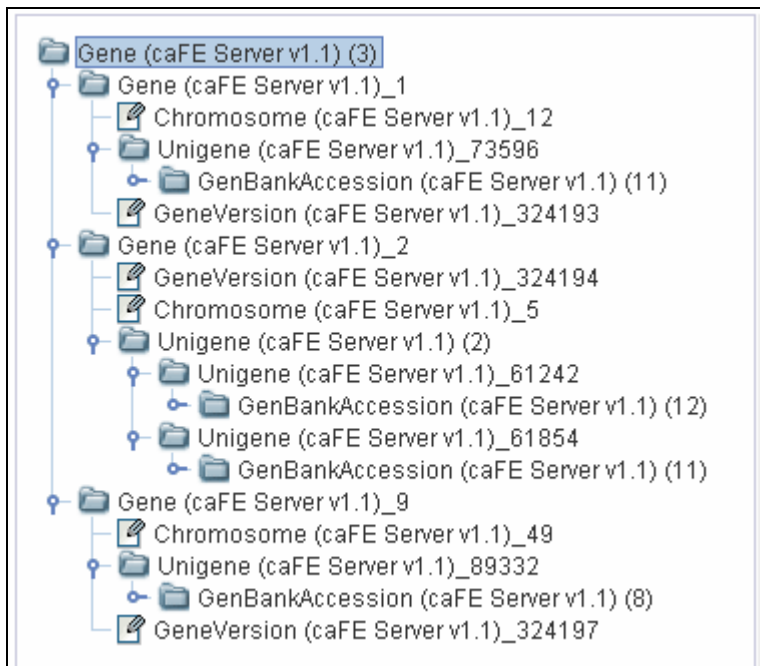


Figure 19: Example 3- Apply Data List

As seen from above figure, following new related data has been fetched:

- For *Gene\_1*, the system fetches *GeneVersion* (as *Gene\_2* had *GeneVersion*).
- For *Gene\_2*, the system fetches *Chromosome*, *Unigene*, and *GenBankAccession*, as these were the related data for *Gene\_1*.
- For *Gene\_9*, the system fetches all of *GeneVersion*, *Chromosome*, *Unigene*, and *GenBankAccession*.

As a result, each gene contains the related data for *GeneVersion*, *Chromosome*, *Unigene*, and *GenBankAccession*.

Thus, the **Apply Data List** operation results in a homogenous structure in the data list. The system fetches related data for all the other records like the related data present for one record.

## The Next and Previous Buttons

- Click **Next** to view the contents of the data list.
- Click Previous to go back to Choose Search Category tab.

## Viewing and Saving Data List

---

After adding the records of your interest to the data list, you can get the consolidated view of the data list. You can also export the data list into a CSV file or create an Experiment using the contents of the data list.

The following figure shows the data list tab:

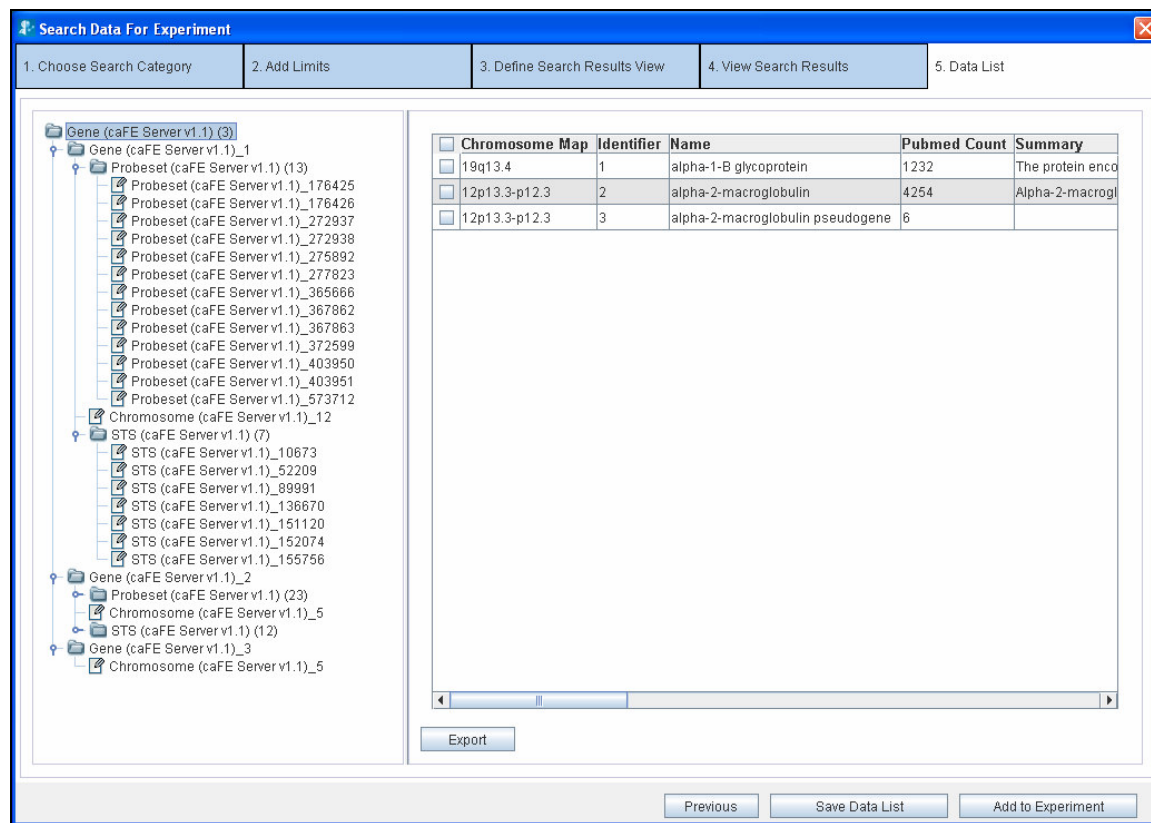


Figure 20: Data List

The left-hand side pane shows all the records that you have added to the data list in a tree format. Each node in the tree represents either a category or a record of a category.

- For a node representing a category:
  - The number of records for that category is shown in parentheses. For example *Gene (3)* means that you have added 3 records for the *Gene* category.
  - Clicking on the node updates the right hand side pane to show a spread sheet containing the records of that category (see figure above).
- For a node representing a record
  - The unique identifier for that record is displayed. For example, *Gene\_1* represents the record with identifier 1.
  - Click the node updates on the right hand side pane to show the details of that record.

## Operations on the Data List

You can do the following operations on the data list:

- Save the data list – Click the **Save Data List** button.
- Export the data list into a CSV file – Click the **Export** button.

- Add the data list to an Experiment – Click the **Add To Experiment** button.

To save the data list:

Click the **Save Data List** button.

Type the title and description for the data list.

Click the **Save** button. The system displays a message in the status bar indicating that the data list is saved.



# Chapter 3 Experiments

## In this Chapter

---

After you search and add some data of interest to the data list, you can create an experiment using that data. This chapter explains the various operations that you can perform on the data sets that you collected.

The following sections are described in this chapter:

- What are Experiments and Projects?
- Creating an Experiment
- Viewing the Existing Experiments

Working with an Experiment

- Filtering Data
- Analyzing Data

## What are Experiments and Projects?

---

An experiment is a collection of data. After you create an experiment, you can perform the following:

- Perform various analyses on the data using the grid-enabled analytical services
- Visualize the analysis results using various viewers such as bar charts, scattered plots.
- Create new data sets by applying filters on the existing datasets

A project is a collection of experiments. A project can contain many Experiments or other sub-projects. The grouping of experiments into projects helps you manage the multiple experiments easily.

Example of an experiment

**Aim:** Find out the micro-array data for a nonmalignant brain tissue. Perform **Comparative Marker Selection (CMS)** on this data to determine the expression values that are most closely correlated with a class template. View the correlation among the expression values as a scattered plot.

You need to perform the following steps using caB2B:

Step no.	Description	Related Section
1	Search for micro array data	Search data – The Query Wizard
2	Create experiment with this data	Creating an Experiment
3	Open the experiment you have created	Opening an Experiment
4	Filter the data further if desired	Filtering Data
5	Save the filtered data	How to save filtered data?
6	Perform CMS analysis on selected data	Analyzing Data
7	Plot analysis result as a scattered plot	Visualizing Data

## Creating an Experiment

---

To create an experiment, you need to have a saved data list with the required data. See Viewing and Saving Data List for details on how to do this.

After you have saved the data list, do the following to create an experiment:

1. Click the **Add to Experiment** button (Figure 20: Data List). This opens the **Create New Experiment** window.

**Create New Experiment**

\* Experiment Name : FE gene Trials

\* Project :

Add New

- My Projects
  - Gene Analysis
  - MicroArrays
    - Cell Free Nucleic Acid Detection
    - Texture Analysis
  - Gene Analysis
  - Participants analysis
    - Participants analysis

Description : This is the experiment on genes and chromosomes from FE application

Cancel Save

Figure 21: Create New Experiment

2. Give an appropriate name to the experiment.
3. Select the project in which you wish to create this experiment (see note below).
4. Provide a description of the experiment.
5. Click **Save**.

You can now close the **Search Data** wizard to return to the **Home** page and open the experiment.

	<ul style="list-style-type: none"> <li>• To create a new project, perform the following:               <ol style="list-style-type: none"> <li>1. Select the parent project under which you wish to create the new project</li> <li>2. Click the <b>Add New</b> button. This adds a new sub project under the selected project with the default name— <i>New Project</i>.</li> </ol> </li> <li>• To rename the new project               <ol style="list-style-type: none"> <li>1. Select the project.</li> <li>2. Press F2.</li> <li>3. Type the desired name.</li> <li>4. Press ENTER.</li> </ol> </li> </ul>
--	--

## Viewing the Existing Experiments

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On the caB2B Home page, click the Experiment tab. This opens the My Experiments page.

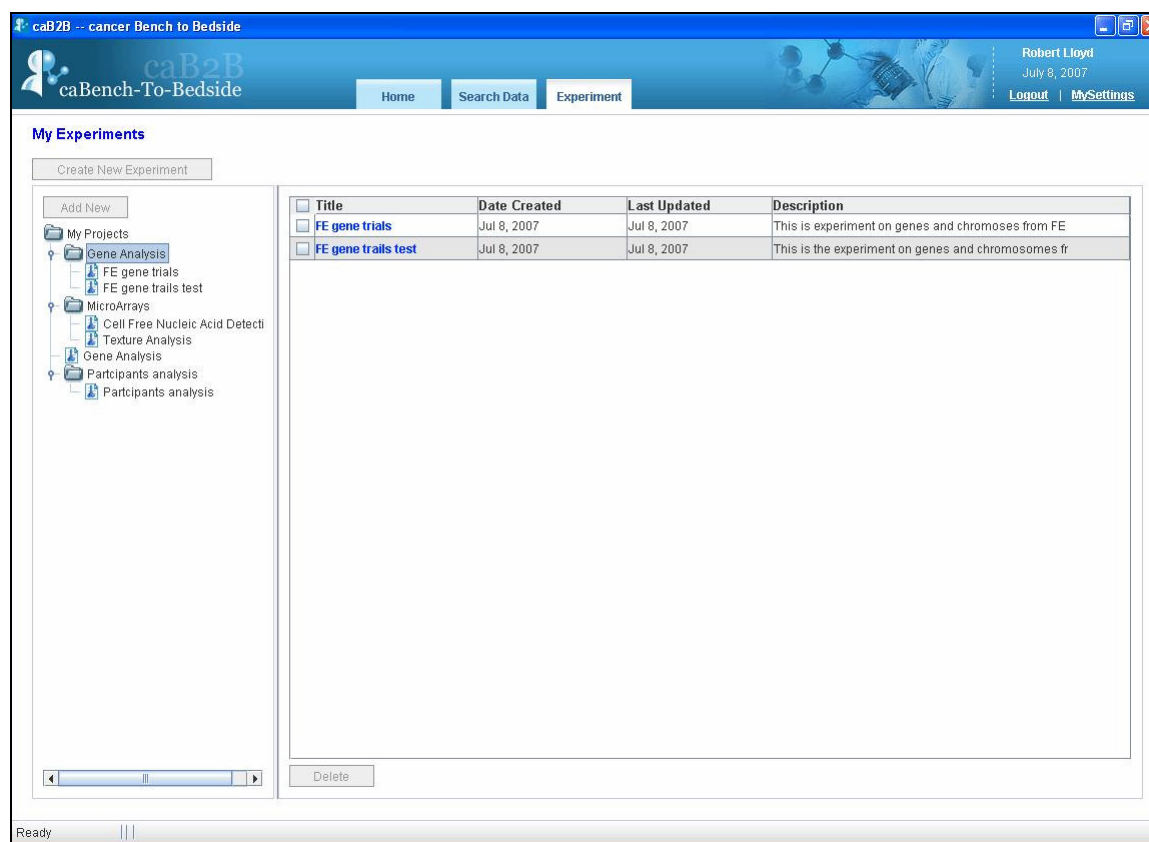


Figure 21: My Experiments

You can see all the projects and experiments that you created in the left panel.

When you select a project in the left hand side pane, the system displays a list of the experiments in the project in right hand side pane.

## Opening an Experiment

---

To open an experiment, go to the My Experiments page and click on the experiment title seen in the right panel (see Figure 21: My Experiments).

When you open an experiment, you see the Experiment Details page.

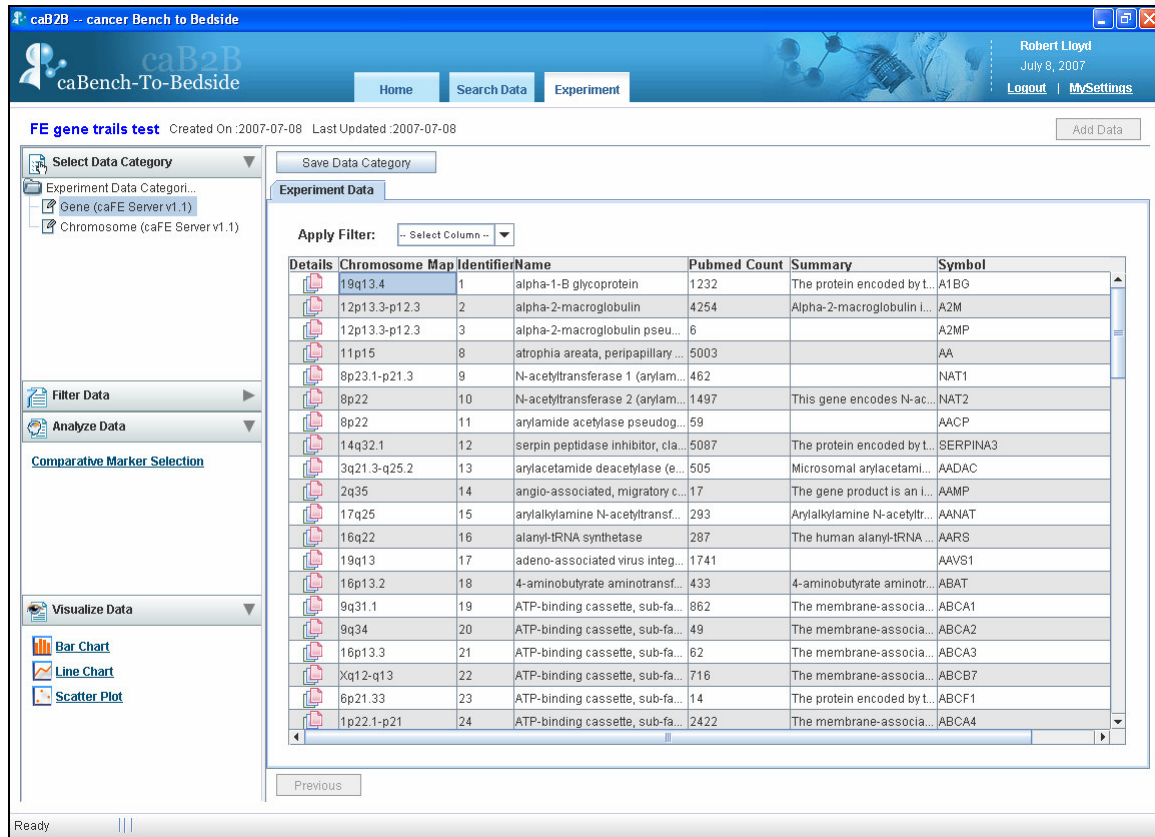


Figure 22: Experiment Details

## Working with an Experiment





The **Experiment Details** page consists of the following sections:

- The **Operations** panel on the left hand side
- The **Visualization** panel on the right hand side

### The Operations panel

The **Operations** panel contains the following collapsible boxes.

Table 1: Operations on the Experiment Page

UI Elements	Description
 <b>Select Data Category</b> ▼	Displays a list of all the data categories present in the experiment. See <i>How to save filtered data?</i>
 <b>Filter Data</b> ▼	Shows all the filters that are currently applied to the data of the selected data-category. See <i>Filtering Data</i> for details.
 <b>Analyze Data</b> ▼	Shows the links to call analytical services that are applicable to the selected data-category. See <i>Analyzing Data</i> for details.
 <b>Visualize Data</b> ▼	Shows the visualization options available for the selected data-category. See <i>Visualizing Data</i> for details.

## Visualization panel

This is the right hand side panel on the **Experiment Details** page (see Figure 22: Experiment Details). This panel can contain several pages at a time (see figure below). You can switch between the pages by clicking on the **tabs** at the top of this panel.

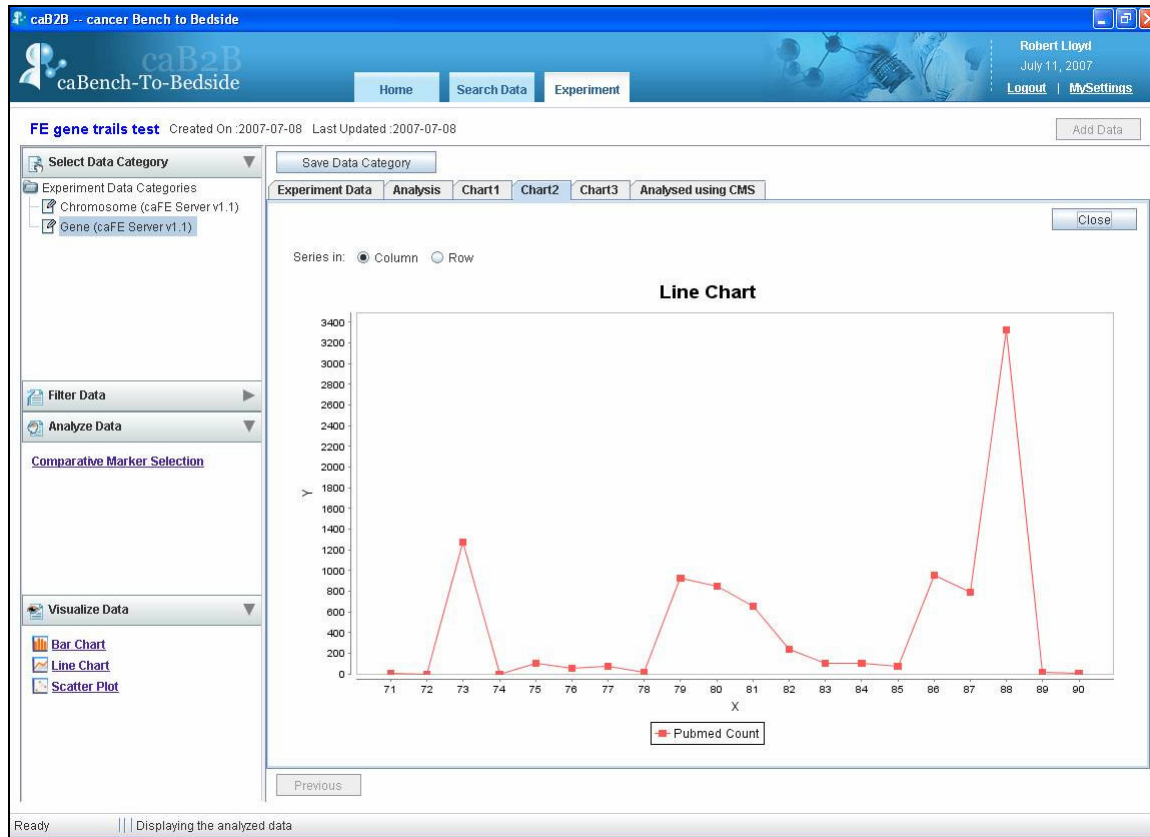


Figure 23: Visualization Pane

The visualization pane is updated based on the operations you do in the operations pane. For example,

Operations pane	What happens in Visualization pane
Click a data-category in the <b>Select Data Category</b> box	The <b>Experiment Data</b> tab is updated to show the records of that data-category
Choose a visualization from the <b>Visualize Data</b> pane	A new tab is created to display the desired visualization

## Filtering Data

The purpose of creating experiments is to perform analysis of the data. To aid the analysis, caB2B provides features to filter the data so that you can zero in on the data of your interest.

After you filter the data, you can save the filtered data as a **data-category**. For example, if you have created an experiment with all female Participants, you can now create different data categories based on age less than 50, age between 50 and 65 and age greater than 65.

## How to filter data?

1. From the **Apply Filter** dropdown list, (located at the top of the **Experiment Data** tab), select the

column of interest.

2. System displays appropriate filter controls.
3. Specify the values that the filtered data must satisfy.
4. The data in the **Experiment Data** tab is updated to show the filtered data.
5. The filter that you have applied is also shown in the **Filter data** box in the Operations panel on the left hand side.

You can now save the filtered data as a new data-category and use it to perform analyses or visualization.



You can filter on multiple columns by successively applying filters on those columns. For example, to obtain *female participants between age 30 and 40*

1. Apply the filter “Gender = female”.
2. Then apply the filter “age between 30 and 40”.

For details of the various filter controls and how to use them, see Types of Filters.

## How to edit a filter?

1. From the **Apply Filter** dropdown, choose the column whose filter you wish to edit.
2. An appropriate filter control is shown with the values that you previously entered.
3. Specify desired values of the filter (see Types of Filters).
4. The data in the **Experiment Data** tab is updated to show data based on the new filter.
5. The filter criteria shown in the **Filter data** box in the operations pane is also updated.

## How to remove a filter?

1. From the **Apply Filter** dropdown, choose the column whose filter you wish to remove.
2. An appropriate filter control is shown with the values that you previously entered.
3. Remove the values that you had specified (see Types of Filters).
4. The data in the **Experiment Data** tab is updated to show data on removing the filter.
5. The filter is also removed from the **Filter data** box in the operations panel.

## How to save filtered data?

Once you apply filters to a data set, you can save the filtered data as a **data-category**. You can create as many data-categories as you want. The data-categories can be further used for data analysis.

Once you have obtained filtered data, you might wish to save it as a new data-category.

To do this,

1. Click the **Save Data Category** button (located at the top of the Visualization panel).



2. The **Save as Data category** panel is displayed.
3. In the **Title** field, type the title of the new data-category.
4. Click **Save**.

The new data-category will appear under **Custom Data Categories** section in **Select Data Category** box of the operations pane.

## Analyzing Data

---

After you searched the data of interest and created experiments from it, you can analyze that data. To do this you can use various analytical services that are available. Typically they accept data, perform analyses on it and return the result. You can also pass configuration parameters along with the data to the analytical services.

When you are viewing the data, the services that can operate on that data are shown in the **Analyze Data** box. In the current version one analytical service **Comparative Marker Selection**, from gene pattern is available.

How to analyze data?

1. Select the data category from **Select Data Category** box, for example *Bioassay*.
2. In the **Analyze Data** box, click on the link to call the service, for example **Comparative Marker Selection** link.
3. It will open a popup that accepts configuration parameters for the service. Figure 24: Configuration parameters for **CMS**.
4. Enter the **Title** for this analysis and values for the various parameters
5. Click the **Finish** button to submit this analysis.

Comparative Marker Selection Parameter Set

Analysis Title : CMS for Hu95Av2

Balanced : ☒ True ☐ False

Complete : ☐ True ☒ False

Min Std : 2

Number Of Permutations : 1000

Phenotype Test : one-versus-all

Random Seed : 5

Smooth Pvalues : ☐ True ☒ False

Test Direction : two-sided

Test Statistic : SNR-minstd

Finish

Figure 24: Configuration parameters for CMS

You can see the new **Analysis** tab added in the right hand side panel. It contains following fields:

Field	Description
Data Category	The data category on which you performed the analysis.
Analysis Title	The title you provided for the analysis. It is a link to the result of the analysis.
Date	The date on which you performed the analysis.
Status	Indicated whether analysis is <b>completed</b> or <b>pending</b> .

You can view the result on **completed** analysis by clicking the link in Analysis **Title** field.



## Visualizing Data




You can visualize the data in the experiment using various graphical components like charts and scatter plots. These options provide a graphical summary of the data allowing comparison, variation and co-relational analysis of the data.

Some Terms that are used:

**Data series:** Related data points that are plotted in a chart and originate from data rows or data columns. Each data series in a chart has a unique color or pattern. This is represented by a *Legend*. You can plot one or more data series in a chart.


**Legend:** A small color box that identifies each series in the chart.

The current version of caB2B supports following visualization options in **Visualize Data** box:

Visualize option	Description
 <a href="#">Bar Chart</a>	This is a chart with rectangular bars of lengths proportional to the data value it represents.
 <a href="#">Line Chart</a>	This is a chart with a line joining the points that represents data value
 <a href="#">Scatter Plot</a>	A scatter plot will show a linear or non-linear relationship between the variables (column selected). It also helps in finding odd-mans in the data.

*Table 2: Types of charts supported*

How to plot data series:

1. Select the data that you want to plot from **Experiment tab**.
2. Click on the link for type of the chart you wanted, for example  [Bar Chart](#)
3. It will open the chart in a new tab in right hand side panel.
4. By default data series are from columns on the **Experiment Data** tab.

Following screen shots represents the various charts for **pubmed count** for few Genes from FE server).

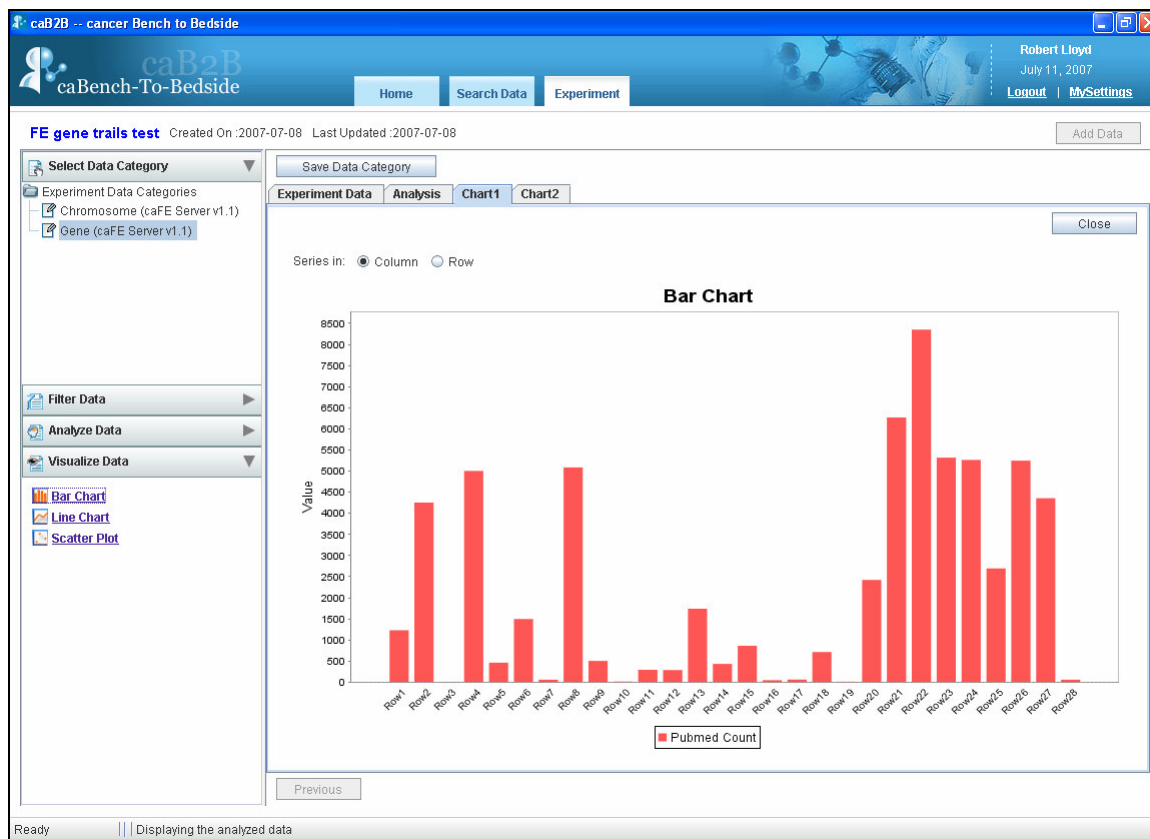


Figure 27: Bar chart example

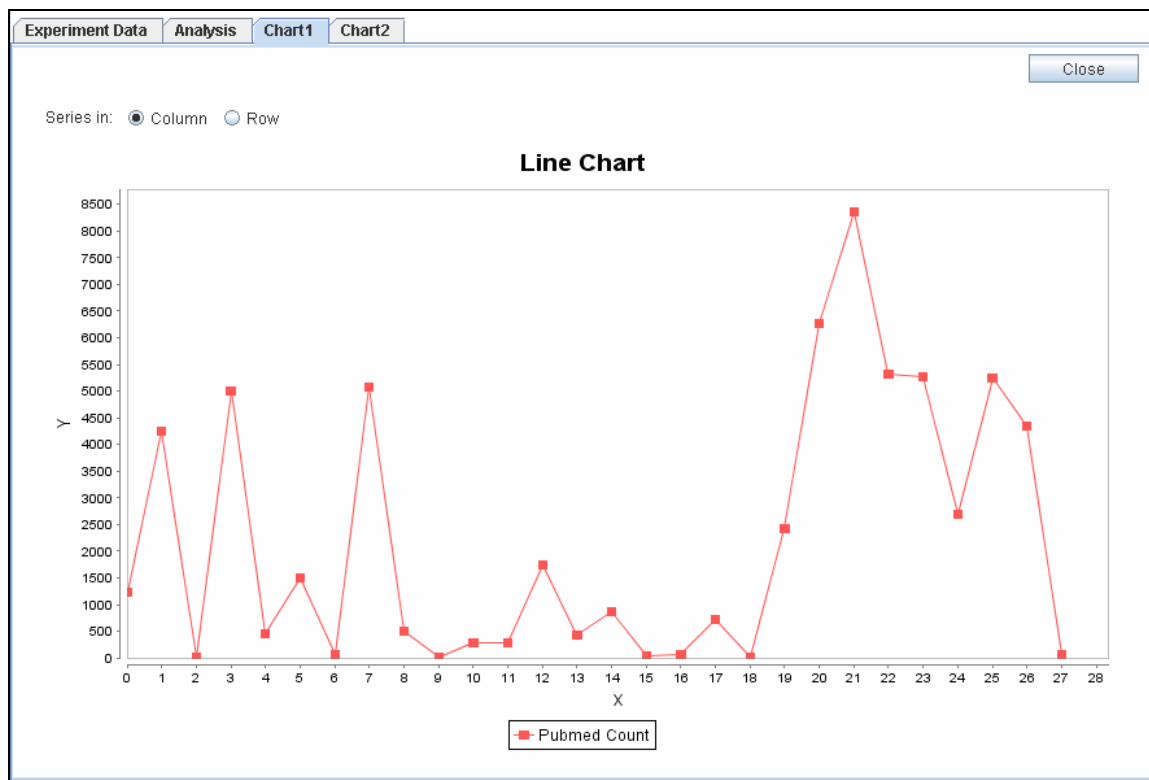


Figure 28: Line chart example

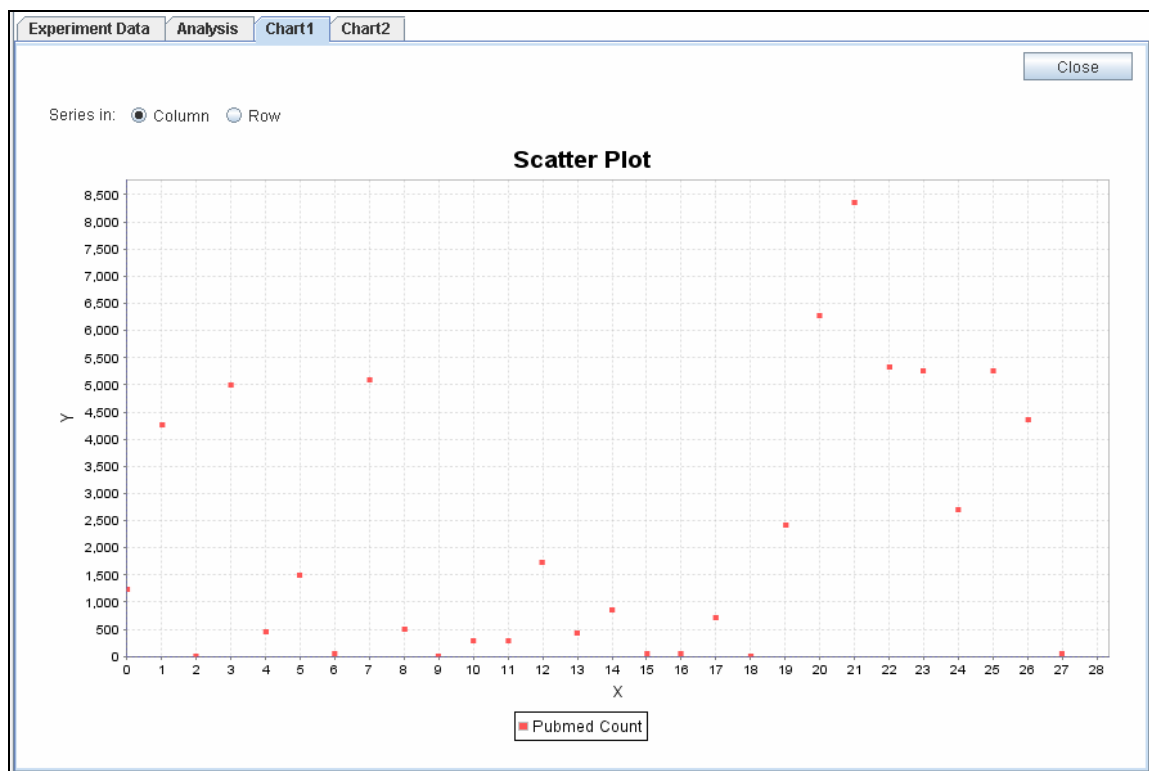


Figure 29: Scatter Plot example

How to change data series from rows to column and vice versa?

You can configure whether data series are from rows or columns by selecting appropriate **Series In** options.

- To have the data columns to represent the data series, select ☐ Column option.
- To have the data rows to represent the data series, select ☒ Row option.

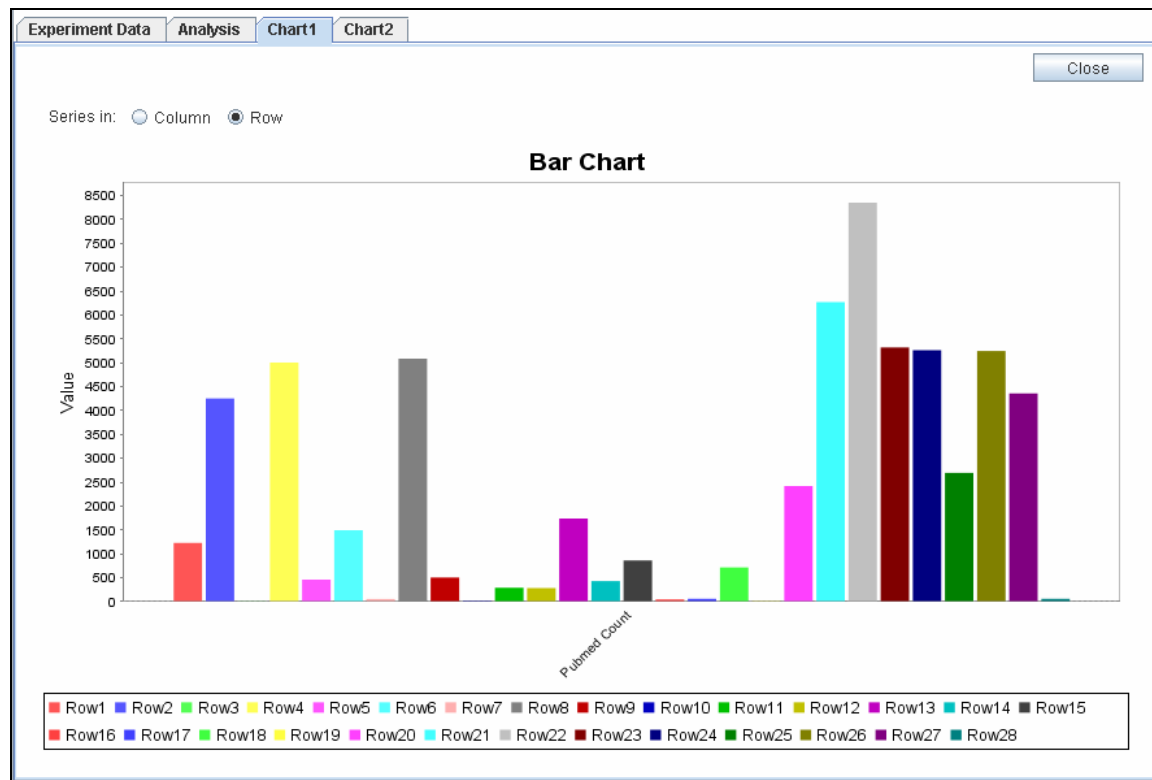


Figure 30: Bar chart with data series from rows



You can change the type of the chart you are currently viewing by selecting required chart link from **Visualize Data** box.

You can create multiple charts for the data.

The name of the tab added for each chart is “chart” followed by a unique number for that chart. For example *chart1*, *chart2* and so on.

# Chapter 4      Appendix 1

## Examples of category search

---

This appendix provides examples of the advanced search when you search for categories.

### Text-based Search - Example 1

To search categories having *gene* in their name, you need to do following:

1. In the **Search** box, type *gene*.
2. Select the **Category** check box.
3. Click the **Text** option button.
4. Click the **Search** button.

The results of this search are as shown below. All the categories shown below have *gene* in their names.



(E.g. Participant, Gene, Experiment, Protein, Specimen)

**Advanced Search**

☒ Category    ☐ Include Description  
☐ Attribute    ☐ Permissible Values  
☒ Text    ☐ Concept Code

**Search Results :- Total results ( 16 )**

[Gene Annotation](#)  
 Gene annotation includes information about a gene such as its symbol, gene name(s), c....

[Genomic Identifiers](#)  
 Genomic identifiers from many publicly available databases (e.g. Entrez, UniGene, Gen....

[Literature-based Gene Association](#)  
 Genes that are co-mentioned in the same PubMed abstracts have been curated. Each pai...

[Mi](#)  
 Mi Genes that are co-mentioned in the same PubMed abstracts have been curated. ro...  
 Each pair of genes as well as their correlation, calculated by squaring the  
 Or number of abstracts where the two genes are co-mentioned divided by the product  
 Ca of the number of abstracts mentioning each of the genes, is reported. f....

[EnsemblGene \(GeneConnect v1\)](#)  
 This class representing the Ensembl Gene ID.

<< < 1 2 3 > >>

Figure 31: Search Result of Example 1

## Text-based Search - Example 2

To search the categories having `Protein` in their name or description or to search the attributes having `Protein` in their name or description, you need to do following:

1. In the **Search** box, type **Protein**
2. Select the **Category** check box.
3. Select the **Attribute** check box.
4. Select the **Include Description** check box.
5. The **Text** option button is selected by default.
6. Click the **Search** button.

The result of this search is as shown in the screenshot below.

The screenshot displays a web-based search interface. At the top, there is a search input field containing the text 'protein' and a 'Search' button to its right. Below the input field, a hint text reads '(E.g. Participant, Gene, Experiment, Protein, Specimen)'. An 'Advanced Search' panel is open, showing several options: 'Category' and 'Include Description' are checked; 'Attribute' is checked and 'Permissible Values' is unchecked; 'Text' is selected with a radio button, while 'Concept Code' is unselected. Below this panel, a blue header bar indicates 'Search Results :- Total results ( 11 )'. The results are listed as follows:   
1. [Gene Annotation](#): Gene annotation includes information about a gene such as its symbol, gene name(s), c....   
2. [Genomic Identifiers](#): Genomic identifiers from many publicly available databases (e.g. Entrez, UniGene, Gen....   
3. [Microarray Annotation](#): Microarray annotation includes information about a probe or probeset found on a micro....   
4. [BioMaterial \(caArray v1.1\)](#): BioMaterial is an abstract class that represents the important substances such as cel....   
5. [BioSequence \(caArray v1.1\)](#): A BioSequence is a representation of a DNA, RNA, or protein sequence. It can be repr....   
6. [GenBankAccession \(caFE Server v1.1\)](#): The GenBank Accession for a Gene   
At the bottom of the results, there is a pagination control showing '<< < 1 2 > >>' with the number '2' highlighted in red.

Figure 32: Search Result of Example 2

## Concept Code Based Search - Example 3

To search categories having concept code c29867:

1. In the **Search** box, type c29867.
2. Select the **Category** check box.
3. Select the **Concept Code** option button.
4. Click the **Search** button.

The result of this search is as shown in the screenshot below.

The screenshot displays a search interface. At the top, a search box contains the text 'c29867' and a 'Search' button is to its right. Below the search box is a hint '(E.g. Participant, Gene, Experiment, Protein, Specimen)'. A section titled 'Advanced Search' contains several checkboxes: 'Category' (checked), 'Include Description' (unchecked), 'Attribute' (unchecked), and 'Permissible Values' (unchecked). Below these are two radio buttons: 'Text' (unchecked) and 'Concept Code' (checked). Below the 'Advanced Search' section is a blue header for 'Search Results :- Total results ( 3 )'. The results are listed as follows: 1. [CollectionProtocolRegistration \(caTissue Core v1.1\)](#) with the description 'A registration of a Participant to a Collection Protocol'. 2. [Participant \(caTissue Core v1.1\)](#) with the description 'An individual from whom a specimen is collected'. 3. [ParticipantMedicalIdentifier \(caTissue Core v1.1\)](#) with the description 'A medical record identification number that refers to a Participant'.

Figure 33: Search Result of Example 3

## Concept code based search - Example 4

To search categories whose attribute has concept code C42614

1. In the **Search** box, type C42614.
2. Select the **Attribute** check box.
3. Select the **Concept Code** option button.
4. Click the **Search** button.

The result of this search is as shown in the screenshot below.

(E.g. Participant, Gene, Experiment, Protein, Specimen)

**Advanced Search**

☐ Category    ☐ Include Description  
☒ Attribute    ☐ Permissible Values  
☐ Text    ☒ Concept Code

**Search Results :- Total results ( 110 )**

[Gene Annotation](#)  
 Gene annotation includes information about a gene such as its symbol, gene name(s), c....

[Literature-based Gene Association](#)  
 Genes that are co-mentioned in the same PubMed abstracts have been curated. Each pai...

[Microarray Annotation](#)  
 Microarray annotation includes information about a probe or probeset found on a micro....

[Orthologous Gene](#)  
 Category providing details of orthologous genes associated with given gene obtained f...

[Array \(caArray v1.1\)](#)  
 The physical substrate along with its features and their annotation

[ArrayDesign \(caArray v1.1\)](#)  
 Describes the design of an gene expression layout. In some cases this might be virtu....

<< < 1 2 3 4 5 > >>

Figure 34: Search Result of Example 4

## Define Limit: Operators and Values


This appendix explains the various operators and how to specify values while defining limits on a category.

The following table explains the different operators and provides examples as to how values are to be specified.

Table 3

Operator	Data types for which applicable	Sample condition	Expected Results
Equals	Numeric Date String	Name <b>equals</b> "John"	Returns only John and not john.
Not equals	Numeric Date String	Identifier <b>not equals</b> 32	Returns all records except those having identifier = 32
Less than	Numeric Date	Participant's birth date <b>less than</b> 2000/1/1	Returns all Participants born before January 1 <sup>st</sup> , 2000
Less than or equal	Numeric Date	Signal value less than or equals to 0.5	Returns all records for which signal value is not more than 0.5
Greater than	Numeric Date	Cell count is <b>greater than</b> 10000	Returns all records with Cell count > 10000
Greater than or equals	Numeric Date	Specimen's collection-date <b>greater than or equal to</b> 2005/5/1	Returns all specimens collected on or after May 1 <sup>st</sup> , 2005
Between	Numeric String Date	Patient's admission date <b>between</b> 2000/1/1 and 2000/12/31	Returns all Patients admitted in the year 2000
Is null	Numeric String Date	Patient's contact number <b>is null</b>	Returns all patients who do not have any contact number
Is not null	Numeric Date	Participant' middle name <b>is not null</b>	Returns all Participants for whom middle name is not specified
In	Numeric String Enumerated	Signal value <b>in</b> 0.1,0.5,0.7	Returns all records whose signal value is 0.1 or 0.5 or 0.7
Not in	Numeric String Enumerated	Participant's gender <b>not in</b> male, unspecified	Returns all participants whose gender is either not specified or gender is not male.

Starts with	String	Participant's first name <b>starts with</b> Jo	Returns all participants whose first name starts with Jo like John, Jona.  Does not return the participant with name Scott, Henry, Jen
Ends with	String	Participant's last name <b>ends with</b> n	Returns all participants whose last name ends with n like John, Jon, Jen. Does not return participant with name Scott, Henry
Contains	String	Participant's first name <b>contains</b> ann	Returns all participants whose first name is Joanna, Anna, and Johanna. Does not return participant with name Jen, Denny

- For attributes with enumerated values and Boolean attributes, clear a value by clicking on the value with the CTRL key pressed.
  - If you use the **In** operator for a non-enumerated attribute, you can specify multiple values as follows:
  - Multiple values should be separated using a comma. For example, to specify the constraint **Identifier IN 2, 4, 5, 7**, you should type the value as **2,4,5,7**.
- If a value itself contains a comma, you can enclose the value in double quotes. For example, to specify the constraint **Name IN "Einstein, Albert", "Newton, Isaac"** the value that you should enter is **"Einstein, Albert", "Newton, Isaac"**.
- For attributes that requires a date value, you can click the  icon to launch a date selector. You can also type a date string directly in the text box. The format of this string must be **YYYY/MM/DD**. A valid date string becomes **green** whereas an invalid date string turns **red**. An invalid date string will be ignored.

## Record Details View

---

The details of a record usually consist of the values of the attributes of the category. See Figure 15: Results' Details for an example.

This section provides examples of special categories that result in a slightly different view of the record's details.

## Administrator defined categories

---

These categories are built by grouping relevant attributes from one or more existing categories.

For each record of such a category the following information is shown:

Values of the attributes in a table

Related information as a tree. The leaf nodes of this tree are attributes; you can see the values of those in the **value** column.

Path: [Genomic Identifiers](#) >> **Genomic Identifiers\_18667**

Attribute	Value
Ensembl Gene ID	ENSG00000120738
Entrez Gene ID	1958
Uni Gene Cluster ID	Hs.326035

Associated Information	
✚ MessengerRNA (3)	
✚ MessengerRNA_6174	
✚ MessengerRNA_6175	
✚ MessengerRNA_198617	
GenBank Nucleotide Accession Number	
RefSeq mRNA Accession Number	NM_001964
Ensembl Transcript ID	
✚ Protein (5)	
✚ Protein_372670	
Ensembl Peptide ID	ENSP00000239938
UniProtKB Primary Accession	P18146
GenBank Protein Accession Number	
RefSeq Protein Accession Number	NP_001955
✚ Protein_372672	
✚ Protein_3435049	
✚ Protein_5676098	
✚ Protein_5852919	

Figure 35: One record of an administrator defined category (Genomic Identifiers)

## BioDataCube

A biodatacube is a three-dimensional array representing micro-array data. The system displays a record containing a biodatacube (for example, the *BioAssayData* category of caArray) as shown in the screen below:

Attribute			Value		
Identifier			1		
Name			1		
	Pairs 1	Pairs Used 1	Signal 1	Detection 1	Detection P-value 1
92555_at	20.0	Absent	0.13876513	2.188886E-4	0.0030666848
92558_at	16.0	Present	0.3276513	3.188886E-4	0.0030666848
92559_at	20.0	Present	0.5645876513	4.188886E-4	0.0030666848
92568_at	16.0	Marginal	0.464376513	5.188886E-4	0.0030666848
92574_at	20.0	Absent	0.235876513	6.188886E-4	0.0030666848
92555_at	20.0	Absent	0.13876513	2.188886E-4	0.0030666848
92558_at	16.0	Present	0.3276513	3.188886E-4	0.0030666848
92559_at	20.0	Present	0.5645876513	4.188886E-4	0.0030666848
92568_at	16.0	Marginal	0.464376513	5.188886E-4	0.0030666848
92574_at	20.0	Absent	0.235876513	6.188886E-4	0.0030666848
92555_at	20.0	Absent	0.13876513	2.188886E-4	0.0030666848
92558_at	16.0	Present	0.3276513	3.188886E-4	0.0030666848
92559_at	20.0	Present	0.5645876513	4.188886E-4	0.0030666848
92568_at	16.0	Marginal	0.464376513	5.188886E-4	0.0030666848
92574_at	20.0	Absent	0.235876513	6.188886E-4	0.0030666848
92555_at	20.0	Absent	0.13876513	2.188886E-4	0.0030666848
92558_at	16.0	Present	0.3276513	3.188886E-4	0.0030666848

Figure 36: BioDataCube Record

This table displays the values of the attributes of the category, in a table at the top. A separate two-dimensional array shows the contents of the BioDataCube (the third dimension of the cube is transformed into multiple columns).

## Types of Filters

A filter control is shown when you choose to filter the data of a data-category (see How to filter data).

The type of filter control upon the column based on which you wish to filter data.

Table 4: Column Type and Applicable Filter

Data type of the column	Applicable filter
Numeric	Range filter
Text	Pattern filter
Column with permissible values	Enumerated filter
Boolean	Enumerated filter



## Using the Range Filter

The system shows a **Range Filter** if the column selected as a basis for the filter has numeric values.. It allows you to select the desired minimum and maximum values of the column.

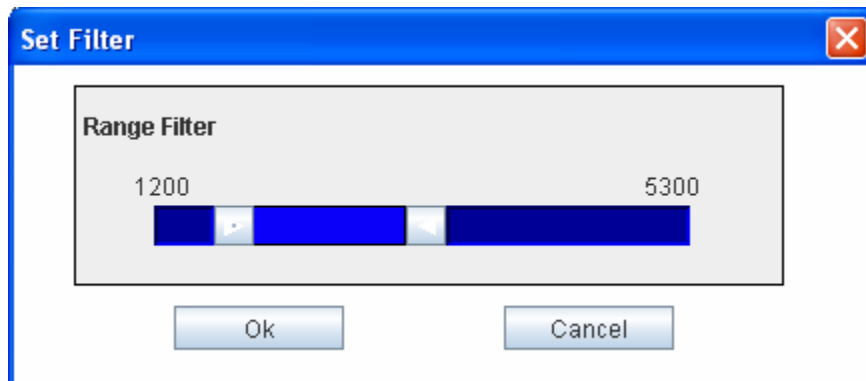


Figure 37: Set Filter for Range

There are two sliders, the left slider and the right slider. The value denoted by each slider is shown at the two ends.

1. Position the left slider at the minimum value desired.
2. Position the right slider at the maximum value desired.
3. Click **Ok** to apply the filter.

## Using the Pattern Filter

The system shows a **Pattern Filter** If the column selected as a basis for the filter has text values. It allows you to specify a pattern that the values of that column should satisfy.

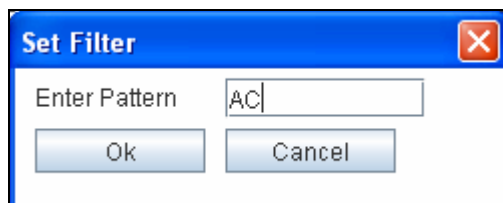
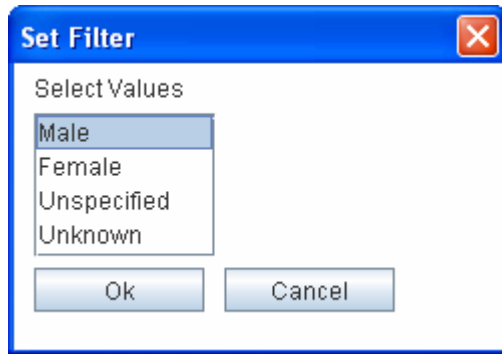


Figure 38: Pattern Filter

In the **Enter Pattern** field, type the desired pattern and click **Ok**.

## Using the Enumerated Values Filter

The system shows an **Enumerated Values Filter** if the column selected as a basis for the filter has a set of permissible values. It allows you to specify the values that the column should satisfy.



*Figure 39: Enumerated Values Filter for the column gender*

Select the desired permissible values and click **Ok**.