
DrugMatrix Reference Guide

Release 2.4

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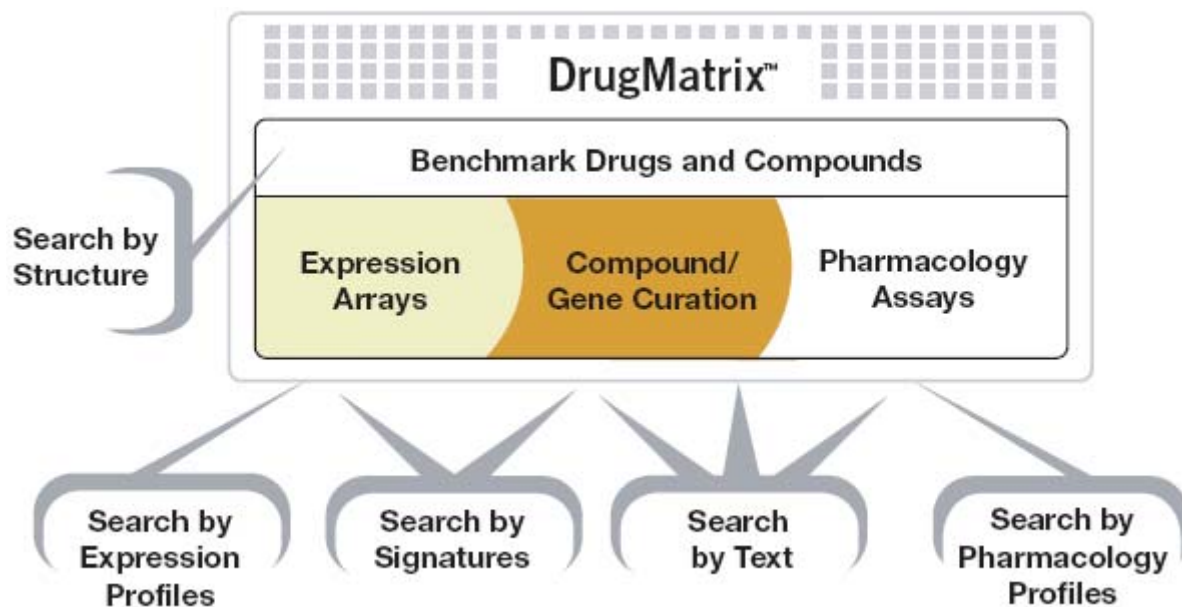
DrugMatrix Overview

The DrugMatrix application is a comprehensive suite of tools that integrate algorithmically extracted experimental data from the proprietary DrugMatrix database with curated information from the scientific literature, reference material and online databases.

Information is presented through seven Major Domains—**GENE**, **COMPOUND**, **ASSAY**, **EXPRESSION EXPERIMENT**, **PATHWAY**, **EXPRESSION STUDY**, and **SIGNATURE**.

Two primary data domains, **GENE** products, and **COMPOUNDS**, are connected via change to chemogenomic-based secondary domains: **ASSAY** activities (a direct measure of interaction between a compound and a target) and **EXPRESSION** array profiles (a measurement of the indirect effects of a compound on the genome). Two secondary domains, **PATHWAY** and **EXPRESSION STUDY**, provide amplifications of these domains. An additional secondary, **SIGNATURE** provides patterns of gene expression that can be used to classify compounds or a set of common experiments reliably compared to the experiment population, or a defined set of control experiments.

The diagram below provides a graphical representation of ways you can enter the database and conduct your queries.



DrugMatrix Desktop Computer Requirements

DrugMatrix requires a minimum of a Pentium 3 computer at 750MHz with 256 Mbytes of RAM. A Pentium 4 processor at 1.5GHz with 384Mbytes of RAM is recommended.

Windows 2000. Internet Explorer version 5.5 SP2, or newer.

To do compound structure searches, you need the Chime PRO plugin, available by licensing from MDL Information Systems (Version 2.6 SP3, or newer).

The DrugMatrix Graphical User Interface

The Graphical User Interface to the DrugMatrix application consists of:

- A set of **sophisticated querying tools** that allow you to query by expression profile, by chemical structure, by gene and compound names or by the presence of any attribute (e.g. a compound that induces a specific gene and has a specific bioactivity).
- **Comprehensive reporting** tools that provide integrated information including automatically generated links to information from other data domains. For example, the **COMPOUND** Domain Report provides, among other things, links to expression experiments (and the associated array technology) in which the query compound has been used and links to all genes (and related assays) that have been significantly impacted by the query compound.
- **Sophisticated data visualizations** to provide extensive detail about query items. The DrugMatrix application uses a number of sophisticated, predefined algorithmic searches to extract, and graphically present, detailed information relevant to the query item.

Organization of Information

Information, extracted from the database, is organized into seven **Domain Reports** that represent each of the DrugMatrix data domains (**GENE**, **COMPOUND**, **ASSAY**, **EXPRESSION**, **PATHWAY**, and **EXPRESSION STUDY**, and **SIGNATURE**).

Each Domain Report contains a subset of **Chemogenomic Data Reports** and **Detail Reports** that present cross referenced experimental data from the proprietary DrugMatrix database and curated information from the scientific literature, reference material and online databases.

The screenshot shows the DrugMatrix 2.3 web application interface. The browser title is "DrugMatrix 2.3 - Microsoft Internet Explorer". The page header includes "DrugMatrix" and "HELP". The main navigation bar contains tabs for "GENE", "COMPOUND", "ASSAY", "EXPRESSION", "PATHWAY", "EXPR. STUDY", and "SIGNATURE". Below this is a search bar with "FIND TEXT" and "WITHIN DOMAIN" options. The central content area displays "ESTROGEN RECEPTOR 1" with sub-tabs for "ACCESSION", "SYNONYMS", and "DETAILS". Below this is a table with columns "GENE", "METHOD", "SCORE", and "SPECIES". The right sidebar contains "GO DATA" and "GO DATA" sections. The bottom right corner shows "SERVER STATUS: PROCESSING" and a list of socket connections for various domains.

As you execute operations within the DrugMatrix framework (for example conduct queries, save lists, or access previously saved lists) the Server Status Messages appear at the bottom right of the User Interface indicate the progress of the requested operation.

Search and List Management Tools

The Search and List area of the DrugMatrix Application consists of tools for generating **Simple Searches** and **Advanced Searches** of the database as well as a **Workspace** with tools for the management of lists generated by these searches.

Lists that have been generated by database searches, previously saved lists that have been retrieved, **Data Objects**, **Favorite** items are all displayed in the **Workspace** area.



SEARCH

This tab accesses the **SIMPLE SEARCH** features of the DrugMatrix application which enables you to search each of the DrugMatrix domains. For more information see [‘Simple Search Panel’ on page 116](#).

ADVANCED

This tab accesses the DrugMatrix suite of **ADVANCED SEARCH** tools which enable you to conduct customized queries base on numerous predefined criteria. For more information see [‘Advanced Search Panel’ on page 118](#).

WORKSPACE

This tab accesses the DrugMatrix **WORKSPACE** area where you can save and organize list generated in your research. The DrugMatrix **TOOLBOX** is also accessed from this tab. For more information about the **WORKSPACE** area, see [‘Workspace Panels’ on page 123](#).

For more information about the DrugMatrix toolbox, see [‘The DrugMatrix Toolbox’ on page 135](#)

The Dataview Panel

The **DATAVIEW** panel, accessed via the DATAVIEW tab on the right side of the User Interface, displays additional information and visualizations derived using the DrugMatrix toolbox.

The DrugMatrix application provides a suite of software tools to define very specific database queries and help you work with generated lists that are relevant to your research.

The **TOOLBOX** button, located on the **WORKSPACE** panel, launches a toolbox containing these tools. For more information about these tools, see [‘Toolbox Functionality’ on page 136](#).



Getting Started

Populating Domain Reports

When you first open the DrugMatrix Application, all reports will be empty. Domain Reports can be populated with information in several ways:

- Use the DrugMatrix query tools.
- Select an item from a previously saved list, or from a favorites list.
- Use the **<| BACK** and **>| FORWARD** buttons at the top left of the Domain Report panel to access lists that have been generated in the current session.
- Click a hyperlinked item from a record within a previously populated Domain Report.
- Upload array data using the **LOAD DATA** tool in the **DATA/IMPORT EXPORT** section of the DrugMatrix toolbox.

Simple Search

The easiest way to extract information from the database is a simple search. To conduct a simple search:

- Select the **SEARCH** tab (selected by default).
- Use the - **Select** - menu to select the domain for the query.
- In the **FIND TEXT** field, enter the text string to define your search.
- Click the **DISPLAY** button.
 - DrugMatrix will retrieve and display all records from the database that contain the name you have entered.
 - Example: “**FIBRA**” will retrieve and display a list of all compounds in the database that include “**FIBRA**” in the name (e.g. **CIPROFIBRATE**, **CLOFIBRATE**, and **FENOFIBRATE** as well as others).
- Click on an item from this list.
 - This will populate the appropriate Domain Report with relevant information from the database about this selection.
 - Example: **CLOFIBRATE** selected from a retrieved list, will populate a **COMPOUND** report with all relevant information about **CLOFIBRATE** from database.

By selecting hyperlinked items within a given Domain Report, you can populate other data domains. For example, the **ACTIVITIES** panel of the **GENE** Domain Report presents a list of compounds that bind to, or inhibit, a specific gene product in the context of a specific bioassay. If you select a compound name from this report, it will generate a **COMPOUND** Domain Report for that compound. Similarly, if you select an assay name from the same **GENE: ACTIVITIES** report, it will generate an **ASSAY** Domain Report for that assay.

Advanced Search

The DrugMatrix suite of query tools enable you to conduct a number of sophisticated queries to filter for drug/target interactions and mine data relevant to your research. These tools are discussed in ‘[Search and List Area](#)’ on page 113.

Global Navigation Features

Global Navigational features function in the same way throughout the application. This section describes the behavior (i.e. “opens dialog box”) but not the specific action (i.e. opens popup containing gene sequence) of the global navigation features of the DrugMatrix application.

Menus

Menus appear on the List Display panel of the Search and List area, on each of the Domain Reports, and on each panel within the Chemogenomic Data Reports.



Display Menus

Menus that launch displays of additional information appear on the List Display panel and at the top of all Domain Reports.

MENU

Used to print the current Domain Report.

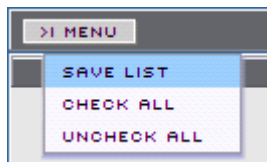


DISPLAY FOR PRINTING

Opens a new browser window containing a printable version of the current domain report. Use the browser's Print command to print the document.

List Menus

MENU



Save the currently displayed list and specify records to be saved with the list. List menus appear on all **Domain Report** panels and in the list display area of the **Search and List** tools.

Some panels allow you to save more than one of the lists that appear on the panel. The **MENU** button on any panel will indicate which lists can be saved.

SAVE

Save all checked records in the list.

CHECK ALL

Check all records in the list. All records will be saved.

UNCHECK ALL

Remove all checks. No records will be saved.

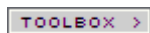
Window Controls



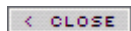
Expand the current panel.



Collapse the current panel.



Open the DrugMatrix List Tool Box.



Close the DrugMatrix List Tool Box.



Expand compound structure image in all rows of current table.



Minimize compound structure image in all rows of current table.

Buttons

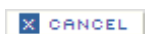
All buttons in the DrugMatrix application include the name of the associated action as well as one of several symbols intended to help indicate the associated action.



Buttons of this type initiate operations such as **DISPLAY**, or **IMPORT** present additional information, for example popup windows, dialogs or lists.



Buttons that are 'grayed out' are inactive on input forms or dialogs until appropriate data has been specified.



Cancel the current action and close the associated form or dialog box.

Icons

Icons in the DrugMatrix application provide a visual representation of the associated action.



Open a popup window displaying an expanded image of the query molecule, or molecule in the selected record.

This image can be copied and used with the **COMPOUND SEARCH/COMPARE** tool found on the **TOOLBOX**.













If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.



Display the referenced publication (from the scientific literature, reference material and online databases) in a new browser window.



Icons - Workspace

There are several icons on the **WORKSPACE** panel that enable you to manage lists. Drag a list onto an icon, or click on the icon (with the exception of the **DISPLAY LIST** icon) to initiate the indicated operation.

- | | | |
|---|-----------------------|--|
|  | DISPLAY LIST | <p>Display a SAVED LIST in the LIST DISPLAY panel below the WORKSPACE, or display a DATA OBJECT (with the  icon attached) in a domain report. See ‘Data Object’ on page 225.</p> <p>This feature is unavailable for FAVORITES items.</p> |
|  | DUPLICATE LIST | <p>This feature is available for SAVED LISTS only, not for FAVORITES items or DATA OBJECTS (with the  icon attached). See ‘Data Object’ on page 225.</p> |
|  | EDIT ITEM | <p>Launches a dialog window that allows you to rename and/or give a new description of a list you select from the WORKSPACE.</p> <p>This feature is available for SAVED LISTS only, not for FAVORITES lists or DATA OBJECTS (with the  icon attached). See ‘Data Object’ on page 225.</p> |
|  | DELETE ITEM | <p>Launches a dialog window that allows you to delete a list you select from the WORKSPACE.</p> <p>This feature is available for all types of lists.</p> |
|  | SIZE WORKSPACE | <p>Select this icon, hold down the mouse button and drag to resize the WORKSPACE panel.</p> |
|  | | <p>In the workspace area DATA OBJECTS will appear with this icon attached to the list type icon.</p> <p>For example:  indicates a DATA OBJECT for an Expression Experiment report. See ‘Data Object’ on page 225.</p> |
|  | | <p>In the WORKSPACE area, FAVORITES will appear with this icon attached to the list type icon.</p> <p>For example:  indicates a FAVORITE Gene Report.</p> |




Icons - Popup Window controls

All popup windows have 3 icons with which to manage popup display.

- | | | |
|---|-----------------|--|
|  | MINIMIZE | Minimizes or maximizes the popup window. |
|  | CLOSE | Closes the popup window. |

Icons - Toolbox Dialogs

All **TOOLBOX** dialogs have 3 icons that allow you to manage folders in the **WORKSPACE**.

- | | | |
|---|-------------------|---|
|  | NEW FOLDER | Launches a dialog window that allows you to create a new folder in the WORKSPACE . |
|  | ZIP ALL | Closes all folders in folder display area of the dialog window. |
|  | UNZIP ALL | Opens or expands all folders in the display area of the dialog window. |

Popup Windows

Popup windows present detailed information about the specified record. For example, the **ACCESSION**, **SYNONYMS** and **DETAILS** buttons on the **GENE** domain report will launch popups containing additional information about the query gene.

Hovers

Additional information about many items within the DrugMatrix application is provided via a **hover**, as you mouse over the item.

<input checked="" type="checkbox"/>	SULFAPHENAZO-5d-1...	SULFAPHENAZOLE	
<input checked="" type="checkbox"/>	SAFROLE-3d-488mg/...	SAFROLE	
<input checked="" type="checkbox"/>	SPARFLOXACIN-.25d...	SPARFLOXACIN	
<input checked="" type="checkbox"/>	RALOXIFENE	Experiment: SPARFLOXACIN-.25d-450mg/kg-LI-RATM-RU1 Description: Transcriptional profile of a 0.25d timepoint for treatment of Rat, Male, CD-IGS, Sprague Dawley with 450.0mg/kg of SPARFLOXACIN on RU1 arrays. Array Technology: BIOCHIP	
<input checked="" type="checkbox"/>	FENOFIBRAT		
<input checked="" type="checkbox"/>	HYDRAZINE-		
<input checked="" type="checkbox"/>	FENOFIBRAT		
<input checked="" type="checkbox"/>	MELATONIN-		
<input checked="" type="checkbox"/>	AZATHIOPR		
<input checked="" type="checkbox"/>	AMANTADINE-3d-220...	AMANTADINE	
<input checked="" type="checkbox"/>	ITRACONAZOLE-.25d...	ITRACONAZOLE	

Selecting and Sorting

Many of the columns on panels in the Chemogenomic Data Reports are sortable, either alphabetically or numerically. Click on a column name in the currently displayed chemogenomic data report to toggle the order (ascending or descending) in which data in that column is sorted. You can also sort lists by items checked (or unchecked).

METHOD	SCORE	PROBABILITY
--------	-------	-------------

↑ click and drag to
modify column width

To modify the width of a column, mouse over the column separator to the right of that column, then when the cursor changes to a cross, hold down the left mouse button and drag to change the column width.

Selecting Records

You can specify records in a displayed list to save as a new list using the check boxes on the left of the list.

Click a single record to check or uncheck →

The screenshot shows a web application interface with a navigation bar at the top containing tabs: SIMILAR, INDUCED, REPRESSED, EXPERIMENTS, ACTIVITIES, LITER., and TARG. Below the navigation bar is a green header with a dropdown menu icon and the text 'BIO-ACTIVITIES'. A table is displayed with columns: ASSAY, INHIBITION, IC50, and KI. The table contains several rows of data. A context menu is open over the first two rows, showing options: SAVE LIST, CHECK ALL, and UNCHECK ALL. The 'UNCHECK ALL' option is highlighted in blue. The first two rows have their checkboxes checked, while the others are unchecked.

ASSAY	INHIBITION	IC50	KI
<input checked="" type="checkbox"/> Dopamine Transporter	36.0%		
<input checked="" type="checkbox"/> Cyclooxygenase COX-2	35.0%		
<input type="checkbox"/> CYP450-2D6 Inhibition	32.0%		
<input checked="" type="checkbox"/> Muscarinic M5	24.0%		
<input checked="" type="checkbox"/> Neuropeptide Y1	24.0%		
<input checked="" type="checkbox"/> CYP450-2C19 Inhibition	23.0%		
<input checked="" type="checkbox"/> Serotonin 5-HT2C	23.0%		
<input checked="" type="checkbox"/> Adrenergic beta1	21.0%		
<input checked="" type="checkbox"/> Testosterone	21.0%		
<input checked="" type="checkbox"/> Adrenergic, Norepinephrin...	21.0%		
<input checked="" type="checkbox"/> Tachykinin NK1	19.0%		

To select a sequence of multiple records:

1. Click the checkbox for a record to specify the beginning of the sequence.
2. Hold down the shift key.
3. Click the checkbox for another record that will end the sequence.

Selected records using steps above

The screenshot shows the same web application interface as the previous one. The table is displayed with the same columns: ASSAY, INHIBITION, IC50, and KI. The table contains the same rows of data. The checkboxes for the following rows are checked: CYP450-2D6 Inhibition, Muscarinic M5, Neuropeptide Y1, CYP450-2C19 Inhibition, Serotonin 5-HT2C, Adrenergic beta1, and Testosterone. A vertical bracket on the left side of the table groups these seven rows together, indicating they are the selected records.

ASSAY	INHIBITION	IC50	KI
<input type="checkbox"/> Dopamine Transporter	36.0%		
<input type="checkbox"/> Cyclooxygenase COX-2	35.0%		
<input checked="" type="checkbox"/> CYP450-2D6 Inhibition	32.0%		
<input checked="" type="checkbox"/> Muscarinic M5	24.0%		
<input checked="" type="checkbox"/> Neuropeptide Y1	24.0%		
<input checked="" type="checkbox"/> CYP450-2C19 Inhibition	23.0%		
<input checked="" type="checkbox"/> Serotonin 5-HT2C	23.0%		
<input checked="" type="checkbox"/> Adrenergic beta1	21.0%		
<input checked="" type="checkbox"/> Testosterone	21.0%		
<input type="checkbox"/> Adrenergic, Norepinephrin...	21.0%		
<input type="checkbox"/> Tachykinin NK1	19.0%		

Domain Reports

Information extracted from the DrugMatrix database is presented in one of seven Domain Reports. Each Domain Report presents information from the perspective of a particular data domain (**GENE**, **COMPOUND**, **ASSAY**, **EXPRESSION**, **EXPRESSION EXPERIMENT**, **PATHWAY**, **EXPRESSION STUDY** and **SIGNATURE**) and allows you to explore relationships between the selected data domain and information in other domains.

The screenshot displays the 'Domain Reports' interface for the query item 'CLOFIBRATE'. The interface is organized into several sections:

- Navigation Bar:** Features color-coded tabs for different data domains: GENE (blue), COMPOUND (yellow), ASSAY (green), EXPRESSION (orange), PATHWAY (blue), EXPRESSION STUDY (orange), and SIGNATURE (blue).
- Sub-panels:** Includes tabs for SIMILAR, INDUCED, REPRESSED, EXPERIMENTS, ACTIVITIES, LITER, TARGET, SUM, and TRANK.
- Main Table:** A table titled 'STRUCTURALLY SIMILAR COMPOUNDS' with columns for COMPOUND, METHOD, SCORE, and PROBABILITY. The first row is highlighted with a red box and labeled 'Record in Report'. The second row is highlighted with a red box and labeled 'Item in record'.
- Detail Panel:** A 'DETAIL' panel for CLOFIBRATE, showing its molecular structure, molecular weight (243), formula (C12 H15 Cl O3), and development status (US FDA Approved).

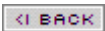
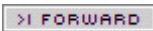
Data Domains are color coded to provide additional visual cues. For example, the **GENE** and **PATHWAY** Data Domains are both blue since they both present information that relates to genes. The **EXPRESSION** and **EXPRESSION STUDY** Data Domains are the same color since they both present information about gene expression experiments.

Each Domain Report contains a subset of **Chemogenomic Data Reports** and **Detail Reports** that present cross referenced experimental data from the proprietary DrugMatrix database and curated information from the scientific literature.

A single line of a subpanel in a chemogenomic report is referred to as a **record**. Each record can contain several different **items**.

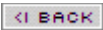
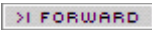
NOTE: In some cases the terms record and item are used interchangeably, for example in the case of a list in which each record contains only a single item.

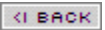
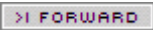
Report panels are also cross referenced with the primary data domain by colors. For example, within the **COMPOUND** Domain Report, the **ACTIVITIES** panel has the green color associated

with the **ASSAY** domain, since it presents information about assays that were affected by a particular compound. These same color codes apply to **SAVED LISTS**, and **FAVORITES** as well as the temporarily available lists accessed via the  and  menus on Domain Report panels.

Populating Domain Reports

Domain Reports can be populated with information in several ways:

- Use the DrugMatrix query tools.
- Select an item from a previously saved list or from a favorites list, or using the  and  menus on Domain Report panels.
- Click a hyperlinked item from within a previously populated Domain Report.
- Upload array data by using the **LOAD DATA** menu option on the **EXPRESSION** report panel.

If a Domain Report is already populated with data when you generate a new report, the existing report will be available until the current session is closed. You can access lists generated in this session using the  and  buttons at the top left of the Domain Report panel. This allows you to quickly retrieve reports you have previously generated in a given session.

Domain Report Menus

These menu buttons appear at the top left of Domain Report panels.



MENU



Used to print the current Domain Report or upload files to be used in populating an **EXPERIMENT** Domain Report.

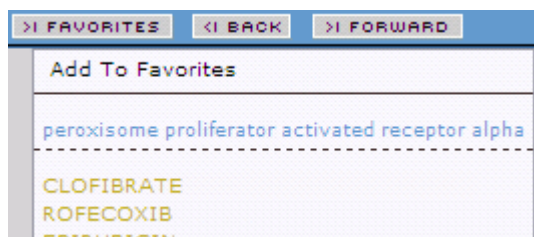
DISPLAY FOR PRINTING

Open a new browser window containing a printable version of the current domain report. Use the browser's Print command to print the document.

LOAD DATA

Launches a dialog window to specify parameters for uploading microarray experiments, from outside the DrugMatrix database, to be used in populating an **EXPERIMENT** Domain Report. This data will be stored in the **WORKSPACE**.

FAVORITES



Save frequently used domain reports of Compounds, Assays, Genes, Expression Experiments, Gene Pathways, Expression Studies and Signatures as favorites.

This saves time by eliminating the need to repeat searches.

The **FAVORITES** list is available from within the Domain Report or via the **LIST MODE** option on the **WORKSPACE** popdown menu on the **WORKSPACE** panel in the Search and List area.

ADD TO FAVORITES

Add the selected item to the appropriate section (**GENE, COMPOUND...**) of the **FAVORITES** list. Each section of the favorites list is associated with one of the DrugMatrix data domains and is color coded accordingly.

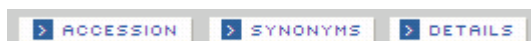


The **<| BACK** and **>| FORWARD** menus on the Domain Report panels allow you to display Domain Reports you have populated in a given session.

Note: When you exit a session this history will be erased. To permanently store a Domain Report, use the **ADD TO FAVORITES** selection from the **FAVORITES** menu.

Domain Report Buttons

Buttons just below the query item in each Domain Report launch popup windows that contain very specific information about the query item.



Gene Report

The **GENE** Domain Report presents all relevant information from the database, for the query gene. You can investigate cross referenced chemogenomic data that comes from other domains. You can also review curated information about the query gene from several different sources.

3-HYDROXY-3-METHYLGLUTARYL-COENZYME A REDUCTASE

ACCESSION | SYNONYMS | DETAILS

SIMILAR | INDUCED | REPRESSED | ACTIVITIES | LITER.

SIMILAR EXPRESSIONS

GENE	METHOD	CORR. COEFF	SPECIES
<input checked="" type="checkbox"/> 3-hydroxy-3-methylglutaryl-Co...	Pearson	0.72	RATTUS N...
<input checked="" type="checkbox"/> 3-hydroxy-3-methylglutaryl-Co...	Pearson	0.72	RATTUS N...
<input checked="" type="checkbox"/> squalene epoxidase (NM_0171...	Pearson	0.62	RATTUS N...
<input checked="" type="checkbox"/> 3-hydroxy-3-methylglutaryl-Co...	Pearson	0.6	RATTUS N...
<input checked="" type="checkbox"/> Protein phosphatase 2a, cataly...	Pearson	0.59	RATTUS N...
<input checked="" type="checkbox"/> COX15 gene product (DBSS) (...	Pearson	0.59	RATTUS N...
<input checked="" type="checkbox"/> sterol-C4-methyl oxidase-like ...	Pearson	0.59	RATTUS N...
<input checked="" type="checkbox"/> lamin B receptor (rc_A1145490...	Pearson	0.59	RATTUS N...
<input checked="" type="checkbox"/> squalene epoxidase (D37920 ...	Pearson	0.58	RATTUS N...
<input checked="" type="checkbox"/> epidermal Langerhans cell prot...	Pearson	0.58	RATTUS N...
<input checked="" type="checkbox"/> tropomyosin 4 (1368838_at)0...	Pearson	0.58	RATTUS N...

GO DATA | PATHWAY | ASSAY | CHIP

GO DATA

Molecular Function:
 HYDROXYMETHYLGLUTARYL-COA REDUCTASE (NADPH) ACTIVITY
 OXIDOREDUCTASE ACTIVITY

Cellular Component:
 ENDOPLASMIC RETICULUM
 ENDOPLASMIC RETICULUM MEMBRANE
 INTEGRAL TO MEMBRANE

Biological Process:
 BIOSYNTHESIS
 LIPID METABOLISM
 CHOLESTEROL BIOSYNTHESIS

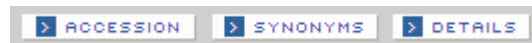
GENE Detail

The Gene Detail area provides aggregated information about the query gene. Items found in lists displayed here link to additional sources of information about the query gene.

GENE Buttons

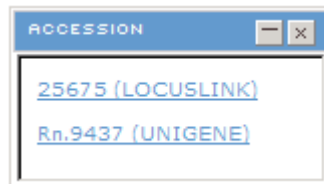
Behavior

These buttons launch popup windows containing specific information about the query gene.



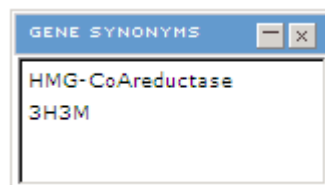
ACCESSION Button

This button displays a list of accession numbers that are hyperlinks to GenBank, UniGene, and other public databases. When you click on a GenBank reference from this list, the associated GenBank page will be displayed in a new browser window.



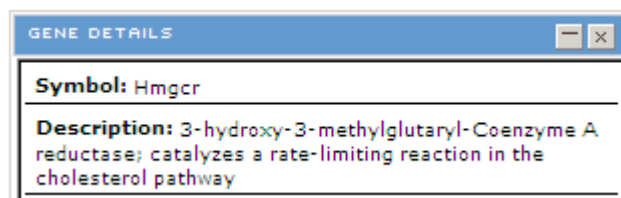
SYNONYMS Button

This button launches a popup window with a list of synonyms for the query gene.



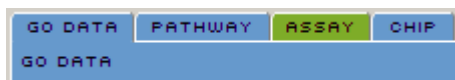
DETAILS Button

This panel launches a popup window that indicates the gene symbol and provides a brief description of the gene function.




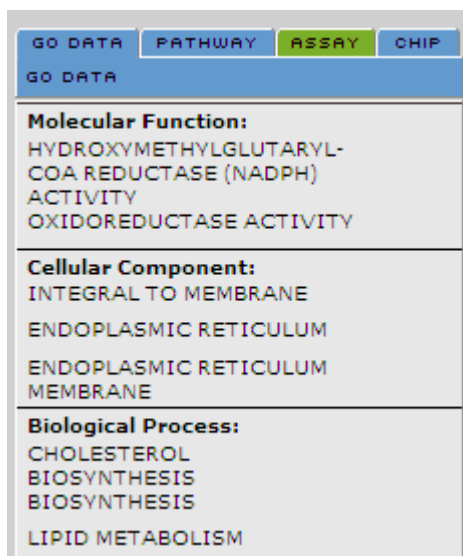
GENE Detail Panels

The Gene Detail panels provide aggregated information about the query gene. Items found in the lists displayed here link to additional sources of information about the query gene.



GENE: GO Data Panel

This panel presents information, curated from the scientific literature, that relates to the query gene. Information is categorized according to standardized nomenclature of the Gene Ontology Consortium. The publication icon  is a link to the named article.



Molecular Function:	Describes known molecular function of the query gene product.
Cellular Components:	Describes cellular components with which the query gene product is known to be associated.
Biological Process:	Describes known biological processes for the query gene product.

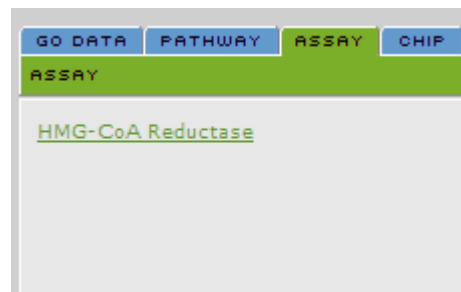
GENE: Pathway Panel

This panel presents a list of pathways in which the query gene is known to be a participant. Click on a pathway name in this panel to populate a **PATHWAY** Domain Report with information about that pathway.



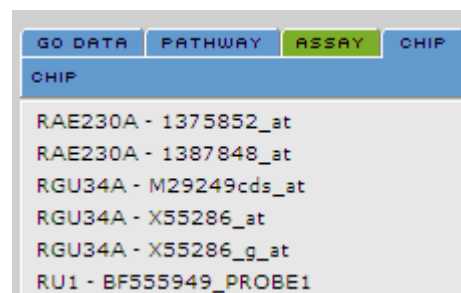
GENE: Assay Panel

This panel displays a list of different bioassays with which the query gene is associated. Click on an assay name in this list to populate an **ASSAY** Domain Report with information about that assay.



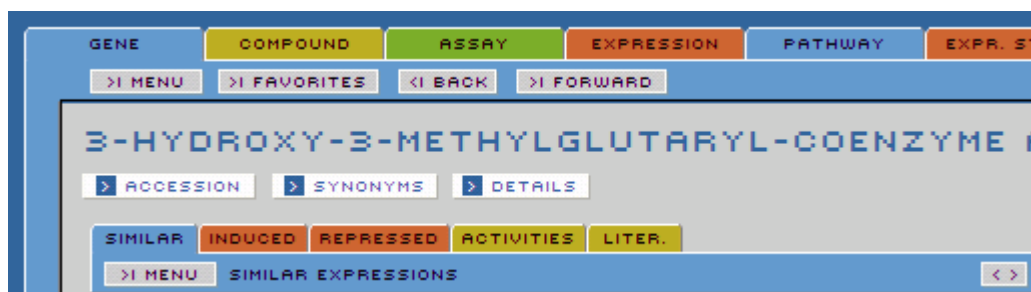
GENE: Chip Panel

This panel displays a list of probes for this gene and the short name for the microarray platform chip type which uses this probe.



GENE Chemogenomic Data Report

This panel presents cross referenced Chemogenomic Data, extracted from the database, that relates to the query gene.



Interactive Elements




Sorting Columns

Many columns on panels in the **GENE** Chemogenomic Data Reports are sortable, either alphabetically or numerically. Click on a column name in the currently displayed Chemogenomic Data Report panel to toggle the order (ascending or descending) in which data in that column is sorted. You can also sort lists by items checked (or unchecked).



To modify the width of a column, mouse over the column separator to the right of that column, then when the cursor changes to a cross, hold down the left mouse button and drag to change the column width.

Expandable images

You can expand  or contract  all molecular structure images in a column containing the molecular structure icon  or click on individual icons for an expanded image of the compound in the selected record.

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

Hyperlinks

Hyperlinked items, appearing in the Gene Chemogenomic data reports, will either populate associated domain reports or link to published information about the selected gene. For example, if you click on a compound name on the **INDUCED** panel of the **GENE** report, it will populate a **COMPOUND** domain report for that compound.

Saving Lists

Each **GENE** Domain Report you create will be available until the current session is closed. You can access **GENE** Domain Reports generated in this session using the **<| BACK** and **>| FORWARD** menus at the top left of the Domain Report panel. Use the **MENU > SAVE** option on any panel in the **GENE** report to permanently save a list of checked records on that panel.

You can also use the **FAVORITES>ADD FAVORITE** option to add the current query item (named at the top of the domain report panel) to the **FAVORITES** list.

Some panels allow you to save more than one of the lists that appear on the panel. The **MENU** button on any panel will indicate which lists can be saved.

GENE: Similar Panel

This panel presents information about genes that show similarity to the query gene (the subject of the report) based on transcriptional changes. The scoring is Pearson's correlation coefficient and represents the correlation of the transcriptional changes for each gene in the **GENE** column, compared to the query gene, across all experiments in the database.

GENE	METHOD	CORR. COEFF	SPECIES
<input checked="" type="checkbox"/> 3-hydroxy-3-methylglutaryl-Co...	Pearson	0.72	RATTUS N...
<input checked="" type="checkbox"/> 3-hydroxy-3-methylglutaryl-Co...	Pearson	0.72	RATTUS N...
<input checked="" type="checkbox"/> squalene epoxidase (NM_0171...	Pearson	0.62	RATTUS N...
<input checked="" type="checkbox"/> 3-hydroxy-3-methylglutaryl-Co...	Pearson	0.6	RATTUS N...

GENE

A list of genes whose transcriptional profiles, correlate to the transcriptional profile of the query gene, when compared across all experiments in the database. The list is ordered by default with the highest scores at the top of the table.

Each gene name in this column is a hyperlink that will populate a **GENE** Domain Report with information about that gene.

METHOD

The method used to establish similarity.

CORR. COEFF

The Pearson's correlation coefficient for transcriptional changes (ratios of treated to control) across all experiments.

See '[Pearson's Correlation Coefficient](#)' on page 227.

Click on the column name to toggle the order of the list.

SPECIES

The species of the gene sample in the currently selected record (i.e. the gene sample in a selected row of the table).

GENE: Induced Panel

This panel displays all experiments, and their associated compounds, in which the query gene has been significantly up regulated.

EXPERIMENT	COMPOUND	P-VALUE	CONFIDENCE INTERVAL	INTENSITY
LOVASTATIN-1d-1500mg...	LOVASTATIN	0.0		
LOVASTATIN-5d-1500mg...	LOVASTATIN	0.0		
LOVASTATIN-1d-450mg/...	LOVASTATIN	0.0		
FLUVASTATIN-5d-94mg/k...	FLUVASTATIN	0.0		
BENZOTHIAZYL-3d-2600...	BENZOTHIAZYL DISULFIDE	0.0		
ATORVASTATIN-5d-300m...	ATORVASTATIN	0.0		
LOVASTATIN-5d-450mg/...	LOVASTATIN	0.0		
LOVASTATIN-5d-450mg/...	LOVASTATIN	0.0		

TISSUES Menu



Selections from this menu will filter for the type of tissue used in experiments listed in the **EXPERIMENT** column of the **INDUCED** panel.

Each selection will populate the **INDUCED** panel with experiments in which the specified tissue was used.

The specified tissue filter is indicated next to the **TISSUES** menu.

EXPERIMENT

Experiment: SAFROLE-3d-488mg/kg-LI-RATM-RU1

Description: Transcriptional profile of a 3.0d timepoint for treatment of Rat, Male, CD-IGS, Sprague Dawley with 488.0mg/kg of SAFROLE on RU1 arrays.

Array Technology: BIOCHIP

This column lists experiments in which the subject gene is most perturbed.

Each experiment name in this column is a hyperlink that will populate an **EXPRESSION** Domain Report with information about that particular experiment.



The hover for this item provides the experiment name, a detailed description of the experiment, and the array technology (type of chip) used.


COMPOUND

The name of the compound with which the sample was treated in the selected experiment. (i.e. the experiment in a selected row of the table).

Each compound name in this column is a hyperlink that will populate a **COMPOUND** Domain Report with information about that particular compound.

COMPOUND IMAGE

Click the icons at the top of this column to expand  or contract  all molecular structure images in the column.

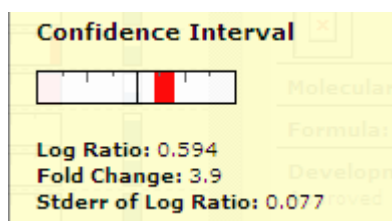
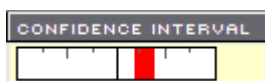
Click the molecular structure icon  for a popup window that displays an expanded image for the compound in the selected record. (i.e. the compound in a selected row of the table).

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

P VALUE

Indicates the statistical significance of the perturbation of this gene in the treated arrays compared to the control arrays.

The score is a **p value** (the probability that the results observed can happen by chance) computed from the log ratio and its standard error.

CONFIDENCE INTERVAL

A visual representation of statistics for the expression perturbation of the query gene in the selected experiment (i.e. the experiment in a selected row of the table).

The position and color of the bar indicate the **Log Ratio** of the specified gene in the selected experiment (i.e. the experiment in a selected row of the table). The greater the log ratio, the further the bar is from the center of the display.

A positive log ratio will appear red and to the right of the central point. A negative log ratio will appear green and to the left of the central point.

The width of the bar represents the confidence of the result. (2.8 standard errors of the log ratio = 99.5% confidence limit).

The **Confidence Interval** hover displays numeric values of statistics for the expression perturbation of the query gene in the selected experiment (i.e. the experiment in a selected row of the table).

Log Ratio:

The log of the ratio of gene expression levels for compound treated vs. control condition (no compound treatment) in the selected experiment (i.e. the experiment in a selected row of the table).

Fold Change:

The fold change of expression levels for the compound treated over the control condition (no compound treatment) in the selected experiment (i.e. the experiment in a selected row of the table). Fold values are within the range

$$1 < x < \infty$$

Stderr of Log Ratio:

The standard error of the log ratio (based on the pairwise log ratios of compound treated vs control for all arrays in an experiment).

INTENSITY



A bar chart indicating the approximate level of the average expression values for a specific gene across all the arrays in the experiment.

The height of the bar indicates increasing intensity.

This measure gives a rough indication of relative transcript abundance.

GENE: Repressed Panel

This panel displays all experiments, and their associated compounds, in which the query gene has been significantly down regulated.

EXPERIMENT	COMPOUND	P VALUE	CONFIDENCE INTERVAL	INTENSITY
LIMENHYDRINA-1d-150mg...	LIMENHYDRINATE	1.0E-6		
TRIACETIN-1d-1200mg/k...	TRIACETIN	1.0E-6		
BROMHEXINE-1d-1200mg...	BROMHEXINE	2.0E-6		
TORSEMIDE-5d-110mg/k...	TORSEMIDE	4.0E-6		
MELOXICAM-5d-.6mg/kg...	MELOXICAM	8.0E-6		



Selections from this menu will filter for the type of tissue used in experiments listed in the **EXPERIMENT** column of the **REPPRESSED** panel.

Each selection will populate the **REPPRESSED** panel with experiments in which the specified tissue was used.

The specified tissue filter is indicated next to the **TISSUES** menu.

EXPERIMENT

Experiment: [METHOTREXATE-3d-.3mg/kg-LI-RATM-RU1](#)

Description: Transcriptional profile of a 3.0d timepoint for treatment of Rat, Male, CD-IGS, Sprague Dawley with 0.3mg/kg of METHOTREXATE on RU1 arrays.

Array Technology: BIOCHIP

This column lists experiments in which the subject gene is most perturbed.

Each experiment name in this column is a hyperlink that will populate an **EXPRESSION** Domain Report with information about that particular experiment.



The hover for this item provides the experiment name, a detailed description of the experiment, and the array technology (type of chip) used.


COMPOUND

The name of the compound with which the sample was treated in the selected experiment. (i.e. the experiment in a selected row of the table).

Each compound name in this column is a hyperlink that will populate a **COMPOUND** Domain Report with information about that particular compound.

COMPOUND IMAGE

Click the icons at the top of this column to expand  or contract  all molecular structure images in the column.

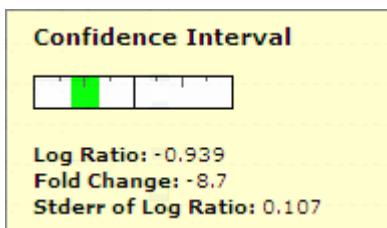
Click the molecular structure icon  for a popup window that displays an expanded image for the compound in the selected record (i.e. the compound in a selected row of the table).

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

P VALUE

Indicates the statistical significance of the perturbation of this gene in the treated arrays compared to the same gene in control arrays.

The score is a **p value** (the probability that the results observed can happen by chance) computed from the log ratio and its standard error.

CONFIDENCE INTERVAL

A visual representation of statistics for the expression perturbation of the query gene in the selected experiment (i.e. the experiment in a selected row of the table).

The position and color of the bar indicate the **Log Ratio** of the specified gene in the selected experiment (i.e. the experiment in a selected row of the table). The greater the log ratio, the further the bar is from the center of the display.

A positive log ratio will appear red and to the right of the central point. A negative log ratio will appear green and to the left of the central point.

The width of the bar represents the confidence of the result. (2.8 standard errors of the log ratio = 99.5% confidence limit).

The **Confidence Interval** hover displays numeric values of statistics for the expression perturbation of the query gene in the selected experiment (i.e. the experiment in a selected row of the table).

Log Ratio:

The log of the ratio of gene expression levels for compound treated vs. control condition (no compound treatment) in the selected experiment (i.e. the experiment in a selected row of the table).

Fold Change:

The fold change of expression levels for the compound treated over the control condition (no compound treatment) in the selected experiment (i.e. the experiment in a selected row of the table). Fold values are within the range $-\infty < x < -1$

Stderr of Log Ratio:

The standard error of the log ratio (based on the pairwise log ratios of compound treated vs control for all arrays in an experiment).

INTENSITY

A bar chart indicating the approximate level of the average expression values for a specific gene across all the arrays in the experiment.

The height of the bar indicates increasing intensity.

This measure gives a rough indication of relative transcript abundance.

GENE: Activities Panel



The activities panel of the Gene Chemogenomic Data Report presents a list of compounds tested in bioassays that measure the binding to, or activity of, the query gene's product.


COMPOUND	INHIBITION	IC50	KI
<input checked="" type="checkbox"/> FLUVASTATIN	100.0%	3.53E-4...	
<input checked="" type="checkbox"/> CERIVASTATIN	100.0%	8.5E-5uM	
<input checked="" type="checkbox"/> ATORVASTATIN	100.0%	2.27E-4...	
<input checked="" type="checkbox"/> PRAVASTATIN	100.0%	0.00559...	

COMPOUND

This column lists the names of the compounds shown to effect the query gene, when tested with the assay listed on the **ASSAY** panel to the right of this report.

COMPOUND IMAGE

Click the icons at the top of this column to expand  or contract  all molecular structure images in the column.

Click the molecular structure icon  for a popup window that displays an expanded image for the compound in the selected record (i.e. the compound in a selected row of the table).

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

INHIBITION

The bioactivity of the selected compound in the tested assay expressed as % inhibition. (i.e. The extent (in %) the compound inhibits an enzyme reaction, or the binding of a ligand to a protein).

IC50

The bioactivity of each compound in the tested assay expressed as an IC50 (50% inhibitory concentration).

KI

The bioactivity of each compound in the tested assay expressed as a KI (a measure of the extent an inhibitor inhibits the function of a protein. It is the equilibrium constant for the dissociation of protein-inhibitor complexes).

GENE: Literature Panel

This literature panel of the Chemogenomic Data Report presents public literature about known experimentally determined impacts of compounds on the query gene product.

COMPOUND	ACTIVITY	DESCRIPTION	PUBLICATION
LOVASTATIN	0.15uM	inhibits, enzyme activity, H...	
LOVASTATIN	0.012uM	inhibits, synthesis (mevalo...	
LOVASTATIN	0.07uM	inhibits, synthesis (cholest...	
MEVASTATIN	6.5uM	inhibits, production (meval...	
MEVASTATIN	0.03uM	inhibits, incorporation ([1-...	
SIMVASTATIN	0.0108uM	inhibits, enzyme activity, h...	
SIMVASTATIN	0.0075uM	inhibits, enzyme activity, r...	
SIMVASTATIN	0.013uM	inhibits, synthesis (sterol)...	
PRAVASTATIN	0.026uM	inhibits, enzyme activity, r...	
PRAVASTATIN	5.9uM	inhibits, biosynthesis (chol...	

COMPOUND

The name of the compound with which a particular assay that relates to the query gene was treated as described in the publication named in the **PUBLICATION** column of this table.

COMPOUND IMAGE

Click the icons at the top of this column to expand or contract all molecular structure images in the column.

Click the molecular structure icon for a popup window that displays an expanded image for the compound in the selected record (i.e. the compound in a selected row of the table).

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

ACTIVITY

The bioactivity of the query compound in the assay described in the selected record.

DESCRIPTION

Describes the activity of the assay identified in the selected publication.

PUBLICATION

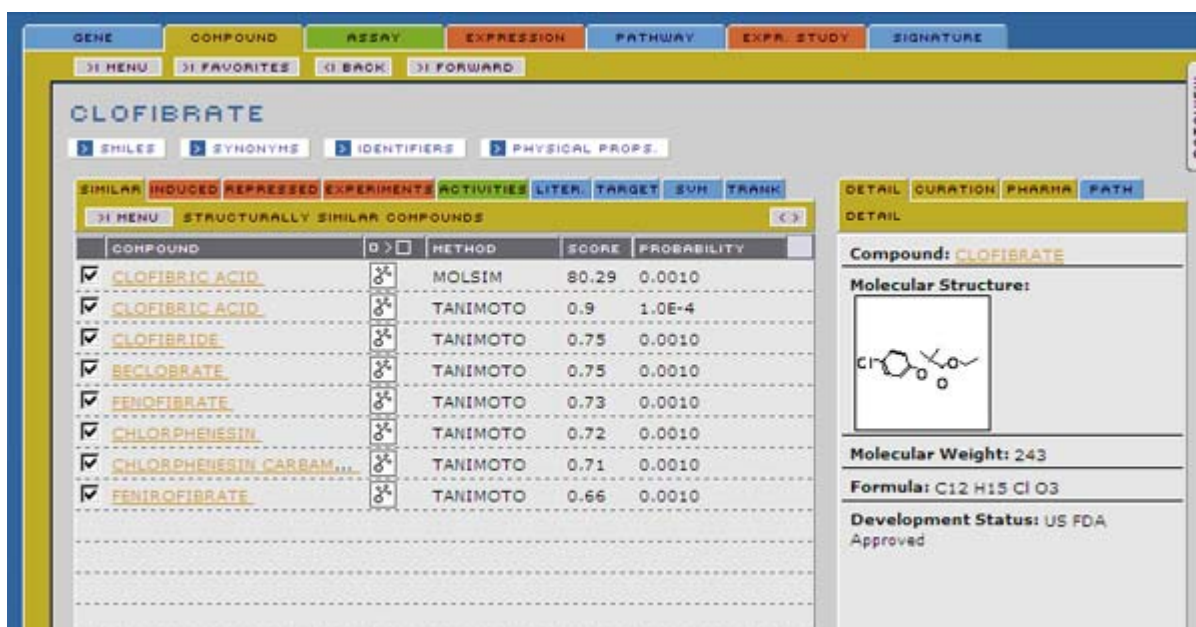


The publication in which the experiment in question was described.

Click on the publication icon to open a new browser window displaying the publication.

Compound Report

The **COMPOUND** Domain Report presents all relevant information from the database, for the query compound. You can investigate cross referenced chemogenomic data that comes from other domains. You can also review curated information about the query compound from several different sources.



CLOFIBRATE

SMILES SYNONYMS IDENTIFIERS PHYSICAL PROPS

SIMILAR INDUCED REPRESSED EXPERIMENTS ACTIVITIES LITER TARGET SUB TRANK

STRUCTURALLY SIMILAR COMPOUNDS

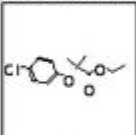
COMPOUND	METHOD	SCORE	PROBABILITY
<input checked="" type="checkbox"/> CLOFIBRIC ACID	MOLSIM	80.29	0.0010
<input checked="" type="checkbox"/> CLOFIBRIC ACID	TANIMOTO	0.9	1.0E-4
<input checked="" type="checkbox"/> CLOFIBRATE	TANIMOTO	0.75	0.0010
<input checked="" type="checkbox"/> BECLOBRATE	TANIMOTO	0.75	0.0010
<input checked="" type="checkbox"/> FENOFIBRATE	TANIMOTO	0.73	0.0010
<input checked="" type="checkbox"/> CHLORPHENESIN	TANIMOTO	0.72	0.0010
<input checked="" type="checkbox"/> CHLORPHENESIN CARBAM...	TANIMOTO	0.71	0.0010
<input checked="" type="checkbox"/> FENIROFIBRATE	TANIMOTO	0.66	0.0010

DETAIL CURATION PHARMA PATH

DETAIL

Compound: **CLOFIBRATE**

Molecular Structure:



Molecular Weight: 243

Formula: C₁₂ H₁₅ Cl O₃

Development Status: US FDA Approved

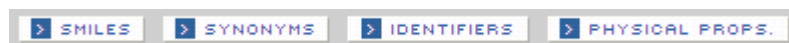
COMPOUND Detail

Aggregated information about the query compound is displayed in the Detail area of the **COMPOUND** report. Items found in lists displayed here link to additional sources of information about the query compound.

COMPOUND Buttons

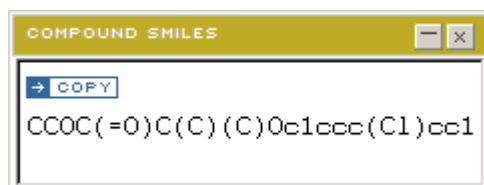
Behavior

These buttons launch popup windows containing specific information about the query compound.



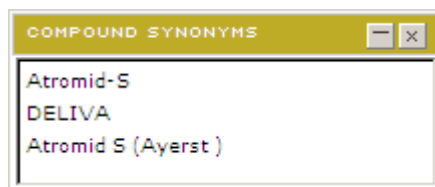
SMILES Button

A **SMILES** string is a formalized way to describe a structure of a compound using a simple string. This button launches a popup that displays the **SMILES** string for the query compound. You can use the **COPY** button to copy this string and use it with the **SIMILAR COMPOUNDS** tool. For more information, see [‘Glossary’ on page 225](#).



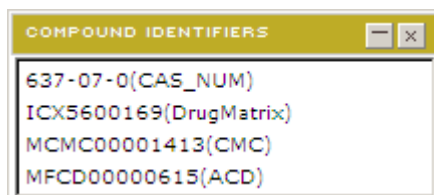
SYNONYMS Button

This button launches a popup that displays a list of industry standard database compound identifier synonyms for the query compound.

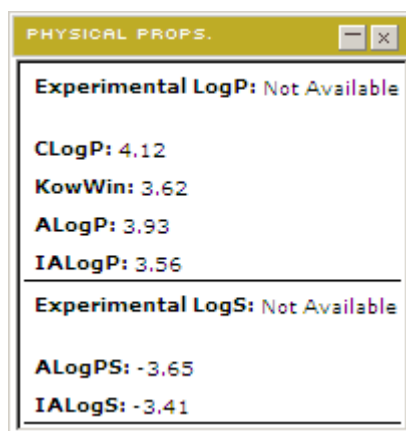


IDENTIFIERS Button

This button launches a popup that displays a list of identifiers from several industry chemical structure databases for the query compound.

**PHYSICAL PROPERTIES Button**

This button launches a popup that displays the physical properties of the query compound.

**Experimental LogP**

The lipophilicity (in kg/liter) of a compound expressed in log scale.

CLogP**KowWin****ALogP****IALogP**

CLogP, **KowWin** (LogKow), **ALogP**, and **IALogP** are the predicted lipophilicity of a compound based on molecular formula using various computational chemistry programs.

Experimental LogS

The aqueous solubility (in kg/liter) of a compound expressed in log scale.

ALogPS**IALogS**

ALogPS and **IALogS** are the predicted aqueous solubility of a compound based on molecular formula using various computational chemistry programs.

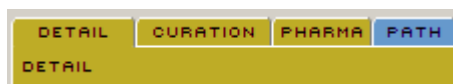
NOTE: The various LogP and LogS and aqueous solubility values in DrugMatrix were obtained using ALOGPS2.1 available at the Virtual Computational Chemistry Laboratory website (<http://vcclab.org>).

All calculated values were recorded since no one computational program appears to be superior for all compounds based on available experimental values which are shown where available.

COMPOUND Detail Panels

Detailed demographic information about the query compound is displayed in four Detail panels of the **COMPOUND** report.

Items found in the lists displayed here link to additional sources of information about the query compound.



COMPOUND: Detail Panel

This panel presents specific information about the molecular nature and developmental status of the query compound if it is intended for therapeutic use.

- Compound Name:** The name of the query compound.
- Molecular Structure:** A two dimensional representation of the query compound's structure. Left click on the image for a popup window that displays an expanded image.
- Molecular Weight:** The molecular weight of the query compound.
- Formula:** The molecular formula for the query compound.
- Development Status:** A categorization of the drug development status for the query compound. Drugs can be "Approved" or "Withdrawn". Compounds which are not drugs may be "Toxicants" or "Biochemical" standards.

COMPOUND: Curation Panel

This panel presents curated information from the scientific literature, reference material and online databases about known activities of the query compound.

The screenshot shows a web interface with four tabs: DETAIL, CURATION, PHARMA, and PATH. The CURATION tab is active, displaying a scrollable list of classification categories and their values:

- Product Class:** Cardiovasculars
- Therapeutic Class:** Hypolipidemic Agents
- Indication:** Hypertriglyceridemia, Hypercholesterolemia, Hyperlipidemia, Hyperlipoproteinemia
- Mechanism:** Increase lipid catabolism
- Mode Class:** Receptor Agonist, selective
- Known Toxicity:** Hepatotoxicity, Miscellaneous, Cardiovascular Toxicity

For a list of Chemical Ontology terms, see [‘Appendix - Chemical Ontology’ on page 231](#)

- Product Class:** One or more terms commonly used to classify pharmaceuticals (based on their use) and other chemicals.
- Therapeutic Class:** One of a list of 120 terms, established in DrugMatrix, used to classify a compound based on its therapeutic uses.
- Indication:** One or more approved drug indications for marketed drugs; intended drug indications for drugs at various stages of clinical trials.
- Mechanism:** One or more descriptive phrases established in DrugMatrix to classify a compound based on its phenotypic or physiological effect.
- Mode Class:** One or more descriptive phrases established in Drug Matrix to describe a compound based on how it affects its molecular target.
- Known Toxicity:** One or more common terms used to highlight serious adverse effects associated with a compound.
- Tissue Toxicity:** One or more serious adverse effects associated with the query compound.
- Adverse Effect:** One or more adverse effects of a drug as listed in the Physicians Desk Reference, prefixed with the organ code and frequency (1 for most common, 2 for less frequent, 3- for rare) of occurrence associated with the adverse effect.

Structure Activity: A description of the compound's structure as it relates to the class of similar compounds or the mode of action of a class or classes of compounds.

COMPOUND: Pharmacology Panel

This panel presents information from the scientific literature, reference material and online databases about the pharmacology of the query compound. Hovers provide additional information for truncated items in this list as you move the cursor over the item.

DETAIL	CURATION	PHARMA	PATH
COMPOUND PHARMACOLOGY			
ANTOX, LD50		> 500 m...	
ANTOX, LD50		540 mg/...	
ANTOX, LD50		910 mg/...	
ANTOX, LD50		940 mg/...	
ANTOX, LD50		1220 mg...	
ANTOX, LD50		1280 mg...	
ANTOX, LD50		1370 mg...	
ANTOX, LD50		2400 mg...	
ANTOX, TDLo (Time...		1698 mg...	
ANTOX, TDLo (Time...		3750 mg...	
ANTOX, TDLo (Time...		4200 mg...	
ANTOX, TDLo (Time...		7000 mg...	
ANTOX, TDLo (Time...		14000 m...	
ANTOX, TDLo (Time...		14700 m...	
ANTOX, TDLo (Time...		140000 ...	

PHARMACOLOGY

The category of the pharmacological effects of the query compound, curated from a specific publication.



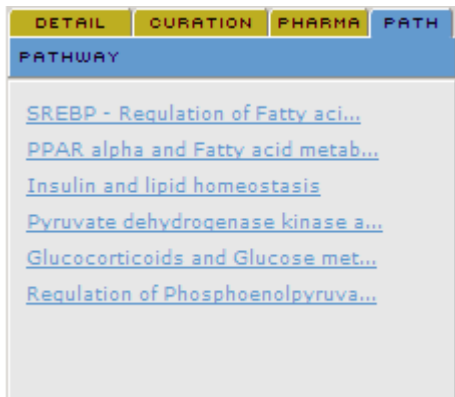
Click on the publication icon to open a new browser window displaying the publication.

VALUE

The concentration required for the specified pharmacological effect or the key values from the referenced paper.

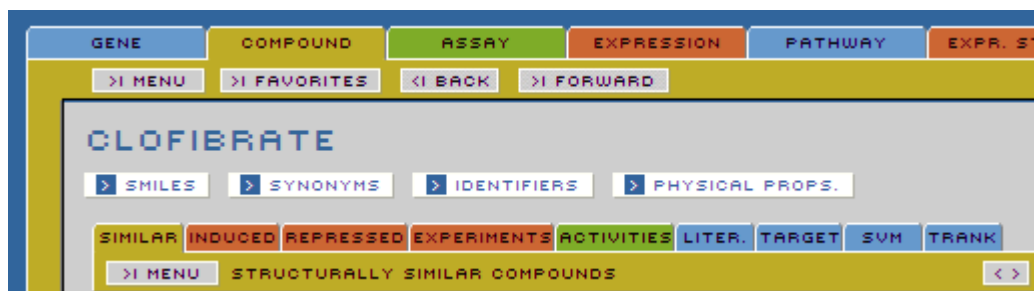
COMPOUND: Pathway Panel

This panel will provide a list of pathways when the compound is either a chemical substrate, an intermediate, or where the compound is known to have an effect. Click on the name of the pathway for a view of the pathway.



COMPOUND Chemogenomic Data Report

This panel presents cross referenced chemogenomic data, extracted from the database, that relates to the query compound.






Interactive Elements

Sorting Columns

Many columns on panels in the **COMPOUND** Chemogenomic Data Reports are sortable, either alphabetically or numerically. Click on a column name in the currently displayed Chemogenomic Data Report panel to toggle the order (ascending or descending) in which data in that column is sorted. You can also sort lists by items checked (or unchecked).



To modify the width of a column, mouse over the column separator to the right of that column, then when the cursor changes to a cross, hold down the left mouse button and drag to change the column width. **Expandable images**

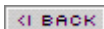
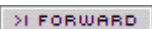
You can expand  or contract  all molecular structure images in a column containing the molecular structure icon  or click on individual icons for an expanded image of the compound in the selected record.

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

Hyperlinks

Hyperlinked items, appearing in the **COMPOUND** Chemogenomic Data Reports, will either populate associated domain reports or link to published information about the selected compound. For example, if you click on an experiment name on the **INDUCED RESPONSE** panel of the **COMPOUND** report, it will populate an **EXPRESSION** domain report for that experiment.

Saving Lists

Each **COMPOUND** Domain Report you create will be available until the current session is closed. You can access **COMPOUND** Domain Reports generated in this session using the  and  menus at the top left of the Domain Report panel.

Use the **MENU > SAVE** option on any panel in the **COMPOUND** report to permanently save a list of checked records on that panel. You can also use the **FAVORITES>ADD FAVORITE** option to add the current query item (named at the top of the domain report panel) to the **FAVORITES** list.

Some panels allow you to save more than one of the lists that appear on the panel. The **MENU** button on any panel will indicate which lists can be saved.

COMPOUND: Similar Panel

This panel presents a list of compounds that have been identified as similar in structure to the query compound by various similarity scoring methods.



COMPOUND	METHOD	SCORE	PROBABILITY
<input checked="" type="checkbox"/> CLOFIBRIC ACID	MOLSIM	80.29	0.0010
<input checked="" type="checkbox"/> CLOFIBRIC ACID	TANIMOTO	0.9	1.0E-4
<input checked="" type="checkbox"/> CLOFIBRIDE	TANIMOTO	0.75	0.0010
<input checked="" type="checkbox"/> BECLOBRATE	TANIMOTO	0.75	0.0010
<input checked="" type="checkbox"/> FENOFIBRATE	TANIMOTO	0.73	0.0010
<input checked="" type="checkbox"/> CHLORPHENESIN	TANIMOTO	0.72	0.0010
<input checked="" type="checkbox"/> CHLORPHENESIN CARBAM...	TANIMOTO	0.71	0.0010


COMPOUND

A list of compounds that have been identified as similar in structure to the query compound by various similarity scoring methods.

Each compound name in this column is a hyperlink that will populate a **COMPOUND** Domain Report with information about that particular compound.

COMPOUND IMAGE

Click the icons at the top of this column to expand  or contract  all molecular structure images in the column.

Click the molecular structure icon  for a popup window that displays an expanded image for the compound in the selected record (i.e. the compound in a selected row of the table).

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

METHOD

The method used to determine the similarity in chemical structure between the query compound and compounds displayed in the table. The methods currently used are, the industry standard Daylight Tanimoto method, the Isis molecular similarity (**MOLSIM**) method, or the DrugMatrix proprietary **3DMI** method.

SCORE

This is a measure of the similarity between the query compound and the selected compound (i.e. the compound in a row of the table).

PROBABILITY

The probability that this score would occur by chance in the database.

This is derived by determination of the distribution of all pairwise scores. The **p value** is the cumulative probability in the tail closest to the perfect match score and the actual distance.

The lower the **p value**, the lower the probability that this similarity score would occur by chance in the database.

Click on **PROBABILITY** at the top of this column to toggle the list order between most similar and least similar.

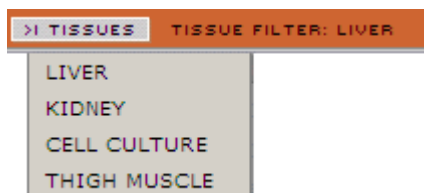
COMPOUND: Induced Panel

This panel presents information about genes that have been up regulated by the query compound. It displays a list of experiments with the gene, in which a significant transcriptional response has occurred.

The screenshot shows the 'CLOFIBRATE' Induced Panel. At the top, there are tabs for GENE, COMPOUND, ASSAY, EXPRESSION, PATHWAY, EXPR. STUDY, and SIGNATURE. Below these are navigation buttons: MENU, FAVORITES, BACK, FORWARD. The main title is 'CLOFIBRATE' with sub-tabs for SMILES, SYNONYMS, IDENTIFIERS, and PHYSICAL PROPS. Below that are tabs for SIMILAR, INDUCED, REPRESSED, EXPERIMENTS, ACTIVITIES, LITER., TARGET, SVM, and TRANK. A 'TISSUES' menu is open, showing 'TISSUE FILTER: LIVER'. The main table has the following columns: EXPERIMENT, GENE, P VALUE, CONFIDENCE INTERVAL, and INTENSITY. The table contains several rows of data, each with a checkmark in the first column and a red bar in the Intensity column.

EXPERIMENT	GENE	P VALUE	CONFIDENCE INTERVAL	INTENSITY
<input checked="" type="checkbox"/> CLOFIBRATE-.25d-500m...	transport-secretion protein 2.2...	0.0		
<input checked="" type="checkbox"/> CLOFIBRATE-3d-500mg/...	transcription termination factor...	0.0		
<input checked="" type="checkbox"/> CLOFIBRATE-3d-500mg/...	islet cell autoantigen 1, 69 kD...	0.0		
<input checked="" type="checkbox"/> CLOFIBRATE-.25d-500m...	camitine acetyltransferase (13...	0.0		
<input checked="" type="checkbox"/> CLOFIBRATE-3d-500mg/...	RIKEN cDNA 1110014F24 (DBS...	0.0		
<input checked="" type="checkbox"/> CLOFIBRATE-1d-500mg/...	camitine acetyltransferase (13...	0.0		
<input checked="" type="checkbox"/> CLOFIBRATE-1d-500mg/...	acetyl-Coenzyme A acyltransfe...	0.0		

TISSUES Menu



Selections from this menu will filter for the type of tissue used in experiments listed in the **EXPERIMENT** column of the **INDUCED** panel.

Each selection will populate the **INDUCED** panel with experiments in which the specified tissue was used.

The specified tissue filter is indicated next to the **TISSUES** menu.

EXPERIMENT

Experiment: CLOFIBRATE-.25d-500mg/kg-LI-RATM-RU1

Description: Transcriptional profile of a 0.25d timepoint for treatment of Rat, Male, CD-1GS, Sprague Dawley with 500.0mg/kg of CLOFIBRATE on RU1 arrays.

Array Technology: BIOCHIP

A list of experiments in the database that showed a significant transcriptional response when the query compound was applied.

Each experiment name in this column is a hyperlink that will populate an **EXPRESSION** Domain Report with information about that particular experiment.

The hover for this item provides the experiment name, a brief description of the experiment, and the array technology (type of chip) used.

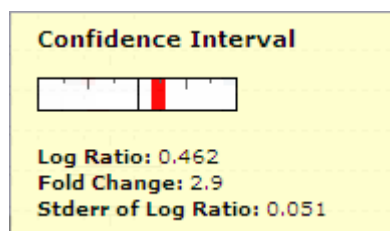
GENE

The gene that was up regulated in the experiment named in the selected record (i.e. the experiment in a selected row of the table).

P VALUE

Indicates the statistical significance of the perturbation of this gene in the treated arrays compared to the same gene in control arrays.

The score is a **p value** (the probability that the results observed can happen by chance) computed from the log ratio and its standard error.

CONFIDENCE INTERVAL

A visual representation of statistics for the expression perturbation of the query gene in the selected experiment (i.e. the experiment in a selected row of the table).

The position and color of the bar indicate the **Log Ratio** of the specified gene in the selected experiment (i.e. the experiment in a selected row of the table). The greater the log ratio, the further the bar is from the center of the display.

A positive log ratio will appear red and to the right of the central point. A negative log ratio will appear green and to the left of the central point.

The width of the bar represents the confidence of the result. (2.8 standard errors of the log ratio = 99.5% confidence limit).

The **Confidence Interval** hover displays numeric values of statistics for the expression perturbation of the query gene in the selected experiment (i.e. the experiment in a selected row of the table).

Log Ratio:

The log of the ratio of gene expression levels for compound treated vs. control conditions (no compound treatment) in the selected experiment (i.e. the experiment in a selected row of the table).

Fold Change:

The fold change of expression levels for the gene in the compound treated vs. the control condition (no compound treatment) in the selected experiment. Fold values are within the ranges $1 < x < \infty$

Stderr of Log Ratio:

The standard error of the log ratio (based on the pairwise log ratios of compound treated vs control for all arrays in an experiment).

INTENSITY

A bar chart indicating the approximate level of the average expression values for a specific gene across all the arrays in the experiment.

The height of the bar indicates increasing intensity.

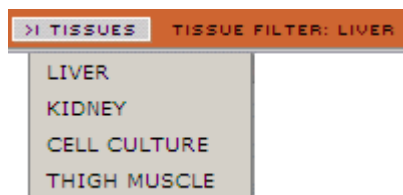
This measure gives a rough indication of relative transcript abundance.

COMPOUND: Repressed Panel

This panel presents information about genes that have been down regulated by the query compound. It displays a list of experiments with the gene, in which a significant transcriptional response has occurred.

EXPERIMENT	GENE	P VALUE	CONFIDENCE INTERVAL	INTENSITY
CLOFIBRATE-3d-500mg/...	latent transforming growth fact...	0.0		
CLOFIBRATE-3d-500mg/...	myosin Ib (1369720_at.X6819...	0.0		
CLOFIBRATE-3d-500mg/...	v-maf musculoaponeurotic fibr...	0.0		
CLOFIBRATE-3d-500mg/...	RIKEN cDNA 5730454B08 (DBS...	0.0		
CLOFIBRATE-3d-500mg/...	endothelin receptor type A (M6...	0.0		
CLOFIBRATE-3d-500mg/...	hepatocyte growth factor (NM ...	0.0		
CLOFIBRATE-3d-500mg/...	TRAP-complex gamma subunit...	0.0		

TISSUES Menu



Selections from this menu will filter for the type of tissue used in experiments listed in the **EXPERIMENT** column of the **REPRESSED** panel.

Each selection will populate the **REPRESSED** panel with experiments in which the specified tissue was used.

The specified tissue filter is indicated next to the **TISSUES** menu.

EXPERIMENT

Experiment: CLOFIBRATE-.25d-500mg/kg-LI-RATM-RU1

Description: Transcriptional profile of a 0.25d timepoint for treatment of Rat, Male, CD-IGS, Sprague Dawley with 500.0mg/kg of CLOFIBRATE on RU1 arrays.

Array Technology: BIOCHIP

A list of experiments in the database that showed a significant transcriptional response when the query compound was applied.

Each experiment name in this column is a hyperlink that will populate an **EXPRESSION** Domain Report with information about that particular experiment.

The hover for this item provides the experiment name, a brief description of the experiment, and the array technology (type of chip) used.

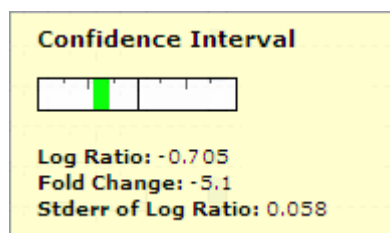
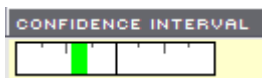
GENE

The gene that was down regulated in the experiment named in the selected record (i.e. the experiment in a selected row of the table).

P VALUE

Indicates the statistical significance of the perturbation of this gene in the treated arrays compared to the same gene in control arrays.

The score is a **p value** (the probability that the results observed can happen by chance) computed from the log ratio and its standard error.

CONFIDENCE INTERVAL

A visual representation of statistics for the expression perturbation of the query gene in the selected experiment (i.e. the experiment in a selected row of the table).

The position and color of the bar indicate the **Log Ratio** of the specified gene in the selected experiment (i.e. the experiment in a selected row of the table). The greater the log ratio, the further the bar is from the center of the display.

A positive log ratio will appear red and to the right of the central point. A negative log ratio will appear green and to the left of the central point.

The width of the bar represents the confidence of the result. (2.8 standard errors of the log ratio = 99.5% confidence limit).

The **Confidence Interval** hover displays numeric values of statistics for the expression perturbation of the query gene in the selected experiment (i.e. the experiment in a selected row of the table).

Log Ratio:

The log of the ratio of gene expression levels for compound treated vs. control conditions (no compound treatment) in the selected experiment (i.e. the experiment in a selected row of the table).

Fold Change:

The fold change of expression levels for the gene in the compound treated vs the control condition (no compound treatment) in the selected experiment (i.e. the experiment in a selected row of the table). Fold values are within the range $-\infty < x < -1$

Stderr of Log Ratio:

The standard error of the log ratio (based on the pairwise log ratios of compound treated vs. control for all arrays in an experiment).

INTENSITY

A bar chart indicating the approximate level of the average expression values for a specific gene across all the arrays in the experiment.

The height of the bar indicates increasing intensity.

This measure gives a rough indication of relative transcript abundance.

COMPOUND: Experiments Panel

This panel presents information on experiments in which the query compound has been used and the array technology used.

EXPERIMENT	TYPE	ORGANISM	TISSUE	TIME	DOSE	INDUCED	REPRESSED	PERTURBED
CLOFIBRATE-7d-500mg/...	BIOCHIP	RATM	THIGH ...	7.0d	500.0mg/...	5.5%	6.6%	12.1%
CLOFIBRATE-7d-500mg/...	BIOCHIP	RATM	LIVER	7.0d	500.0mg/...	3.1%	2.1%	5.2%
CLOFIBRATE-7d-500mg/...	BIOCHIP	RATM	KIDNEY	7.0d	500.0mg/...	0.9%	1.1%	2.0%
CLOFIBRATE-7d-130mg/...	BIOCHIP	RATM	LIVER	7.0d	130.0mg/...	1.7%	1.0%	2.7%
CLOFIBRATE-3d-500mg/...	BIOCHIP	RATM	THIGH ...	3.0d	500.0mg/...	6.5%	6.4%	12.9%
CLOFIBRATE-3d-500mg/...	BIOCHIP	RATM	LIVER	3.0d	500.0mg/...	14.3%	17.9%	32.2%
CLOFIBRATE-3d-500mg/...	BIOCHIP	RATM	LIVER	3.0d	500.0mg/...	6.0%	4.4%	10.4%

EXPERIMENT

Experiment: CLOFIBRATE-.25d-500mg/kg-LI-RATM-RU1

Description: Transcriptional profile of a 0.25d timepoint for treatment of Rat, Male, CD-IGS, Sprague Dawley with 500.0mg/kg of CLOFIBRATE on RU1 arrays.

Array Technology: BIOCHIP

The names of the experiments in which the query compound was used.

Each experiment name in this column is a hyperlink that will populate an **EXPRESSION** Domain Report with information about that particular experiment.

The hover for this item provides the experiment name, a detailed description of the experiment, and the array technology (type of chip) used.

TYPE

The array technology upon which the experiment in the selected record was performed.

ORGANISM

The animal or the source of the cell line used in the experiment.

TISSUE

The tissue or cell line array from which the sample was extracted.

TIME

The time period for the experiment, (e.g. 5 days).

DOSE

The dose administered per day.

INDUCED

The percent of genes in this experiment that were up regulated with a **p value** ≤ 0.02 .

REPRESSED

The percent of genes in this experiment that were down regulated with a **p value** ≤ 0.02 .

PERTURBED

The percent of genes in this experiment that were up or down regulated with a **p value** ≤ 0.02 .

COMPOUND: Activities Panel

This panel displays a list of all assays and that have been significantly impacted by the query compound.

The screenshot shows the 'ACTIVITIES' tab for the compound CLOFIBRATE. The table lists the following assays and their corresponding inhibition percentages:

ASSAY	INHIBITION	IC50	KI
<input checked="" type="checkbox"/> Dopamine Transporter	36.0%		
<input checked="" type="checkbox"/> Cyclooxygenase COX-2	35.0%		
<input checked="" type="checkbox"/> CYP450-2D6 Inhibition	32.0%		
<input checked="" type="checkbox"/> Muscarinic M5	24.0%		
<input checked="" type="checkbox"/> Neuropeptide Y1	24.0%		
<input checked="" type="checkbox"/> CYP450-2C19 Inhibition	23.0%		
<input checked="" type="checkbox"/> Serotonin 5-HT2C	23.0%		

ASSAY

This column lists the names of the assays in which the compound in the selected record was tested.

This is a hyperlink to populate an **ASSAY** domain report.

INHIBITION

The bioactivity of the selected compound in the tested assay expressed as % inhibition. (i.e. The extent (in %) the compound inhibits an enzyme reaction, or the binding of a ligand to a protein).

IC50

The bioactivity of each compound in the tested assay expressed as an IC50 (50% inhibitory concentration).

KI

The bioactivity of each compound in the tested assay expressed as a KI (a measure of the extent an inhibitor inhibits the function of a protein. It is the equilibrium constant for the dissociation of protein-inhibitor complexes).

COMPOUND: Literature Panel

The compound literature panel presents information from the public sources about gene activity produced by the query compound.

GENE	TYPE	ACTIVITY	DESCRIPTION	PUBLICATION
<input checked="" type="checkbox"/> peroxisome proliferator activat...	EC50	50.0uM	induces, secretion (placent...	
<input checked="" type="checkbox"/> peroxisome proliferator activat...	EC50	50.0uM	induces, secretion (placent...	

GENE

The name of a particular gene that is associated with the assay identified in the selected publication (i.e. the publication in a selected row of the table).

Each gene name in this column is a hyperlink that will populate a **GENE** Domain Report with information about that particular gene.

TYPE

The type of measurement used in the selected publication (i.e. the publication in a selected row of the table).

ACTIVITY

The bioactivity of the query compound in the tested assay.

DESCRIPTION

Describes the method of action of the assay identified in the selected publication (i.e. the publication in a selected row of the table).

PUBLICATION



The publication in which the activity was described. Click on the publication icon to open a new browser window displaying the publication.

COMPOUND: Target Panel

This panel presents the known protein target of the compound.

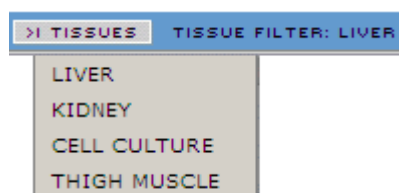
The screenshot displays a web interface for the compound CLOFIBRATE. At the top, there are navigation tabs: GENE, COMPOUND, ASSAY, EXPRESSION, PATHWAY, and EXPR. ST. Below these are buttons for >| MENU, >| FAVORITES, <| BACK, and >| FORWARD. The main title is CLOFIBRATE. Below the title are buttons for >| SMILES, >| SYNONYMS, >| IDENTIFIERS, and >| PHYSICAL PROPS. A secondary row of tabs includes SIMILAR, INDUCED, REPRESSED, EXPERIMENTS, ACTIVITIES, LITER., TARGET, SVM, and TRANK. The 'TARGET' tab is selected, showing a sub-header >| MENU PROTEIN TARGET <>. Underneath, there is a table with a 'GENE' column. The first entry is checked and labeled 'peroxisome proliferator a...'. The table has dashed lines below it, indicating more entries.

COMPOUND: SVM

This panel presents the **SVM** signatures that are positive hits for this compound. The signatures are restricted to the tissues and platforms of the experiments that have been run with this compound.

SIGNATURE NAME	MAX SP SCORE	ALGORITHM	PLATFORM
<input checked="" type="checkbox"/> PPAR alpha Agonist LIVER_RU1_SPLP	2.712	SPLP	RU1
<input checked="" type="checkbox"/> Cholesterol Decrease LIVER_RU1_SPLP	1.642	SPLP	RU1
<input checked="" type="checkbox"/> Hepatocyte Enlargement LIVER_RU1_SPLP	1.293	SPLP	RU1
<input checked="" type="checkbox"/> Liver Weight Increase LIVER_RU1_SPLP	1.262	SPLP	RU1
<input checked="" type="checkbox"/> Liver Weight Increase - Early LIVER_RU1_S...	0.721	SPLP	RU1
<input checked="" type="checkbox"/> Increased Eosinophilic Granular Cytoplasm...	0.68	SPLP	RU1
<input checked="" type="checkbox"/> Albumin Increase LIVER_RU1_SPLP	0.677	SPLP	RU1

TISSUES Menu



Selections from this menu will filter for the type of tissue used in the experiment set classified by the signatures listed in the **SIGNATURE** column of the **SVM** panel.

The specified tissue filter is indicated next to the **TISSUES** menu.

SIGNATURE NAME

The name of the signature.

PLATFORM

The array technology applicable to the signature.

MAX SP SCORE

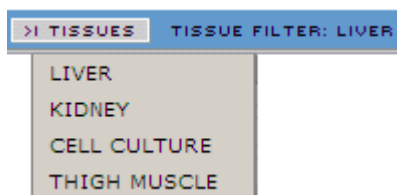
The maximum signature score across all doses/times for the query compound in the selected tissue on the specified platform for this signature type.

COMPOUND: TRANK

This panel presents the **TRANK** signatures that score highly against this compound. The signatures are restricted to the tissues and platforms of the experiments that have been run with this compound.

<input type="checkbox"/>	SIGNATURE NAME	MAX SPS SCORE	PLATFORM
<input checked="" type="checkbox"/>	Sigma Binding LIVER RU1 TRANK	88.374	RU1
<input checked="" type="checkbox"/>	PPAR alpha Aqonist LIVER RU1 TRANK	88.331	RU1
<input checked="" type="checkbox"/>	Albumin Increase LIVER RU1 TRANK	75.488	RU1
<input checked="" type="checkbox"/>	Estrogen Modulation LIVER RU1 TRANK	71.983	RU1
<input checked="" type="checkbox"/>	Increased Eosinophilic Granular Cytoplasm...	69.045	RU1
<input checked="" type="checkbox"/>	Hepatocyte Enlargement LIVER RU1 TRANK	69.045	RU1
<input checked="" type="checkbox"/>	Liver Weight Increase - Early LIVER RU1 T...	64.936	RU1

TISSUES Menu



Selections from this menu will filter for the type of tissue used in the experiment set classified by the signatures listed in the **SIGNATURE** column of the **TRANK** panel.

The specified tissue filter is indicated next to the **TISSUES** menu.

SIGNATURE NAME

The name of the signature.

PLATFORM

The array technology applicable to the signature.

MAX SPS SCORE

The maximum signature score across all doses/times for the query compound in the selected tissue on the specified platform for this signature type.

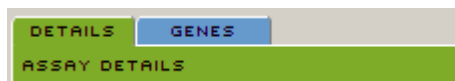
Assay Report

The **ASSAY** Domain Report presents all relevant information from the database, for the query assay. You can investigate cross referenced experimental data that comes from other domains. You can also review curated information about the query assay from several different sources.

The screenshot displays the 'ASSAY' domain report for 'TESTOSTERONE'. The interface includes a navigation bar with tabs for GENE, COMPOUND, ASSAY, EXPRESSION, PATHWAY, EXPR. STUDY, and SIGNATURE. Below the navigation bar, there are buttons for 'MENU', 'FAVORITES', 'BACK', and 'FORWARD'. The main content area is titled 'TESTOSTERONE' and features a 'COMPOUND ACTIVITIES' table. The table has columns for 'COMPOUND', 'D', 'INHIBITION', 'IC50', and 'KI'. The 'COMPOUND' column lists various compounds, and the 'INHIBITION' column shows 100.0% for most, with 99.0% for 17-METHYL TESTOSTERONE and 98.0% for BETA-ESTRADIOL. The 'IC50' and 'KI' columns provide numerical values for each compound. To the right of the table, there is a 'DETAILS' panel with 'ASSAY DETAILS' showing 'Type: BINDING', 'Species: RATTUS NORVEGICUS', and 'Catalog:'. A 'DATAVIEW' button is visible on the far right edge of the interface.

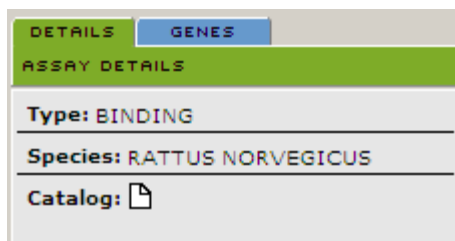
COMPOUND	D	INHIBITION	IC50	KI
NORETHINDRONE	♂	100.0%	0.022uM	0.015uM
NORGESTREL	♂	100.0%	0.00639...	0.00426...
MEGESTROL ACETATE	♂	100.0%	0.03uM	0.02uM
STANZOLOL	♂	100.0%	0.022uM	0.015uM
ETHINYLESTRADIOL	♂	100.0%	1.634uM	1.09uM
MIFEPRISTONE	♂	100.0%	0.00834...	0.00556...
DANAZOL	♂	100.0%	0.012uM	0.00799...
STANDOLONE	♂	100.0%	0.00230...	0.00153...
TESTOSTERONE	♂	100.0%	0.00616...	0.00411...
17-METHYL TESTOSTERONE	♂	99.0%	0.00639...	0.00426...
NANDROLONE	♂	99.0%	0.00314...	0.00209...
BETA-ESTRADIOL	♂	98.0%	0.353uM	0.235uM

ASSAY Detail



ASSAY: Detail Panel

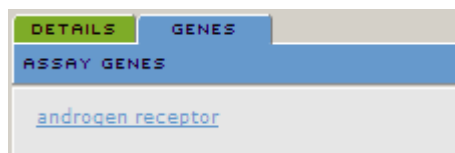
This panel provides aggregated information about the query assay, including links to additional sources of information.



Type:	The type of assay.
Species:	The species from which the gene product for the assay originated.
Catalog:	Link to the MDS Pharma Services online assay catalog (www.mdsp.com).

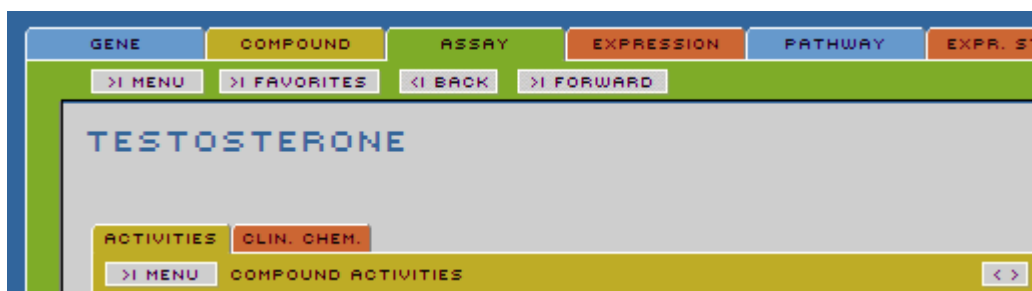
ASSAY: Genes Panel

This panel provides a list of genes or gene products for which this assay is testing compound interactions. Items in this list are links that will populate a **GENE** domain report.



ASSAY Chemogenomic Data Report

This panel presents cross referenced chemogenomic data extracted from the database, that relates to the query assay.



ASSAY: Activities Panel

This panel presents a list of compounds that have shown activity in the query assay to some specified level.



COMPOUND	INHIBITION	IC50	KI
<input checked="" type="checkbox"/> NORETHINDRONE	100.0%	0.022uM	0.015uM
<input checked="" type="checkbox"/> NORGESTREL	100.0%	0.00639...	0.00426...
<input checked="" type="checkbox"/> MEGESTROL ACETATE	100.0%	0.03uM	0.02uM


COMPOUND

The name of the compound whose activity was measured in the query assay.

Each compound name in this column is a hyperlink that will populate a **COMPOUND** Domain Report with information about that particular compound.

COMPOUND IMAGE

Click the icons at the top of this column to expand  or contract  all molecular structure images in the column.

Click the molecular structure icon  for a popup window that displays an expanded image for the compound in the selected record (i.e. the compound in a selected row of the table).

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

INHIBITION

The bioactivity of the selected compound in the tested assay expressed as % inhibition. (i.e. The extent (in %) the compound inhibits an enzyme reaction, or the binding of a ligand to a protein).

IC50

The bioactivity of each compound in the tested assay expressed as an IC50.

KI

The bioactivity of each compound in the tested assay expressed as a KI (a measure of the extent an inhibitor inhibits the function of a protein. It is the equilibrium constant for the dissociation of protein-inhibitor complexes).

ASSAY: Clin Chem Panel

This panel presents the results of an assay or test, for the query compound, used in the clinical setting, (e.g. Red blood cell count in whole blood).

EXPERIMENT	TYPE	P VALUE	CONFIDENCE INTERVAL
<input checked="" type="checkbox"/> 1-NAPHTHYL I-7d-30mg/...	BLOOD_CHEM	0.0	
<input checked="" type="checkbox"/> CARBON TETRA-7d-400m...	BLOOD_CHEM	0.0	
<input checked="" type="checkbox"/> CARBON TETRA-7d-1175...	BLOOD_CHEM	0.0	

EXPERIMENT

Experiment: CLOFIBRATE-1d-500mg/kg-LI-RATM-RU1

Description: Transcriptional profile of a 1.0 d timepoint for treatment of Rat, Male, CD-IGS, Sprague Dawley with 500.0 mg/kg of on RU1 arrays.

The experiment for which the assay was performed.

Each experiment name in this column is a hyperlink that will populate an **EXPRESSION** Domain Report with information about that particular experiment.

The hover for this item provides the experiment name, and a brief description of the experiment.

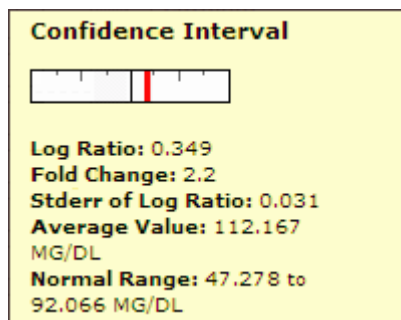
TYPE

The type of assay used for the experiment. (e.g. blood).

P VALUE

Indicates the statistical significance of the perturbation of this assay in the treated animals compared to the same assay in control animals.

The score is a **p value** (the probability that the results observed can happen by chance) computed from the log ratio and its standard error.

CONFIDENCE INTERVAL

A visual representation of statistics for the expression perturbation of the query assay in the selected experiment (i.e. the experiment in a selected row of the table).

The position and color of the bar indicate the **Log Ratio** of the specified assay in the selected experiment (i.e. the experiment in a selected row of the table). The greater the log ratio, the further the bar is from the center of the display.

A positive log ratio will appear red and to the right of the central point. A negative log ratio will appear green and to the left of the central point. The range of the graphic is ± 2 logs (-100 fold to +100 fold).

The width of the bar represents the confidence of the result. (2.8 standard errors of the log ratio = 99.5% confidence limit).

The **Confidence Interval** hover displays numeric values of statistics for the expression perturbation of the query assay in the selected experiment (i.e. the experiment in a selected row of the table).

Log Ratio:

The log of the ratio of assay levels for compound treated vs. control conditions (no compound treatment) in the selected experiment (i.e. the experiment in a selected row of the table).

Fold Change:

The fold change of expression levels for the for the assay ratio in the compound treated assay vs. the control condition in the selected experiment (i.e. the experiment in a selected row of the table). Fold values are within the ranges $-\infty < x < -1$ or $1 < x < \infty$

Stderr of Log Ratio:

The standard error of the log ratio (based on the pairwise log ratios of compound treated vs control for all animals in an experiment).

Average Value:

The average value of the assay in the control.

Normal Range:

The expected normal range of this value.

Expression Report

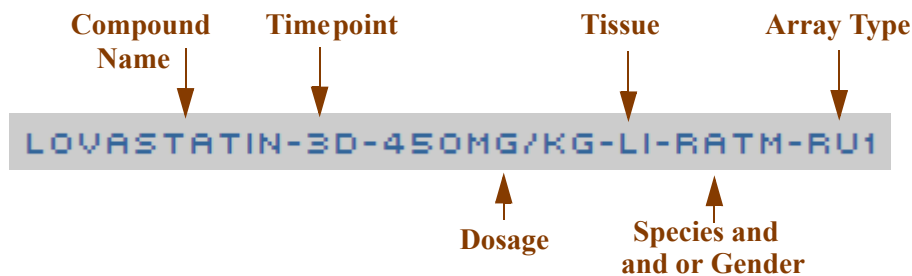
The **EXPRESSION** Domain Report presents all relevant information from the database, for the query experiment. You can investigate cross referenced chemogenomic data that comes from other domains.

The screenshot displays the 'EXPRESSION' domain report for the experiment 'LOVASTATIN-3D-450MG/KG-LI-RATM-RU1'. The interface includes navigation tabs (GENE, COMPOUND, ASSAY, EXPRESSION, PATHWAY, EXPR. STUDY, SIGNATURE) and a 'SIMILAR' section with a table of related experiments. The table columns are 'COMPOUND', 'EXPERIMENT', and 'CORR. COEFF'. The detail panel on the right provides a description, compound name (LOVASTATIN), molecular structure, and array technology (BIOCHIP).

COMPOUND	EXPERIMENT	CORR. COEFF
LOVASTATIN	LOVASTATIN-5d-450mg/...	0.5959206
SIMVASTATIN	SIMVASTATIN-3d-1200m...	0.54973677
LOVASTATIN	LOVASTATIN-3d-1500mg...	0.54321503
FLUVASTATIN	FLUVASTATIN-3d-94mg/k...	0.531171
PRAVASTATIN	PRAVASTATIN-3d-1200m...	0.52607777
SIMVASTATIN	SIMVASTATIN-1d-1200m...	0.50113677
ATORVASTATIN	ATORVASTATIN-3d-300m...	0.49312107
GEMFIBROZIL	GEMFIBROZIL-1d-700mg...	0.46591875
LOVASTATIN	LOVASTATIN-5d-1200mg...	0.45419714
FLUVASTATIN	FLUVASTATIN-5d-94mg/k...	0.45079444
PRAVASTATIN	PRAVASTATIN-5d-1200m...	0.44824978

Naming System for Drug Matrix Expression Experiments.

The following example describes the different parts of a DrugMatrix experiment name.



NOTE: For long compound names only the first 12 characters are used in the experiment name.

EXPRESSION Detail

The Expression Detail area provides aggregated information about the query experiment. Some items displayed here link to additional sources of information about the query experiment.

EXPRESSION Buttons

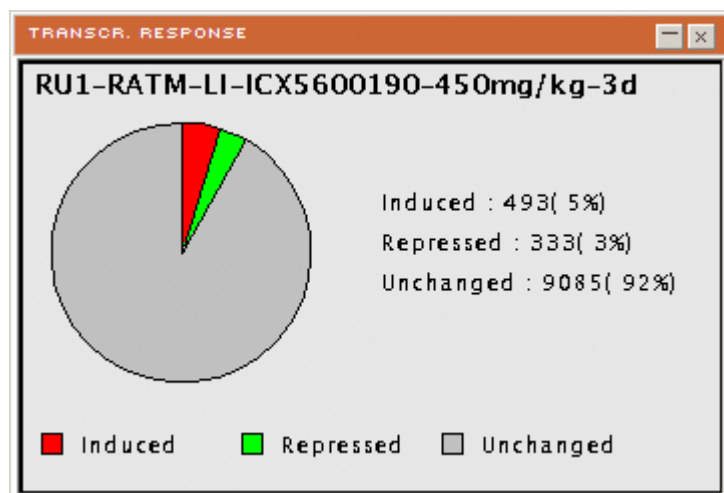


Behavior

These buttons launch popup windows containing specific information about the query experiment.

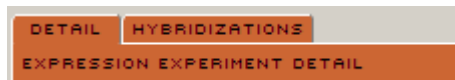
TRANSCRIPTIONAL RESPONSES Button

This chart provides a graphical representation of statistics for the transcriptional changes in the query experiment to help quickly identify the number and percent of induced, repressed, and unchanged genes in the experiment (gene is induced if the log ratio minus 2.8 standard errors is > 0 ; gene is repressed if the log ratio plus 2.8 standard errors is < 0).



EXPRESSION Detail Panels

The Expression Detail panels provide aggregated information about the query experiment. Some items found in the lists displayed here link to additional sources of information about the query experiment.



EXPRESSION: Detail Panel

This panel presents a synopsis of the experimental conditions for the query experiment, including information about time, dose, and species, as well as information about the associated compound.

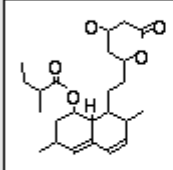
DETAIL **HYBRIDIZATIONS**

EXPRESSION EXPERIMENT DETAIL

Description:
Transcriptional profile of a 3.0d timepoint for treatment of Rat, Male, CD-IGS, Sprague Dawley with 450.0mg/kg of LOVASTATIN on RU1 arrays.

Compound:
[LOVASTATIN](#)

Molecular Structure:



Array Technology: BIOCHIP

Dose Level: LO

Vehicle: CORN OIL 100 %

Administration Route: ORAL GAVAGE

Administration Frequency: DAILY

Strain Name: RATM

CTL Label: S-Alexa

EXP Label: S-Alexa

Study: [LOVASTATIN-RATM](#)

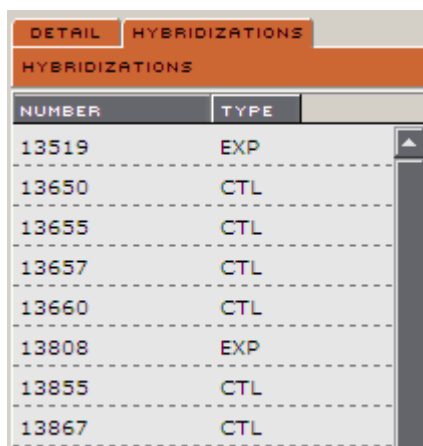
Description:

A synopsis of the experimental conditions for the query experiment, providing information about time, dose, and species.

Compound:	The name of the compound investigated in the query experiment. This is a hyperlink will populate a Compound domain report.
Molecular Structure:	The 2 dimensional rendered image of the chemical structure of the compound used in the query expression experiment.
Array Technology:	The array technology upon which the query experiment was performed.
Strain Name:	The species and sex of animal or the specific strain of cell line used in the query experiment.
CTL Label:	Fluorescent label that is used for the mock treated sample.
EXP Label:	Fluorescent label used for the compound treated sample.
Study:	This is a link that populates an EXPRESSION STUDY Domain Report (the collection of experiments for all the dose, time and tissue experiments done for a particular compound during a narrow window of time). See ' Expression Study Report ' on page 93.

EXPRESSION: Hybridization

This panel displays a list of hybridizations for the query experiment.

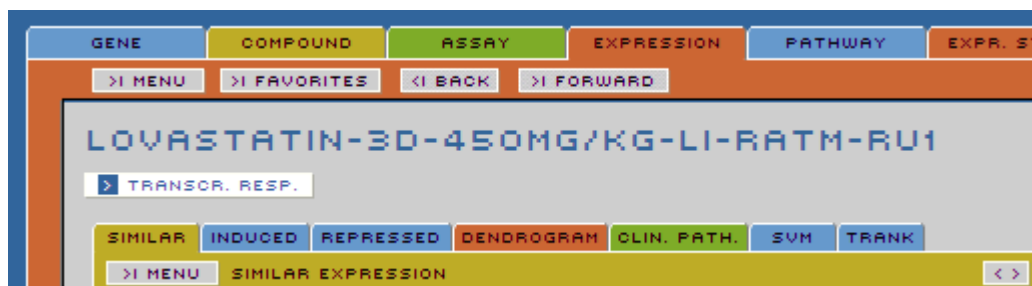


HYBRIDIZATIONS	
NUMBER	TYPE
13519	EXP
13650	CTL
13655	CTL
13657	CTL
13660	CTL
13808	EXP
13855	CTL
13867	CTL

NUMBER	The hybridization number.
TYPE	CTL (control) or EXP (experimental).

EXPRESSION Chemogenomic Data Report

This panel presents cross referenced chemogenomic data extracted from the database, that relates to the query experiment.



Interactive Elements




Sorting Columns

Many columns on panels in the **EXPRESSION** Chemogenomic Data Reports are sortable, either alphabetically or numerically. Click on a column name in the currently displayed Chemogenomic Data Report panel to toggle the order (ascending or descending) in which data in that column is sorted. You can also sort lists by items checked (or unchecked).



To modify the width of a column, mouse over the column separator to the right of that column, then when the cursor changes to a cross, hold down the left mouse button and drag to change the column width.

Expandable images

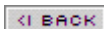
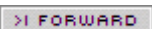
You can expand  or contract  all molecular structure images in a column containing the molecular structure icon  or click on individual icons for an expanded image of the compound in the selected record.

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

Hyperlinks

Hyperlinked items, appearing in the **EXPRESSION** Chemogenomic Data Reports, will either populate associated domain reports or link to published information about the selected compound. For example, if you click on a gene name on the **INDUCED** panel of the **EXPRESSION** report, it will populate a **GENE** domain report for that gene.

Saving Lists

Each **EXPRESSION** Domain Report you create will be available until the current session is closed. You can access **EXPRESSION** Domain Reports generated in this session using the  and  buttons at the top left of the Domain Report panel.

Use the **MENU > SAVE** option on any panel in the **EXPRESSION** report to permanently save a list of checked records on that panel. You can also use the **FAVORITES>ADD FAVORITE** option to add the current query item (named at the top of the domain report panel) to the **FAVORITES** list.

Some panels allow you to save more than one of the lists that appear on the panel. The **MENU** button on any panel will indicate which lists can be saved.

EXPRESSION: Similar Panel

This panel presents experiments from the database, and their associated compounds, in which the transcriptional response profile shows significant similarity to the transcriptional response profile for the query experiment as measured by a distance metric.



COMPOUND	EXPERIMENT	CORR. COEFF
<input checked="" type="checkbox"/> LOVASTATIN	LOVASTATIN-5d-450mg/...	0.5959206
<input checked="" type="checkbox"/> SIMVASTATIN	SIMVASTATIN-3d-1200m...	0.54973677
<input checked="" type="checkbox"/> LOVASTATIN	LOVASTATIN-3d-1500mg...	0.54321503
<input checked="" type="checkbox"/> FLUVASTATIN	FLUVASTATIN-3d-94mg/k...	0.531171


COMPOUND

A list of compounds that have caused gene expression profiles similar to the gene expression profiles caused by the compound used in the query experiment.

Each compound name in this column is a hyperlink that will populate a **COMPOUND** Domain Report with information about that particular compound.

COMPOUND IMAGE

Click the icons at the top of this column to expand  or contract  all molecular structure images in the column.

Click the molecular structure icon  for a popup window that displays an expanded image for the compound in the selected record (i.e. the compound in a selected row of the table).

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

EXPERIMENT

A list of experiments in which the gene expression profiles are similar to the gene expression profile in the query experiment.

Each experiment name in this column is a hyperlink that will populate a **EXPRESSION** Domain Report with information about that particular experiment.

CORR COEFF

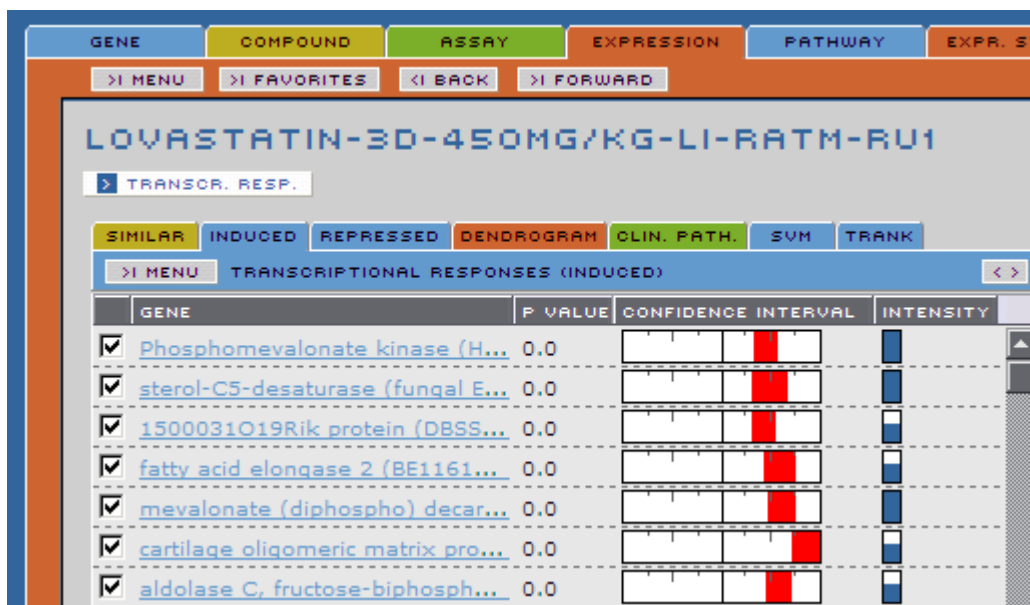
A measure of similarity between the expression profiles for the query experiment and the experiment in the selected record (i.e. the experiment in a selected row of the table).

This is the R-value from the Pearson's Correlation Coefficient for transcriptional changes (ratios of treated to control) across all experiments. See '[Pearson's Correlation Coefficient](#)' on page 227.

Values closest to 1.0 are the closest match to the query experiment.

EXPRESSION: Induced Panel

This panel presents a list of genes that were up regulated in the query experiment.



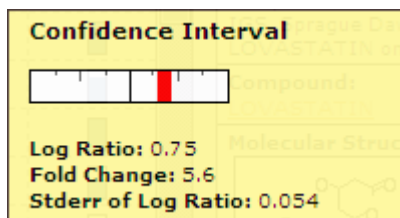
GENE

A list of genes that were up regulated in the query experiment.

P VALUE

Indicates the **p value** of the measurements of the perturbation of this gene in the treated arrays compared to the same gene in control arrays.

CONFIDENCE INTERVAL



A visual representation of statistics for the expression perturbation of the query gene in the selected experiment (i.e. the experiment in the selected row of the table).

The position and color of the bar indicates the **Log Ratio** of the specified gene in the selected experiment (i.e. the experiment in the selected row of the table). The greater the log ratio, the further the bar is from the center of the display.

A positive log ratio will appear red and to the right of the central point. A negative log ratio will appear green and to the left of the central point. Since this table displays induced genes, the bar will always be red and to the right of center.

The width of the bar represents the confidence of the result. (2.8 standard errors of the logratio = 99.5% confidence limit).

The **Confidence Interval** hover displays numeric values of statistics for the expression perturbation of the query gene in the selected experiment (i.e. the experiment in the selected row of the table).

Log Ratio: The log of the ratio the ofgene expression level for compound treated over control condition for the selected gene in the query experiment (i.e. the gene in a selected row of the table).

Fold Change: The fold change of expression levels for the gene in the compound treated vs the control condition in the query experiment.
Fold values for the induced report are within the range $1 < x < \infty$

Stderr of Log Ratio: The standard error of the log ratio (based on the pairwise log ratios of compound treated vs control for all arrays in an experiment).

INTENSITY



A bar chart indicating the approximate level of the average expression values for a specific gene across all the arrays in the experiment.

The height of the bar indicates increasing intensity.

EXPRESSION: Repressed Panel

This panel presents a list of genes that were down regulated in the query experiment.

GENE	P VALUE	CONFIDENCE INTERVAL	INTENSITY
<input checked="" type="checkbox"/> serine dehydratase (J03865m...	0.0		
<input checked="" type="checkbox"/> HMBA-inducible (Hs.) (DBSS) (...	1.0E-6		
<input checked="" type="checkbox"/> solute carrier family 37 (glycer...	2.0E-6		
<input checked="" type="checkbox"/> mitochondrial DNA polymerase...	3.0E-6		
<input checked="" type="checkbox"/> hydroxysteroid (17-beta) dehy...	2.4E-5		
<input checked="" type="checkbox"/> ESTs (AW921162_PROBE1,137...	4.4E-5		
<input checked="" type="checkbox"/> hypothetical protein MGC2793 ...	4.7E-5		

GENE

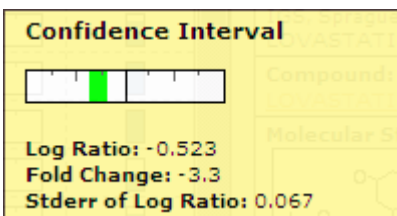
A list of genes that were down regulated in the query experiment.

Each gene name in this column is a hyperlink that will populate a **GENE** Domain Report with information about that particular gene.

P VALUE

Indicates the **p value** of the measurements of the perturbation of this gene in the treated arrays compared to the same gene in control arrays.

CONFIDENCE INTERVAL



A visual representation of statistics for the expression perturbation of the selected gene (i.e. the gene in a selected row of the table) in the query experiment.

The position and color of the bar indicate the **Log Ratio** of the specified gene in the query experiment. The greater the log ratio, the further the bar is from the center of the display.

A positive log ratio will appear red and to the right of the central point. A negative log ratio will appear green and to the left of the central point. Since this table displays repressed genes, the bar will always be green and to the left of center.

The width of the bar represents the confidence of the result. (2.8 standard errors of the log ratio = 99.5% confidence limit).

The **Confidence Interval** hover displays numeric values of statistics for the expression perturbation of the query gene in the query experiment.

Log Ratio: The log of the ratio the of gene expression level for compound treated over control condition—for the selected gene (i.e. the gene in a selected row of the table) in the query experiment.

Fold Change: The fold change of expression levels for the compound treated over the control condition (no compound treatment) in the selected experiment.

Fold values for the repressed report are within the range $-\infty < x < -1$

Stderr of Log Ratio: The standard error of the log ratio (based on the pairwise log ratios of compound treated vs control for all arrays in an experiment).

INTENSITY



A bar chart indicating the approximate level of the average expression values for a specific gene across all the arrays in the experiment.

The height of the bar indicates increasing intensity.

EXPRESSION: Dendrogram Panel

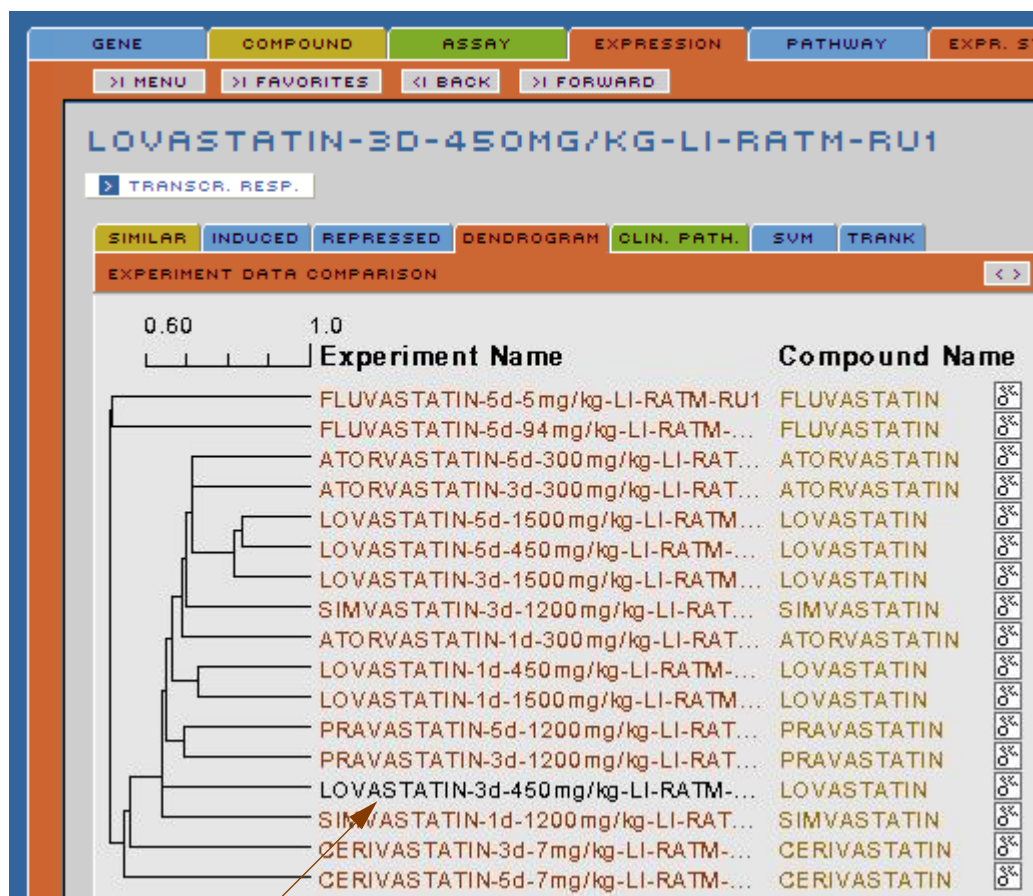
The dendrogram button that appears on this panel, allows you to load a dendrogram that graphically represents a hierarchical clustering of experiments with transcriptional response profiles similar to the query experiment.

The query profile appears in black. If it is from the database, it is labelled with the relevant experiment name.

NOTE: If the query profile is uploaded from a data file external to the database, it is labeled **CustomerDataSet1** for the first upload of the session, **CustomerDataSet2** for the second upload and so on.

The dendrogram represents hierarchical clustering, using Pearson's correlation coefficient as the similarity metric (scores approaching 1.0 indicate the highest similarity while scores approaching -1 indicate the least similarity). In this example, the lowest scores are near 0, indicating these nodes are poorly correlated.

The experiments with the highest scores (i.e. approaching 1.0) are the most similar to the **QUERY EXPERIMENT**. Similarity between other experiments in the table is also indicated by the clustering.



Query Experiment



A scale representing the similarity for experiments in the dendrogram.

Experiment Name


The name of the experiment represented by this position in the dendrogram. Each experiment is a link that will populate an **EXPRESSION** domain report.

Compound Name

The name of the compound used in the named experiment. Each compound is a link that will populate a **COMPOUND** domain report.

Structure

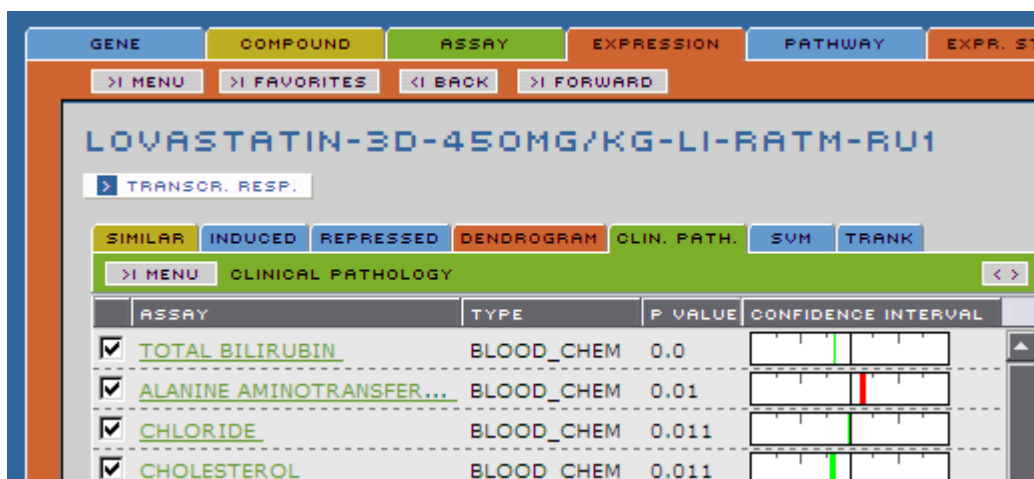
The 2 dimensional rendered image of the compound used in the named experiment.

Click the molecular structure icon  for a popup window that displays an expanded image for the compound.

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

EXPRESSION: Clin Path Panel

This panel presents information for a list of assays, used in the clinical setting, for the compound in the query expression experiment.



ASSAY

A list of assays in which the compound in the query expression experiment was tested.

This is a hyperlink to populate an ASSAY domain report.

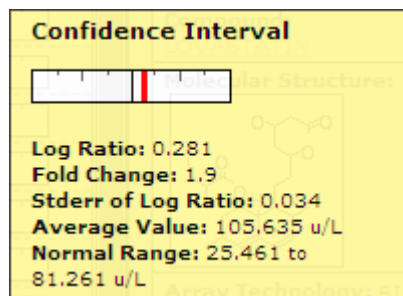
TYPE

The type of assay used for the experiment. (e.g. blood chem).

P VALUE

Indicates the **p value** of the measurements of the perturbation of this assay in the treated arrays compared to the same assay in control arrays.

CONFIDENCE INTERVAL



A visual representation of the statistics for the perturbation of the selected assay (i.e. the assay in a selected row of the table) in the query experiment.

The position and color of the bar indicate the **Log Ratio** of the specified assay (i.e. the assay in a selected row of the table) in the query experiment. The greater the log ratio, the further the bar is from the center of the display.

A positive log ratio will appear red and to the right of the central point. A negative log ratio will appear green and to the left of the central point. The range of the graphic is ± 2 logs (-100 fold to +100 fold).

The width of the bar represents the confidence of the result. (2.8 standard errors of the log ratio = 99.5% confidence limit).

The **Confidence Interval** hover displays numeric values of statistics for the perturbation of the selected assay (i.e. the assay in a selected row of the table) in the query experiment.

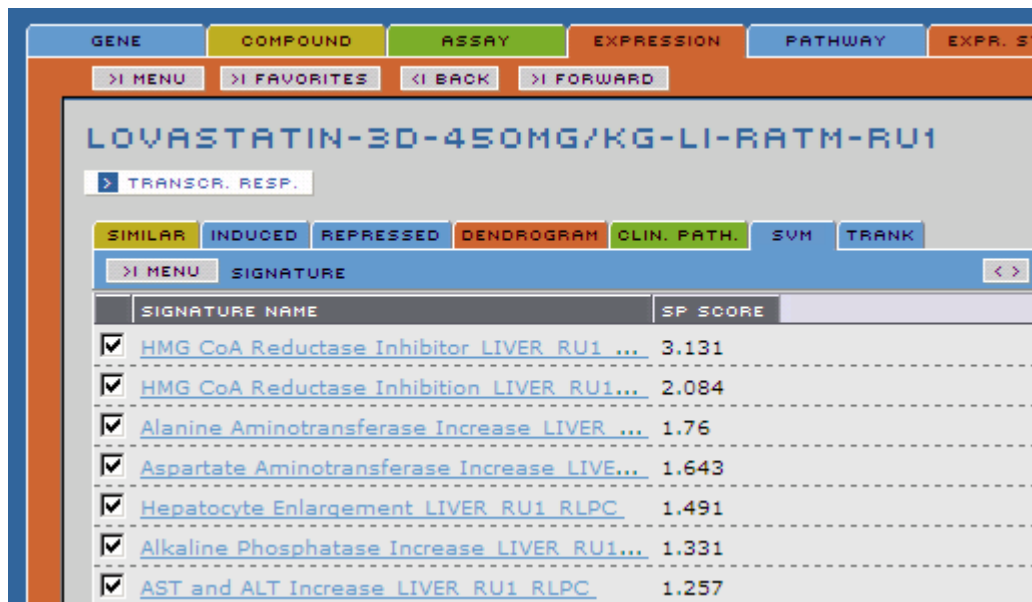
Log Ratio:

The log of the ratio of assay measurement levels for compound treated vs. control conditions (no compound treatment) in the selected experiment.

Fold Change:	The fold change of assay measurement levels in the compound treated vs the control condition in the selected experiment. Fold values are within the ranges $-\infty < x < -1$ or $1 < x < \infty$
Stderr of Log Ratio:	The standard error of the log ratio (based on the pairwise log ratios of compound treated vs control for all assays in an experiment).
Average Value:	The average value of the assay in the control.
Normal Range:	The expected normal range of the assay values in the controls.

EXPRESSION: SVM

This panel presents the **SVM** signatures that have a positive score against this experiment. The signatures are restricted to the tissues and platforms of the experiments that have been run with this compound.



The screenshot shows a web interface for the EXPRESSION: SVM panel. At the top, there are tabs for GENE, COMPOUND, ASSAY, EXPRESSION, PATHWAY, and EXPR. ST. Below these are navigation buttons: >| MENU, >| FAVORITES, <| BACK, and >| FORWARD. The main title is LOVASTATIN-3D-450MG/KG-LI-RATM-RU1. Below the title is a dropdown menu for TRANSCR. RESP. and a row of tabs: SIMILAR, INDUCED, REPRESSED, DENDROGRAM, CLIN. PATH., SVM, and TRANK. Below these is another navigation bar with >| MENU, SIGNATURE, and < >. The main content is a table with two columns: SIGNATURE NAME and SP SCORE. The table lists seven signatures, each with a checked checkbox in the first column.

SIGNATURE NAME	SP SCORE
<input checked="" type="checkbox"/> HMG CoA Reductase Inhibitor LIVER RU1 ...	3.131
<input checked="" type="checkbox"/> HMG CoA Reductase Inhibition LIVER RU1...	2.084
<input checked="" type="checkbox"/> Alanine Aminotransferase Increase LIVER ...	1.76
<input checked="" type="checkbox"/> Aspartate Aminotransferase Increase LIVE...	1.643
<input checked="" type="checkbox"/> Hepatocyte Enlargement LIVER RU1 RLPC	1.491
<input checked="" type="checkbox"/> Alkaline Phosphatase Increase LIVER RU1...	1.331
<input checked="" type="checkbox"/> AST and ALT Increase LIVER RU1 RLPC	1.257

SIGNATURE NAME The name of the signature.

SP SCORE The scalar product score for this experiment against the signature in this row.

EXPRESSION: TRANK

This panel presents the **TRANK** signatures that score highly against this experiment. The signatures are restricted to the tissues and platforms of the experiments that have been run with this compound.

The screenshot shows a web application interface for the experiment **LOVASTATIN-3D-450MG/KG-LI-RATM-RU1**. The interface includes navigation tabs for GENE, COMPOUND, ASSAY, EXPRESSION, PATHWAY, and EXPR. ST. Below these are navigation buttons: >| MENU, >| FAVORITES, <| BACK, and >| FORWARD. A dropdown menu is open for TRANSCR. RESP., showing options: SIMILAR, INDUCED, REPRESSED, DENDROGRAM, CLIN. PATH., SUM, and TRANK. The TRANK option is selected, and a sub-menu is open showing >| MENU and <|. Below this is a table of signatures.

SIGNATURE NAME	SPS SCORE
<input checked="" type="checkbox"/> HMG CoA Reductase Inhibitor LIVER RU1 ...	81.391
<input checked="" type="checkbox"/> HMG CoA Reductase Inhibition LIVER RU1...	77.984
<input checked="" type="checkbox"/> TBI, ALP, and ALT Increase LIVER RU1 TR...	58.574
<input checked="" type="checkbox"/> AST and ALT Increase LIVER RU1 TRANK	55.661
<input checked="" type="checkbox"/> Aspartate Aminotransferase Increase LIVE...	55.46
<input checked="" type="checkbox"/> TBI and ALT Increase LIVER RU1 TRANK	55.456
<input checked="" type="checkbox"/> Cholesterol Decrease LIVER RU1 TRANK	40.024

SIGNATURE NAME

The name of the signature.

SPS SCORE

The signature projection score for this experiment against the signature in this row.

Pathway Report

The **PATHWAY** Domain Report provides hand curated information about a biochemical, metabolic, or signal transduction pathway.

The screenshot displays a web-based Pathway Report interface. At the top, there are navigation tabs: GENE, COMPOUND, ASSAY, EXPRESSION, PATHWAY, EXPR. STUDY, and SIGNATURE. Below these are buttons for MENU, FAVORITES, BACK, and FORWARD. The main title of the report is "Ca++ Signaling, Cytochrome c Release, & Apoptosis".

On the left side, there is a sub-section titled "PATHWAY" with tabs for GENES, COMPOUNDS, and PATHWAYS. Under the "GENES" tab, there is a list of genes in the pathway, each with a checkbox and a truncated name:

GENE
<input checked="" type="checkbox"/> transforming growth factor, bet...
<input checked="" type="checkbox"/> mitogen activated protein kina...
<input checked="" type="checkbox"/> mitogen activated protein kina...
<input checked="" type="checkbox"/> Kirsten rat sarcoma viral oncop...
<input checked="" type="checkbox"/> mitogen activated protein kina...
<input checked="" type="checkbox"/> voltage-dependent anion chan...
<input checked="" type="checkbox"/> voltage-dependent anion chan...

On the right side, there is a "PATHWAY DETAIL" section with tabs for DETAIL, ANNOTATION, and LITERATURE. It features a diagram of the pathway, showing various molecules and their interactions, with a legend on the right side of the diagram.

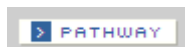
PATHWAY Detail

The Pathway Detail area provides information about the query pathway.

PATHWAY Buttons

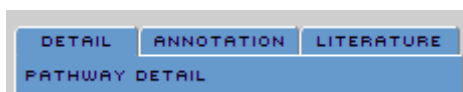
PATHWAY Button

This button will launch a popup window containing a full size image of the pathway. You can use this to inspect the pathway in more detail or to save the image.



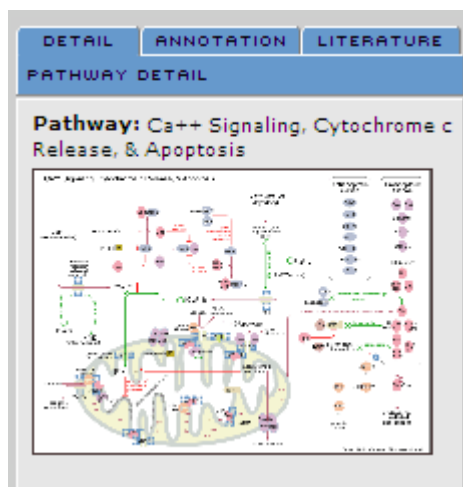
Pathway Detail Panels

The Pathway Detail panel provides information about the pathway.



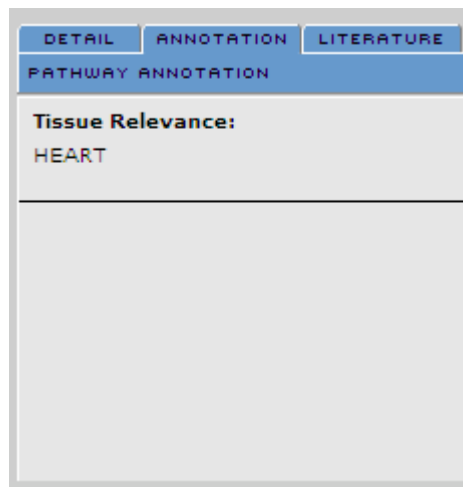
Pathway: Detail

This panel displays a thumbnail image that represents the pathway. Click on this image for a popup window with an expanded image of the pathway.



Pathway: Annotation

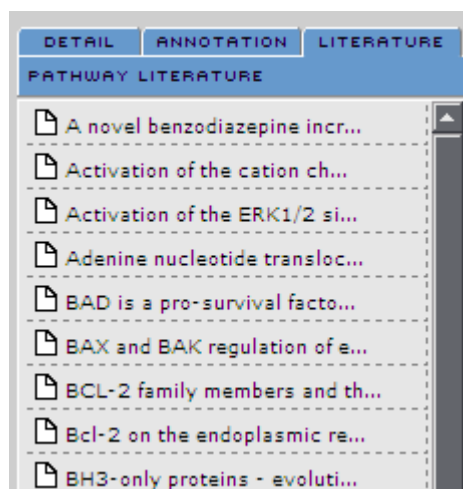
This panel displays the literature annotations about the pathway.



Tissue relevance: The tissue in which the pathway is dominant (i.e. most relevant).

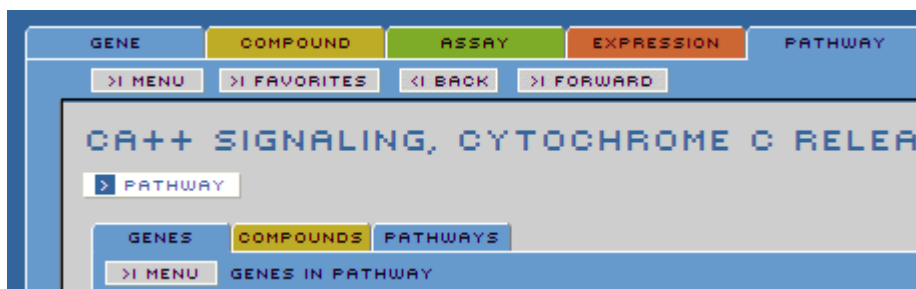
Pathway: Literature

This panel displays the literature sources of information used to construct the pathway.



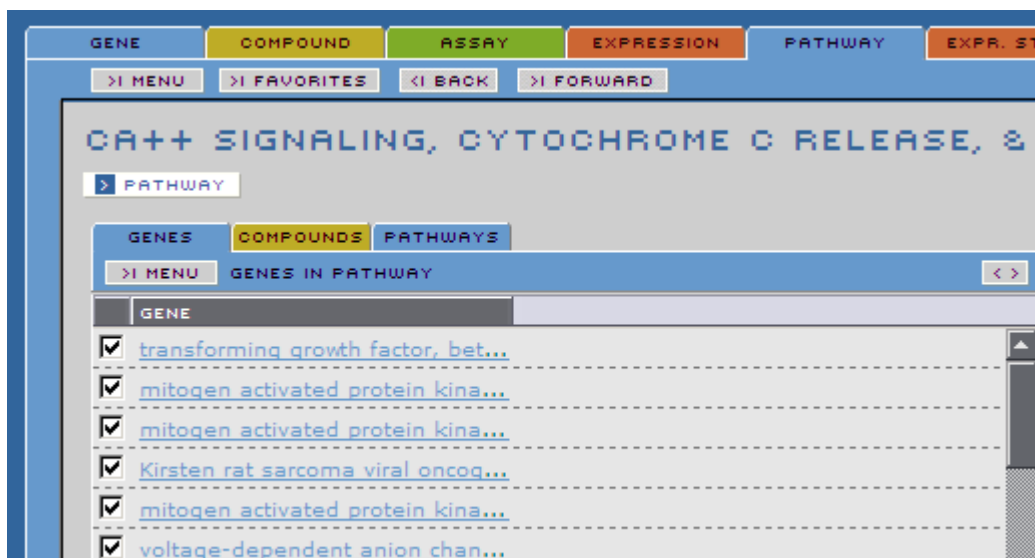
Pathway Chemogenomic Data Report

This panel presents cross referenced chemogenomic data extracted from the database, that relates to the query pathway.



Pathway: Genes Panel

This panel lists the genes from the database that are known to be in the pathway based on the curated information used to construct the pathway.



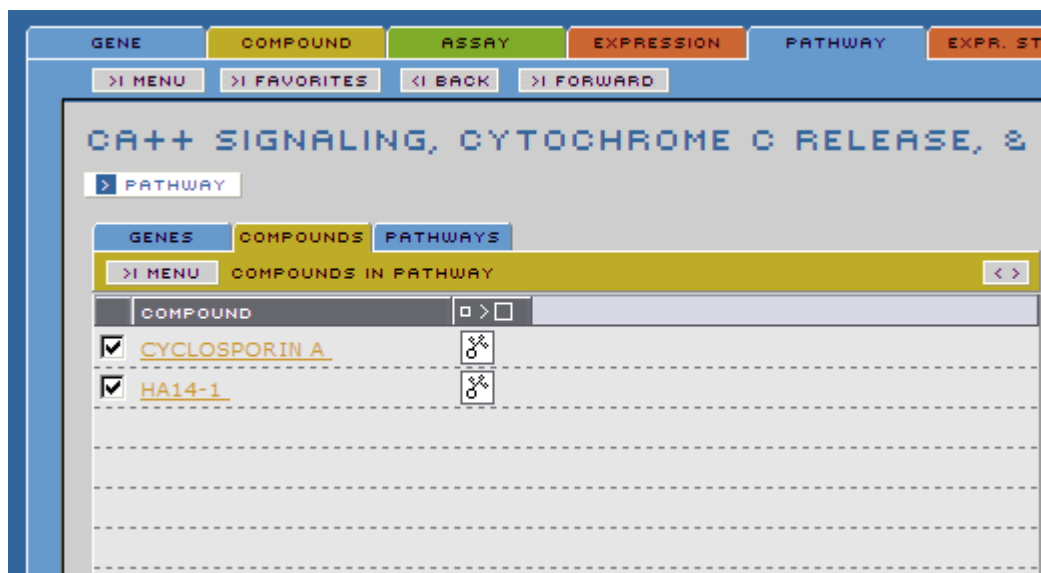
GENE

A list of the genes in the query pathway.

Click on the gene name to populate a **GENE** Domain Report with information about that gene.

Pathway: Compounds Panel

This panel displays a list of compounds that are known to act on the pathway of the query gene.






COMPOUND

A list of compounds that are associated with or known to affect the query pathway.

Each compound name in this column is a hyperlink that will populate a **COMPOUND** Domain Report with information about that particular compound.

COMPOUND IMAGE

Click the icons at the top of this column to expand  or contract  all molecular structure images in the column.

Click the molecular structure icon  for a popup window that displays an expanded image for the compound in the selected record (i.e. the compound in a selected row of the table).

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

Pathway: Pathways Panel

This panel displays a list of pathways which are links to other pathways related to the query pathway.

The screenshot displays a web interface for a pathway report. At the top, there are tabs for GENE, COMPOUND, ASSAY, EXPRESSION, PATHWAY, and EXPR. ST. Below these are navigation buttons: >| MENU, >| FAVORITES, <| BACK, and >| FORWARD. The main title is "CA⁺⁺ SIGNALING, CYTOCHROME C RELEASE, &". Below the title is a "PATHWAY" button. A sub-panel has tabs for GENES, COMPOUNDS, and PATHWAYS, with "PATHWAYS" selected. Below this sub-panel are buttons for >| MENU and PATHWAY LINKS, and a <> button. The main content area is titled "PATHWAY" and contains a list of related pathways, each with a checked checkbox and a blue hyperlink:

- [Angiotensin II Regulated...](#)
- [Apoptosis](#)
- [Calcium Signaling in Non...](#)
- [Cardiac Hypertrophy & Ce...](#)
- [Cardiolipin & Mitochondri...](#)
- [Glycolysis](#)
- [G-Protein Gq Signaling](#)

Expression Study Report

The **EXPRESSION STUDY** Domain Report presents a list of experiments related to the query study.

EXPERIMENT	TYPE	TISSUE	TIME	DOSE	LEVEL
LOVASTATIN-5d-450mg/...	BIOCHIP	LIVER	5.0d	450.0mg/...	LO
LOVASTATIN-5d-1500mg...	BIOCHIP	THIGH ...	5.0d	1500.0m...	
LOVASTATIN-5d-1500mg...	BIOCHIP	LIVER	5.0d	1500.0m...	HI
LOVASTATIN-5d-1500mg...	BIOCHIP	KIDNEY	5.0d	1500.0m...	HI
LOVASTATIN-3d-450mg/...	BIOCHIP	LIVER	3.0d	450.0mg/...	LO
LOVASTATIN-3d-450mg/...	BIOCHIP	KIDNEY	3.0d	450.0mg/...	LO
LOVASTATIN-3d-1500mg...	BIOCHIP	THIGH ...	3.0d	1500.0m...	
LOVASTATIN-3d-1500mg...	BIOCHIP	LIVER	3.0d	1500.0m...	HI
LOVASTATIN-3d-1500mg...	BIOCHIP	KIDNEY	3.0d	1500.0m...	HI
LOVASTATIN-1d-450mg/...	BIOCHIP	LIVER	1.0d	450.0mg/...	LO

Expression Study Detail

The Expression Study Detail area provides aggregated information about the query study. Some items found in the lists displayed here link to additional sources of information about the query study.

Expression Study Buttons

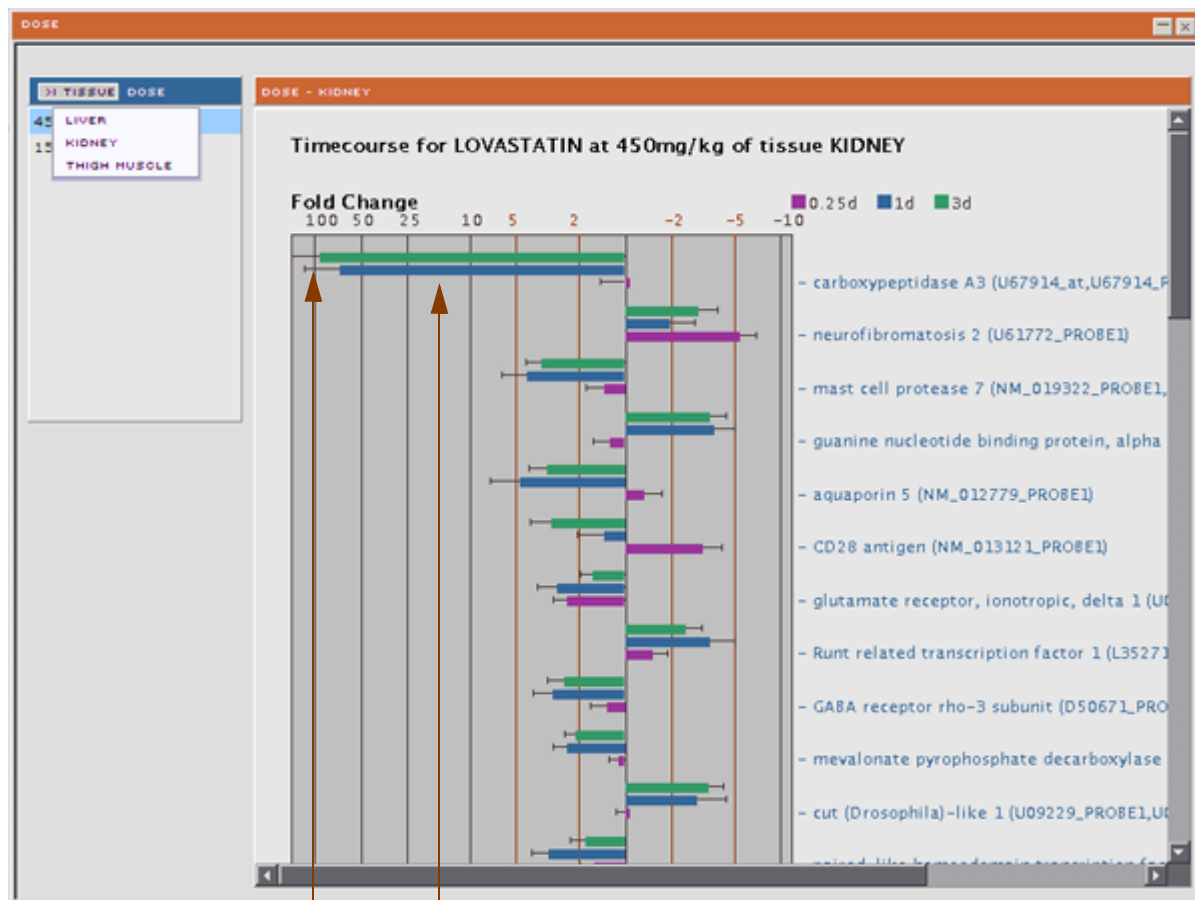
Behavior

These buttons launch popup windows containing reports or graphical representations of various predefined data sets.



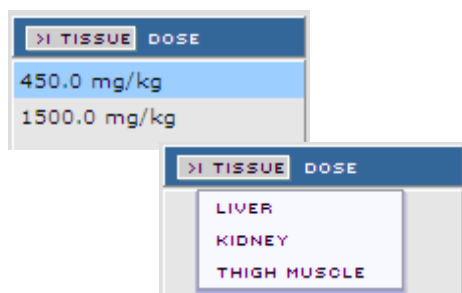
TIME COURSE Button

This is a chart of the most consistent significant gene expression changes for the experimental compound in the subset of experiments in the query study, where the dose is fixed and the time periods are varied. Each gene name on this chart is a hyperlink to a **GENE** Domain Report.



Standard error of
Fold Change Fold Change

NOTE: Each bar represents the fold change (colored portion) and the standard error of the fold change (black portion) for the gene for each experiment in the time course set.

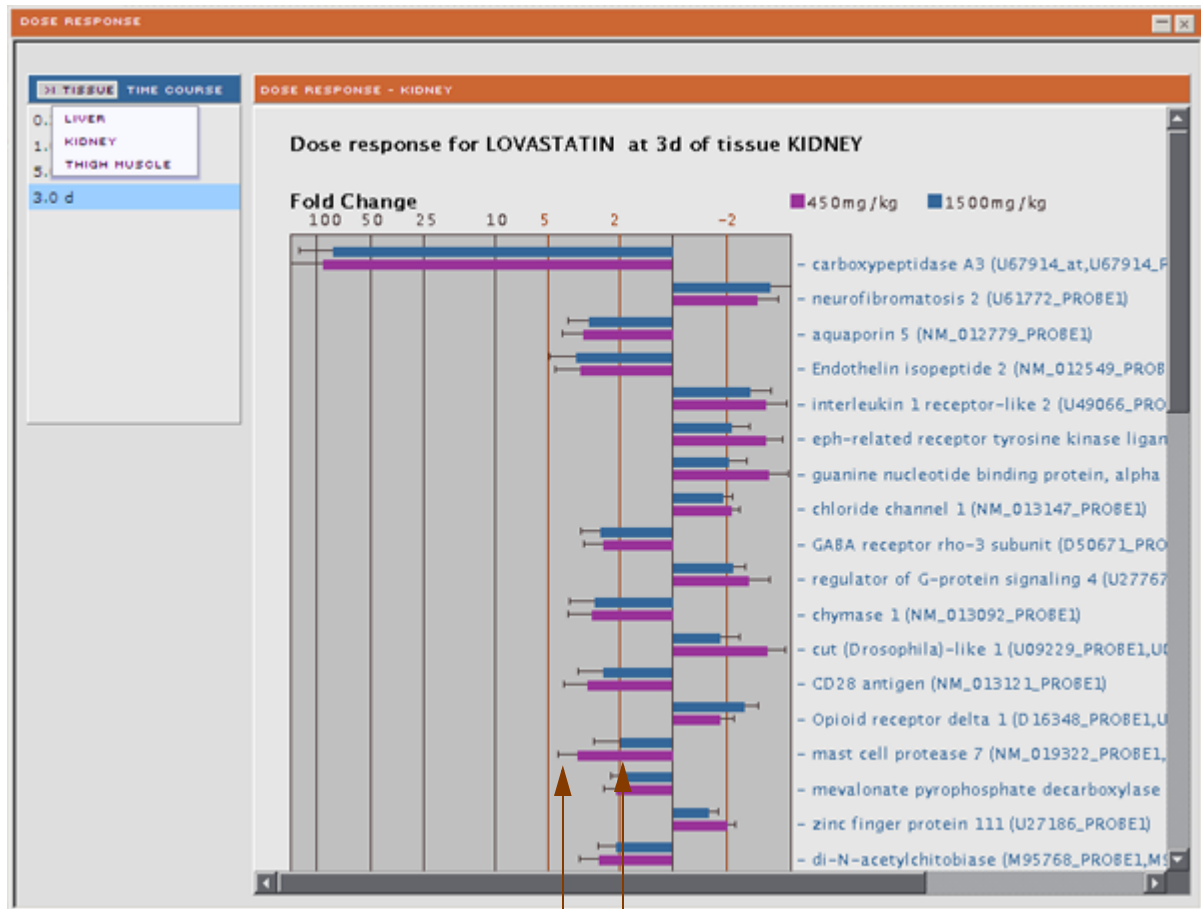


The menu on the left of this panel allows you to display results for different doses used in the experiments.

Selections from this menu will filter for the type of tissue used in the experiments.

DOSE RESPONSE Button

This is a chart of the most consistent significant gene expression changes for the experimental compound in the subset of experiments in the query study, over several compound doses, with time held constant. Each gene name on this chart is a hyperlink to a **GENE** Domain Report.



Standard error of Fold Change

Fold Change

NOTE: Each bar represents the fold change (colored portion) and the standard error of the fold change (black portion) for the gene for each experiment in the time course set.



The menu on the left of this panel allows you to display results for experiments at different time intervals.

Selections from this menu will filter for the type of tissue used in the experiments.

PATHLAB REPORT Button

This will launch a **Histopathology and Clinical Pathology Report** for the live animals used in the query study. The report is presented in PDF format and provides Selected Clinical Chemistry data, Selected Clinical hematology (blood measurements), Clinical observations including weight changes of the animal over time, Selected organ weight changes over time, a Histopathology report with example tissue images as well as links to clinical chemistry and hematology assay information.

Clinical Pathology - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Norton AntiVirus

DrugMatrix™

LOVASTATIN

Histopathology and Clinical Pathology Report

This report summarizes clinical chemistry, hematology, clinical observations, and histopathology findings from an expression array study run on LOVASTATIN. The study was conducted with 6-8 week old male Sprague-Dawley rats (Charles River), which were quarantined for 3-5 days before initiation of the study. LOVASTATIN was delivered in 100 % corn oil PO daily for a maximum of 5 days. Animals were sacrificed by exsanguination under carbon dioxide anesthesia and tissues were collected 3 days, and 5 days after the start of treatment.

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Clinical Chemistry

Blood samples were collected from animals at the time of sacrifice and the following parameters were assayed using a Hitachi 911 instrument. Further information about the Hitachi 911 and these assays are available

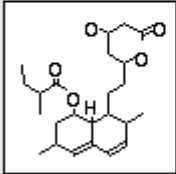
Dose Justify Button


This panel displays a detailed rationale for High Dose and Low Dose for animal treatments in this study.



Expression Study: Detail Panel

This panel presents a synopsis of the query study and information about the associated compound.

DETAIL	
EXPRESSION STUDY DETAIL	
Description:	Transcriptional profiles resulting from the treatment of Rat, Male, CD-1GS, Sprague Dawley with LOVASTATIN.
Compound:	LOVASTATIN
Molecular Structure:	
Salt Form:	Lovastatin
Purity:	98.8%
Strain Name:	RATM

- Description:** A synopsis of the query study.
- Compound:** The name of the compound investigated in the query study. Click on the compound name in this panel to open a new browser window with additional information about the compound.
- Molecular Structure:** The 2 dimensional rendered image of the chemical structure of the compound used in the query study. Click the molecular structure icon  for a popup window that displays an expanded image for the compound in the selected record (i.e. the compound in a selected row of the table). If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.
- Salt Form:** Refers to whether the sample used is a salt and what the counter ion is, if it is a salt. Compounds prepared with no counter ions are called "Salt Free". See '[Salt Form](#)' on page 227 for more details.
- Purity:** A measure of how clean the sample is. Drug matrix uses data provided by the compound supplier for purity. See '[Purity](#)' on page 227 for more detail.
- Strain Name:** The species and sex of animal or the specific cell line used in the study.

Expression Study Chemogenomic Data Report

The Expression Study chemogenomic information report presents a list of experiments in the query study.



Expression Study: Experiments Panel

This panel presents a list of experiments in the query study, and the type of microarray with which the study was performed.

EXPERIMENT	TYPE	TISSUE	TIME	DOSE	LEVEL	VEHICLE	ROUTE	FREQUENCY
LOVASTATIN-5d-450mg/...	BIOCHIP	LIVER	5.0d	450.0mg/...	LO	CORN OIL...	ORAL GAV...	DAILY
LOVASTATIN-5d-1500mg/...	BIOCHIP	THIGH ...	5.0d	1500.0m...		CORN OIL...	ORAL GAV...	DAILY
LOVASTATIN-5d-1500mg/...	BIOCHIP	LIVER	5.0d	1500.0m...	HI	CORN OIL...	ORAL GAV...	DAILY
LOVASTATIN-5d-1500mg/...	BIOCHIP	KIDNEY	5.0d	1500.0m...	HI	CORN OIL...	ORAL GAV...	DAILY
LOVASTATIN-3d-450mg/...	BIOCHIP	LIVER	3.0d	450.0mg/...	LO	CORN OIL...	ORAL GAV...	DAILY
LOVASTATIN-3d-450mg/...	BIOCHIP	KIDNEY	3.0d	450.0mg/...	LO	CORN OIL...	ORAL GAV...	DAILY
LOVASTATIN-3d-1500mg/...	BIOCHIP	THIGH ...	3.0d	1500.0m...		CORN OIL...	ORAL GAV...	DAILY
LOVASTATIN-3d-1500mg/...	BIOCHIP	LIVER	3.0d	1500.0m...	HI	CORN OIL...	ORAL GAV...	DAILY
LOVASTATIN-3d-1500mg/...	BIOCHIP	KIDNEY	3.0d	1500.0m...	HI	CORN OIL...	ORAL GAV...	DAILY

EXPERIMENT

Each experiment name in this column is a hyperlink that will populate an **EXPRESSION** Domain Report with information about that particular experiment.

TYPE

The type of microarray with which the study was performed.

TISSUE

The type of tissue used in the selected experiment (i.e. the experiment in a selected row of the table).

TIME

The time period for the experiment, (e.g. 5 days).

DOSE

The dose administered daily.

LEVEL

Indicates whether the dose was high or low.

VEHICLE	The fluid that is used to dissolve the compound to make it both deliverable to the animal and absorbable by the organism's cells.
ROUTE	The method or dosing the animal or cell line, e.g. by intra-venous injection.
FREQUENCY	The timing of the dose. Usually daily.
INDUCED	The percent of genes in this experiment that were up regulated with a p value ≤ 0.02 .
REPRESSED	The percent of genes in this experiment that were down regulated with a p value ≤ 0.02 .
PERTURBED	The percent of genes in this experiment that were either up or down regulated with a p value ≤ 0.02 .

Signature Report

The Signature Domain Report presents information from the data base about experiments and compounds identified by a specified Signature. A signature is a classifier that separates the feature class of experiments from the control population. (see [‘Signature’ on page 228](#))

PPAR ALPHA AGONIST_LIVER_RAE230A_TRANK

EXPERIMENT	COMPOUND	SPS SCORE
FENOFIBRATE-5d-215mg/...	FENOFIBRATE	99.887
FENOFIBRATE-3d-215mg/...	FENOFIBRATE	98.707
BEZAFIBRATE-3d-617mg/...	BEZAFIBRATE	95.729
NAFENOPIN-5d-338mg/k...	NAFENOPIN	95.541
BEZAFIBRATE-7d-617mg/...	BEZAFIBRATE	95.473
FENOFIBRATE-3d-100mg/...	FENOFIBRATE	92.775
NAFENOPIN-3d-338mg/k...	NAFENOPIN	92.066
PIRINIXIC AC-3d-354mg...	PIRINIXIC ACID	89.536
FENOFIBRATE-1d-215mg/...	FENOFIBRATE	89.174
FENOFIBRATE-7d-100mg/...	FENOFIBRATE	87.546

CLASS DESCRIPTION

Universe: (Tissue=LIVER) Not (STRUCTURE_ACTIVITY =***Blank***)

Positive Class Description: (STRUCTURE_ACTIVITY = PPAR alpha agonist

Negative Class Description: All else

Excluded Class Description: (Zero_Class =***Blank***) Or (Zero_Class =V)

Label Description: PPAR alpha agonist IN LIVER

Signature Detail Panels

The Signature Detail area provides aggregated information about the specified Signature. Some items displayed here link to additional sources of information about the Signature.

CLASS DESC. **TRUTH** **DETAILS**

CLASS DESCRIPTION

Signature: Class Desc Panel

This panel presents information about the descriptions of the experiments comprising treatment and the control classes.

CLASS DESC.	TRUTH	DETAILS
CLASS DESCRIPTION		
Universe: (Tissue =LIVER) Not (STRUCTURE_ACTIVITY =***Blank***)		
Positive Class Description: (STRUCTURE_ACTIVITY = PPAR alpha agonist		
Negative Class Description: All else		
Excluded Class Description: (Zero_Class =***Blank***) Or (Zero_Class =Y)		
Label Description: PPAR alpha agonist IN LIVER		

Universe:	Describes the set of experiments from which treatment and control class sets are selected.
Positive Class Description:	Describes the set of experiments that comprise the treatment class.
Negative Class Description:	Describes the set of experiments that comprise the control class.
Label Description:	An explanation of the signature.

Signature: Truth Panel

This panel presents information about the signature performance. For more information on signature technology see **DrugMatrix Calculations** in the online **HELP** files.

CLASS DESC.	TRUTH	DETAILS
TRUTH TABLE		
Average Log Odds: 7.77		
Average True Positive: 100.0 %		
Average True Negative: 98.0 %		
Positive Class Size: 25		
Negative Class Size: 733		
Excluded Class Size: 22.0		
Total Size: 780		

Average Log Odds:	The score metric for the signature performance. This metric is computed and averaged over 20 different test results. (see DrugMatrix Calculations in the online HELP files)
Average True Positive:	The percent of experiments that are correctly predicted to be in the positive class.
Average True Negative:	The percent of experiments that are correctly predicted to be in the negative class.
Positive Class Size:	The number of experiments in the positive class.
Negative Class Size:	The number of experiments in the negative class.
Excluded Class Size:	The number of experiments in the universe that are not in the positive or negative classes.
Total Size:	The total number of experiments in the universe.

Signature: Details Panel

This panel presents information about the methods used to define the signature.

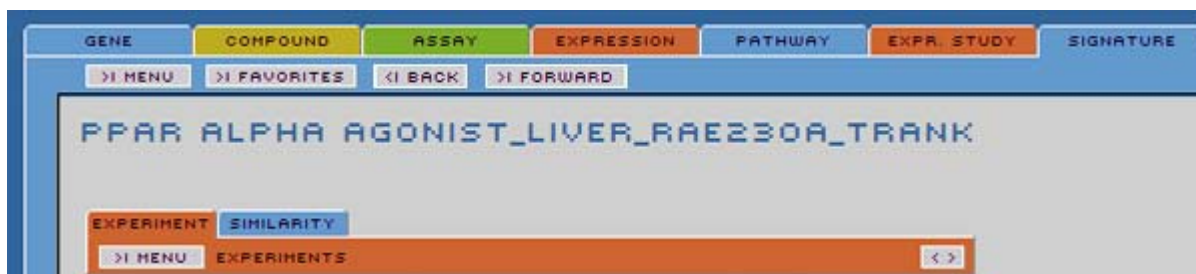


CLASS DESC.	TRUTH	DETAILS
SIGNATURE DETAILS		
Identifier:	SV112122TBEU	
Tissue:	LIVER	
Algorithm:	TRANK	
Platform:	RAE230A	
Type:	Structure Activity	

Identifier:	The unique simple string identifier for the signature.
Tissue:	The tissue used in the universe of experiments from which the signature was derived.
Algorithm:	The algorithm used to derive the signature.
Platform:	The chip technology used in the universe of experiments from which the signature was derived.
Type:	The type of feature used to derive the positive and negative classes.

Signature Chemogenomic Data Report

This panel presents cross referenced Chemogenomic Data, extracted from the database, that relates to the query signature.



Interactive Elements




Sorting Columns

Many columns on panels in the **Signature** Chemogenomic Data Reports are sortable, either alphabetically or numerically. Click on a column name in the currently displayed Chemogenomic Data Report panel to toggle the order (ascending or descending) in which data in that column is sorted. You can also sort lists by items checked (or unchecked).



To modify the width of a column, mouse over the column separator to the right of that column, then when the cursor changes to a cross, hold down the left mouse button and drag to change the column width.

Expandable images

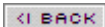
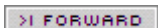
You can expand  or contract  all molecular structure images in a column containing the molecular structure icon  or click on individual icons for an expanded image of the compound in the selected record.

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

Hyperlinks

Hyperlinked items, appearing in the **SIGNATURE** Chemogenomic Data Reports, will either populate associated domain reports or link to published information about the selected compound. For example, if you click on a compound name on the **EXPERIMENT** panel of the **SIGNATURE** report, it will populate a **COMPOUND** domain report for that compound.

Saving Lists

Each **Signature** Domain Report you create will be available until the current session is closed. You can access **Signature** Domain Reports generated in this session using the  and  buttons at the top left of the Domain Report panel.

Use the **MENU > SAVE** option on any panel in the **Signature** report to permanently save a list of checked records on that panel. You can also use the **FAVORITES>ADD FAVORITE** option to add the current query item (named at the top of the domain report panel) to the **FAVORITES** list.

Some panels allow you to save more than one of the lists that appear on the panel. The **MENU** button on any panel will indicate which lists can be saved.

Signature: Experiment Panel

This panel presents information about the experiments that are predicted as positive by the signature.

EXPERIMENT	COMPOUND	SPS SCORE
FENOFIBRATE-5d-215mg/...	FENOFIBRATE	99.887
FENOFIBRATE-3d-215mg/...	FENOFIBRATE	98.707
BEZAFIBRATE-3d-617mg/...	BEZAFIBRATE	95.729
NAFENOPIN-5d-338mg/k...	NAFENOPIN	95.541
BEZAFIBRATE-7d-617mg/...	BEZAFIBRATE	95.473
FENOFIBRATE-3d-100mg/...	FENOFIBRATE	92.775
NAFENOPIN-3d-338mg/k...	NAFENOPIN	92.066
PIRINIXIC AC-3d-364mg...	PIRINIXIC ACID	89.536
FENOFIBRATE-1d-215mg/...	FENOFIBRATE	89.174
FENOFIBRATE-7d-100mg/...	FENOFIBRATE	87.546

EXPERIMENT

Experiment: SAFROLE-3d-488mg/kg-LI-RATM-RU1

Description: Transcriptional profile of a 3.0d timepoint for treatment of Rat, Male, CD-1GS, Sprague Dawley with 488.0mg/kg of SAFROLE on RU1 arrays.

Array Technology: BIOCHIP

This column lists experiments identified by the signature.

Each experiment name in this column is a hyperlink that will populate an **EXPRESSION** Domain Report with information about that particular experiment.



The hover for this item provides the experiment name, a detailed description of the experiment, and the array technology (type of chip) used.


COMPOUND

The name of the compound with which the sample was treated in the selected experiment. (i.e. the experiment in a selected row of the table).

Each compound name in this column is a hyperlink that will populate a **COMPOUND** Domain Report with information about that particular compound.

COMPOUND IMAGE

Click the icons at the top of this column to expand  or contract  all molecular structure images in the column.

Click the molecular structure icon  for a popup window that displays an expanded image for the compound in the selected record. (i.e. the compound in a selected row of the table).

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

SP SCORE

The signature score for the query experiment on the specified platform for this signature type. This column appears if the signature is based **SVM** signature algorithm.

SPS SCORE

The signature score for the query experiment on the specified platform for this signature type. This column appears if the signature is based on the **TRANK** signature algorithm.

Signature: Similarity Panel

This panel presents information about the similarity between the query and the signature in the selected record. The score is based on the correlation of these two experiment score profiles.

SIGNATURE NAME	CORR. COEFF
<input checked="" type="checkbox"/> PPAR_alpha_agonist_LIVER_RAE230A_TRANK	1.0
<input checked="" type="checkbox"/> PPAR_alpha_agonist_fibrate-like_LIVER_RA...	0.983
<input checked="" type="checkbox"/> Peroxisome_proliferator_LIVER_RAE230A_T...	0.977
<input checked="" type="checkbox"/> Hypolipidemic_agent-like_LIVER_RAE230A_...	0.951
<input checked="" type="checkbox"/> PPAR_alpha_agonist_fibrate-like_early_gen...	0.949
<input checked="" type="checkbox"/> Hepatotoxicity_hepatocellular_hypertrophy...	0.87
<input checked="" type="checkbox"/> Hyperalbuminemia_early_gene_expression...	0.837
<input checked="" type="checkbox"/> Carbonic_anhydrase_inhibition_LIVER_RAE2...	0.627
<input checked="" type="checkbox"/> Hypoglycemia_LIVER_RAE230A_TRANK	0.623

CLASS DESCRIPTION

Universe: (Tissue (STRUCTURE_ACT =***Blank***)

Positive Class Des
(STRUCTURE_ACT: agonist

Negative Class De

Excluded Class De
(Zero_Class =***B (Zero_Class =Y)

Label Description:
IN LIVER

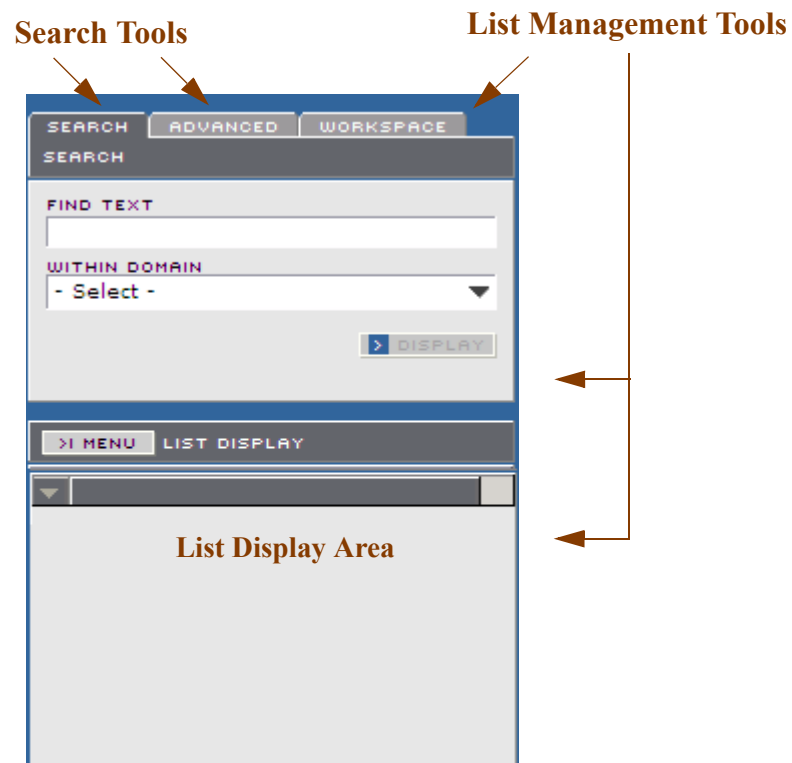
SIGNATURE NAME The name of the signature.

CORR. COEFF Correlation coefficient of adjusted signature scores for each experiment profile.

Search and List Area

The Search and List area of the DrugMatrix Application consists of tools for generating **Simple Searches** and **Advanced Searches** of the database as well as a **Workspace** with tools for the management of lists generated by these searches.

Lists that have been generated by database searches, previously saved lists that have been retrieved, **Data Objects**, and **Favorite** items are all displayed in the **Workspace** area.



Displayed Lists

Lists that you generate using DrugMatrix **SEARCH** tools, or lists that you select from previously **SAVED LISTS** can be displayed in the List Display area below the Search and List panels.

Use this menu to save the displayed list

You can check or uncheck items and save the modified list.

Select items from this displayed list to populate major domains

Item	Checked
<input checked="" type="checkbox"/> CHECK ALL	Yes
<input checked="" type="checkbox"/> UNCHECK ALL	Yes
<input checked="" type="checkbox"/> ALRESTATIN	Yes
<input checked="" type="checkbox"/> ATORVASTATIN	Yes
<input checked="" type="checkbox"/> AURISTATIN PE	Yes
<input checked="" type="checkbox"/> BERVASTATIN	Yes
<input checked="" type="checkbox"/> BRYOSTATIN 1	Yes
<input checked="" type="checkbox"/> BRYOSTATIN-1	Yes

Search and List Tabs



Simple Search

Allows you to search any of the seven DrugMatrix data domains by name. Lists generated by a simple search can be displayed and saved. You can select items from displayed lists to populate associated domain reports. For more information, see [‘Simple Search Panel’ on page 116](#).

Advanced Search

Allows you to generate lists of Compounds, Assays, Genes, Expression Experiments, Gene Pathways, Expression Studies and Signatures by filtering the database on one or more parametric and logical criteria. These lists can be displayed in the list display area, and saved. You can select items from displayed lists to populate associated domain reports. For more information, see [‘Advanced Search Panel’ on page 118](#).

Workspace

You can save lists of items that have been generated by the DrugMatrix query tools, or that have been extracted from the database for primary Domain Reports. These lists can be managed in the **WORKSPACE** area. Lists of **FAVORITE** items (with the  icon attached), and **DATA OBJECTS** (with the  icon attached) also appear in the **WORKSPACE** area. See [‘Data Object’ on page 225](#).

For more information, see [‘Workspace Panels’ on page 123](#).

The DrugMatrix application provides several tools for working with lists you generate while conducting your research. The **TOOLBOX** button, located on **WORKSPACE** panel, launches a toolbox containing these tools. For more information about the DrugMatrix **TOOLBOX**, see [‘Toolbox Functionality’ on page 136](#).

Simple Search Panel

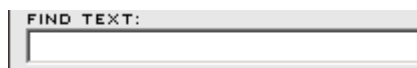
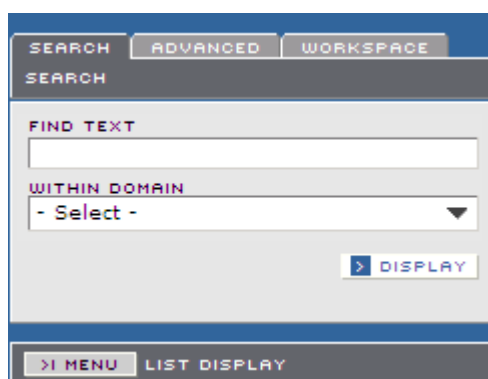
The **SEARCH** panel allows you to conduct the most straight forward search of the DrugMatrix database. You can use this panel to search by all or part of item names in any of the top level data domains. The DrugMatrix application will retrieve and display all record from the database that contain the name you have entered.

For example, a search for the text string “fibra”, within the **COMPOUND** domain, will retrieve and display a list of all compounds in the database that include “fibra” in the name (e.g. **CIPROFIBRATE**, **CLOFIBRATE**, and **FENOFIBRATE** as well as others).

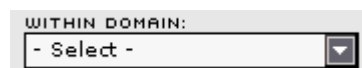
When you search the **COMPOUND** domain using brand names or other synonyms, DrugMatrix will retrieve the actual compound name (e.g. a search for “Vioxx” will retrieve the compound “**ROFECOXIB**” for which Vioxx is a brand name).

Once you have retrieved records from the database, you can select an item from the displayed list to populate the appropriate Domain Report for that item. For example, **CLOFIBRATE**, selected from a retrieved list, will populate a **COMPOUND** report with all relevant information about **CLOFIBRATE** from database.

See ‘**Getting Started**’ on page 7 for step by step instructions on how to conduct a simple search.

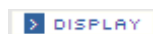


Use this field to enter a string of characters for a **Simple Search**.

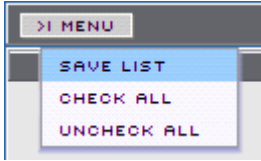


Note: the wildcard character “%” used by itself, will retrieve all records from the specified domain. If it is used in combination with other characters, it will have no effect on the search.

Use this - **Select** - menu to choose the domain within which to conduct a **Simple Search**.



Display a retrieved list in the list display area below the Search and List panels.

MENU

Save the currently displayed list and specify records to be saved with the list.

SAVE

Save all checked records in the list.

CHECK ALL

Check all records in the list. All records will be saved.

UNCHECK ALL

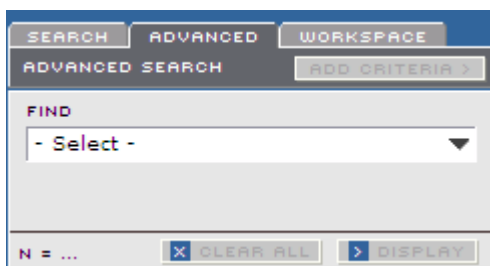
Remove all checks. No records will be saved.

Advanced Search Panel

The **ADVANCED** search panel allows you to define very specific queries of the DrugMatrix database using one or more predefined criteria. You can refine your search by applying increasingly specific search criteria for the kind of information you wish to retrieve from the database.

Once you have retrieved records from the database, you can display a list of those records, and then select an item from the displayed list to populate the appropriate Domain Report for that item. You can save a list of records retrieved from the database (see [‘Toolbox Functionality’ on page 136](#)). Saved lists can be manipulated and/or modified using the DrugMatrix Toolbox (see [‘Toolbox Functionality’ on page 136](#)).

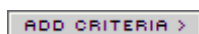
The **ADVANCED** search tab displays the top level advanced search panel. This panel provides a drop down menu from which you can select an initial search criterion. As you add criteria, additional panels will be displayed, offering more criteria for further refinement of your search.



The criteria available at each level, parallels the levels of detail provided in the Domain Report associated with the top level criteria you have chosen.

Advanced Search Panel Buttons

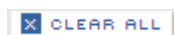
Some buttons listed below will appear as you add criteria or as search results are displayed.



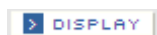
Add additional criteria to further refine your search.

N = ...

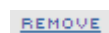
Displays the number of records found. This will change as additional criteria are added.



Clear all search results on the panel. This button will highlight when search results appear in the advanced search panel.



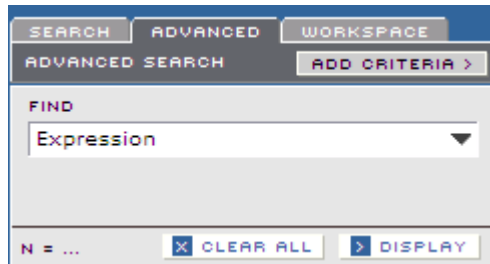
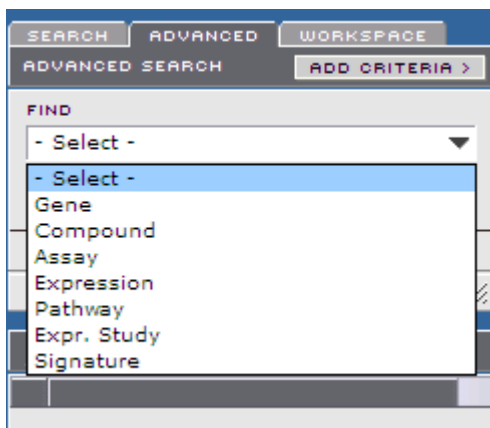
Display the results of the most recently calculated search in the display area below the advanced search panel. This button will highlight when search results appear in the advanced search panel.



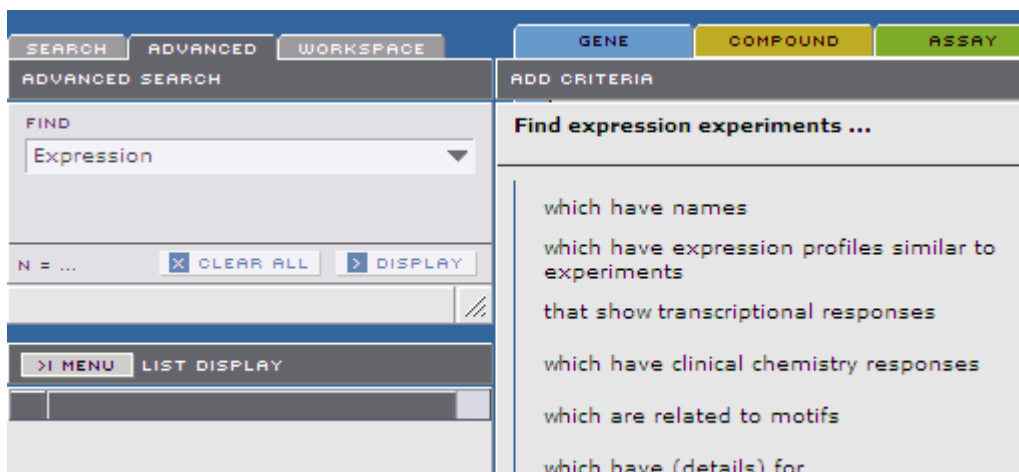
Remove a specific set of search criteria from the search.

Advanced Search Sub Panels

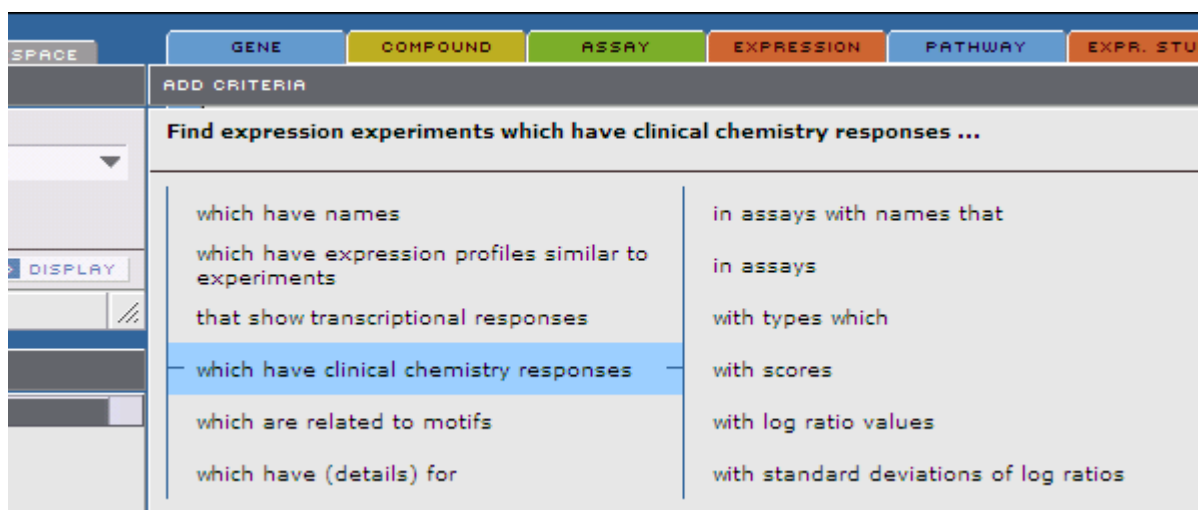
The initial **ADVANCED SEARCH** criteria reflect the primary data domains of the DrugMatrix application—Compounds, Assays, Genes, Expression Experiments, Gene Pathways, and Expression Studies.



Click the **ADD CRITERIA** button to begin adding criteria with which to refine your search. This will present the first level of the **ADD CRITERIA** panel.



When you select a criterion from that panel, it will expand to present a subset of additional criteria with which to refine your search.



This process continues until the panel is fully expanded (three levels of refinement). When all required criteria for a search have been entered, the **RUN QUERY** button becomes active (it displays blue rather than gray).

GENE COMPOUND ASSAY EXPRESSION PATHWAY EXPR. STUDY MOTIF SIGNATURE

ADD CRITERIA CLOSE

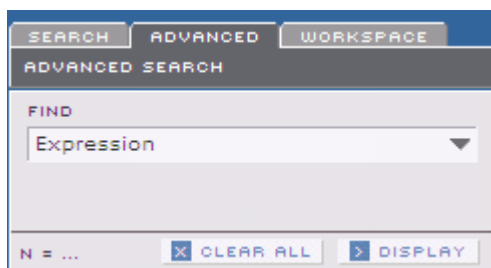
Find expression experiments which have clinical chemistry responses in assays with names that contain ...

which have names	in assays with names that	exactly match
which have expression profiles similar to experiments	in assays	begin with
that show transcriptional responses	with types which	end with
which have clinical chemistry responses	with scores	contain
which are related to motifs	with log ratio values	
which have (details) for	with standard deviations of log ratios	

Leukocyte count

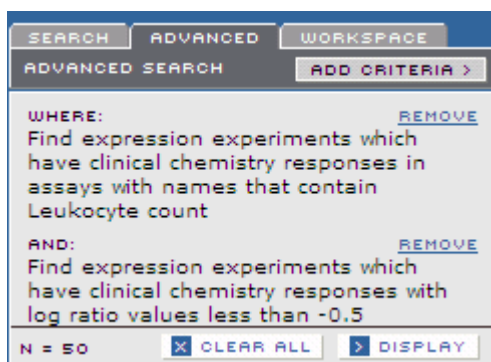
RUN QUERY

When you click the **RUN QUERY** button, the search will be processed. A description of the search, and the number of records retrieved from the database is displayed on the **Advanced Search** panel.



Once an **Advanced Search** has been processed, you can narrow the results by selecting an additional set of criteria. A description of the search, and the number of records retrieved from the database as a result of successive searches, is displayed on the panel.

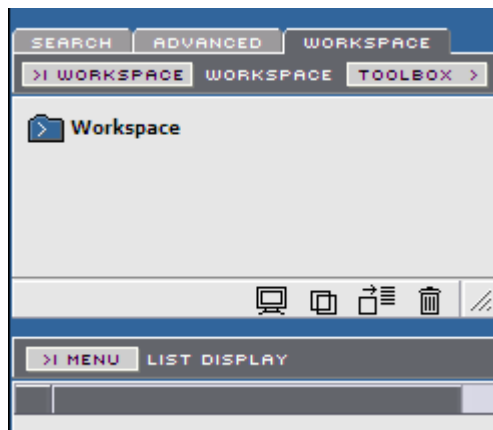
You can use the **REMOVE** button to remove a specific set of criteria and re-process your search. You can use the **CLEAR ALL** button to remove all search criterion from the panel.



The results of the search will be displayed in the **List Display** area when you click the **DISPLAY** button. If the number of records retrieved is greater than 2000, results will not be displayed. You will need to further refine your search.








Workspace Panels






You can save lists of records that have been generated by the DrugMatrix query tools, or that have been extracted from the database from primary Domain Reports. These lists can be managed in the **WORKSPACE** area. The DrugMatrix **TOOLBOX**, accessed from the **WORKSPACE** area enables you to perform a number of sophisticated operations with lists to further refine your research. See [‘Toolbox Functionality’ on page 136](#) for information on working with saved lists.



Workspace Icons








There are several icons on the **WORKSPACE** panel that enable you to manage lists. Drag a list onto an icon, or click on the icon (with the exception of the **DISPLAY LIST** icon) to initiate the indicated operation.

- | | |
|---|--|
|  DISPLAY LIST | <p>Display a SAVED LIST in the LIST DISPLAY panel below the WORKSPACE, or display a DATA OBJECT (with the  icon attached) in a domain report. See ‘Data Object’ on page 225.</p> <p>This feature is unavailable for FAVORITES items.</p> |
|  DUPLICATE LIST | <p>This feature is available for SAVED LISTS only, not for FAVORITES items or DATA OBJECTS (with the  icon attached). See ‘Data Object’ on page 225.</p> |
|  EDIT ITEM | <p>Launches a dialog window that allows you to rename and/or give a new description of a list you select from the WORKSPACE.</p> <p>This feature is available for SAVED LISTS only, not for FAVORITES lists or DATA OBJECTS (with the  icon attached). See ‘Data Object’ on page 225.</p> |
|  DELETE ITEM | <p>Launches a dialog window that allows you to delete a list you select from the WORKSPACE.</p> <p>This feature is available for all types of lists.</p> |

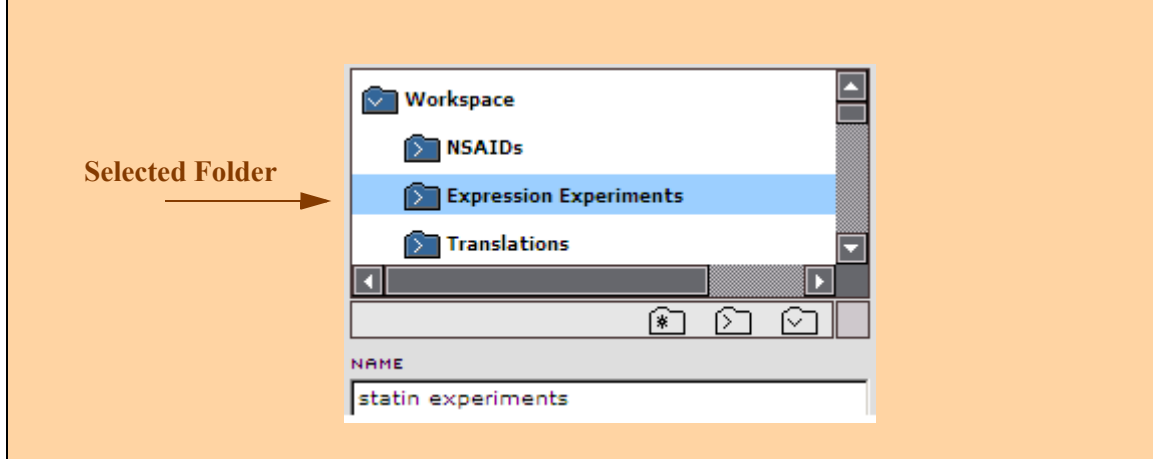
-  **SIZE WORKSPACE** Select this icon, hold down the mouse button and drag to resize the **WORKSPACE** panel.
-  In the **WORKSPACE** area **DATA OBJECTS** will appear with this icon attached to the list type icon.
For example:  indicates a **DATA OBJECT** for an Expression Experiment report. See '[Data Object](#)' on [page 225](#).
-  In the **WORKSPACE** area, **FAVORITES** will appear with this icon attached to the list type icon.
For example:  indicates a **FAVORITE** Gene Report.

Domain Icons

Each of the DrugMatrix data domains has an associated icon which shows up in the **WORKSPACE** area.

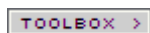
ICON	DOMAIN
	GENE DOMAIN
	COMPOUND DOMAIN
	ASSAY DOMAIN
	EXPRESSION EXPERIMENT DOMAIN
	PATHWAY DOMAIN
	EXPRESSION STUDY DOMAIN
	GENE SIGNATURE DOMAIN
	For information about signatures see ' Signature ' on page 228

NOTE: Within any of the DrugMatrix dialogs that allow you to save a list to a specific folder, that folder must be selected so that it displays a blue background. You can either directly select the folder or left mouse click on a list in the folder (the folder background will turn blue).

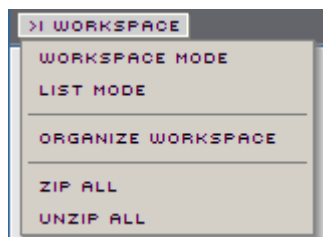


Workspace Buttons and Menus

Buttons on the **WORKSPACE** panel access tools for managing lists as well as a suite of tools in the DrugMatrix **TOOLBOX**.



Open the DrugMatrix **TOOLBOX** to perform a number of list operations. For more information on the DrugMatrix **TOOLBOX**, see [‘The DrugMatrix Toolbox’ on page 135](#)



Selections from the **WORKSPACE** menu allow you to present different groupings of lists and to organize lists in the **WORKSPACE**.

WORKSPACE MODE

Displays saved lists as they were saved (in top level **WORKSPACE** folder or user defined folders).

LIST MODE

Displays lists in two top level folders, a **Saved Lists** folder a **Favorites** folder. Each of these contains seven sub-folders, one for each of the DrugMatrix domains.

ORGANIZE WORKSPACE

This menu selection launches an **ORGANIZE WORKSPACE** dialog window that allows you to create new **WORKSPACE** folders, delete folders, move lists between folders, and edit or remove lists.

ZIP ALL

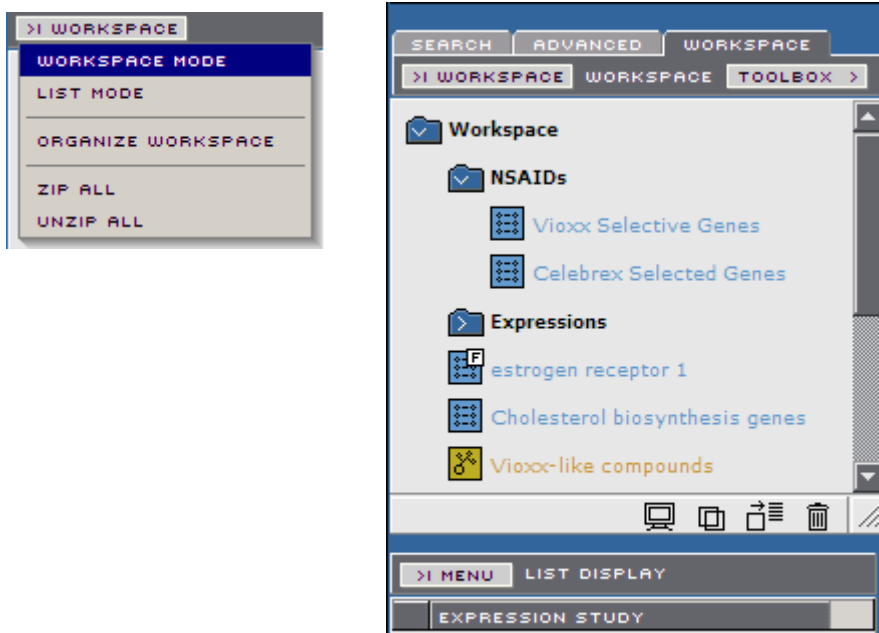
Collapses all folders to their top level. This feature works in both **WORKSPACE** and **LIST** modes.

UNZIP ALL


Expands all folders as a directory tree. This feature works in both **WORKSPACE** and **LIST** modes.

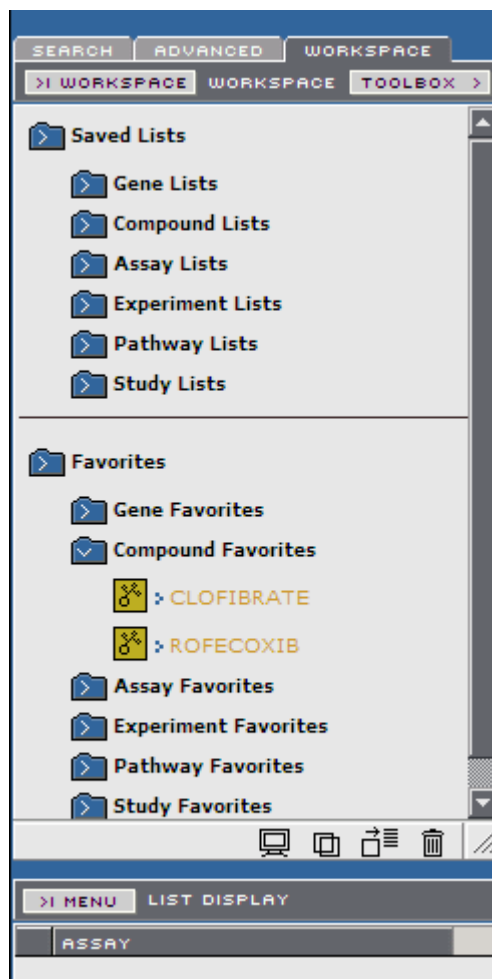
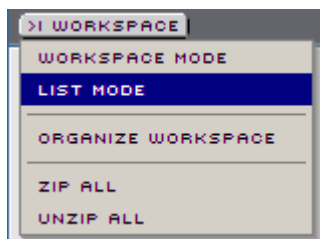
Workspace - WORKSPACE MODE

This mode presents lists as you have organized them using the **ORGANIZE WORKSPACE** dialog accessed from the same menu.



Workspace - LIST MODE

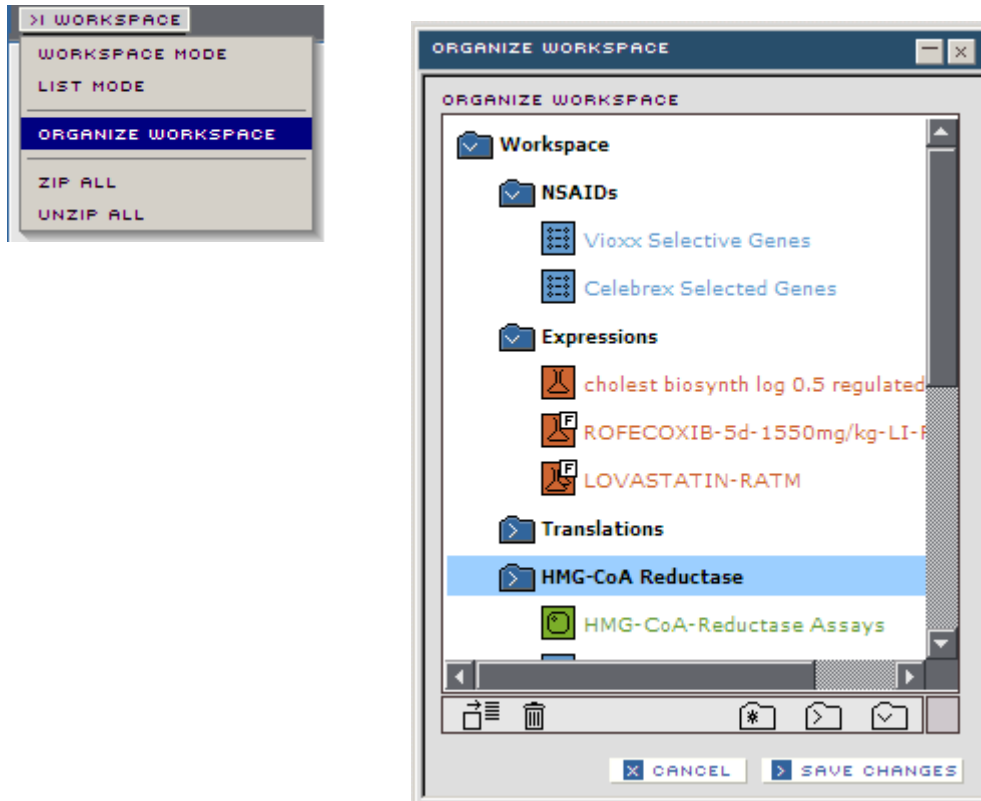
In this mode, **Saved Lists** and **Favorites** are categorized and displayed according to their domain. **Favorites** are displayed without the  icon attached.



NOTE: Signatures and Data Objects will not appear in this mode in the current version of DrugMatrix.

Workspace - ORGANIZE WORKSPACE

The **ORGANIZE WORKSPACE** dialog window allows you to organize lists according to your own requirements. It represents how lists will be organized and displayed in **WORKSPACE MODE**.



EDIT ITEM

Launches a dialog window that allows you to rename and/or give a new description of a list you select from the **WORKSPACE**.



DELETE ITEM

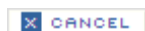
Launches a dialog window that allows you to delete a list or folder you select from the **WORKSPACE**.

Note: If you delete a folder, all lists within that folder will also be deleted.

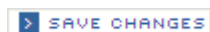


NEW FOLDER

Launches a dialog window the allows you to create a new folder in the **WORKSPACE**.




Close the dialog window without saving changes.



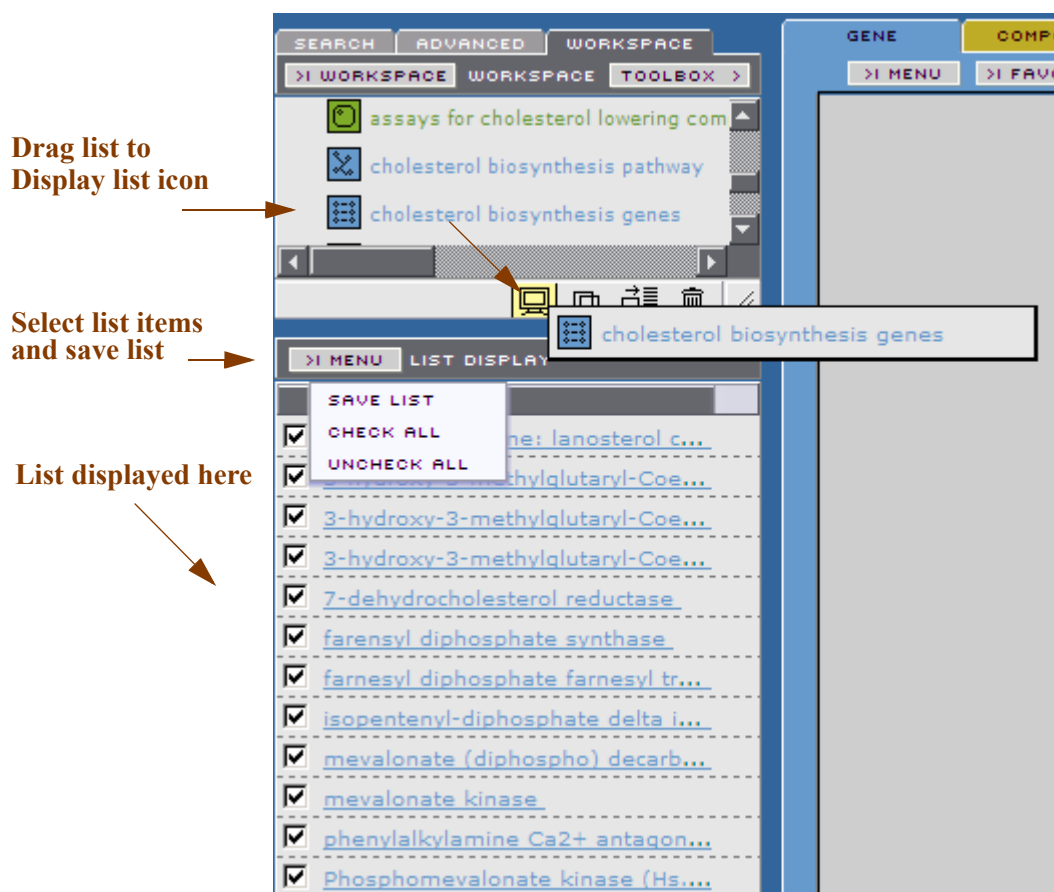
Saves changes made to **WORSPACE** and closes the dialog window.

Display Lists

 The **DISPLAY LIST** feature allows you to display the contents of a list. You can create a new list from this list by using the check boxes on the left to specify new list items, and then save the new list with a new name (see '**MENU**' on page 117).

This tool does not present a dialog. You must drag and drop the list you wish to display from **WORKSPACE** area onto this icon to display the list.

Individual items from the displayed list will populate appropriate Domain reports.

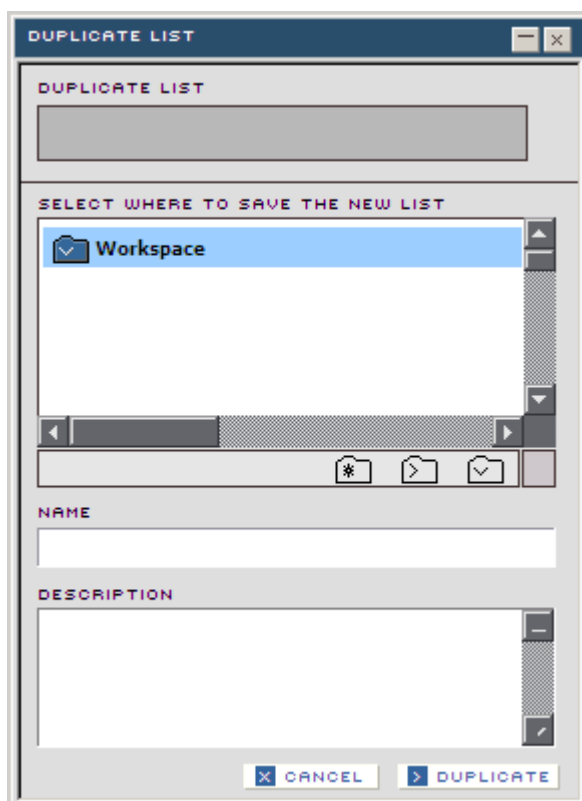
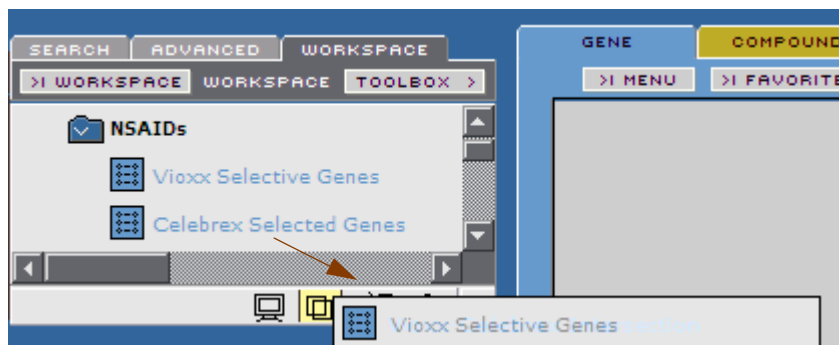


If you drag a **Data Object** (with the  icon attached), the information for that Data Object will populate an appropriate domain report. See '**Data Object**' on page 225.

This feature is unavailable for **Favorites** items.

Duplicate Lists


-  The **DUPLICATE LIST** feature allows you to create a duplicate copy of a list. This feature is unavailable for **Favorites** items or **Data Objects**.



DUPLICATE LIST

The name of the list to be duplicated (drag from **WORKSPACE**).

FOLDER

The name of the folder in which the new list will be placed. You can navigate to the desired folder, or create a new folder with the  **New Folder** icon.

NAME

The name of the new list.

DESCRIPTION

Use this text area to describe the new list. This description will appear in a hover when you mouse over the list name in the **WORKSPACE**.




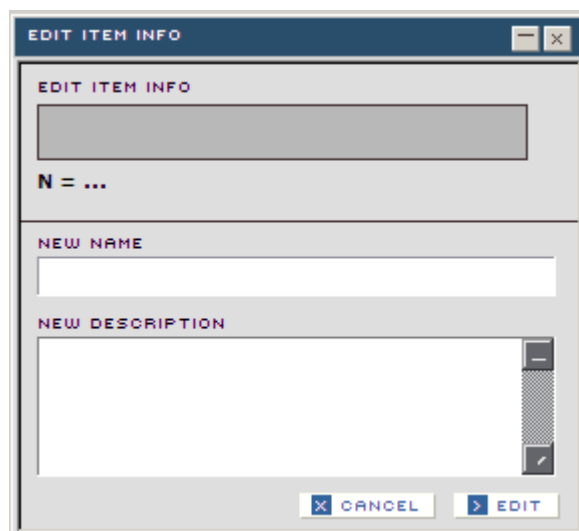
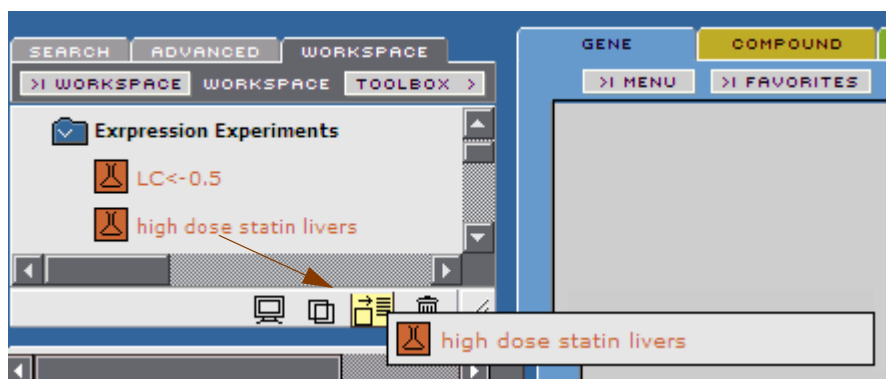
Close the dialog window without saving changes.



Duplicate the list and save it in the specified **WORKSPACE** folder.

Edit Item

-  The **EDIT ITEM** feature allows you to change the name and description of an existing list. This feature is available for **Lists** and **Data Objects**, but not for **Favorites** items.



EDIT ITEM

The list to be edited (drag from **WORKSPACE**).

N = ...

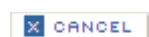
The number of records in the list.

NEW NAME:

Give the selected list a new name.

NEW DESCRIPTION:

Change the description of the selected list.




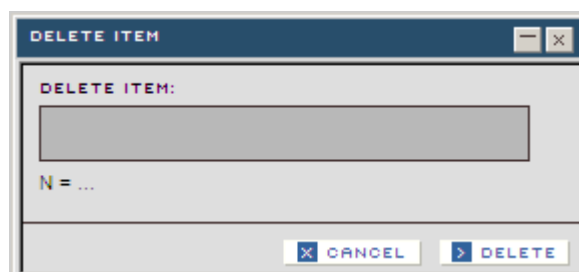
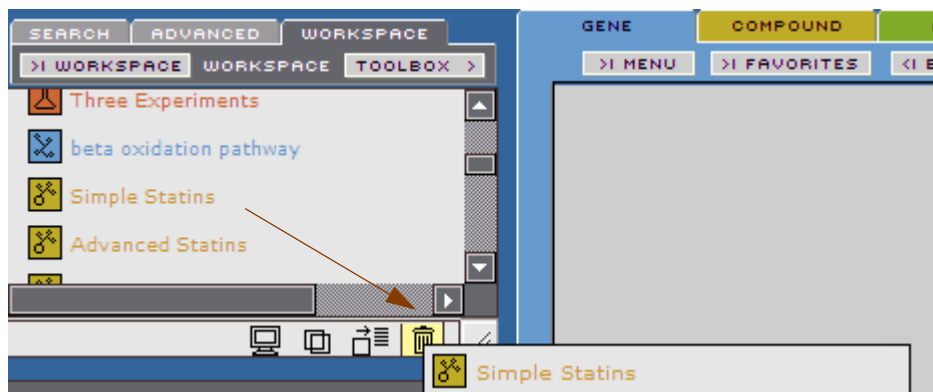
Close the dialog window without saving changes.



Save the list with modifications.

Delete Item

-  The **DELETE ITEM** feature allows you to remove a list from the **WORKSPACE**. This feature is available for **SAVED LISTS**, **FAVORITES** and **Data Objects** lists.

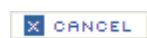


DELETE ITEM

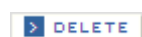
The list to be deleted (drag from **WORKSPACE**).

N = ...

The number of records in the list.



Close the dialog window without saving changes.

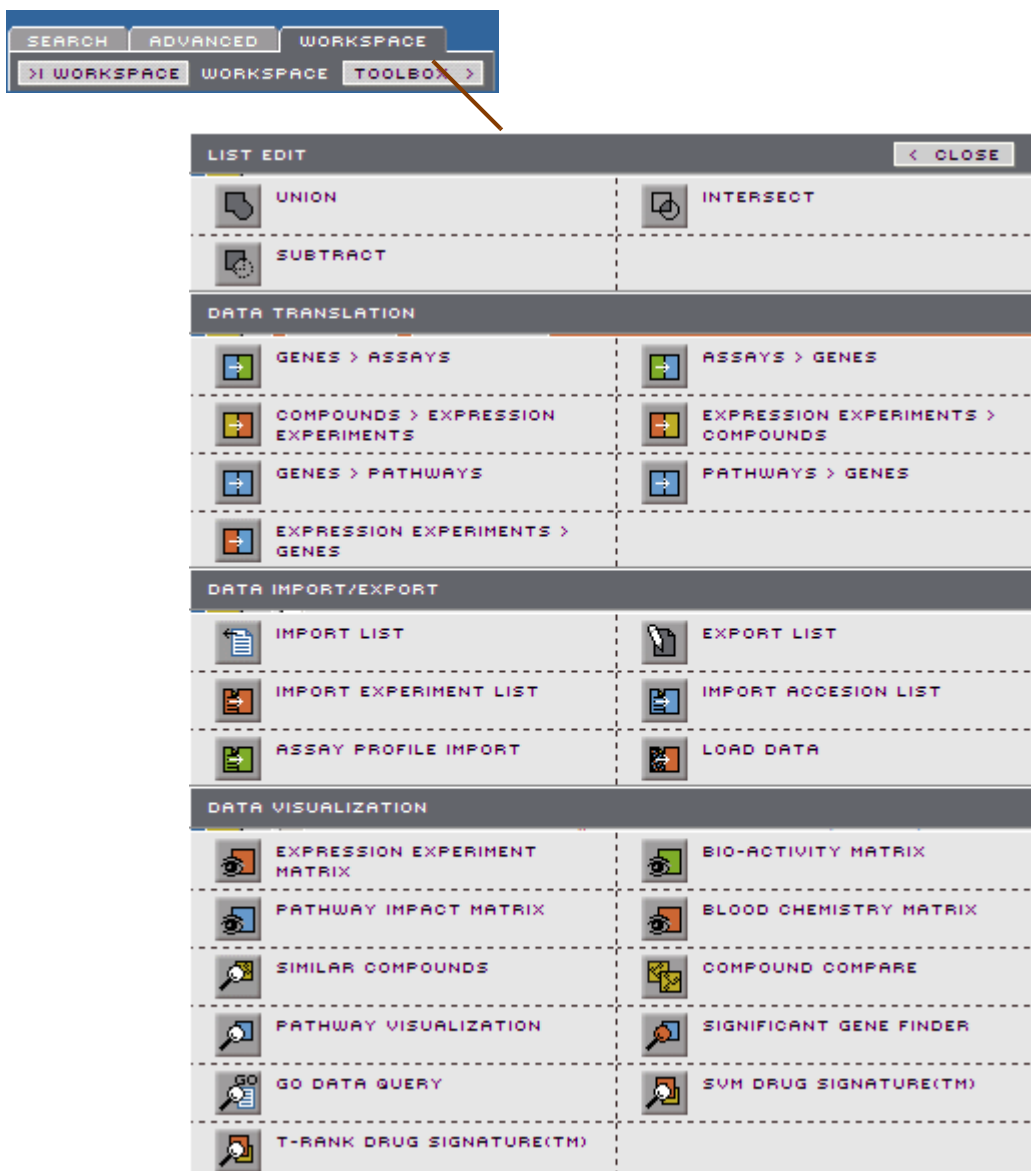


Delete the selected list.

The DrugMatrix Toolbox

The DrugMatrix application provides a suite of software tools to define very specific database queries and help you work with generated lists that are relevant to your research.

The **TOOLBOX** button, located on the **WORKSPACE** panel, launches a toolbox containing these tools. For more information see the next section.



TOOLBOX >



This button, located on the **WORKSPACE** panel, launches the DrugMatrix **TOOLBOX**.

< CLOSE

This button, located on the upper right corner of the DrugMatrix **TOOLBOX**, closes the **TOOLBOX**.

Toolbox Functionality

Each tool in the DrugMatrix **TOOLBOX** has a dialog box that allows you to enter information and perform the specified task.

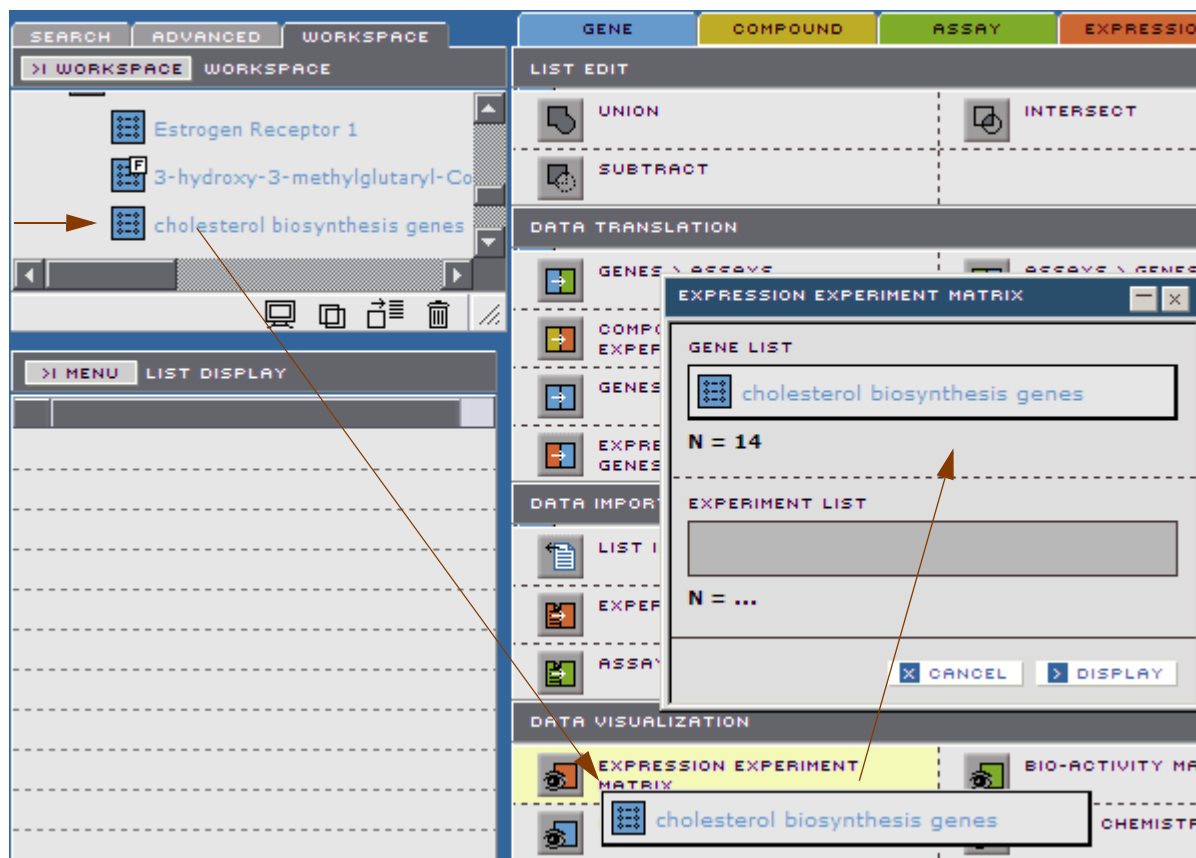
NOTE: FAVORITES lists (showing the  icon) will only be accepted by specific fields in DrugMatrix tool dialogs. The fields that accept **FAVORITES** will include the word 'FAVORITES' in the name of the field. Some, but not all DrugMatrix tool dialogs will also accept **DATA OBJECTS** (with the  icon attached). See 'Data Object' on page 225.

The **TOOLBOX** consists of 4 different sections relating to different types of functionality. These sections are **LIST EDIT**, **DATA TRANSLATION**, **DATA IMPORT/EXPORT**, and **DATA VISUALIZATION**. You can launch a **TOOLBOX** dialog window in one of two ways:

- In the DrugMatrix **TOOLBOX**, click the icon for the tool you wish to use.

Or Drag and Drop a List

- In the **WORKSPACE** area, move the cursor over a list name.
 - Hold down the left mouse button and drag the list name over the icon for the tool you wish to use.
- Note:** The cursor must be placed over the list name, not the icon, in order to drag and drop. You are able to drag the list when the cursor changes to a diamond shape.
- When the textbox background becomes yellow, release the mouse button (If the box does not highlight in yellow, the wrong list or item type is being used).
The tool's dialog box will pop up with the selected list or item in the appropriate field.



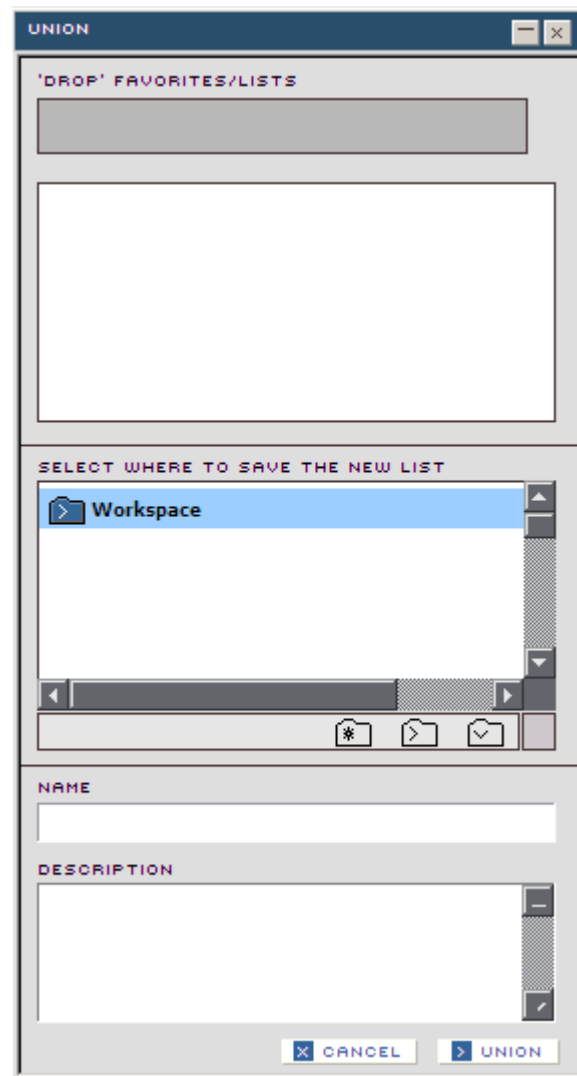
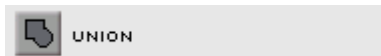
List Editing Tools

The **LIST EDIT** tools allow you to perform such operations as subtract a list or group of lists from a list, combine lists, or generate a list of common items between lists.

List Editing: Union

The **UNION** tool allows you to combine lists and create a new list of unique items. All lists used with this tool must be of the same domain type (e.g. all **GENE** lists).

LIST 1	=	A, B, C
LIST 2	=	C, D, E
LIST 3	=	B, E, F
UNION	=	A, B, C, D, E, F



'DROP' FAVORITES/LISTS

Drag lists or **FAVORITES** from **WORKSPACE** into this field. All lists must be of the same domain type (e.g. all **GENE** lists).




All items from the lists in the area below the **'DROP' FAVORITES/LISTS** field will be combined and any items that are not unique will be removed.

The number of items in each list appears, in brackets, next to the list name.

Click on [remove](#) to remove the list from this area and exclude it from the **UNION** operation.

**SELECT WHERE TO
SAVE
THE NEW LIST**

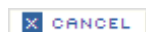
Specify the folder in which to save the new list. You can navigate to the desired folder, or create a new folder with the  **New Folder** icon.

NAME

A text field in which you can enter the name for the new list you will save.

DESCRIPTION

A text entry field in which you can enter a description of the new list.



Cancel without performing the **UNION** operation.



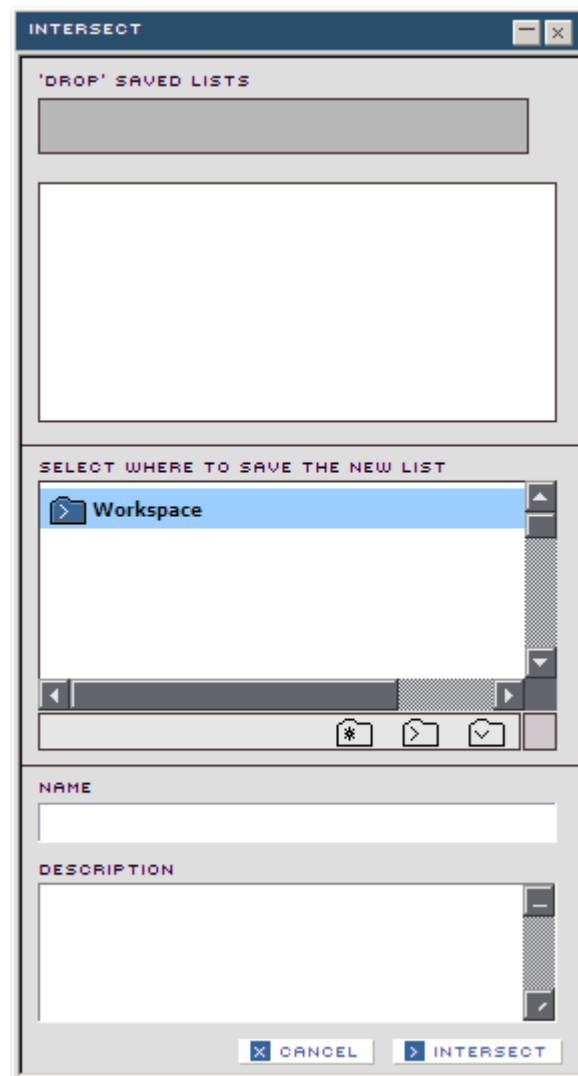
Create and display a new list, with a new name and description, showing the results of the specified operation.

NOTE: You can convert a **FAVORITES** list to a saved list by dropping it into the **UNION** tool **'DROP' FAVORITES/LISTS** field and saving it with a new name. This is useful as a work around for the **PATHWAY VISUALIZATION** tool that requires a list of 1 record for the **PATHWAYS LIST** field in the present version of the DrugMatrix software.

List Editing: Intersect

The **INTERSECT** tool allows you to compare several lists and create a new list with the items that are common to those lists. All lists must be of the same domain type (e.g. all **GENE** lists).

LIST 1	=	A, B, C
LIST 2	=	C, D, E
LIST 3	=	C, D, F
INTERSECTION	=	C



'DROP' FAVORITES/LISTS Drag lists from **WORKSPACE** into this field. All list must be of the same domain type (e.g. all **GENE** lists).




The **INTERSECT** operation will be performed with all items from the lists in the area below the '**DROP**' **FAVORITES/LISTS** field.

The number of items in each list appears, in brackets, next to the list name.

Click on [remove](#) to remove the list from this area and exclude it from the **INTERSECT** operation.

SELECT WHERE TO SAVE THE NEW LIST

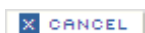
Specify the folder in which to save the new list. You can navigate to the desired folder, or create a new folder with the  **New Folder** icon.

NAME

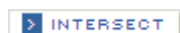
A text field in which you can enter the name for the new list you will save.

DESCRIPTION

A text entry field in which you can enter a description of the new list.



Cancel without performing the **INTERSECT** operation.

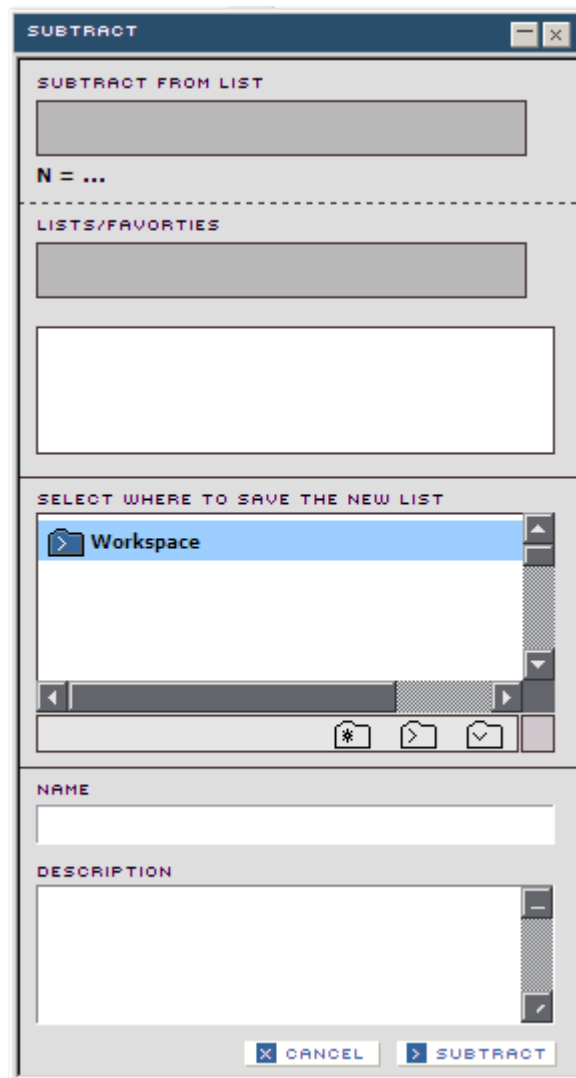


Create and display a new list, with a new name and description, showing the results of the **INTERSECT** operation.

List Editing: Subtract

The **SUBTRACT** tool allows you to compare several lists and create a new list consisting of items from the first list minus items from the other selected lists. All lists must be of the same domain type (e.g. all **GENE** lists).

LIST 1	=	A, B, C, F, G
LIST 2	=	C, D, E
LIST 3	=	E, F
SUBTRACT	=	A, B, G



SUBTRACT FROM LIST

Drag lists from **WORKSPACE** into this field. All lists must be of the same domain type (e.g. all **GENE** lists). Only lists can be used in this field.

N = ...

Indicates the number of records in the list placed in the **SUBTRACT FROM LIST** field.

LIST/FAVORITES

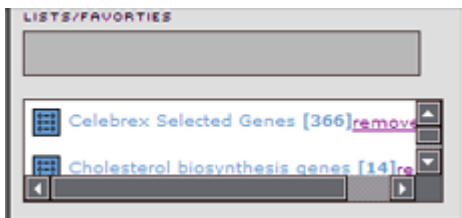
Lists dropped in this field will be placed in the area below the **LIST/FAVORITES** field.


Both lists and **FAVORITES** can be used in this field.

The **SUBTRACT** operation will be performed with all items from the lists in the area below the **LIST/FAVORITES** field. Common items (items found in any of the lists in this field) will be removed from the list in the top field of this dialog box.

The number of items in each list appears, in brackets, next to the list name.

Click on **remove** to remove the list from this area and exclude it from the **SUBTRACT** operation.

**SELECT WHERE TO SAVE THE NEW LIST**

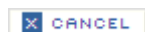
Specify the folder in which to save the new list. You can navigate to the desired folder, or create a new folder with the  **New Folder** icon.

NAME

A text field in which you can enter the name for the new list you will save.

DESCRIPTION

A text entry field in which you can enter a description of the new list.



Cancel without performing the **SUBTRACT** operation.



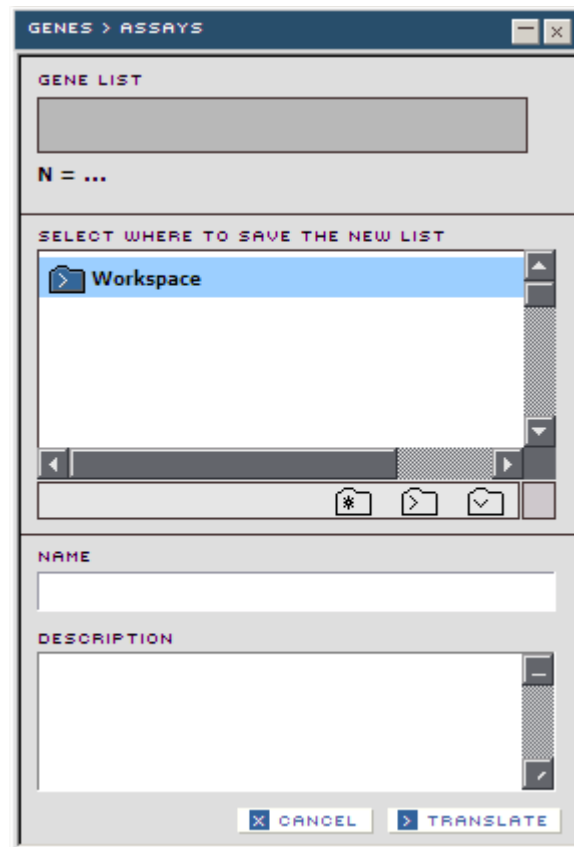
Create and display a new list with a new name and description, showing the results of the **SUBTRACT** operation.

Data Translation Tools

The **DATA TRANSLATION TOOLS** are used to convert one type of list of items to another type of list (e.g. a list of genes to a list of associated assays).

Data Translation: Genes > Assays

This tool translates a specified list of genes to a list of assays that correspond to those genes. For an assay to correspond to a gene, it will be an assay on the gene product or protein. If no genes in the specified list correspond to assays, there will be no list of assays generated.




GENE LIST

The name of the **GENE** list that will be translated to an associated **ASSAY** list.

N = ...

The number of records in the named list.

**SELECT WHERE TO
SAVE THE NEW LIST**

Specify the folder in which to save the new list. You can navigate to the desired folder, or create a new folder with the  **New Folder** icon.

NAME

A text field in which you can enter the name for the new list you will save.

DESCRIPTION

A text entry field in which you can enter a description of the new list.



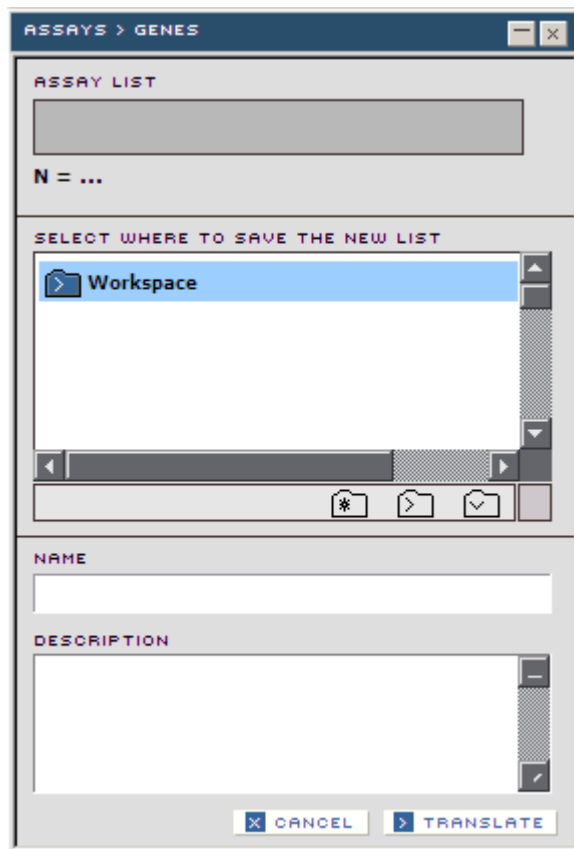
Cancel without performing the list translation.



Translate and save the list.

Data Translation: Assays > Genes

This tool translates a specified list of assays to a list of genes that correspond to those assays.




ASSAY LIST

The name of the **ASSAY** list that will be translated to an associated **GENE** list.

N = ...

The number of records in the named list.

SELECT WHERE TO SAVE THE NEW LIST

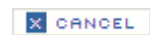
Specify the folder in which to save the new list. You can navigate to the desired folder, or create a new folder with the  **New Folder** icon.

NAME

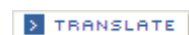
A text field in which you can enter the name for the new list you will save.

DESCRIPTION

A text entry field in which you can enter a description of the new list.



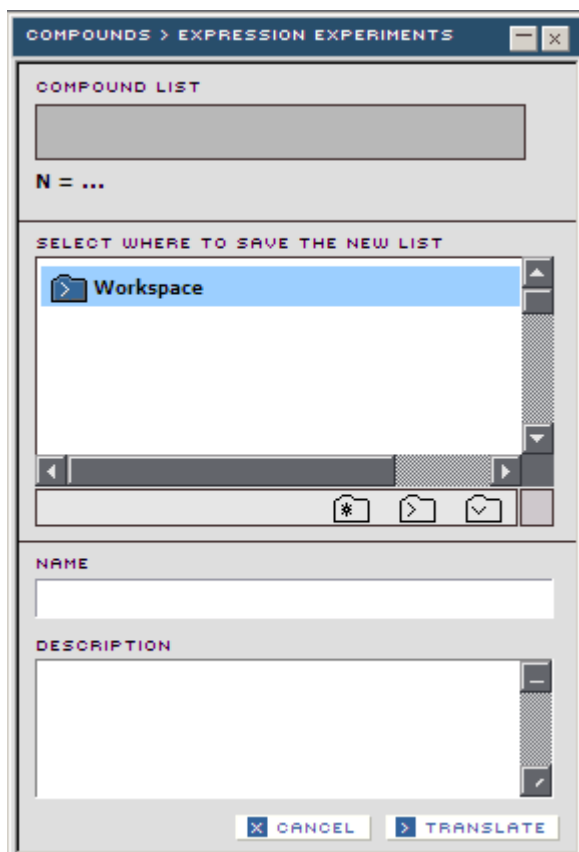
Cancel without performing the list translation.



Translate and save the list.

Data Translation: Compounds > Expression Experiments

This generates list of expression experiments in which the compounds in the specified compound list have been used.


**COMPOUND LIST**

The name of the **COMPOUND** list that will be translated to an associated **EXPERIMENT** list.

N = ...

The number of records in the named list.

SELECT WHERE TO SAVE THE NEW LIST

Specify the folder in which to save the new list. You can navigate to the desired folder, or create a new folder with the  **New Folder** icon.

NAME

A text field in which you can enter the name for the new list you will save.

DESCRIPTION

A text entry field in which you can enter a description of the new list.



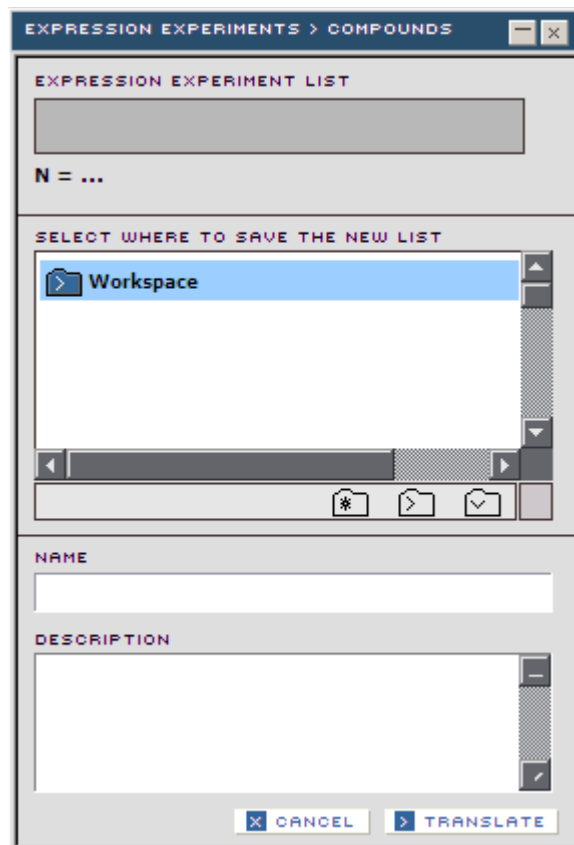
Cancel without performing the list translation.



Translate and save the list.

Data Translation: Expression Experiments > Compounds

This tool translates a specified list of expression experiments to a list of associated compounds. This allows you to generate a list of compounds used in the experiments in the specified expression experiment list.




EXPRESSION EXPERIMENT LIST

The name of the **EXPRESSION EXPERIMENT** list that will be translated to an associated **COMPOUND** list.

N = ...

The number of records in the named list.

SELECT WHERE TO SAVE THE NEW LIST

Specify the folder in which to save the new list. You can navigate to the desired folder, or create a new folder with the  **New Folder** icon.

NAME

A text field in which you can enter the name for the new list you will save.

DESCRIPTION

A text entry field in which you can enter a description of the new list.



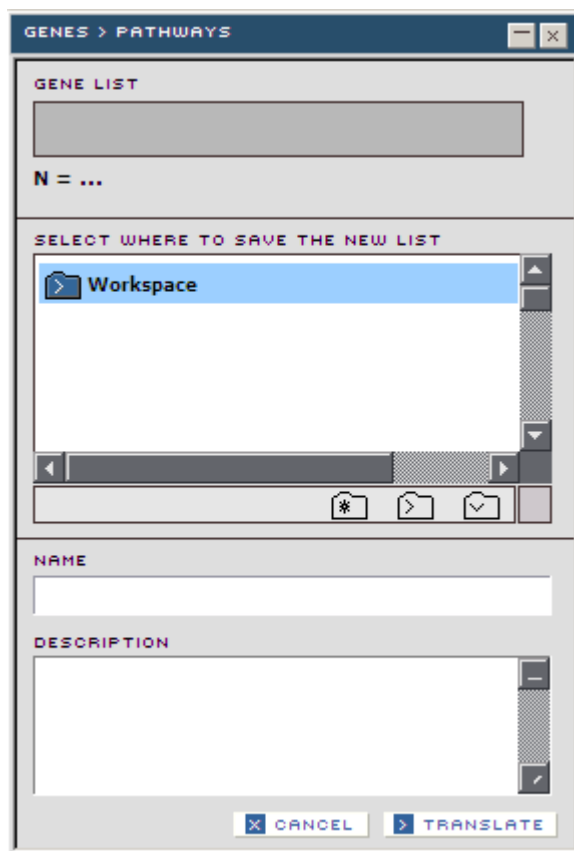
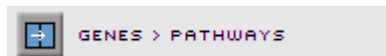
Cancel without performing the list translation.



Translate and save the list.

Data Translation: Genes > Pathways

The translation tool works with the curated pathways in the database. If any gene in the list is curated as being part of a pathway, that pathway will be included in the translated list.




GENE LIST

The name of the **GENE** list that will be translated to an associated **PATHWAYS** list.

N = ...

The number of records in the named list.

SELECT WHERE TO SAVE THE NEW LIST

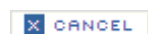
Specify the folder in which to save the new list. You can navigate to the desired folder, or create a new folder with the  **New Folder** icon.

NAME

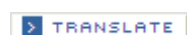
A text field in which you can enter the name for the new list you will save.

DESCRIPTION

A text entry field in which you can enter a description of the new list.



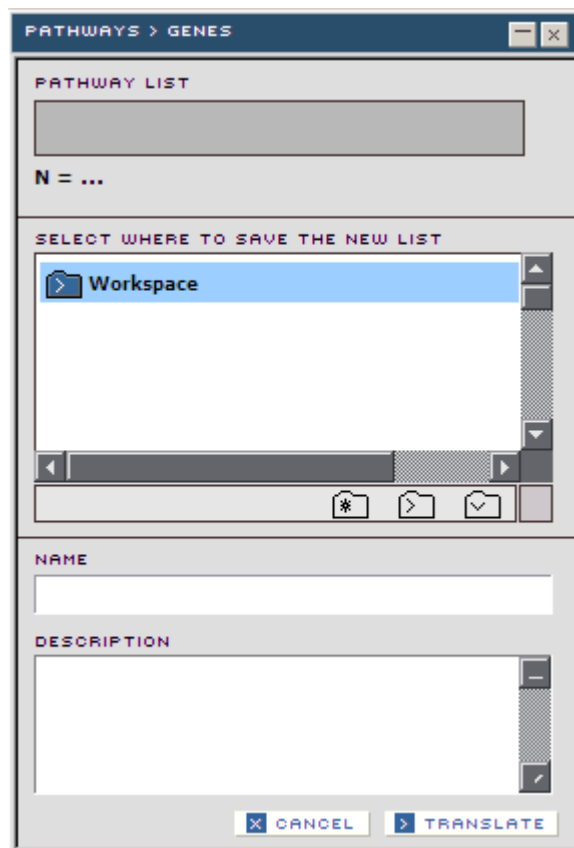
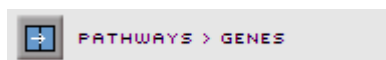
Cancel without performing the list translation.



Translate and save the list.

Data Translation: Pathways > Genes

This tool translates a specified list of pathways to a list of associated genes. Any gene that is curated as being part of a pathway in the specified list of pathways, will be included in the generated list of genes.




PATHWAY LIST

The name of the **PATHWAY** list that will be translated to an associated **GENE** list.

N = ...

The number of records in the named list.

SELECT WHERE TO SAVE THE NEW LIST

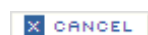
Specify the folder in which to save the new list. You can navigate to the desired folder, or create a new folder with the  **New Folder** icon.

NAME

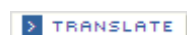
A text field in which you can enter the name for the new list you will save.

DESCRIPTION

A text entry field in which you can enter a description of the new list.



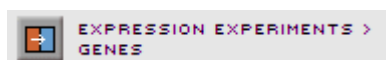
Cancel without performing the list translation.



Translate and save the list.

Data Translation: Expression Experiments > Genes

This tool translates a specified list of expression experiments to a filtered list of associated genes. This allows you to generate a list of genes impacted in the experiments in the specified expression experiment list. With this tool, you can filter either by **p value** (the probability that the expression of each gene would occur by chance), or by top ranked standard deviations.



p value
filter

top ranked
stdevs filter

EXPRESSION EXPERIMENTS > GENES

EXPERIMENT LIST

N = ...

PVALUE < 0.02

INDUCED

REPPRESSED

BOTH

FOR >= 50 % EXPERIMENTS

TOP 500 RANKED STDEVS

SELECT WHERE TO SAVE THE NEW LIST

Workspace

ENTER NEW LIST NAME

ENTER DESCRIPTION

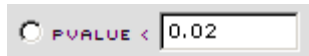
CANCEL TRANSLATE

EXPERIMENT LIST

The name of the **EXPRESSION EXPERIMENT** list that will be translated to an associated **GENE** list.

N = ...

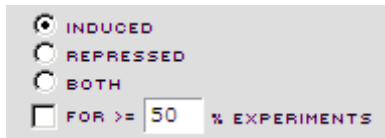
The number of records in the named list.



Selecting this option filters for the probability that the expression of each gene would occur by chance.

Thus this filter will select any gene that has a **p value** less than the specified threshold in any of the experiments in the list (and that also matches other filter terms).

You can change the default value shown here. This filter is mutually exclusive with the **TOP...RANKED STDEVS** described below.



Specify whether to present only up regulated, only down regulated or either up or down regulated genes. These selections are options to the **P VALUE** filter.

INDUCED

Find and display only up regulated genes in the specified **EXPRESSION EXPERIMENT** list.

Note: The gene only has to be induced in ANY one of the experiments in the list, thus it could be downregulated in all but one and upregulated in one and still be selected.

REPRESSED

Find and display only down regulated genes in the specified **EXPRESSION EXPERIMENT** list.

Note: The gene only has to be repressed in ANY one of the experiments in the list, thus it could be upregulated in all but one and downregulated in one and still be selected.

BOTH

Find and display genes that are either up or down regulated in the specified **EXPRESSION EXPERIMENT** list.

FOR >=% EXPERIMENTS

The genes must be consistently perturbed in the same direction for a fraction of the experiments in the list. You can change the default value of 50%.




Filters the genes for the topmost variable genes by standard deviation of the expression ratios across all experiments in the list.

You can change the default. The filter is mutually exclusive with the **PVALUE** filter described above.

This tool can be contrasted with the **SIGNIFICANT GENE FINDER** tool that looks for most consistent change across the experiments in a specified list.

SELECT WHERE TO SAVE THE NEW LIST

Specify the folder in which to save the new list. You can navigate to the desired folder, or create a new folder with the  **New Folder** icon.

ENTER NEW LIST NAME

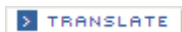
A text field in which you can enter the name for the new list you will save.

ENTER DESCRIPTION

A text entry field in which you can enter a description of the new list.



Cancel without performing the list translation.



Translate and save the list.

Data Import/Export Tools

The **DATA IMPORT/EXPORT** tools allow you to export or import previously saved lists enabling you to archive and/or share lists with colleagues.

Supported List Formats

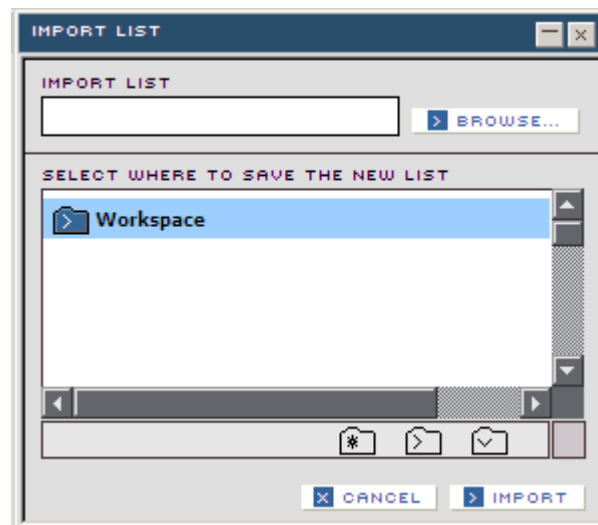
The **LIST EXPORT** tool allows you to export lists in XML format, tab delimited ASCII format, or Spotfire® format.

The **LIST IMPORT** tool allows you to import lists that have been saved or created in XML format.

The **EXPERIMENT IMPORT** and **ACCESSION IMPORT** tools allow you to import line delimited text files.

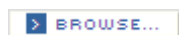
Data Import/Export: List Import

When you select the **LIST IMPORT** tool you will be presented with a standard Windows dialog box for file import. When you import a file, it will automatically be added to your **WORKSPACE** area.




IMPORT LIST

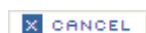
The name of the list to be imported. This field will be populated with the list you select using the browse button. The list must be in XML format.



Launches a standard Windows dialog for file import. The name of the list you select using that dialog will be displayed in the **IMPORT LIST** field.

SELECT WHERE TO SAVE THE NEW LIST

Specify the folder in which to save the new list. You can navigate to the desired folder, or create a new folder with the  **New Folder** icon.




Cancel without importing the list.

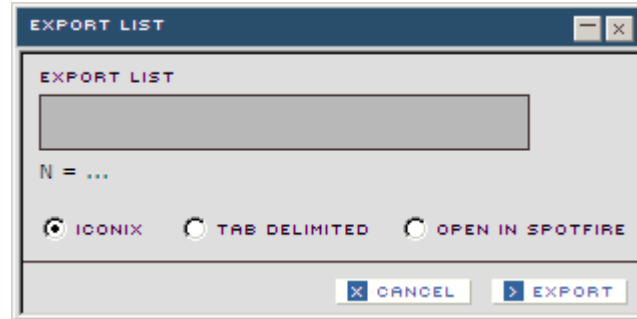


Import the list into the specified location in the **WORKSPACE** area.

Data Import/Export: List Export

This tool allows you to export domain lists of any type in XML PLUS, a data upload type as XML. Lists of this type (called **DATA OBJECTS**) appear with the  icon attached. See [‘Data Object’ on page 225](#).

You can use this feature to archive the list and/or share it with colleagues or to view data in a different display.

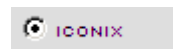


EXPORT LIST

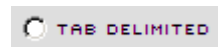
The original list dragged from **WORKSPACE** area.

N = ...

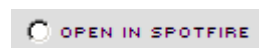
The number of records in the list.



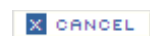
Export the specified list in XML format.



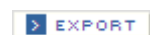
Export the specified list in tab delimited format. (2 columns, each column is TAB separated). Each line has a value for **ID** and **NAME**.



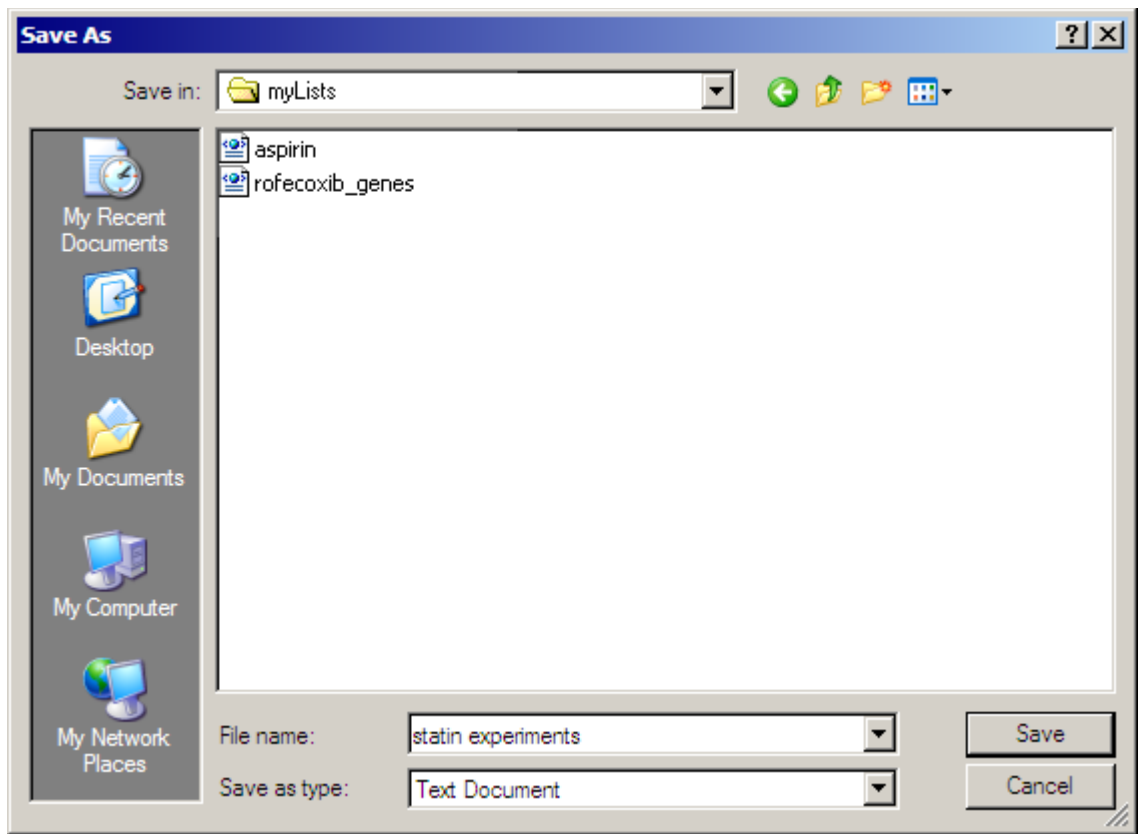
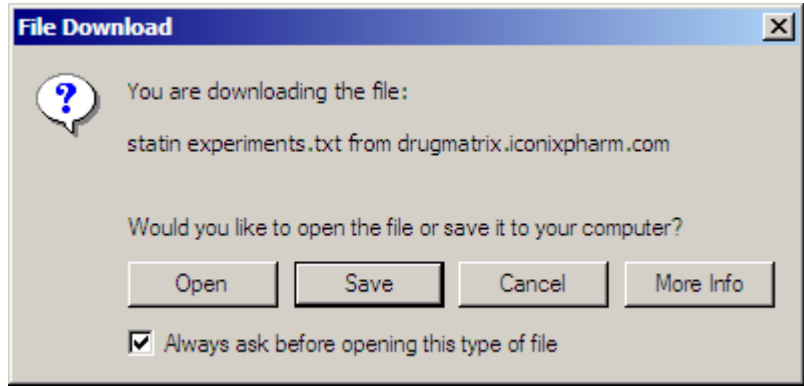
Opens the specified list in Spotfire® data visualization software tool from Spotfire, Inc. If you do not have Spotfire® installed, lists are exported as **TAB DELIMITED** lists with the .sfa format file extension.



Cancel without exporting the file.



Export the list in the specified format. This will launch a standard Windows download popup window that allows you to open or save the file to a folder on your local system.

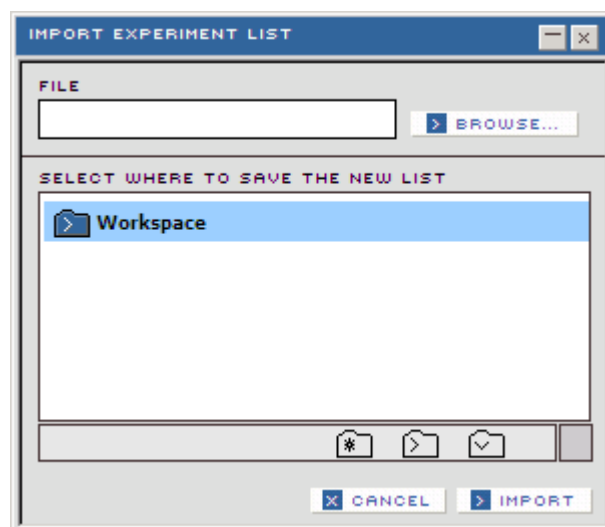


Data Import/Export: Import Experiment List

This tool allows you to import a list of replicate/experiment IDs such as:

```
2575
2576
3031
3033
5201
```

These experiments will be retrieved from the database and the list of experiments will be displayed in the **LIST DISPLAY** area below the **WORKSPACE**.




FILE

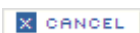
The name of the **EXPERIMENT** list to be imported. This field will be populated with the list you select using the **BROWSE** button.



Launches a standard Windows dialog for file import. The name of the list you select using that dialog will be displayed in the **IMPORT EXPERIMENT LIST** field.

SELECT WHERE TO SAVE THE NEW LIST

Specify the folder in which to save the new list. You can navigate to the desired folder, or create a new folder with the  **New Folder** icon.



Cancel without importing the list.



Import the list into the specified location in the **WORKSPACE** area.

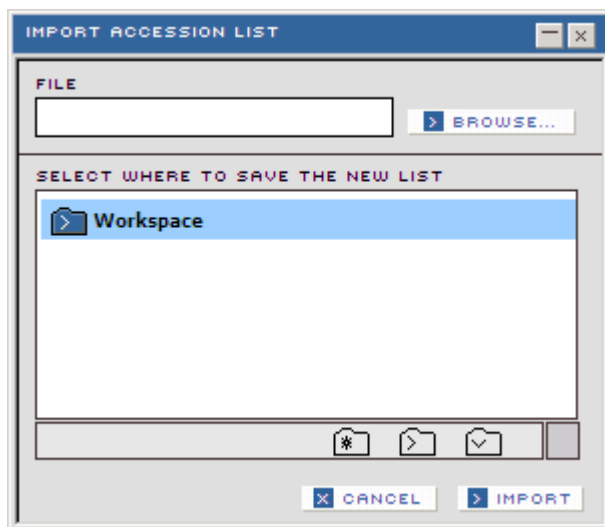
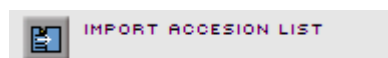
Note: The imported list will have the name **import list**. To rename the list, drag it to the **Edit** icon at the bottom of the **Workspace** panel.

Data Import/Export: Import Accession List

This tool allows you to import a line delimited list of accession numbers from GenBank, such as:

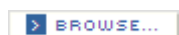
```
AW918717
BE095944
AI102799
AI137413
AI013038
NM_013148
M59742
AA799981
BE113142
```

These experiments will be retrieved from the database and the list of experiments will be displayed in the **LIST DISPLAY** area below the **WORKSPACE**.




FILE

The name of the accession list to be imported. This field will be populated with the list you select using the browse button.



Launches a standard Windows dialog for file import. The name of the list you select using that dialog will be displayed in the **IMPORT LIST** field.

SELECT WHERE TO SAVE THE NEW LIST

Specify the folder in which to save the new list. You can navigate to the desired folder, or create a new folder with the  **New Folder** icon.



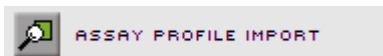
Cancel without importing the list.



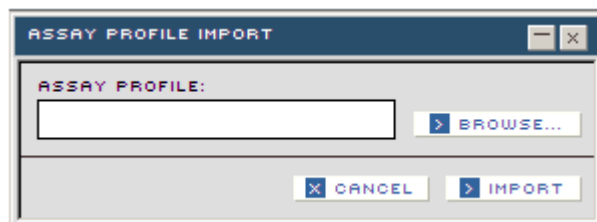
Import the list into the specified location in the **WORKSPACE** area.

Note: The imported list will have the name **import list**. To rename the list, drag it to the **Edit** icon at the bottom of the **Workspace** panel.

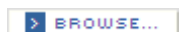
Data Import/Export: Assay Profile Import



The **ASSAY PROFILE IMPORT** tool allows you to import an assay profile in MDS proprietary file format, and search for compounds in the DrugMatrix with similar inhibitory action.

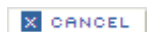


ASSAY PROFILE

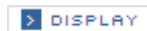


The text file containing the assay profile to be imported.

Launches a standard Windows dialog for file import. The name of the file you select using that dialog will be displayed in the **ASSAY PROFILE** field.



Cancel without generating the data visualization.



Create and display the data visualization.

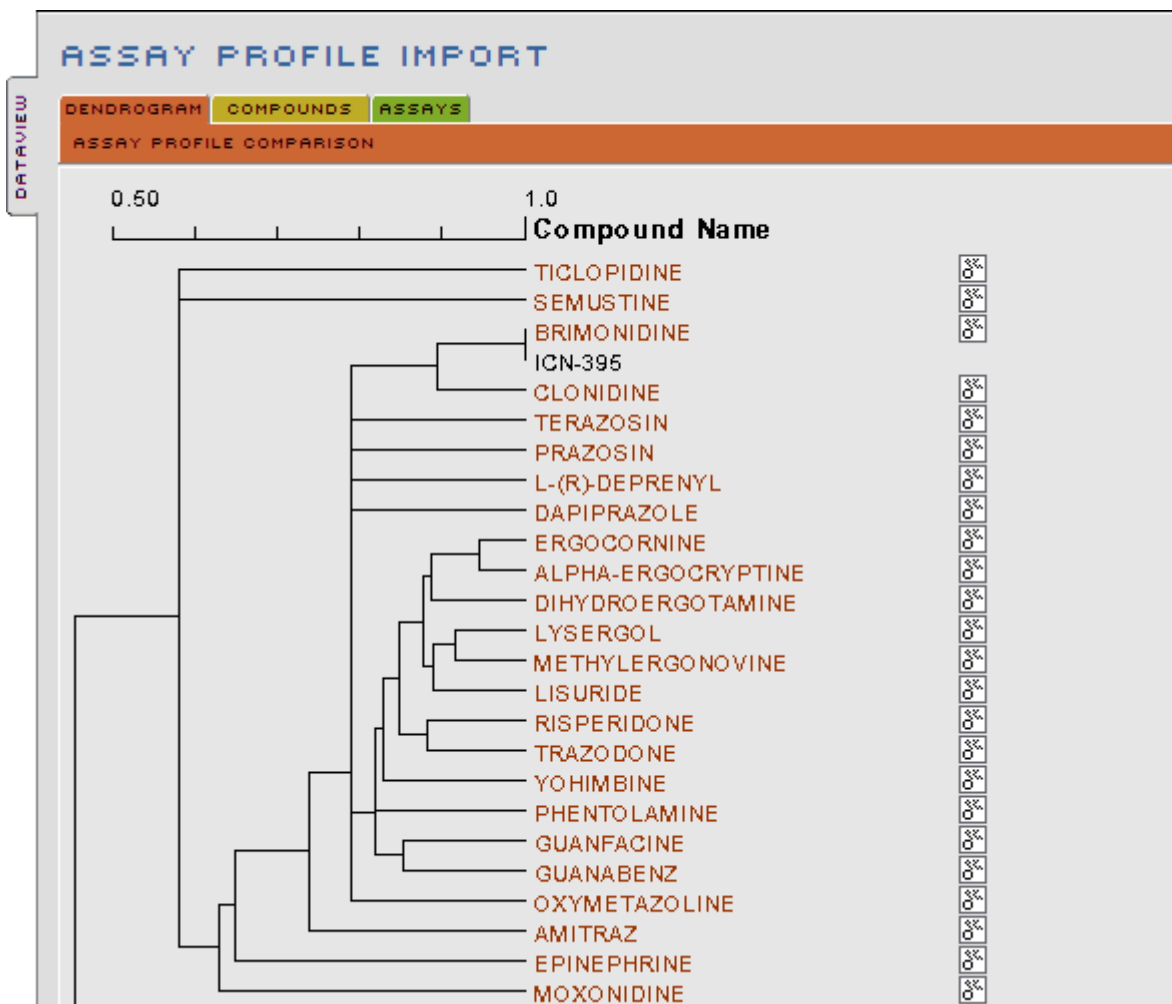
Assay Profile Import Tool - Dendrogram Panel

The panel displays a dendrogram that graphically represents a hierarchical clustering, using Pearson's correlation coefficient as the similarity metric, for compounds based on the assay profile (% inhibition values).

The query profile appears in black. If it is from the database, it is labelled with the relevant compound name. If the query profile is uploaded from a data file external to the database, it is labelled **QUERY**.

The dendrogram represents hierarchical clustering, using Pearson's correlation coefficient as the similarity metric (scores approaching 1.0 indicate the highest similarity while scores approaching -1 indicate the least similarity). The compounds with the highest scores (i.e. approaching 1.0) are the most similar to the **QUERY ASSAY PROFILE**. In this example **BRIMONIDINE** is highly correlated with the query, while the lowest scores are well below 0.5, indicating these nodes are poorly correlated.

Similarity between other compounds in the table is also indicated by the clustering.
















Assay Profile Import Tool - Compounds Panel

This panel displays the compounds that appear in the dendrogram (i.e. the closest matches in the database to the query profile). The compounds in this list are initially in the same order as in the cluster display.

Click on the compound image icon for an expanded image of any compound in the list.

The screenshot shows the 'ASSAY PROFILE IMPORT' interface with the 'COMPOUNDS' tab selected. A table displays a list of compounds with their similarity scores. Each row includes a checkbox, a compound name (underlined as a hyperlink), a molecular structure icon, and a similarity value.



	COMPOUND		SIMILARITY
<input checked="" type="checkbox"/>	TICLOPIDINE		0.6077
<input checked="" type="checkbox"/>	SEMUSTINE		0.6074
<input checked="" type="checkbox"/>	BRIMONIDINE		1
<input checked="" type="checkbox"/>	CLONIDINE		0.8657
<input checked="" type="checkbox"/>	TERAZOSIN		0.748
<input checked="" type="checkbox"/>	PRAZOSIN		0.7038
<input checked="" type="checkbox"/>	L-(R)-DEPRENYL		0.7538
<input checked="" type="checkbox"/>	DAPIPRAZOLE		0.6637
<input checked="" type="checkbox"/>	ERGOCORNINE		0.5909
<input checked="" type="checkbox"/>	ALPHA-ERGOCRYPTINE		0.5885
<input checked="" type="checkbox"/>	DIHYDROERGOTAMINE		0.5785
<input checked="" type="checkbox"/>	LYSERGOL		0.588


COMPOUND

The name of the compound in the database whose activity was measured.

Each compound name in this column is a hyperlink that will populate a **COMPOUND** Domain Report with information about that particular compound.

COMPOUND IMAGE

Click the icons at the top of this column to expand  or contract  all molecular structure images in the column.

Click the molecular structure icon  for a popup window that displays an expanded image for the compound in the selected record (i.e. the compound in a selected row of the table).

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

CORR COEFF

A measure of the assay profile similarity to the query assay profile using the Pearson's Correlation Coefficient. See '[Pearson's Correlation Coefficient](#)' on page 227.

Assay Profile Import Tool - Assays Panel

This panel displays the list of assays in the imported profile specified in the **ASSAY PROFILE** field of the **ASSAY PROFILE IMPORT** dialog window.

The screenshot shows the 'ASSAY PROFILE IMPORT' dialog window with the 'ASSAYS' tab selected. A table lists various assays with columns for CATALOG, ASSAY, INHIBITION, TYPE, TISSUE, and SPECIES. Each row has a checkbox in the left margin.

CATALOG	ASSAY	INHIBITION	TYPE	TISSUE	SPECIES
<input checked="" type="checkbox"/>	265600	Potassium Channel [KATP]	-4.0%	BINDING	PANCRE... CRICETUL...
<input checked="" type="checkbox"/>	265200	Platelet-Derived Growth Fa...	-6.0%	BINDING	3T3 CELLS MUS MUSC...
<input checked="" type="checkbox"/>	265010	Platelet Activating Factor (...)	-1.0%	BINDING	PLATELE... ORYCTOLA...
<input checked="" type="checkbox"/>	264500	Phorbol Ester	-4.0%	BINDING	BRAIN MUS MUSC...
<input checked="" type="checkbox"/>	260410	Opiate mu	4.0%	BINDING	RECOM... HOMO SAP...
<input checked="" type="checkbox"/>	260210	Opiate kappa	1.0%	BINDING	RECOM... HOMO SAP...
<input checked="" type="checkbox"/>	260110	Opiate delta	9.0%	BINDING	RECOM... HOMO SAP...
<input checked="" type="checkbox"/>	257110	Neuropeptide Y2	-5.0%	BINDING	KAN-TS ... HOMO SAP...
<input checked="" type="checkbox"/>	257000	Neuropeptide Y1	5.0%	BINDING	RECOM... HOMO SAP...
<input checked="" type="checkbox"/>	255600	Tachykinin NK2	3.0%	BINDING	RECOM... HOMO SAP...
<input checked="" type="checkbox"/>	255510	Tachykinin NK1	-9.0%	BINDING	RECOM... HOMO SAP...
<input checked="" type="checkbox"/>	253000	Muscarinic M5	3.0%	BINDING	RECOM... HOMO SAP...
<input checked="" type="checkbox"/>	252900	Muscarinic M4	-2.0%	BINDING	RECOM... HOMO SAP...
<input checked="" type="checkbox"/>	252800	Muscarinic M3	-2.0%	BINDING	RECOM... HOMO SAP...
<input checked="" type="checkbox"/>	252700	Muscarinic M2	3.0%	BINDING	RECOM... HOMO SAP...
<input checked="" type="checkbox"/>	252600	Muscarinic M1	3.0%	BINDING	RECOM... HOMO SAP...
<input checked="" type="checkbox"/>	251350	Melanocortin MC4	1.0%	BINDING	RECOM... HOMO SAP...
<input checked="" type="checkbox"/>	243510	Interleukin IL-1 alpha	-11.0%	BINDING	3T3 CELLS MUS MUSC...
<input checked="" type="checkbox"/>	243000	Insulin	1.0%	BINDING	LIVER RATTUS R...

CATALOG

MDS Pharma Services Catalog number.

ASSAY

The assay name identified by the catalog number. Each assay in this column is a hyperlink to an **ASSAY** domain report.

INHIBITION

The bioactivity of the selected compound in the tested assay expressed as % inhibition. (i.e. The extent (in %) the compound inhibits an enzyme reaction, the binding of a ligand to a protein, or the growth of a cell culture).

TYPE

The type of activity for this assay.

TISSUE


The type of tissue used.

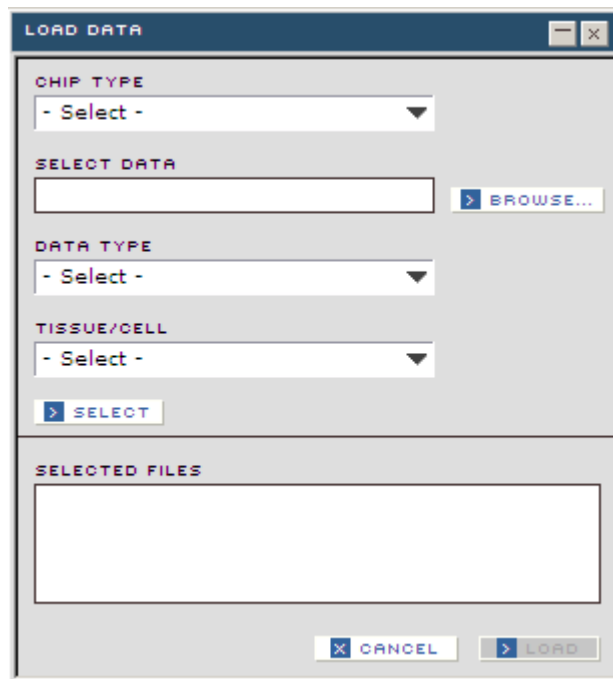
SPECIES

The species from which the tissue was obtained.

Data Import/Export: Load Data

The **LOAD DATA** tool allows you to upload microarray experiments from outside the DrugMatrix database and find the most similar experiments in the DrugMatrix database.

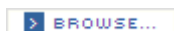
Data will be saved in the **WORKSPACE** area as a **DATA OBJECT** (with the  icon attached), which can populate an **EXPRESSION** report. See [‘Data Object’ on page 225](#).



CHIP TYPE

The type of array technology to be queried.

SELECT DATA



Browse for previously saved microarray experiment files on accessible drives.

DATA TYPE

Control

Specifies that the file to be uploaded is a control. Use for a single color array, such as Amersham BioChip™.

Experiment

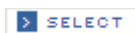
Specifies that the file to be uploaded is an experimental (compound treated) condition. Use for a single color array, such as Amersham BioChip™.

Ratio

Specifies that the file to be uploaded is a ratio type, two color array.

TISSUE/CELL

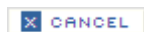
Selections from this menu will filter for the type of tissue or cell line used in the experiments.



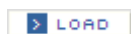
Select the file displayed in the **SELECT DATA** field to be uploaded.

SELECTED FILES

Items you have selected to be uploaded are displayed in this field. You can upload a number of arrays of both two color and single color types. For single color arrays, a minimum of one experiment and one control is required.





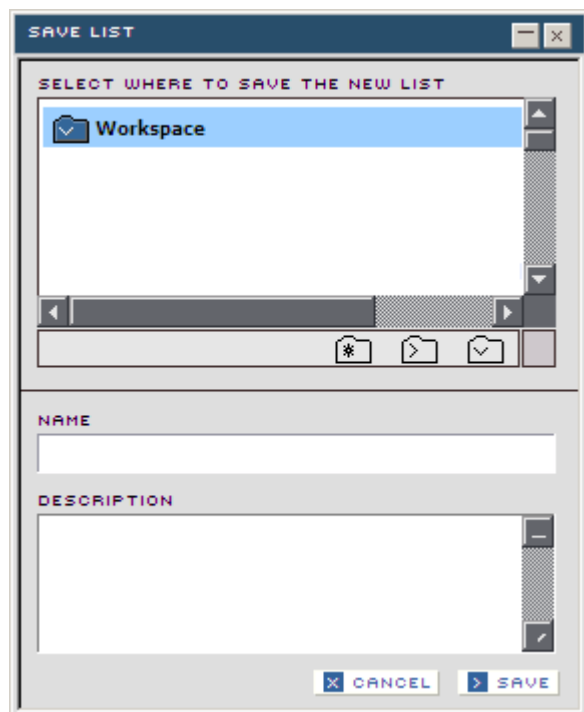
Cancel the operation and close the dialog.



Upload the selected files. This button is inactive until appropriate data and chip type have been specified.

NOTE: With this tool, you must use only chips of the same technology type in uploading files for a given dendrogram (i.e. only GE BioChips or Affymetrix array, but not both types at once).

When you click the **LOAD** button on the **LOAD DATA** dialog, a **SAVE LIST** dialog is displayed allowing you to save the list as a **DATA OBJECT** (with the  icon attached) in the **WORKSPACE** area. When a data object is dragged to the display list icon  in the Workspace area, the information from that list will populate an Expression Domain Report. See '[Data Object](#)' on page 225.

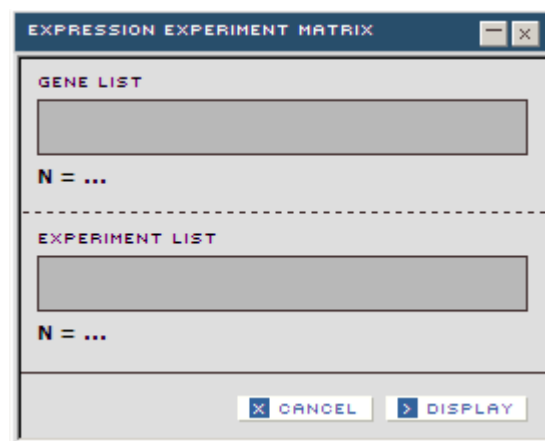


Data Visualization Tools

The Data Visualization Tools provide graphical representations of detailed information extracted from the database presented in visual displays that highlight significant characteristics of the data based on the type of query.

Data Visualization: Expression Experiment Matrix

This tool allows you to generate a graphical matrix, with a heat map type display, to compare expression ratios for a specified list of genes in a specified list of experiments. The data is ordered as a 2 dimensional hierarchical clustering.



GENE LIST

The **GENE** list to be used in the display.

N = ...


The number of records in the named list.

EXPERIMENT LIST


The **EXPERIMENT** list to be used in the display.

N = ...

The number of records in the named list.

 CANCEL

Cancel without generating the data visualization.

 DISPLAY

Create and display the data visualization.

NOTE: In order to show clustering, this tool requires a minimum list size of 5 records with contiguous data for each list entered in the dialog.

Expression Experiment Matrix Tabs

MATRIX	This panel displays a two dimensional clustered visualization of expression data using a heat map format of the values.
GENES	The specified list of genes. Each gene name is a link which will populate a GENE domain report.
EXPERIMENTS	The specified list of expression experiments. Each experiment is a link which will populate an EXPRESSION domain report.

Records listed on the **GENES** panel and on the **EXPERIMENTS** panel are initially in the same order as in the **MATRIX** display. You can check or uncheck records on these lists and then use the **MENU** button on the top left of the panel to save the new list of checked records. The gene or experiment name in each record of these lists is a hyperlink which will populate an appropriate domain report for that item.

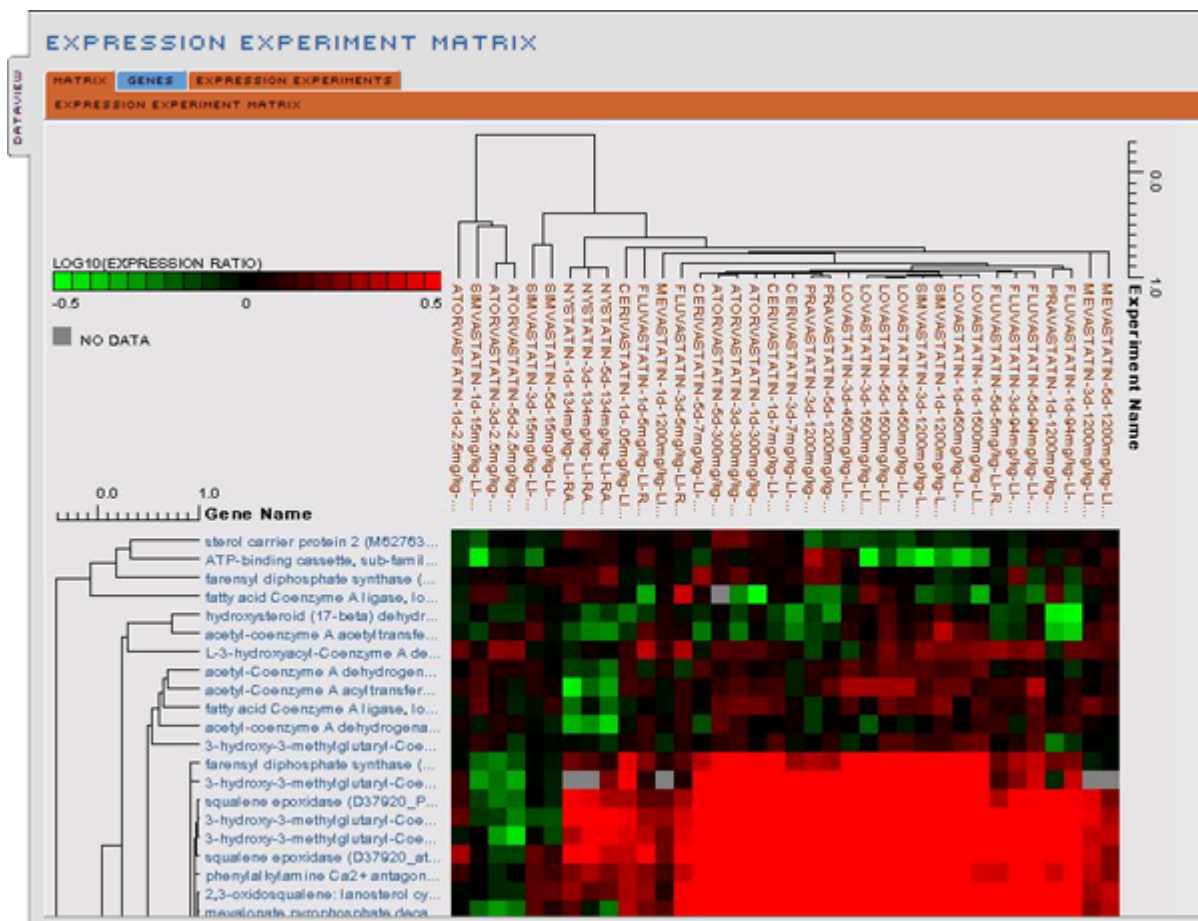


Expression Experiment Matrix - Matrix Panel

This data visualization uses a heat map type display where red indicates up regulated genes and green down regulated genes, of varying intensities.

The dendrogram represents hierarchical clustering, using Pearson's correlation coefficient as the similarity metric (scores approaching 1.0 indicate the highest similarity while scores approaching -1 indicate the least similarity). In this example, the lowest scores are near 0, indicating these nodes are poorly correlated.

NOTE: If data is missing, the color value will be gray. If the row or the column size is less than 5 real (non-blank) data points, no cluster will be generated.



Expression Experiment Matrix - Genes Panel

This panel displays the list of genes specified in the **GENE LIST** field of the **EXPRESSION EXPERIMENT MATRIX** dialog window. The genes in this list are initially in the same order as in the **MATRIX** display. Each gene name in this list is a link which will populate a **GENE** domain report.

The screenshot shows a software window titled "EXPRESSION EXPERIMENT MATRIX". On the left side, there is a vertical tab labeled "DATAVIEW". The main area has three tabs: "MATRIX", "GENES", and "EXPRESSION EXPERIMENTS", with "GENES" currently selected. Below the tabs is a blue header bar with a "> MENU" button and the word "GENES". A table below the header lists genes, each with a checked checkbox in the first column and the gene name in the second column. The gene names are truncated with ellipses. The list includes:

GENE
<input checked="" type="checkbox"/> sterol carrier protein 2 (M6276...
<input checked="" type="checkbox"/> ATP-binding cassette, sub-fam...
<input checked="" type="checkbox"/> farnesyl diphosphate synthase...
<input checked="" type="checkbox"/> fatty acid Coenzyme A ligase, l...
<input checked="" type="checkbox"/> hydroxysteroid (17-beta) dehy...
<input checked="" type="checkbox"/> acetyl-coenzyme A acetyltransf...
<input checked="" type="checkbox"/> L-3-hydroxyacyl-Coenzyme A ...
<input checked="" type="checkbox"/> acetyl-Coenzyme A dehydroge...
<input checked="" type="checkbox"/> acetyl-Coenzyme A acyltransfe...
<input checked="" type="checkbox"/> fatty acid Coenzyme A ligase, l...
<input checked="" type="checkbox"/> acetyl-coenzyme A dehydroge...
<input checked="" type="checkbox"/> 3-hydroxy-3-methylglutaryl-Co...
<input checked="" type="checkbox"/> farnesyl diphosphate synthase...
<input checked="" type="checkbox"/> 3-hydroxy-3-methylglutaryl-Co...
<input checked="" type="checkbox"/> squalene epoxidase (D37920 ...
<input checked="" type="checkbox"/> 3-hydroxy-3-methylglutaryl-Co...
<input checked="" type="checkbox"/> 3-hydroxy-3-methylglutaryl-Co...
<input checked="" type="checkbox"/> squalene epoxidase (D37920 ...
<input checked="" type="checkbox"/> 3-hydroxy-3-methylglutaryl-Co...

Expression Experiment Matrix - Experiments Panel

This panel provides detailed information about the experiments in the experiment list specified in the **EXPRESSION EXPERIMENT MATRIX** tool. The compounds in this list are initially in the same order as in the **MATRIX** display. Each compound name, or experiment name, in this list is a link which will populate an appropriate domain report. You can mouse over compound or experiment names to display additional information.

EXPRESSION EXPERIMENT MATRIX										
EXPRESSION EXPERIMENTS										
EXPERIMENT	COMPOUND		TYPE	TISSUE	TIME	DOSE	INDUCED	REPRESSED	PERTURBED	
<input checked="" type="checkbox"/> MEVASTATIN-5d-1200mg...	MEVASTATIN		BIOCHIP	LIVER	5.0d	1200.0m...	0.6%	0.2%	0.9%	
<input checked="" type="checkbox"/> MEVASTATIN-3d-1200mg...	MEVASTATIN		BIOCHIP	LIVER	3.0d	1200.0m...	2.5%	0.8%	3.4%	
<input checked="" type="checkbox"/> FLUVASTATIN-1d-94mg/k...	FLUVASTATIN		BIOCHIP	LIVER	1.0d	94.0mg/kg	3.3%	4.0%	7.3%	
<input checked="" type="checkbox"/> PRAVASTATIN-1d-1200m...	PRAVASTATIN		BIOCHIP	LIVER	1.0d	1200.0m...	1.3%	1.1%	2.3%	
<input checked="" type="checkbox"/> FLUVASTATIN-5d-94mg/k...	FLUVASTATIN		BIOCHIP	LIVER	5.0d	94.0mg/kg	5.4%	4.7%	10.0%	
<input checked="" type="checkbox"/> FLUVASTATIN-3d-94mg/k...	FLUVASTATIN		BIOCHIP	LIVER	3.0d	94.0mg/kg	10.7%	9.4%	20.1%	
<input checked="" type="checkbox"/> FLUVASTATIN-3d-5mg/kg...	FLUVASTATIN		BIOCHIP	LIVER	5.0d	5.0mg/kg	2.0%	0.6%	2.6%	
<input checked="" type="checkbox"/> LOVASTATIN-1d-1500mg...	LOVASTATIN		BIOCHIP	LIVER	1.0d	1500.0m...	5.4%	4.4%	9.8%	
<input checked="" type="checkbox"/> LOVASTATIN-1d-450mg/...	LOVASTATIN		BIOCHIP	LIVER	1.0d	450.0mg/...	3.9%	1.8%	5.7%	

EXPERIMENT

The list of experiments specified in the **EXPERIMENT LIST** field of the **EXPRESSION EXPERIMENT MATRIX** dialog window.

COMPOUND

The compound used in the selected experiment.

COMPOUND IMAGE

Click the icons at the top of this column to expand or contract all molecular structure images in the column.

Click the molecular structure icon for a popup window that displays an expanded image for the compound in the selected record (i.e. the compound in a selected row of the table).

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

TYPE

The type of microarray used for the experiment (e.g. Codelink BIOCHIP).

TISSUE

The type of tissue used in the selected experiment.

TIME

The time period for the experiment, (e.g. 5 days).

DOSE

The dose administered at the indicated time intervals.

INDUCED

The percent of genes in this experiment that were up regulated with a **p value** ≤ 0.02 .

REPRESSED

The percent of genes in this experiment that were down regulated with a **p value** ≤ 0.02 .

PERTURBED

The percent of genes in this experiment that were up or down regulated with a **p value** ≤ 0.02 .

Data Visualization: Bio-Activity Matrix

This tool allows you to create a graphical matrix, with a heat map type display, to compare the bio-activities from the specified list of assays and compounds.

**COMPOUND LIST**

The **COMPOUND** list to be used in the display.

N = ...

The number of records in the named list.

ASSAY LIST

The **ASSAY** list to be used in the display.

N = ...

The number of records in the named list.

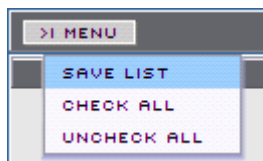
Cancel without generating the data visualization.

Create and display the data visualization.

Bio-Activity Matrix Tabs

MATRIX	This panel displays a two dimensional clustered visualization of bio-activity data using heat map format.
ASSAYS	The specified list of assays. Each assay name is a link that will populate an ASSAY domain report.
COMPOUNDS	The specified list of compounds. Each assay name is a link which will populate a COMPOUND domain report.

Records listed on the **ASSAYS** panel and on the **COMPOUND** panel are initially in the same order as in the **MATRIX** display. You can check or uncheck records on these lists and then use the **MENU** button on the top left of the panel to save the new list of checked records. The assay or compound name in each record of these lists is a hyperlink which will populate an appropriate domain report for that item.

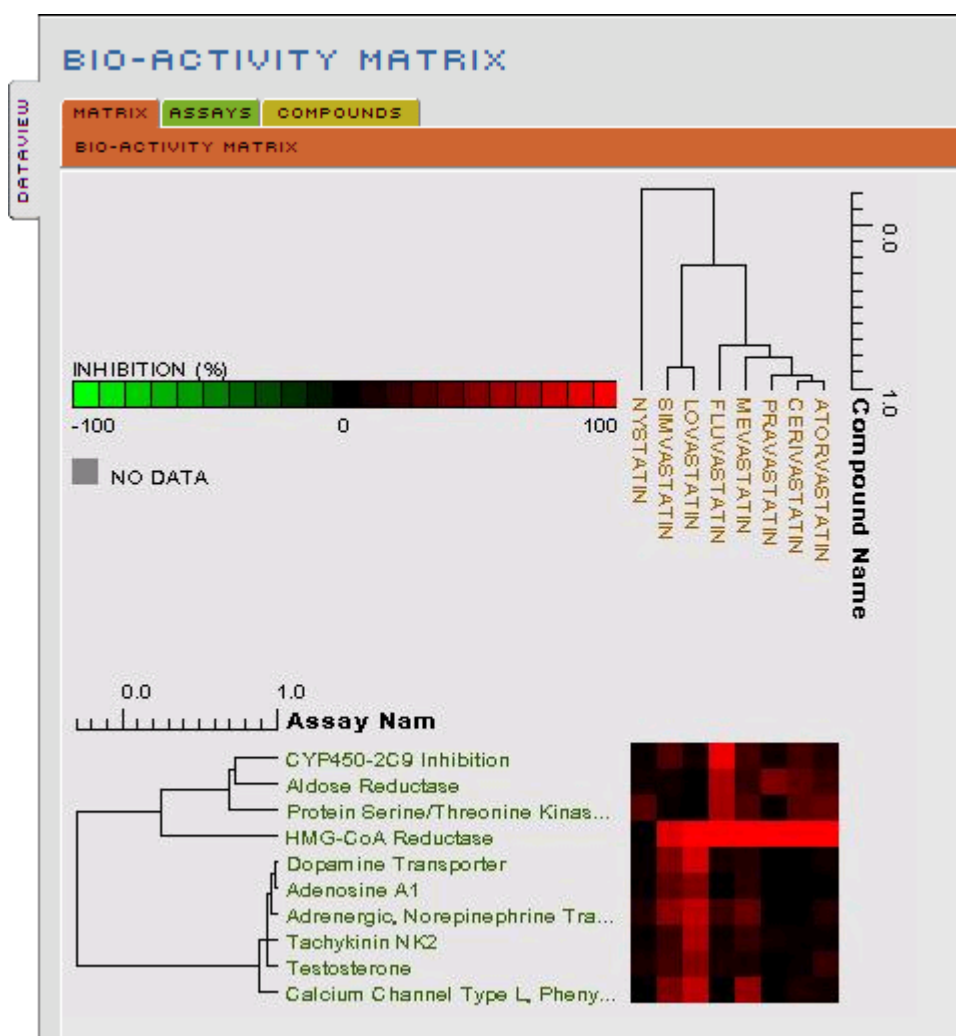


Bio Activity Matrix - Matrix Panel

This data visualization uses a heat map type display format where red indicates the highest % inhibition. Black indicates no effect.

The dendrogram represents hierarchical clustering, using Pearson's correlation coefficient as the similarity metric (scores approaching 1.0 indicate the highest similarity while scores approaching -1 indicate the least similarity). In this example, the lowest scores are near 0, indicating these nodes are poorly correlated.

NOTE: If data is missing, the color value will be gray. If the row or the column size is less than 5 significant elements, no cluster will be generated.



Bio Activity Matrix - Assays Panel

This panel shows the assays in the list specified in the **ASSAY LIST** field of the **BIO-ACTIVITY MATRIX** dialog window. The genes in this list are initially in the same order as in the heat map display. Each assay name in this list is a link which will populate an **ASSAY** domain report. You can save a sublist by selecting and deselecting assays in this list.

BIO-ACTIVITY MATRIX

MATRIX ASSAYS COMPOUNDS

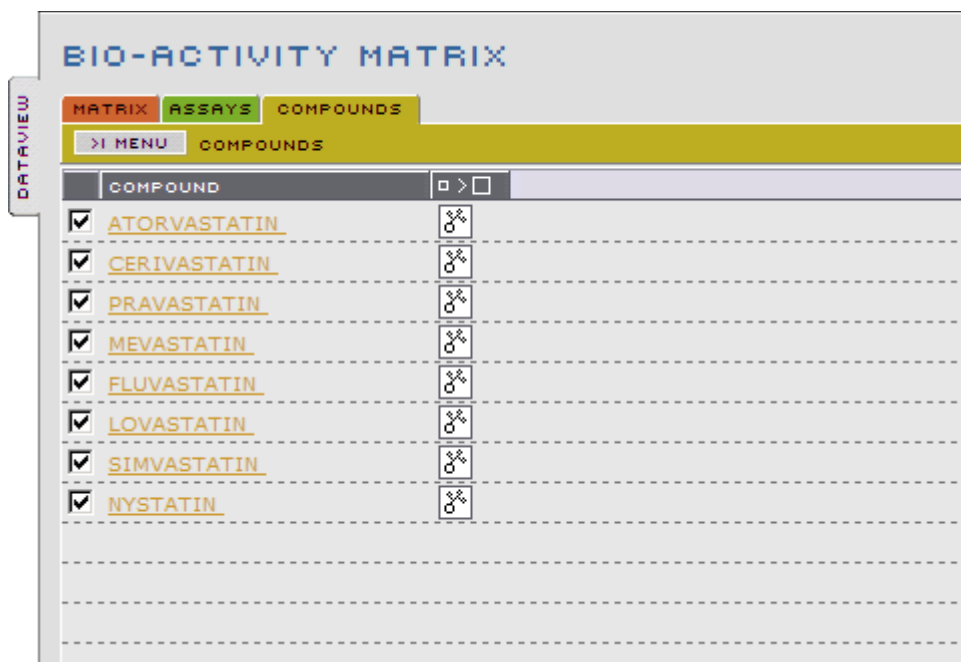
>| MENU ASSAYS

DATAVIEW

ASSAY
<input checked="" type="checkbox"/> CYP450-2C9 Inhibition
<input checked="" type="checkbox"/> Aldose Reductase
<input checked="" type="checkbox"/> Protein Serine/Threonine ...
<input checked="" type="checkbox"/> HMG-CoA Reductase
<input checked="" type="checkbox"/> Dopamine Transporter
<input checked="" type="checkbox"/> Adenosine A1
<input checked="" type="checkbox"/> Adrenergic, Norepinephrin...
<input checked="" type="checkbox"/> Tachykinin NK2
<input checked="" type="checkbox"/> Testosterone
<input checked="" type="checkbox"/> Calcium Channel Type L, ...

Bio Activity Matrix - Compounds Panel

This panel shows the compounds in the list specified in the **COMPOUND LIST** field of the **BIO-ACTIVITY MATRIX** dialog window. The compounds in this list are initially in the same order as in the heat map display (top compound is on the right of the heatmap). You can save a sublist by selecting and deselecting compounds in this list.



Data Visualization: Pathway Impact Matrix



PATHWAY IMPACT MATRIX

The Pathway Impact Matrix tool allows you to examine the impact of compounds, in a specified expression experiment list, on gene pathways.

EXPERIMENT LIST

The **EXPERIMENT** list to be used in the display.

N = ...

The number of records in the named list.

PATHWAY LIST



The **PATHWAY** list to be used in the display.

N = ...

The number of records in the named list.

P VALUE <

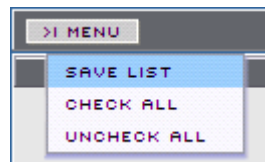
Specify the **p value** for the filter.

INDUCED	Filter for genes that were up regulated in the specified experiment list.
REPRESSED	Filter for genes that were down regulated in the specified experiment list.
BOTH	Filter for genes that were up or down regulated in the specified experiment list.
SCORE TYPE	The type of data to display.
HYPERGEOMETRIC	The statistical method that creates a p value for the perturbed genes in the specified pathway.
% PERTURBED	The number of genes perturbed as a percent of genes in the pathway.
COLOR RANGE	The heat map color scale type to use on the data.
MAX VALUE (- LOG P)	The data value that will cause the highest color saturation.
	Cancel without generating the data visualization.
	Create and display the data visualization.

Pathway Impact Matrix Tabs

MATRIX	This panel displays a two dimensional clustered visualization of bio-activity data using heat map format.
PATHWAYS	The specified list of pathways. Each pathway name is a link that will populate a PATHWAY domain report.
EXPERIMENTS	The specified list of experiments. Each experiment name is a link which will populate a EXPRESSION EXPERIMENT domain report.

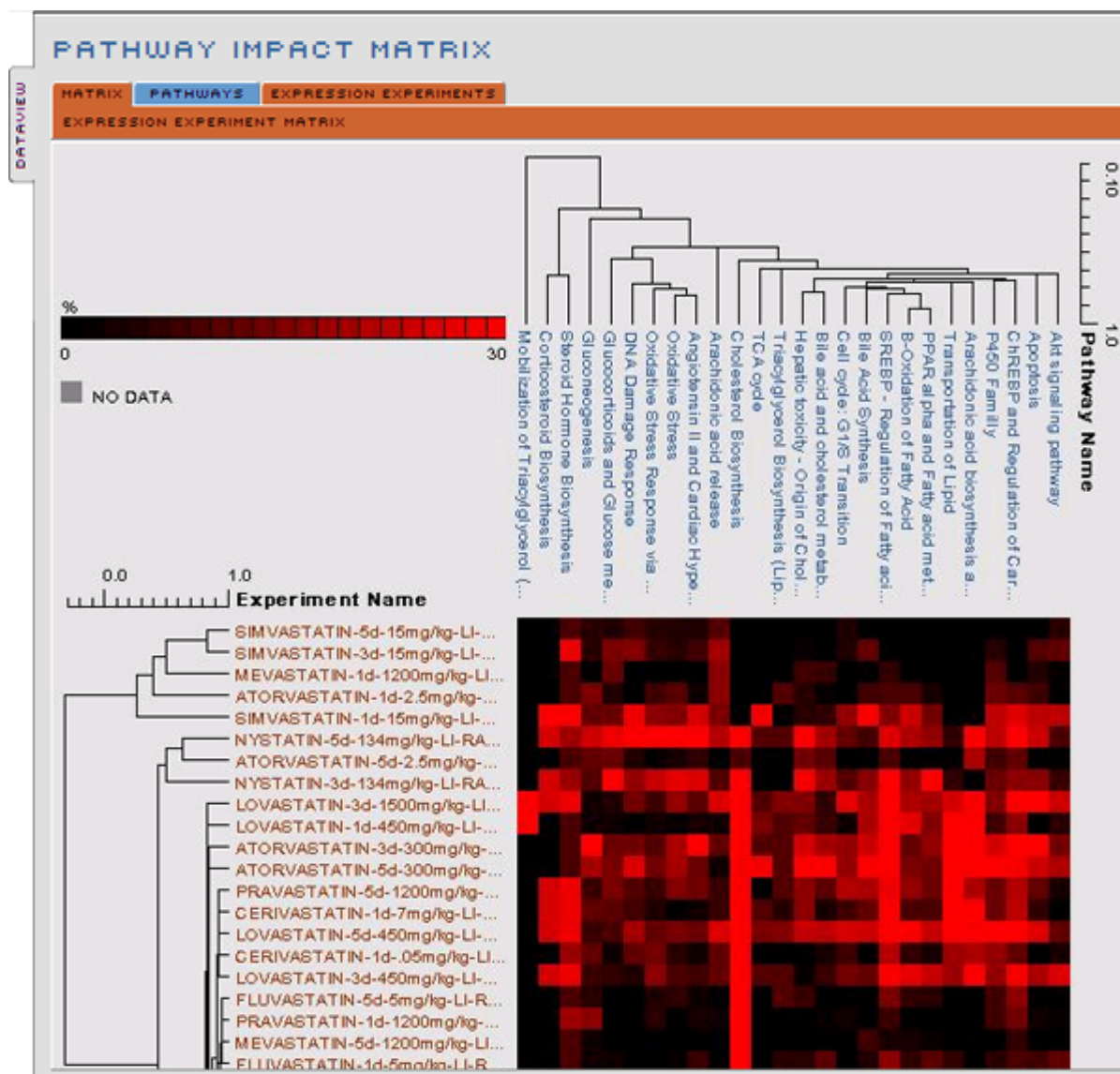
Records listed on the **PATHWAYS** panel and on the **EXPERIMENTS** panel are initially in the same order as in the **MATRIX** display. You can check or uncheck records on these lists and then use the **MENU** button on the top left of the panel to save the new list of checked records. The pathway or experiment name in each record of these lists is a hyperlink which will populate an appropriate domain report for that item.



Pathway Impact Matrix - Matrix Panel

This panel presents a heat map type display format where red indicates significantly perturbed pathways. The scale is a **p value** metric based on the number of genes significantly perturbed (**p value** of log expression ratio < 0.02) in the pathway. The **p value** is not normalized between pathways and therefore is not necessarily an indication of different relative impacts between pathways.

NOTE: If data is missing, the color value will be gray. If the row or the column size is less than 5 real (non-blank) data points, no cluster will be generated.



Pathway Impact Matrix - Pathways Panel

This panel displays the list of pathways specified in the **PATHWAY LIST** field of the **EXPRESSION EXPERIMENT MARTIX** dialog window.

The pathways in this list are initially in the same order as in the **MATRIX** display. Each pathway name in this list is a link which will populate a **PATHWAY** domain report.

PATHWAY
<input checked="" type="checkbox"/> Akt signaling pathway
<input checked="" type="checkbox"/> Apoptosis
<input checked="" type="checkbox"/> ChREBP and Regulation ...
<input checked="" type="checkbox"/> P450 Family
<input checked="" type="checkbox"/> Arachidonic acid biosynth...
<input checked="" type="checkbox"/> Transportation of Lipid
<input checked="" type="checkbox"/> PPAR alpha and Fatty aci...
<input checked="" type="checkbox"/> B-Oxidation of Fatty Acid
<input checked="" type="checkbox"/> SREBP - Regulation of Fa...
<input checked="" type="checkbox"/> Bile Acid Synthesis
<input checked="" type="checkbox"/> Cell cycle: G1/S Transition
<input checked="" type="checkbox"/> Bile acid and cholesterol ...

Pathway Impact Matrix - Experiments Panel

This panel provides detailed information about the experiments in the list specified in the **EXPERIMENT LIST** field of the **PATHWAY IMPACT MATRIX** dialog window. The experiments in this list are initially in the same order as in the **MATRIX** display. Each experiment name, or compound name, in this list is a link which will populate an appropriate domain report. You can mouse over experiment names or compound names to display additional information.

PATHWAY IMPACT MATRIX										
EXPRESSION EXPERIMENTS										
EXPERIMENT	COMPOUND		TYPE	TISSUE	TIME	DOSE	INDUCED	RERESSED	PERTURBED	
<input checked="" type="checkbox"/> SIMVASTATIN-3d-15mg/...	SIMVASTATIN		BIOCHIP	LIVER	5.0d	15.0mg/kg	0.5%	0.8%	1.3%	
<input checked="" type="checkbox"/> SIMVASTATIN-3d-15mg/...	SIMVASTATIN		BIOCHIP	LIVER	3.0d	15.0mg/kg	2.0%	2.2%	4.1%	
<input checked="" type="checkbox"/> MEVASTATIN-1d-1200mg...	MEVASTATIN		BIOCHIP	LIVER	1.0d	1200.0m...	0.3%	0.7%	0.9%	
<input checked="" type="checkbox"/> ATORVASTATIN-1d-2.5m...	ATORVASTATIN		BIOCHIP	LIVER	1.0d	2.5mg/kg	2.4%	1.7%	4.0%	
<input checked="" type="checkbox"/> SIMVASTATIN-1d-15mg/...	SIMVASTATIN		BIOCHIP	LIVER	1.0d	15.0mg/kg	8.1%	7.2%	15.3%	
<input checked="" type="checkbox"/> HYSTATIN-5d-134mg/kg...	HYSTATIN		BIOCHIP	LIVER	5.0d	134.0mg/...	7.6%	6.3%	13.9%	
<input checked="" type="checkbox"/> ATORVASTATIN-5d-2.5m...	ATORVASTATIN		BIOCHIP	LIVER	5.0d	2.5mg/kg	1.4%	0.7%	2.1%	
<input checked="" type="checkbox"/> HYSTATIN-3d-134mg/kg...	HYSTATIN		BIOCHIP	LIVER	3.0d	134.0mg/...	5.5%	2.6%	8.1%	
<input checked="" type="checkbox"/> LOVASTATIN-3d-1500mg...	LOVASTATIN		BIOCHIP	LIVER	3.0d	1500.0m...	9.6%	4.0%	13.6%	
<input checked="" type="checkbox"/> LOVASTATIN-1d-450mg/...	LOVASTATIN		BIOCHIP	LIVER	1.0d	450.0mg/...	3.9%	1.8%	5.7%	
<input checked="" type="checkbox"/> ATORVASTATIN-3d-300m...	ATORVASTATIN		BIOCHIP	LIVER	3.0d	300.0mg/...	14.5%	9.0%	23.5%	

EXPERIMENT

The list of experiments specified in the **EXPERIMENT LIST** field of the **PATHWAY IMPACT MATRIX** tool. Each experiment name is a link that will populate a **EXPRESSION EXPERIMENT** domain report.

COMPOUND

This column displays the name of the compound used in each experiment shown in the **EXPERIMENT** column of this table. Each compound name is a link that will populate a **COMPOUND** domain report.

COMPOUND IMAGE

Click the icons at the top of this column to expand or contract all molecular structure images in the column.

Click the molecular structure icon for a popup window that displays an expanded image for the compound name shown next to the icon.

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

TYPE

The type of microarray used for the experiment (e.g. Codelink BIOCHIP).

TISSUE

The type of tissue used in the selected experiment.

TIME

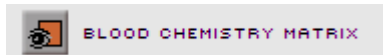
The time period for the experiment, (e.g. 5 days).

DOSE

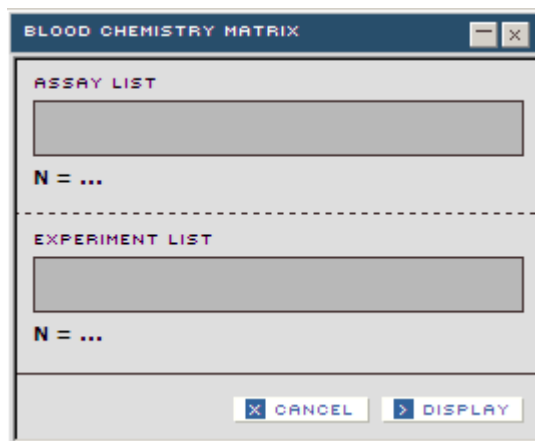
The dose administered at the indicated time intervals.

INDUCED	The percent of genes in this experiment that were up regulated with a p value ≤ 0.02 .
REPRESSED	The percent of genes in this experiment that were down regulated with a p value ≤ 0.02 .
PERTURBED	The percent of genes in this experiment that were up or down regulated with a p value ≤ 0.02 .

Data Visualization: Blood Chemistry Matrix



The Blood Chemistry Matrix tool allows you to create a heat map display to examine the perturbation of blood chemistry assays, in a specified expression experiment list.



ASSAY LIST

The **ASSAY LIST** to be used in the display.

N = ...

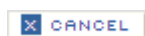
The number of records in the named list.

EXPERIMENT LIST

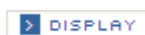
The **EXPERIMENT LIST** to be used in the display.

N = ...

The number of records in the named list.



Cancel without generating the data visualization.

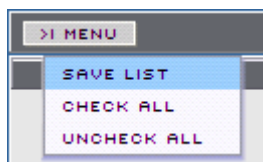


Create and display the data visualization.

Blood Chemistry Matrix Tabs

MATRIX	This panel displays a two dimensional clustered visualization of bio-activity data using heat map format.
ASSAYS	The specified list of assays. Each assay name is a link that will populate an ASSAY domain report.
EXPERIMENTS	The specified list of experiments. Each experiment name is a link which will populate a EXPRESSION EXPERIMENT domain report.

Records listed on the **ASSAYS** panel and on the **EXPERIMENTS** panel are initially in the same order as in the **MATRIX** display. You can check or uncheck records on these lists and then use the **MENU** button on the top left of the panel to save the new list of checked records. The assay or experiment name in each record of these lists is a hyperlink which will populate an appropriate domain report for that item.

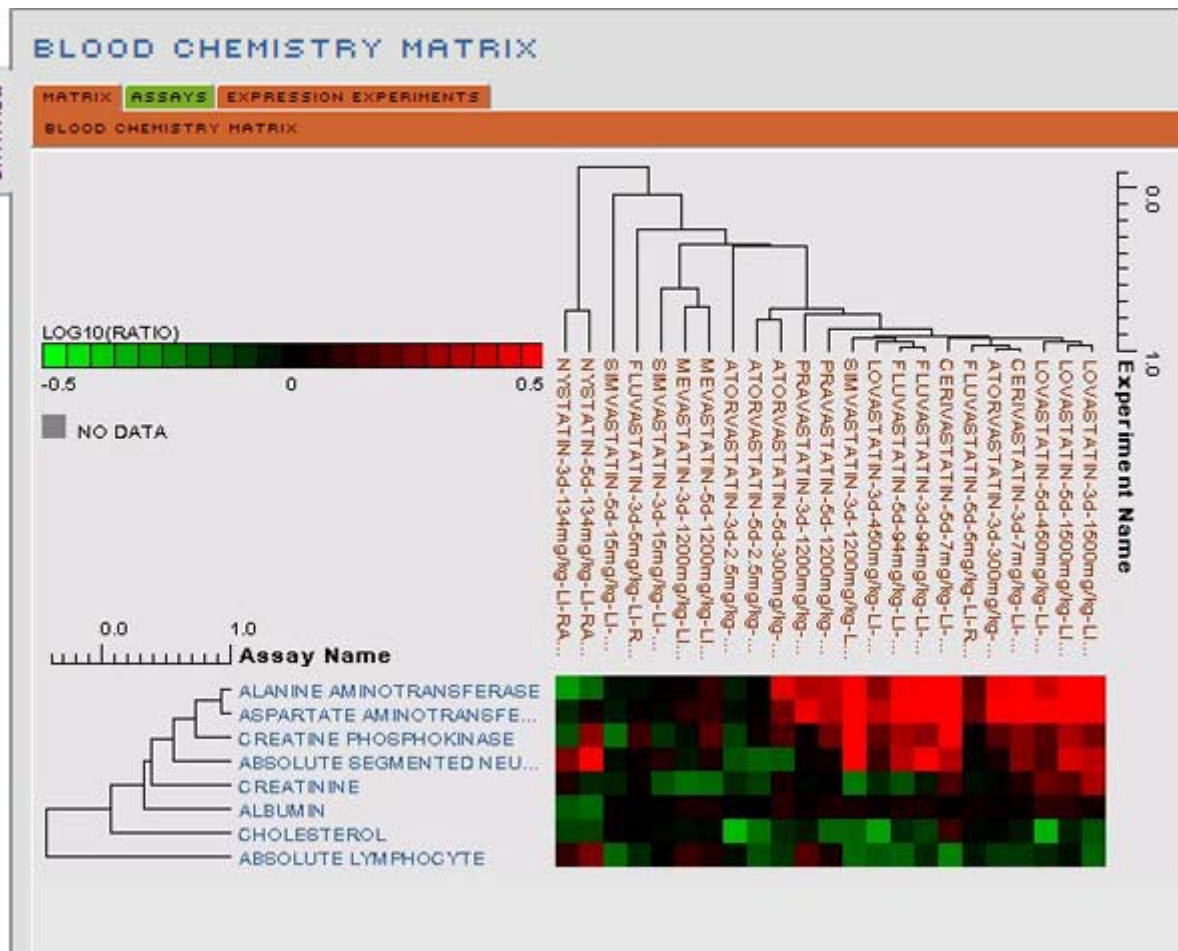


Blood Chemistry Matrix - Experiments Matrix

This data visualization uses a heat map type display format to show the changes for the blood chemistry assays, where red indicates increased values in blood chemistry assays and green indicates decreased values in blood chemistry assays, in the experiments.

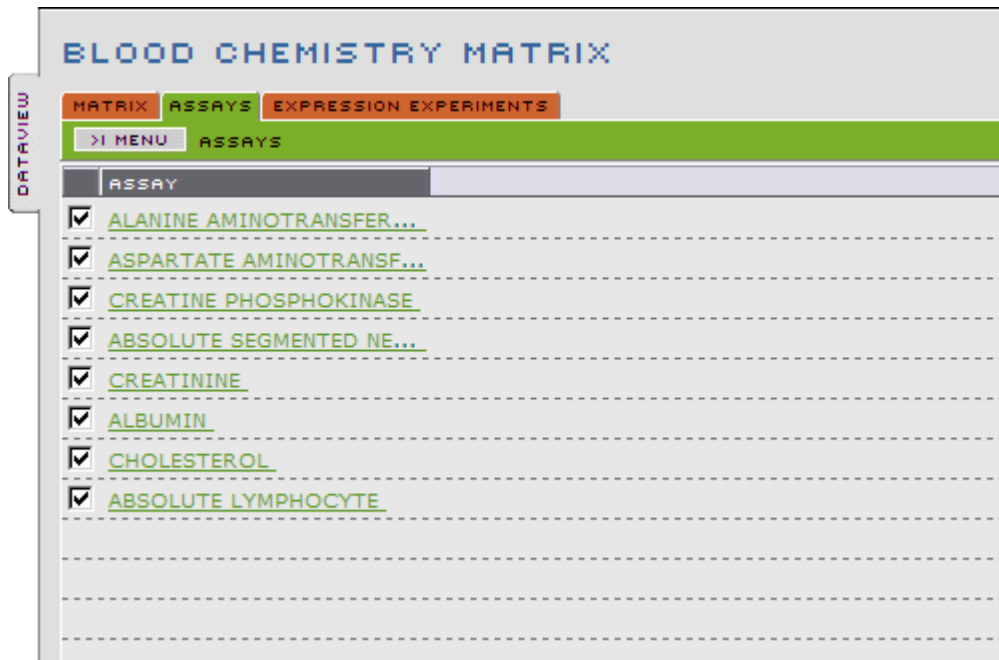
The dendrogram represents hierarchical clustering, using Pearson's correlation coefficient as the similarity metric (scores approaching 1.0 indicate the highest similarity while scores approaching -1 indicate the least similarity). In this example, the lowest scores for experiments are near 0, indicating these nodes are poorly correlated.

NOTE: If data is missing, the color value will be gray. If the row or the column size is less than 5 real (non-blank) data points, no cluster will be generated.



Blood Chemistry Matrix - Experiments Assay

This panel displays the assay list specified in the **ASSAY LIST** field of the **BLOOD CHEMISTRY MATRIX** dialog window. The initial order of assays in this list is the same as on the **MATRIX** panel. Each item in the list is link that will populate new **ASSAY** Domain Report. You can select specific records in the list using the check boxes and then save the checked records as a new list.



The screenshot shows a software interface titled "BLOOD CHEMISTRY MATRIX". On the left, there is a vertical tab labeled "DATAVIEW". The main area has three tabs: "MATRIX", "ASSAYS", and "EXPRESSION EXPERIMENTS", with "ASSAYS" currently selected. Below the tabs is a green bar with a "> MENU" button and the word "ASSAYS". Underneath is a table with a header "ASSAY". The table contains a list of assays, each with a checked checkbox and a link:

ASSAY
<input checked="" type="checkbox"/> ALANINE AMINOTRANSFER...
<input checked="" type="checkbox"/> ASPARTATE AMINOTRANSF...
<input checked="" type="checkbox"/> CREATINE PHOSPHOKINASE
<input checked="" type="checkbox"/> ABSOLUTE SEGMENTED NE...
<input checked="" type="checkbox"/> CREATININE
<input checked="" type="checkbox"/> ALBUMIN
<input checked="" type="checkbox"/> CHOLESTEROL
<input checked="" type="checkbox"/> ABSOLUTE LYMPHOCYTE

Blood Chemistry Matrix - Experiments Panel

This panel provides detailed information about the experiments in the list specified in the **EXPERIMENT LIST** field of the **BLOOD CHEMISTRY MATRIX** dialog window. The experiments in this list are initially in the same order as in the **MATRIX** display. Each experiment name, or compound name, in this list is a link which will populate an appropriate domain report. Additional information will be displayed as you mouse over experiment names or compound names.

EXPERIMENT	COMPOUND	TYPE	TISSUE	TIME	DOSE	INDUCED	RERESSED	PERTURBED
LOVASTATIN-3d-1500mg...	LOVASTATIN	BIOCHIP	LIVER	3.0d	1500.0m...	9.6%	4.0%	13.6%
LOVASTATIN-5d-1500mg...	LOVASTATIN	BIOCHIP	LIVER	5.0d	1500.0m...	9.1%	5.6%	14.7%
LOVASTATIN-5d-450mg/...	LOVASTATIN	BIOCHIP	LIVER	5.0d	450.0mg/...	9.0%	6.3%	15.3%
CERIVASTATIN-3d-7mg/kg...	CERIVASTATIN	BIOCHIP	LIVER	3.0d	7.0mg/kg	8.2%	6.3%	14.4%
ATORVASTATIN-3d-300m...	ATORVASTATIN	BIOCHIP	LIVER	3.0d	300.0mg/...	14.5%	9.0%	23.5%
FLUVASTATIN-5d-5mg/kg...	FLUVASTATIN	BIOCHIP	LIVER	5.0d	5.0mg/kg	2.0%	0.6%	2.6%
CERIVASTATIN-5d-7mg/kg...	CERIVASTATIN	BIOCHIP	LIVER	5.0d	7.0mg/kg	7.8%	5.0%	12.9%
FLUVASTATIN-3d-94mg/kg...	FLUVASTATIN	BIOCHIP	LIVER	3.0d	94.0mg/kg	10.7%	9.4%	20.1%
FLUVASTATIN-5d-94mg/kg...	FLUVASTATIN	BIOCHIP	LIVER	5.0d	94.0mg/kg	5.4%	4.7%	10.0%
LOVASTATIN-3d-450mg/...	LOVASTATIN	BIOCHIP	LIVER	3.0d	450.0mg/...	5.0%	3.4%	8.3%
SIMVASTATIN-3d-1200m...	SIMVASTATIN	BIOCHIP	LIVER	3.0d	1200.0m...	11.7%	10.2%	21.9%
PRAVASTATIN-5d-1200m...	PRAVASTATIN	BIOCHIP	LIVER	5.0d	1200.0m...	7.1%	5.1%	12.2%
PRAVASTATIN-3d-1200m...	PRAVASTATIN	BIOCHIP	LIVER	3.0d	1200.0m...	10.4%	7.2%	17.5%
ATORVASTATIN-5d-300m...	ATORVASTATIN	BIOCHIP	LIVER	5.0d	300.0mg/...	9.4%	5.8%	15.2%



EXPERIMENT


The list of experiments specified in the **EXPERIMENT LIST** field of the **BLOOD CHEMISTRY MATRIX** tool.

COMPOUND

This column displays the name of the compound used in each experiment shown in the **EXPERIMENT** column of this table.

COMPOUND IMAGE

Click the icons at the top of this column to expand  or contract  all molecular structure images in the column.

Click the molecular structure icon  for a popup window that displays an expanded image for the compound in the selected record (i.e. the compound in a selected row of the table).

If you have the MDL Information Systems ChimePro plugin installed in your browser, right click on the expanded image to access the Chime features.

TYPE

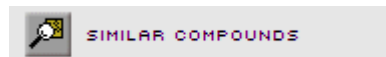
The type of microarray upon which the experiment is stored. (e.g. Codelink BIOCHIP)

TISSUE

The type of tissue used in the selected experiment.

TIME	The time period for the experiment, (e.g. 5 days).
DOSE	The dose administered at the indicated time intervals.
INDUCED	The percent of genes in this experiment that were up regulated with a p value ≤ 0.02 .
REPRESSED	The percent of genes in this experiment that were down regulated with a p value ≤ 0.02 .
PERTURBED	The percent of genes in this experiment that were up or down regulated with a p value ≤ 0.02 .

Data Visualization: Similar Compounds



The **SIMILAR COMPOUNDS** tool allows you to query the DrugMatrix database for compounds that are similar in structure to your target compound.

You can use either an item from your **FAVORITES** list, a chime molecular image (if you have ChimePro plugin installed in your browser), or a mol string.

The data visualization produced by this tool will present a table of two dimensional images of the molecular structures of the compounds similar to your target compound.

MDL ISIS/DIRECT

Comparisons will be made via MDL ISIS technology.

DAYLIGHT

Comparisons will be made via Daylight Chemical Information Systems technology. This requires a Daylight license.

SUBSTRUCTURE RESEARCH

Compares the query compound to compounds in the DrugMatrix database by exact match of substructure.

SIMILARITY SEARCH

Compares the query compound to compounds in the DrugMatrix database by similarity of molecular structure.

COMPOUND ITEM

Query the database for compounds similar to an item from your **FAVORITES** list.

CHIME STRUCTURE

Paste a chime molecular image to query the DrugMatrix database for similar compounds.

Note: This requires the MDL Information Systems ChimePro plugin installed in your browser.

QUERY STRING

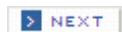
Enter a SMART string to query the DrugMatrix database for similar compounds.



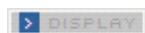
Cancel without generating the data visualization.



Go to previous dialog window. Not active on this dialog.



Go to next dialog window.



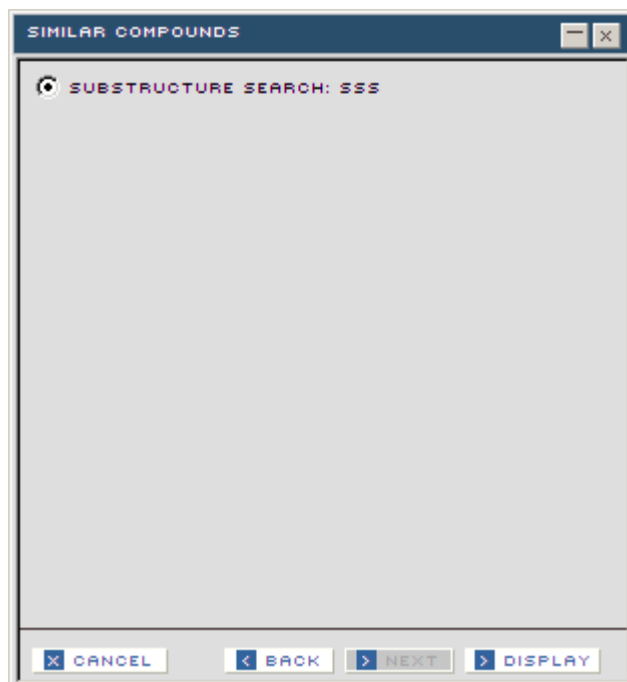
Create and display the data visualization. Not active on this dialog.

NOTE: Depending on the type of query (**SUBSTRUCTURE SEARCH** or **SIMILARITY SEARCH**) specified in the first dialog window of the **SIMILAR COMPOUNDS** tool, one of two second dialog windows will appear.

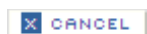
Also, each of the two types of query generates a slightly different data visualization.

Similar Compounds Tool - Substructure Search - 2nd Dialog

If **SUBSTRUCTURE SEARCH** is selected in the 1st dialog of the **SIMILAR COMPOUNDS** tool, this 2nd dialog window will appear.

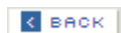


SUBSTRUCTURE SEARCH SSS

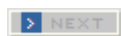


The search is based upon similarity of substructure to the query compound.

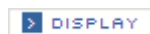
Cancel without generating the data visualization.



Go to previous dialog window.



Go to next dialog window. Not active on this dialog.



Create and display the data visualization.

Similar Compounds Tool - Substructure Search Dataview

The **SIMILAR COMPOUNDS** tool will query the database and present a table of two dimensional images for the molecular structures of compounds which a substructure that is the same as the query compound.

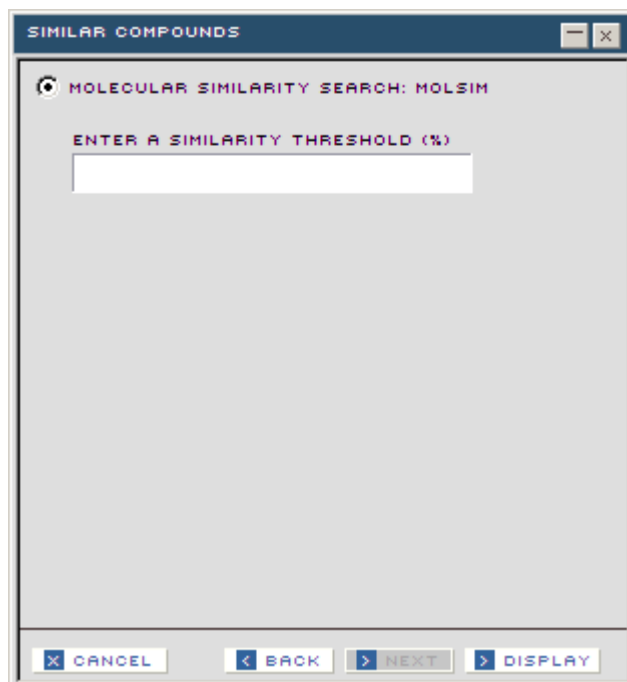
As you mouse over the two dimensional compound structure images on the **COMPOUND COMPARE** data visualization screen, hovers will display detailed information about the specified compound.

You can also check or uncheck items on this panel and save the list of checked items using the **MENU** in the upper left corner of the panel.

The screenshot shows the 'SIMILAR COMPOUNDS' dataview interface. The panel is titled 'SIMILAR COMPOUNDS' and has a 'DATAVIEW' label on the left. At the top, there is a yellow bar with '> MENU' and 'SIMILAR COMPOUNDS'. Below this, six compound cards are displayed in a 2x3 grid. Each card shows a chemical structure, the compound name, and a checked checkbox. The compounds are: PIRIFIBRATE, PICAFIBRATE, CLOFIBRIDE, SALAFIBRATE, THEOFIBRATE, and BINIFIBRATE. To the right of the grid, there are partial views of other compound cards labeled 'ET' and 'RC'.

Similar Compounds Tool - Similarity Search - 2nd Dialog

If **SIMILARITY SEARCH** is selected in the 1st dialog of the **SIMILAR COMPOUNDS** tool, this 2nd dialog window will appear.

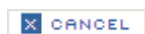


MOLECULAR SIMILARITY SEARCH: MOLSIM

The the ISIS molecular similarity (**MOLSIM**) method will be used to search for similarity in chemical structure between the query compound and compounds in DrugMatrix.

ENTER A SIMILARITY THRESHOLD %

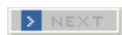
The % of similarity a compound must equal or exceed, compared to the query compound, in order to be included in the displayed list.



Cancel without generating the data visualization.



Go to previous dialog window.



Go to next dialog window. Not active on this dialog.



Create and display the data visualization.

Similar Compounds Tool - Similar Search Dataview

The **SIMILAR COMPOUNDS** tool will query the database and present a table of two dimensional images for the molecular structures of compounds similar to the query compound.

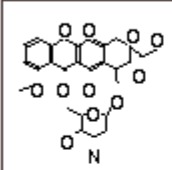
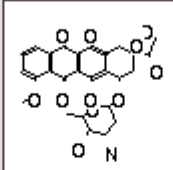
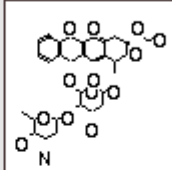
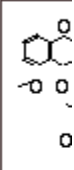
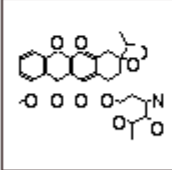
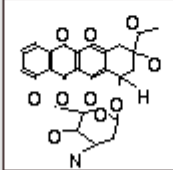
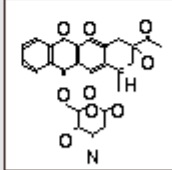
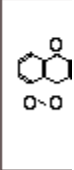
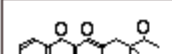
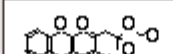
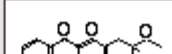

As you mouse over the two dimensional compound structure images on the **COMPOUND COMPARE** data visualization screen, hovers will display detailed information about the specified compound.

You can also check or uncheck items on this panel and save the list of checked items using the **MENU** in the upper left corner of the panel.

Score the score represents the % similarity of molecular structure to the query compound.

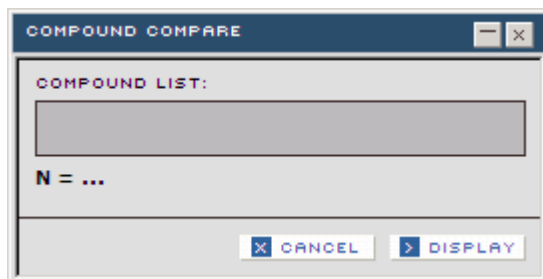
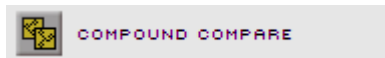
SIMILAR COMPOUNDS

> MENU SIMILAR COMPOUNDS

<p>DOXORUBICIN</p>  <p>Score = 100.0 <input checked="" type="checkbox"/></p>	<p>EPIRUBICIN</p>  <p>Score = 100.0 <input checked="" type="checkbox"/></p>	<p>MEN-10755</p>  <p>Score = 97.22 <input checked="" type="checkbox"/></p>	<p>N,N-DI...</p>  <p>Score</p>
<p>DAUNORUBICIN</p>  <p>Score = 95.51 <input checked="" type="checkbox"/></p>	<p>CARUBICIN</p>  <p>Score = 95.34 <input checked="" type="checkbox"/></p>	<p>IDARUBICIN</p>  <p>Score = 95.23 <input checked="" type="checkbox"/></p>	<p>ESORL...</p>  <p>Score</p>
<p>IDARUBICINOL (METABOLITE)</p> 	<p>LEURUBICIN</p> 	<p>AMRUBICIN HYDROCHLORIDE</p> 	<p>DA-12...</p> 

Data Visualization: Compound Compare

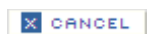
The data visualization produced by **COMPOUND COMPARE** tool presents a table of two dimensional images of the molecular structures of the compounds in the specified list of compounds.

**COMPOUND LIST**

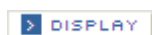
The list of compounds to be displayed in the **COMPOUND COMPARE** visualization.

N = ...

The number of records in the named list.



Cancel without generating the data visualization.



Create and display the data visualization.

Compound Compare Tool - Dataview

The **COMPOUND COMPARE** tool will query the database and present a table of two dimensional images for the molecular structures of all compounds in the specified list.

As you mouse over the two dimensional compound structure images on the **COMPOUND COMPARE** data visualization screen, hovers will display detailed information about the specified compound.

For a list of Chemical Ontology terms, see [‘Appendix - Chemical Ontology’ on page 231](#)

Compound Name:	The name of the compound represented by the two dimensional image.
Compound Identifier:	A list of standard database compound identifier synonyms for the compound.
Molecular Weight:	The molecular weight of the compound.
Formula:	The molecular formula for the compound.
FDA Approval:	The FDA developmental status of the compound. Products on the market are “Approved”.
Smiles:	The SMILES string for the compound.
Product Class:	The therapeutic category in which the drug is used.
Indication:	A list of known indications for the compound.
Mode of Action:	A list of known mechanisms of action for the compound.
Mode Class:	A classification of the actions of the query compound.
Synonyms:	A list of synonyms for the compound.

Data Visualization: Pathway Visualization



PATHWAY VISUALIZATION

This tool allows you to investigate the effects of experiments on the genes in a specified pathway and enables you to see the impact of compounds on the genes in a pathway of interest at various doses and times.

EXPERIMENT LIST	The list of expression experiments you wish to investigate.
N = ...	The number of records in the named list.
PATHWAY FAVORITE	A list consisting of a single pathway.
N = ...	The number of records in the named list.
P VALUE FILTER	The probability that the expression ratio is not significantly perturbed.
DISPLAY TYPE LOG RATIO BINARY	The type of data to display, log ratio or a 3 state, up-, down-regulated or no change.

COLOR RANGE
GREEN-WHITE-RED
GREEN-BLACK-RED

The heat map color scale type to use on the data.

MAX SCORE VALUE

The data value that will cause the highest color saturation.

Note: This option is only available if **LOG RATIO** is selected for **DISPLAY TYPE**. If **BINARY** selected, this control is disabled and grayed out.



Cancel without generating the data visualization.

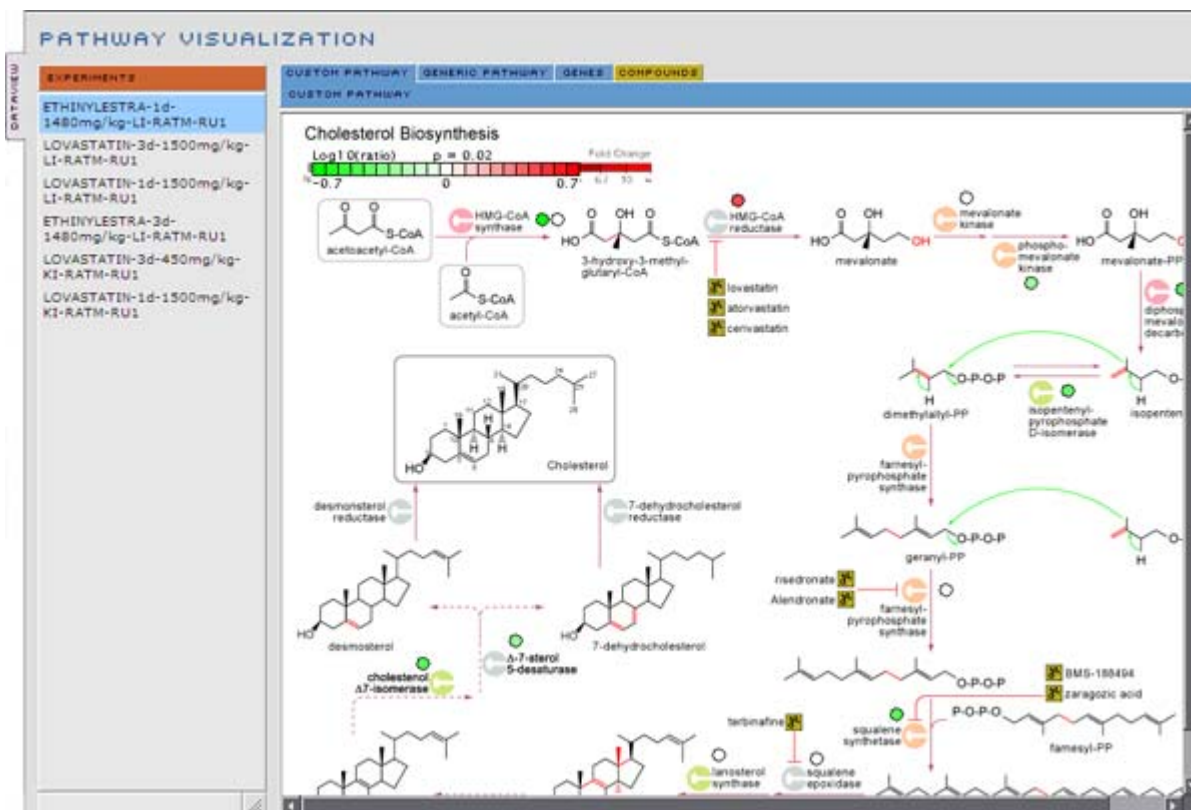


Create and display (or export) the data visualization.

Pathway Visualization Tool - Dataview

This dataview consists of four panels containing detailed information about genes and compounds associated with the specified pathway.

There may be more than one spot associated with the gene. This may be due to different genes being identified with this gene (e.g. isoforms), or due to different probes on the array platform being associated with the gene, but having incompatible transcriptional profiles with each other.



EXPRESSION EXPERIMENT

EXPERIMENTS
ETHINYLESTRA-3d-10mg/kg-LI-RATM-RU1
LOVASTATIN-3d-450mg/kg-LI-RATM-RU1

This panel allows you to select among experiments from the list you specified in your **PATHWAY VISUALIZATION** query.

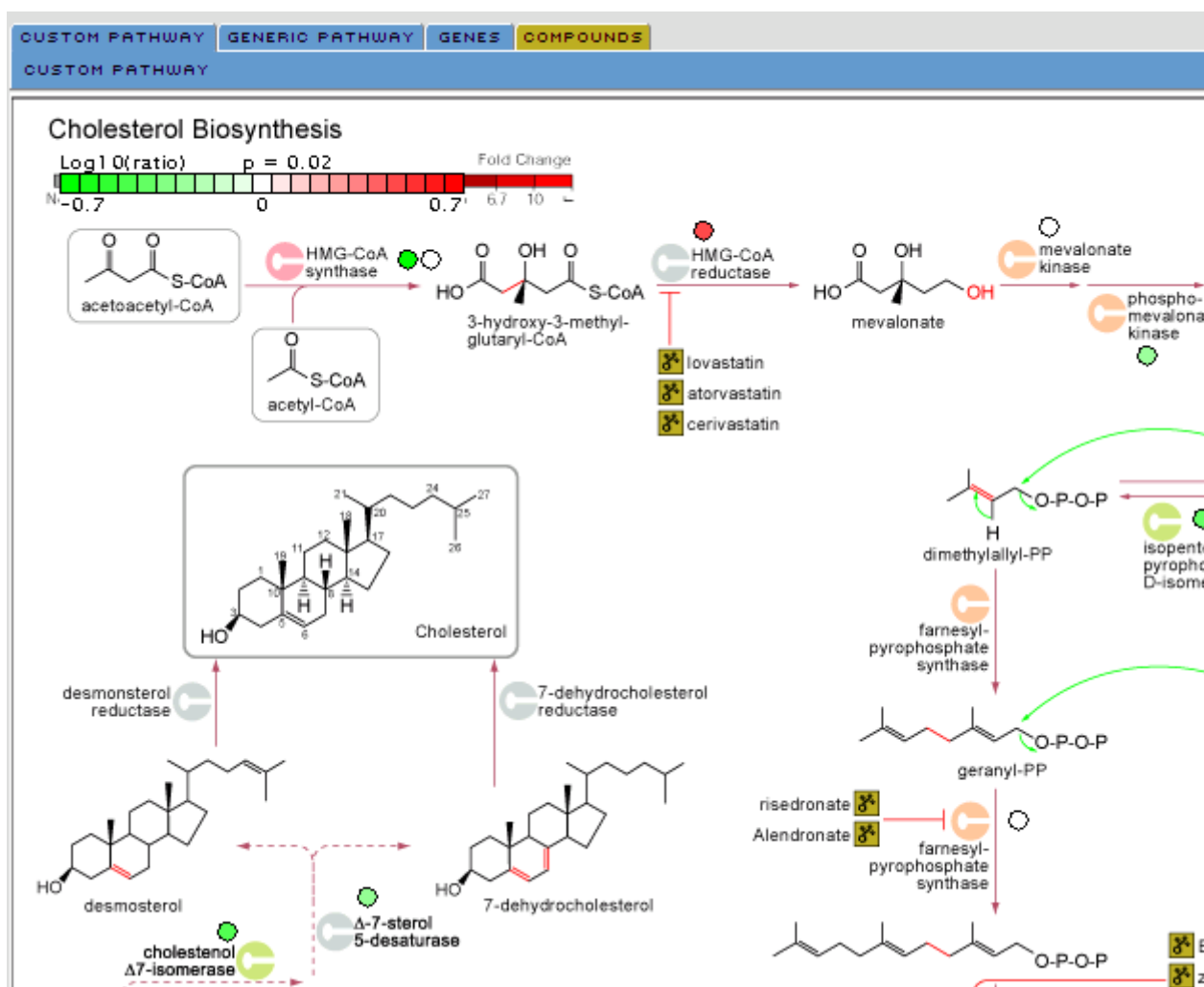
Pathway Visualization Tabs

CUSTOM PATHWAY	Displays the DrugMatrix rendering of the specified gene pathway with the gene expression data.
GENERIC PATHWAY	Displays the DrugMatrix rendering of the pathway.
GENES	Displays a list of genes, found in the DrugMatrix database, that are in the specified pathway.
COMPOUNDS	Displays a list compounds associated with, or known to affect, the specified pathway.

Pathway Visualization Tool - Custom Pathway Panel

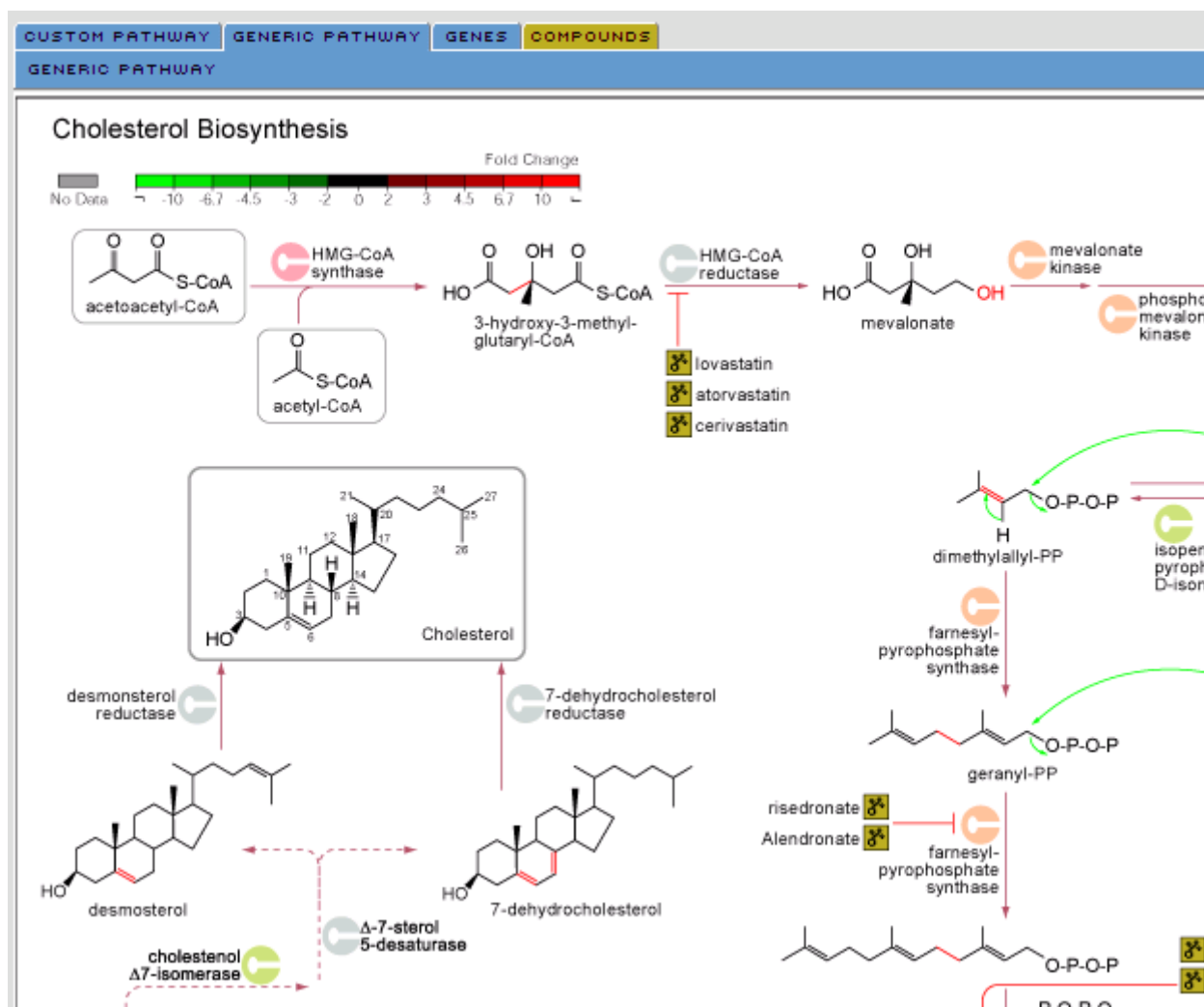
The **CUSTOM PATHWAY** panel displays a pathway map (illustration) overlaid with heat map coloration over genes indicating the expression changes. Intensity of color (darker or lighter red or green) reflects the degree of up or down regulation.

If you mouse position the cursor over a spot, a hover will appear showing its gene name. The spot is also a hyperlink to a **GENE** report. The same behavior applies to the compound icons.



Pathway Visualization Tool - Generic Pathway Panel

The **GENERIC PATHWAY** panel displays the image for the specified pathway. The image is a standard rendering of the hand curated pathway map.



Pathway Visualization Tool - Gene Panel

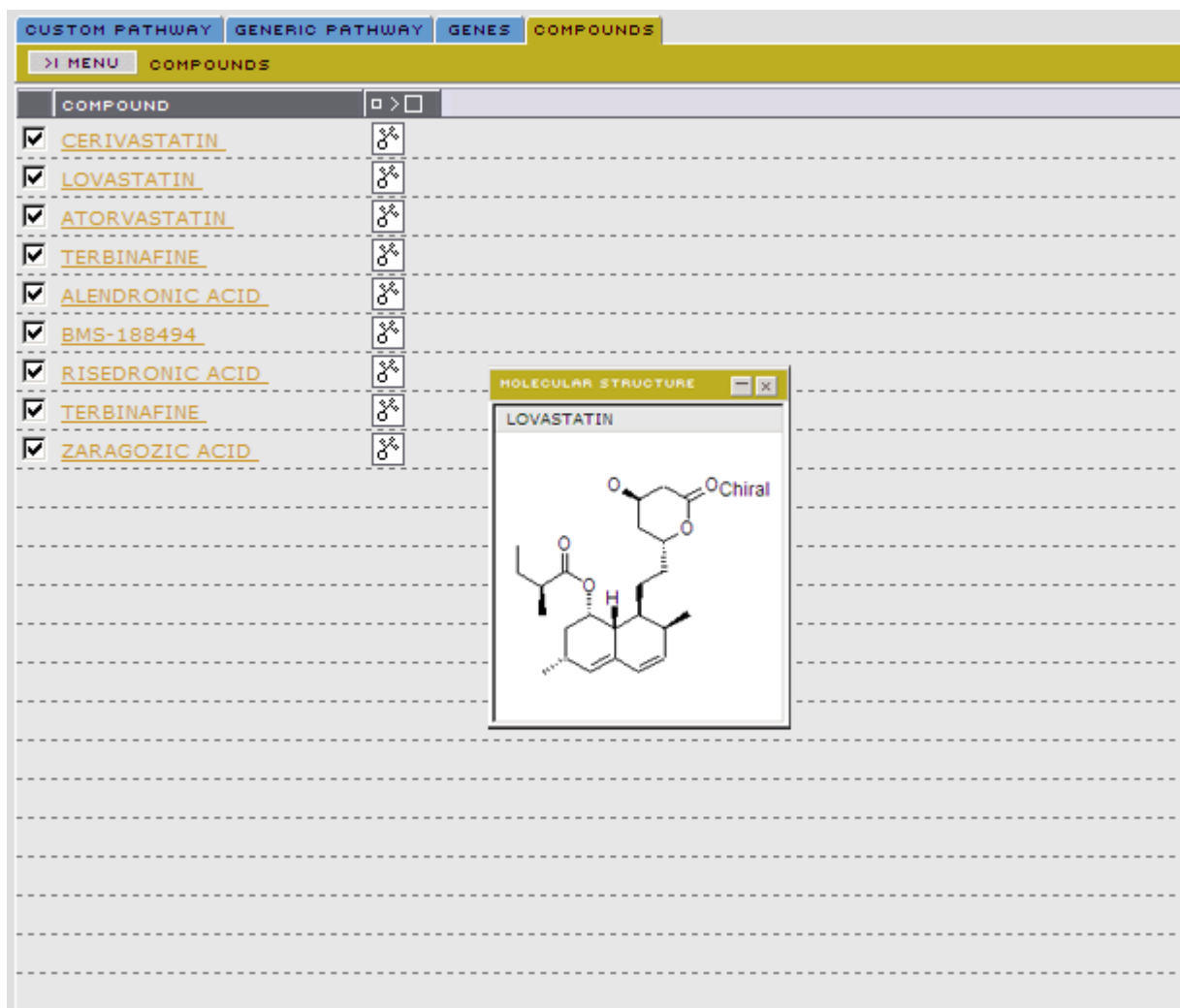
The **GENE** panel displays a list of genes, found in the DrugMatrix database, that are in the pathway for the specified gene. Gene names in this list are links which will populate a **GENE** domain report.












GENE
<input checked="" type="checkbox"/> 2,3-oxidosqualene: lanosterol ...
<input checked="" type="checkbox"/> 2,3-oxidosqualene: lanosterol ...
<input checked="" type="checkbox"/> 2,3-oxidosqualene: lanosterol ...
<input checked="" type="checkbox"/> mevalonate pyrophosphate de...
<input checked="" type="checkbox"/> isopentenyl-diphosphate delta...
<input checked="" type="checkbox"/> sterol-C5-desaturase (fungal E...
<input checked="" type="checkbox"/> phenylalkylamine Ca2+ antag...
<input checked="" type="checkbox"/> 7-dehydrocholesterol reductas...
<input checked="" type="checkbox"/> Phosphomevalonate kinase (H...
<input checked="" type="checkbox"/> farenstyl diphosphate synthase...
<input checked="" type="checkbox"/> farenstyl diphosphate synthase...
<input checked="" type="checkbox"/> farenstyl diphosphate synthase...
<input checked="" type="checkbox"/> 3-hydroxy-3-methylglutaryl-Co...
<input checked="" type="checkbox"/> squalene epoxidase (D37920 ...

Pathway Visualization Tool - Compounds Panel

The **COMPOUNDS** panel displays a list of compounds, found in the DrugMatrix database, that are associated with, or known to affect, the specified pathway. Click on the compound image icon for an expanded image of any compound in the list.

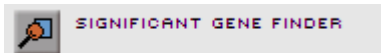


The screenshot shows the 'COMPOUNDS' panel of the Pathway Visualization Tool. The panel has a navigation bar with tabs for 'CUSTOM PATHWAY', 'GENERIC PATHWAY', 'GENES', and 'COMPOUNDS'. Below the navigation bar is a 'MENU' button and the text 'COMPOUNDS'. The main area is a table with a 'COMPOUND' header and a search icon. The table lists the following compounds, each with a checked checkbox and a small image icon:

COMPOUND	Image Icon
<input checked="" type="checkbox"/> CERIVASTATIN	
<input checked="" type="checkbox"/> LOVASTATIN	
<input checked="" type="checkbox"/> ATORVASTATIN	
<input checked="" type="checkbox"/> TERBINAFINE	
<input checked="" type="checkbox"/> ALENDRONIC ACID	
<input checked="" type="checkbox"/> BMS-188494	
<input checked="" type="checkbox"/> RISEDRONIC ACID	
<input checked="" type="checkbox"/> TERBINAFINE	
<input checked="" type="checkbox"/> ZARAGOZIC ACID	

A pop-up window titled 'MOLECULAR STRUCTURE' is open, showing the chemical structure of Lovastatin. The structure is a complex polycyclic molecule with a lactone ring and a side chain. The word 'Chiral' is written in purple next to the structure.

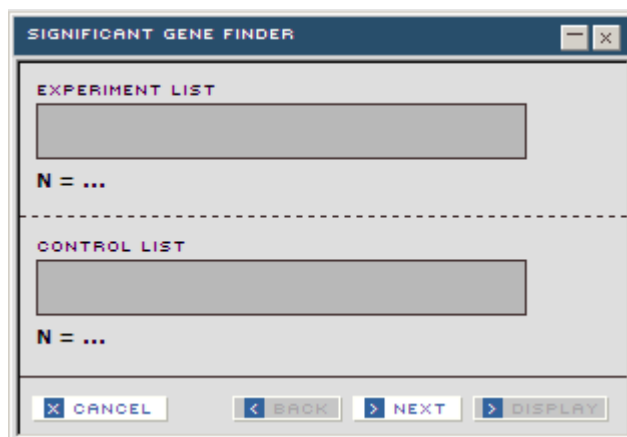
Data Visualization: Significant Gene Finder



This tool extracts the most significant set of genes for a list of experiments and can also use another list as an optional control. The analysis extracts genes that are most consistently perturbed within the set of experiments. The optional control set can be used when determining differences between related compounds.

You can select filters to exclude individual expression readings that are not significant (**p value** > 0.02), the direction of the regulation and the maximum size of the gene list.

The resulting gene list will be displayed with a score that indicates how consistently the expression differs from the control value (or zero if no control) and the direction of the expression change.



EXPERIMENT LIST

The list of expression experiments you wish to examine for significant genes.

N = ...

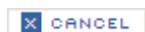
The number of records in the named list.

CONTROL LIST

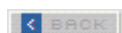
The list of experiments to use as a control population. The control list is optional. This feature can be useful when comparing similar sets for small differences.

N = ...

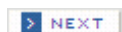
The number of records in the named list.



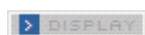
Cancel without generating the data visualization.



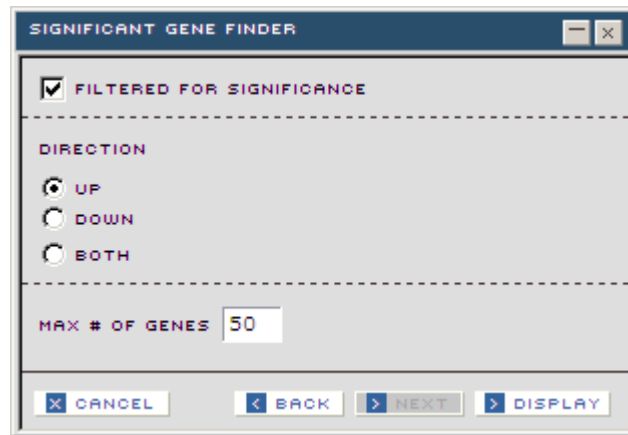
Go to previous dialog window. Not active on this dialog.



Go to next dialog window.



Create and display the data visualization. Not active on this dialog window.



FILTERED FOR SIGNIFICANCE

Filters for an expression ratio **p value** < 0.02 (the filter sets gene expression value to 0 if the experimental value is not significantly perturbed at the 0.02 probability value.)

DIRECTION

Specify the direction of perturbation to filter for.

UP

Filter for genes that are significantly up regulated in the specified list of expression experiments.

DOWN

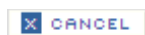
Filter for genes that are significantly down regulated in the specified list of expression experiments.

BOTH

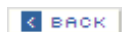
Filter for genes that are significantly perturbed (either up or down regulated) in the specified list of expression experiments.

MAX # OF GENES

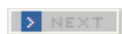
Specify the maximum number of most significantly perturbed genes in the selected list of expression experiments.



Cancel without generating the data visualization.



Go to previous dialog window.



Go to next dialog window. Not active on this dialog.



Create and display the data visualization.

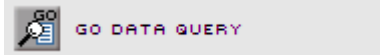
Significant Gene Finder Dataview

This panel displays a list of genes that were significantly perturbed in the specified list of expression experiments. Each gene in the list is a link that will populate a **GENE** Domain Report.

SIGNIFICANT GENE FINDER			
SIGNIFICANT GENE FINDER			
	GENE	SCORE	DIRECTI
<input checked="" type="checkbox"/>	vanin 1 (AW141928 PROBE1,1389253 at)	0.866...	UP
<input checked="" type="checkbox"/>	enoyl-Coenzyme A, hydratase/3-hydroxyacyl Coenzyme A dehydrogenase (1...	0.829...	UP
<input checked="" type="checkbox"/>	acetyl-Coenzyme A acyltransferase 1 (peroxisomal 3-oxoacyl-Coenzyme A th...	0.782...	UP
<input checked="" type="checkbox"/>	peroxisomal biogenesis factor 11A (1387740 at,AJ224120 PROBE1)	0.779...	UP
<input checked="" type="checkbox"/>	pyruvate dehydrogenase kinase, isoenzyme 4 (1369150 at,AF034577 PROB...	0.692...	UP
<input checked="" type="checkbox"/>	hydroxysteroid (17-beta) dehydrogenase 7 (NM 017235 PROBE1,1387233 a...	0.689...	UP
<input checked="" type="checkbox"/>	mevalonate (diphospho) decarboxylase (1368020 at,U53706 at,U53706 PR...	0.688...	UP
<input checked="" type="checkbox"/>	3-hydroxy-3-methylglutaryl-Coenzyme A reductase (BF555949 PROBE1,1375...	0.673...	UP
<input checked="" type="checkbox"/>	carnitine acetyltransferase (1371886 at,AI411979 PROBE1)	0.640...	UP
<input checked="" type="checkbox"/>	farnesyl diphosphate synthase (M89945mRNA at,1367667 at,rc AI180442 a...	0.637...	UP
<input checked="" type="checkbox"/>	isopentenyl-diphosphate delta isomerase (rc AI176778 at,AF003835 at,136...	0.631...	UP
<input checked="" type="checkbox"/>	ADIR1 (DBSS) (AW918222 PROBE1)	0.630...	UP
<input checked="" type="checkbox"/>	mevalonate kinase (M29472 at,M29472 PROBE1)	0.617...	UP
<input checked="" type="checkbox"/>	sterol-C4-methyl oxidase-like (1368275 at,rc AI172293 at,D50559 PROBE1)	0.612...	UP
<input checked="" type="checkbox"/>	ultraviolet B radiation-activated UV96 (BE114586 PROBE1,1388674 at)	0.598...	UP
<input checked="" type="checkbox"/>	cytochrome P450, subfamily 51 (AB004096 at,NM 012941 PROBE1,1387020...	0.595...	UP
<input checked="" type="checkbox"/>	2,3-oxidosqualene: lanosterol cyclase (1372973 at,U31352 at,D45252 s at...	0.589...	UP
<input checked="" type="checkbox"/>	3-hydroxy-3-methylglutaryl-Coenzyme A reductase (1387848 at NM 012134	0.585...	UP

GENE	The list of genes that were significantly perturbed in the specified list of expression experiments.
SCORE	A measure of consistency of expression changes between the experiment and control.
DIRECTION	The direction of regulation for the gene (i.e. up or down).

Data Visualization: GO Data Query



The **GO DATA QUERY** tool allows you to analyze a specified gene list using Gene Ontology annotations to find significantly over-represented terms.

GENE LIST:

The **GENE LIST** for the analysis.

N = ...

The number of genes in the specified list.

MAX P VALUE

The maximum **p value** for any of the displayed **GO** nodes. Nodes greater than this value will be filtered out.

GENE UNIVERSE

This drop down list enables the selection of the chip type to use as the background distribution of genes and **GO** terms for the sample list.

Cancel without generating the data visualization.

Create and display the data visualization.

GO Data Visualization Tabs

MOLECULAR

Molecular function of the selected genes.

CELLULAR

Cellular Location the selected genes.

BIOLOGICAL

Biological Function the selected genes.

GO Data Query - Dataview

The **GO DATA QUERY** Dataview consists of a list of genes on the right, and three panels for three Gene Ontology hierarchies: molecular function, cellular location and biological process.

GO terms are structured as a tree, with the most specific terms at the leaves. Therefore, most of the genes associated with a more specific term are a subset of the genes in the more general parent term. The bold font is used for the most significant term AND the parent terms that lead to that term. Otherwise a plain font is used.

The visualizations in DrugMatrix represent the tree with its root at the upper left corner, and each child term below its parent and indented. The branches can be exposed or hidden by clicking on the icon to the left of the term. Position the cursor over a node to display a hover with the term's annotation.

Each node displays the label of the GO term and 2 values in square brackets. The first value is the number of genes in the query gene list that intersect with that term. The second term is the **p value** of the intersection, after multiple testing correction has been applied.

The gene display table to the right shows all the genes in the list. The name of the imported list is displayed in the table header. Genes in the selected GO node are checked. You can sort this list and save it as with other lists in DrugMatrix.

GO Data Query Tool - Molecular Panel

The view shows a partial tree with the most significant GO terms associated with molecular function. For a description of the DrugMatrix **GO DATA VISUALIZATION**, see [‘GO Data Query - Dataview’](#) on the previous page.

The screenshot displays the 'GO DATA VISUALIZATION' interface. On the left, a tree structure shows the hierarchy of GO terms under 'BIOLOGICAL FUNCTION TAXONOMY' and 'BIOLOGICAL_PROCESS'. The most significant terms are expanded, showing sub-categories like 'metabolism', 'lipid metabolism', and 'lipid biosynthesis'. On the right, a 'GENE' panel lists the corresponding genes for each term, such as '3-hydroxy-3-methylglutaryl-CoA synthetase long-chain', 'acyl-Coenzyme A oxidase 1', and 'sterol carrier protein 2'.

GO DATA VISUALIZATION

MOLECULAR CELLULAR BIOLOGICAL

BIOLOGICAL FUNCTION TAXONOMY

BIOLOGICAL_PROCESS

biological_process [41, 1.0]

physiological process [41, 0.0080]

metabolism [41, 1.01E-9]

alcohol metabolism [14, 1.482E-11]

sterol metabolism [14, 0.0]

cholesterol metabolism [14, 0.0]

sterol biosynthesis [14, 0.0]

biosynthesis [23, 1.295E-10]

macromolecule biosynthesis [23, 1.004E-11]

lipid biosynthesis [23, 0.0]

fatty acid biosynthesis [9, 1.025E-8]

isoprenoid biosynthesis [5, 9.376E-9]

steroid biosynthesis [14, 0.0]

sterol biosynthesis [14, 0.0]

cholesterol biosynthesis [14, 0.0]

organic acid biosynthesis [9, 1.109E-8]

coenzyme and prosthetic group metabolism [5, 0.05]

coenzyme metabolism [5, 0.063]

lipid metabolism [41, 0.0]

lipid biosynthesis [23, 0.0]

fatty acid biosynthesis [9, 1.025E-8]

isoprenoid biosynthesis [5, 9.376E-9]

steroid biosynthesis [14, 0.0]

sterol biosynthesis [14, 0.0]

cholesterol biosynthesis [14, 0.0]

fatty acid metabolism [27, 0.0]

fatty acid biosynthesis [9, 1.025E-8]

acyl-CoA metabolism [3, 0.028]

GENE

3-hydroxy-3-methylglutaryl-CoA synthetase long-chain [1, 0.028]

mevalonate (diphospho) decarboxylase [1, 0.028]

acyl-Coenzyme A oxidase 1, long-chain [1, 0.028]

isopentenyl-diphosphate delta-isomerase [1, 0.028]

hydroxyacyl-Coenzyme A dehydratase [1, 0.028]

carnitine palmitoyltransferase 2 [1, 0.028]

short chain acyl-coenzyme A oxidase [1, 0.028]

3-hydroxyacyl-Coenzyme A dehydratase [1, 0.028]

acyl-Coenzyme A dehydratase [1, 0.028]

sterol-C4-desaturase (human) [1, 0.028]

phenylalanyl-Glutamate Ca2+-antagonist [1, 0.028]

ATP-binding cassette, sub-family A, member 1 [1, 0.028]

Phosphomevalonate kinase (Hs) [1, 0.028]

7-dehydrocholesterol reductase [1, 0.028]

farnesyl diphosphate synthase [1, 0.028]

hydroxysteroid (17-beta) dehydrogenase [1, 0.028]

carnitine palmitoyltransferase [1, 0.028]

3-hydroxy-3-methylglutaryl-CoA synthetase long-chain [1, 0.028]

catalase [1, 0.028]

acyl-CoA synthetase long-chain [1, 0.028]

acyl-Coenzyme A oxidase 1, long-chain [1, 0.028]

sterol carrier protein 2 [1, 0.028]

farnesyl diphosphate farnesyl transferase [1, 0.028]

sterol carrier family 25 (carnitine palmitoyltransferase II) [1, 0.028]

coumarin 4-hydroxylase [1, 0.028]

acyl-CoA synthetase long-chain [1, 0.028]

acyl-Coenzyme A hydratase [1, 0.028]

GO Data Query Tool - Cellular

The view shows a partial tree with the most significant GO terms associated with cellular function. For a description of the DrugMatrix **GO DATA VISUALIZATION**, see [‘GO Data Query - Dataview’ on page 212](#).

The screenshot displays the 'GO DATA VISUALIZATION' interface. On the left, a hierarchical tree shows the following structure:

- cellular_component [38, 1.0]
 - cell [38, 0.052]
 - intracellular [37, 9.981E-6]
 - cytoplasm [37, 9.599E-13]
 - microbody [13, 0.0]
 - peroxisome [13, 0.0]
 - mitochondrion [18, 1.272E-9]
 - membrane [16, 1.0]
 - outer membrane [4, 0.0070]

On the right, a 'GENE' list is shown with the following entries:

- acyl-Coenzyme A oxidase 3, B...
- isopentenyl-diphosphate delta...
- ATP-binding cassette, sub-fam...
- phosphomevalonate kinase 1H...
- catalase
- acyl-CoA synthetase long-chain...
- acyl-Coenzyme A oxidase 1, D...
- sterol carrier protein 2
- acyl-CoA synthetase long-chain...
- acyl-Coenzyme A hydratase/...
- mevalonate kinase
- ATP-binding cassette, sub-fam...
- acetyl-Coenzyme A acyltransfer...
- 2,3-bisdoxqualene lanosterol...
- mevalonate (diphospho) decar...
- hydroxyacyl-Coenzyme A dehy...
- carnitine palmitoyltransferase 2
- short chain acyl-coenzyme A de...
- 1,2-hydroxyacyl-Coenzyme A...
- acetyl-Coenzyme A dehydrogen...
- sterol-C5-desaturase (fungal)...
- phenylethylamine Ca2+ anti...
- 7-dehydrocholesterol reductase
- isoprenyl diphosphate synthase
- hydroxysteroid (17-beta) dehy...
- carnitine palmitoyltransferase...
- 3-hydroxy-2-methylglutaryl-Co...

GO Data Query Tool - Biological

The view shows a partial tree with the most significant GO terms associated with biological process. For a description of the DrugMatrix **GO DATA VISUALIZATION**, see [‘GO Data Query - Dataview’ on page 212](#).

The screenshot displays the 'GO DATA VISUALIZATION' interface. On the left, a tree structure shows the hierarchy of GO terms under the 'BIOLOGICAL' tab. The most significant terms are expanded, showing sub-categories and their associated counts and p-values. On the right, a list of genes is shown, each with a checkbox and a link to its details page.

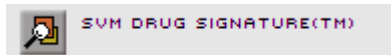
MOLECULAR FUNCTION TAXONOMY

- molecular_function [41, 1.0]
 - binding [14, 1.0]
 - metal ion binding [7, 1.0]
 - magnesium ion binding [7, 7.312E-4]
 - catalytic activity [40, 0.0]
 - isomerase activity [4, 0.305]
 - intramolecular oxidoreductase activity [3, 0.216]
 - intramolecular oxidoreductase activity, transposing C=C bonds [3, 0.014]
 - ligase activity [5, 0.569]
 - ligase activity, forming carbon-sulfur bonds [3, 1.038E-6]
 - fatty-acid ligase activity [5, 8.618E-8]
 - long-chain-fatty-acid-CoA ligase activity [5, 1.41E-7]
 - lyase activity [8, 4.756E-5]
 - carbon-oxygen lyase activity [4, 0.027]
 - hydro-lyase activity [4, 0.03]
 - enoyl-CoA hydratase activity [4, 4.794E-5]
 - long-chain-enoyl-CoA hydratase activity [2, 0.052]
 - oxidoreductase activity [17, 9.847E-9]
 - oxidoreductase activity, acting on CH-OH group of donors [7, 1.428E-4]
 - oxidoreductase activity, acting on the CH-OH group of donors, NAD or NADP as acceptor [7, 1.981E-4]
 - 3-hydroxyacyl-CoA dehydrogenase activity [5, 1.41E-7]
 - oxidoreductase activity, acting on the CH-CH group of donors [7, 3.503E-8]
 - acyl-CoA dehydrogenase activity [3, 0.0090]
 - oxidoreductase activity, acting on the CH-CH group of donors, oxygen as acceptor [3, 0.0060]
 - transferase activity [15, 0.0080]
 - transferase activity, transferring acyl groups [11, 4.846E-11]

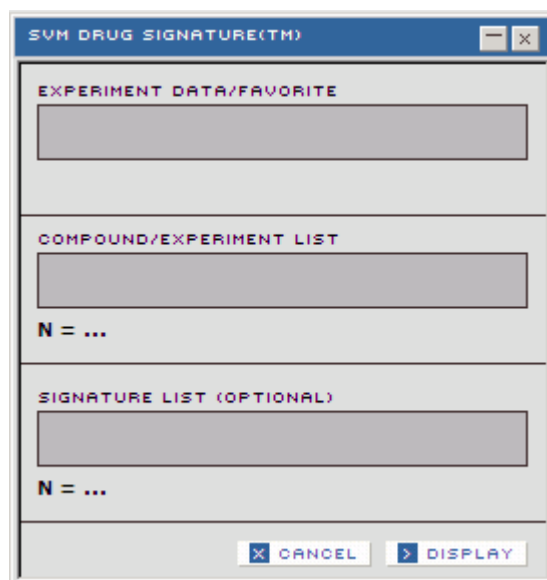
GENE

- acyl-Coenzyme A oxidase 3, B...
- isopentenyl-diphosphate delta...
- ATP-binding cassette, sub-fam...
- phosphomevalonate kinase 1H...
- catalase
- acyl-CoA synthetase long-chain...
- acyl-Coenzyme A oxidase 1, D...
- sterol carrier protein 2
- acyl-CoA synthetase long-chain...
- enoyl-Coenzyme A hydratase...
- mevalonate kinase
- ATP-binding cassette, sub-fam...
- acetyl-Coenzyme A acyltransfer...
- 2,3-oxidosqualene lanosterol...
- mevalonate (diphospho) decar...
- hydroxyacyl-Coenzyme A dehy...
- gamma-linolenic palmitoyltransferase 2
- short chain acyl-coenzyme A d...
- 1,3-hydroxyacyl-Coenzyme A...
- acetyl-Coenzyme A dehydrogen...
- sterol-C5-desaturase (fungal S...
- phenylethylamine Ca2+ anti...
- 7-dehydrocholesterol reductase
- acetyl diphosphate synthase
- hydroxysteroid (17-beta) dehy...
- gamma-linolenic palmitoyltransferase...
- 3-hydroxy-2-methylglutaryl-Co...

Data Visualization: SVM Drug Signature™



This tool allows you to generate a view of SVM signatures displayed as a histogram for the query experiment and the control list. The histogram shows the scalar product value (>0 is significant).



EXPERIMENT DATA/ FAVORITE

A **DATA OBJECT** (See [‘Data Object’ on page 225](#)) or a **FAVORITE** experiment list.

COMPOUND/ EXPERIMENT LIST

A list of experiments or compounds for comparison.

N = ...

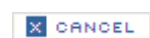
The number of records in the named list.

SIGNATURE LIST (OPTIONAL)

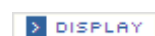
A filter for the signatures to test. You can create signature lists using the **SEARCH** tool.

N = ...

The number of records in the named list.



Cancel without generating the data visualization.



Generate and display the **SVM Drug Signature™** data visualization.

NOTE: Although you can filter thru all signatures, by leaving the **SIGNATURE LIST** field empty, it is advisable to use a defined signature list, since a filter of the entire DrugMatrix **Signature** library is quite time consuming.

Drug Signature™ SVM Histogram Visualization Tabs

SIGNATURE

Displays the list of signatures specified in the optional **SIGNATURE LIST** field.

**COMPOUND/
EXPERIMENT**

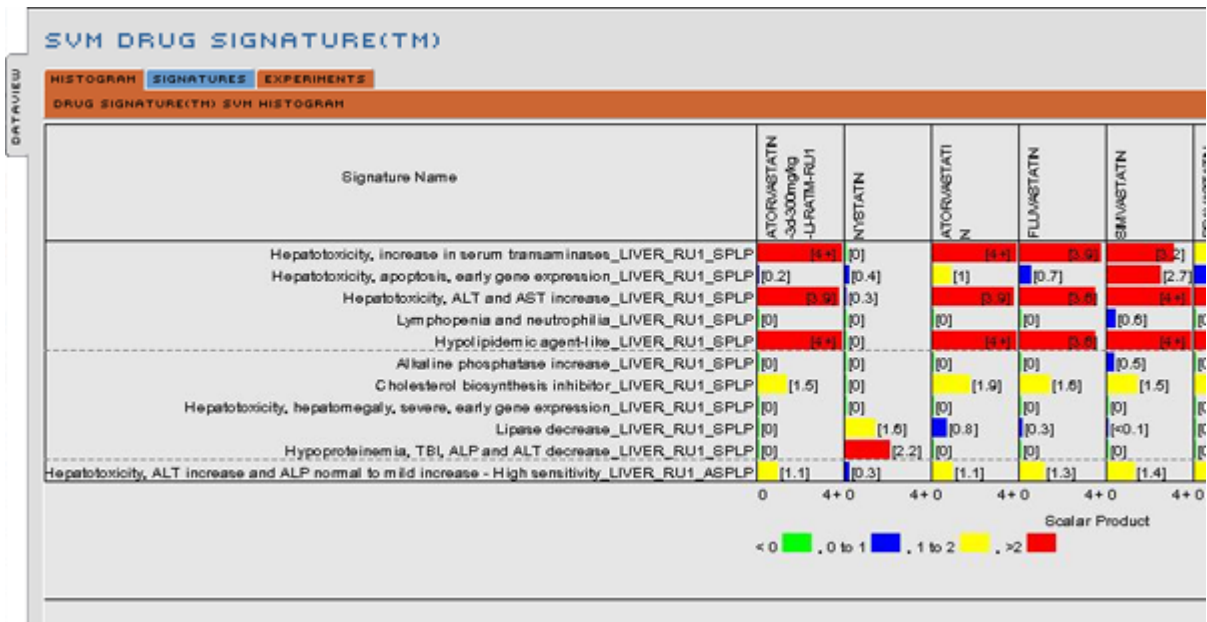
Displays the list of compounds or experiments (experiments if an experiment list used) specified in the **COMPOUND/EXPERIMENT LIST** field.

Drug Signature™ SVM Histogram Visualization - Histogram Panel

This visualization displays the score for each SVM signature technology and experiment or compound that is used to build the display.

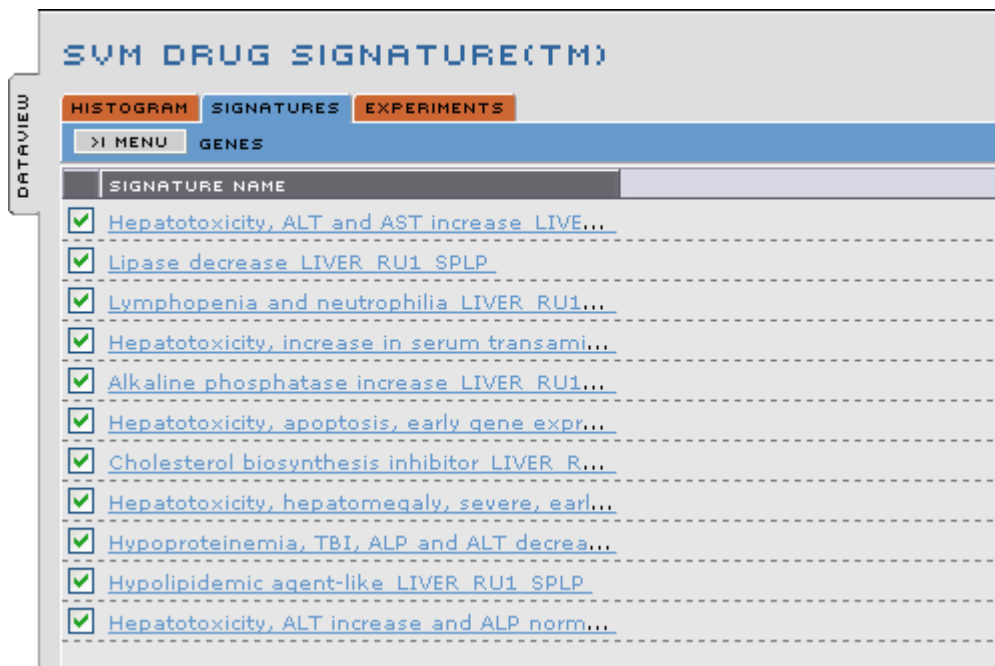
All scores above 0 have some significance, although scores exceeding 1.0 are preferred (The higher the score, the stronger the match to the signature pattern).

The display uses a histogram with the score value in brackets to the right of the bar. The histogram bars are color coded to the scale at the bottom of the display (not shown in this image).



Drug Signature™ SVM Histogram Visualization - Signature Panel

This panel displays the list of signatures specified in the optional **SIGNATURE LIST** field of the **Drug Signature (TM) SVM Histogram** dialog window (or the full list of signatures in the library if no list specified).



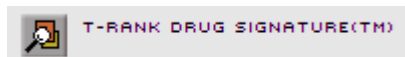
NOTE: The initial order of genes in this list reflects the order of genes in the **HISTOGRAM** panel of this **DATAVIEW**. If you deselect records in this list and/or sort the list, the order will no longer be the same as on the **HISTOGRAM** panel.

Drug Signature™ SVM Histogram Visualization - Experiments Panel

This panel displays the list of compounds specified in the **COMPOUND/EXPERIMENT LIST** field of the **Drug Signature (TM) SVM Histogram** dialog window. If an experiment list is used, the experiment field is also populated.

EXPERIMENT	COMPOUND
<input checked="" type="checkbox"/> -	LOVASTATIN
<input checked="" type="checkbox"/> -	MEVASTATIN
<input checked="" type="checkbox"/> -	SIMVASTATIN
<input checked="" type="checkbox"/> -	NYSTATIN
<input checked="" type="checkbox"/> -	PRAVASTATIN
<input checked="" type="checkbox"/> -	FLUVASTATIN
<input checked="" type="checkbox"/> -	ATORVASTATIN
<input checked="" type="checkbox"/> -	CERIVASTATIN

Data Visualization: T-Rank Drug Signature™



This tool allows you to generate a heatmap view of the signature hits for the experiments and compounds in the two input lists. If a compound list is used, the maximum value for that compound, based on the experiments using that compound, is used. The ordering of data is based on the highest signature hit for the query.

**EXPERIMENT DATA/
FAVORITE**

A **DATA OBJECT** (See [‘Data Object’ on page 225](#)) or a **FAVORITE** experiment list.

**COMPOUND/
EXPERIMENT LIST**

A list of experiments or compounds as controls.

N = ...

The number of records in the named list.

**SIGNATURE LIST
(OPTIONAL)**

A filter for the signatures to test. You can create signature lists using the **SEARCH** tool.

N = ...

The number of records in the named list.

CANCEL

Cancel without generating the data visualization.

GO

Generate and display the **T-Rank Drug Signature™** data visualization.

NOTE: Although you can filter thru all signatures, by leaving the **SIGNATURE LIST** field empty, it is advisable to use a defined signature list, since a filter of the entire DrugMatrix **Signature** library is quite time consuming.

Drug Signature™ T-Rank Heatmap Visualization Tabs

SIGNATURE

Displays a list of signatures.

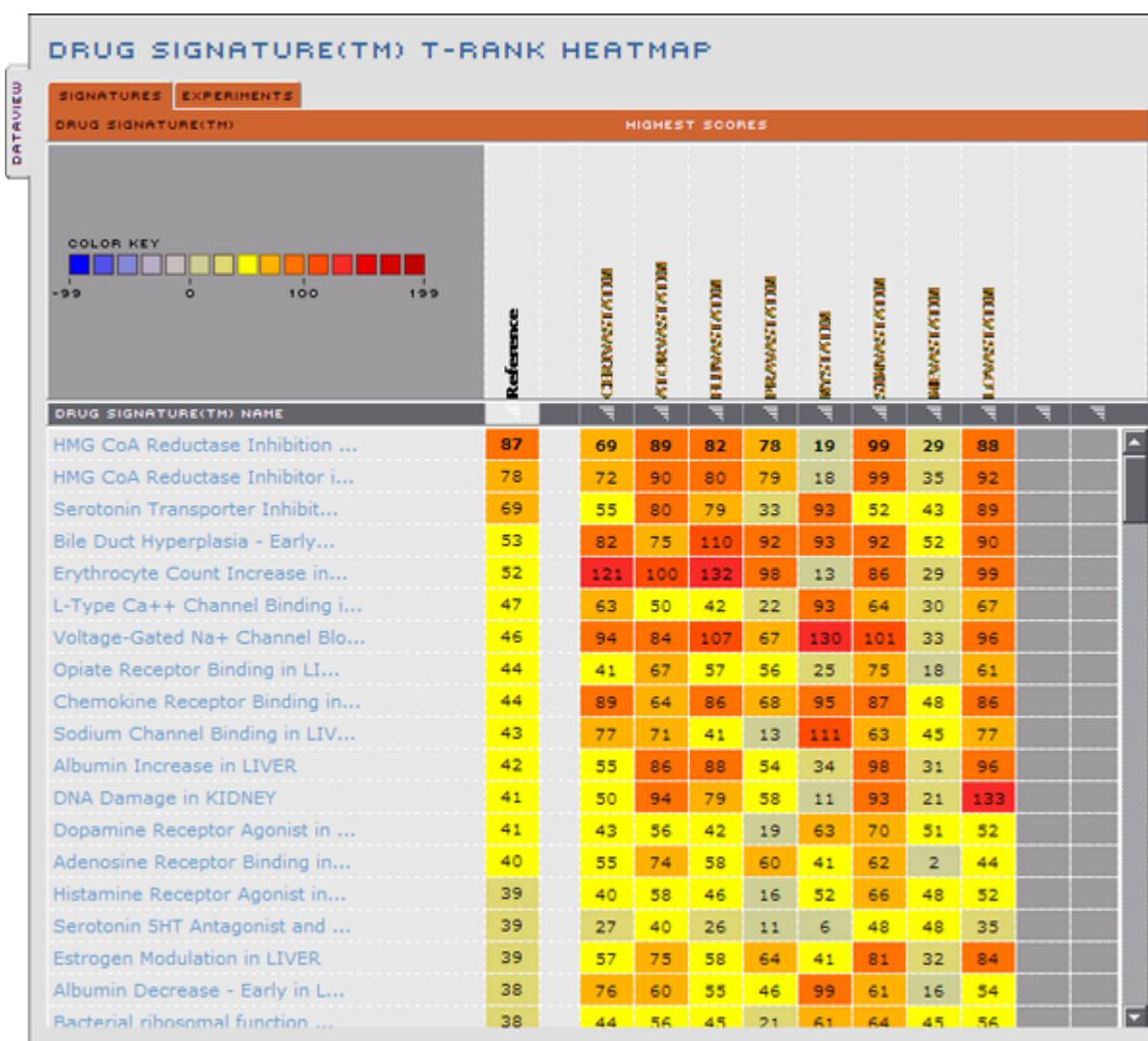
COMPOUND/ EXPERIMENT

Displays a list of compounds and/or experiments (experiments if an experiment list presented). The order of this list is based on the highest signature hit for the query.

Drug Signature™ T-Rank Heatmap Visualization - Signature Panel

This matrix displays both the score value and the heatmap using the color scale shown in the **COLOR KEY**.

The signatures are ordered by the descending score order for the query. Scores very close or above 100 mean a strong match to signature pattern. Positioning the cursor over a value pops up a hover to show details of the experiment.



Drug Signature™ T-Rank Heatmap Visualization - Compound/Experiment Panel

This panel displays the list of compounds specified in the **COMPOUND/EXPERIMENT LIST** field of the **Drug Signature (TM) T-Rank Heatmap** dialog window. The signatures are ordered by the descending score order for the query.

The screenshot shows a software interface titled "DRUG SIGNATURE(TM) T-RANK HEATMAP". It features a "DATAVIEW" sidebar on the left and a main content area. The main area has tabs for "SIGNATURES" and "EXPERIMENTS", with "EXPERIMENTS" selected. Below the tabs is a "MENU" section with "COMPOUNDS/EXPERIMENTS" selected. The main content area displays a table with the following columns: "COMPOUND NAME" and a column with icons. The table contains the following rows:

COMPOUND NAME	Icon
<input checked="" type="checkbox"/> CERIVASTATIN	
<input checked="" type="checkbox"/> ATORVASTATIN	
<input checked="" type="checkbox"/> FLUVASTATIN	
<input checked="" type="checkbox"/> PRAVASTATIN	
<input checked="" type="checkbox"/> NYSTATIN	
<input checked="" type="checkbox"/> SIMVASTATIN	
<input checked="" type="checkbox"/> MEVASTATIN	
<input checked="" type="checkbox"/> LOVASTATIN	
<input checked="" type="checkbox"/>	
<input checked="" type="checkbox"/>	

Glossary

%Inhibition

The extent (in %) a compound inhibits an enzymereaction, the binding of a ligand to a protein, or the growth of a cell culture.

3DMI

A proprietary method of comparing two molecularstructures using their three dimensional shapes and physico-chemical properties.

Accession

Refers to accession numbers from the GenBank® database (NIHdatabase of all publicly available DNA sequences) for query gene.

(<http://www.ncbi.nlm.nih.gov/Genbank/GenbankOverview.html>)



Avg Signal Intensity

The average normalized signal intensity of a probe when measured across all the arrays used in an experiment.

Confidence Interval

The range of values for the log expression ratio that lay within a number of standard errors (e.g. 99.5% probability for 2.8 standard errors).

Data Object

A persistent data object is an item in the workspace that encapsulates all data pertaining to a given domain or data view. This data is separate from DrugMatrix database data and can not currently be included in standard or advanced searches. It can however be used by specific tools (to generate a dataview). Data Objects appear in the Workspace area with the  icon attached. When a data object is dragged to the display list icon  in the Workspace area, the information from that list will populate an Expression Domain Report.

Detail Report

The panels that appear on the right of a Domain Report, as well as buttons that appear just below the name of the query item. Detail Reports present information from scientific literature, reference material and online databases.

Dendrogram

A dendrogram is a representation of a hierarchically clustered data set. The representation is a tree, with nodes and leaves. Each node has 2 branches that terminate in either a another node or a leaf. The nodes are positioned relative to the scale to show similarity. In this case, the Pearson's correlation coefficient metric is used, which has a value of 1.0 when the two branches are exactly correlated. The similarity between any 2 leaves is represented by the similarity value of first common node in the tree.

Domain Report

Top level reports that represent each of the DrugMatrix data domains (**GENE**, **COMPOUND**, **ASSAY**, **EXPRESSION**, **PATHWAY**, and **EXPRESSION STUDY**). Each Domain Report contains a subset of **Chemogenomic Data Reports** and **Detail Reports** that present cross referenced experimental data from the proprietary DrugMatrix database and curated information from the scientific literature, reference material and online databases.

Dose Response

A chart of the effects of an experimental compound, at a known time, on the expression profile over several compound doses. The chart shows the major gene changes observed.

Chemogenomic Data Reports

Cross referenced reports that present all relevant chemogenomic data from the proprietary DrugMatrix database, that pertains to the query item.

Fold Change

The number of times the compound treated expression level differs from the untreated control. Fold values are within the ranges $-\infty < x < -1$ or $1 < x < \infty$

GO (Gene Ontology)

Refers to terminology standardized by the Gene Ontology™ Consortium.
(<http://www.geneontology.org/>)

IC50

The concentration of compound that inhibits an enzyme activity to 50% of its normal level in the context of a bioassay designed to measure this enzyme's activity.

Intensity

A metric that indicates the level of the average spot reading for all the arrays in the experiment within the context of the expected distribution of values.

KI

“Ki” is a measure of the extent an inhibitor inhibits the function of a protein. It is the equilibrium constant for the dissociation of protein-inhibitor complexes.

Log Ratio

The log of the ratio (base 10) of experimental conditions (compound treated) to control (no treatment).

MOLSIM

A proprietary algorithm for determining molecular similarity between structures.

Negative Class:

The diverse set of experiments used as a control to test the positive class.

Pathway

DrugMatrix pathways are hand curated to reflect current scientific understanding of the biological processes and their regulations. Classical metabolic, general signal transduction, and cutting-edge regulatory pathways are included.

In addition to illustrating the genes/proteins involved in a specific process, DrugMatrix pathways illustrate the complex relationships among the genes/proteins within a cellular/physiological context, as well as, the biological outcomes from such relationships.

Genes on each pathway are mapped, where possible, to probes in the microarray platforms DrugMatrix supports, thus, allowing the visualization of gene expression changes of an experiment directly on the pathway drawings.

Pearson's Correlation Coefficient

Pearson's correlation measures the degree of linear relationship between two variables. Ranges are from +1 to -1. A correlation of +1 indicates a perfect positive linear relationship. A correlation of -1 indicates a perfect negative linear relationship. A value of $R = 0$ is random. $R = 0.95$ would be considered a good fit.

Positive Class:

This is the class that contains the experiments that identify the characteristic of interest.

Purity

A measure of how clean the sample is. DrugMatrix uses data provided by the compound supplier for purity. There are many different ways of measuring or estimating purity depending on the chemical properties of the compounds. Purity data provided by standard chemical suppliers is generally acceptable.

p value

The probability that the results observed can happen by chance.

Salt Form

Ionizable compounds are often prepared in a ionized form (salt) with counter ions such as hydrochloride, methane sulfonic acid, or sodium, in order to increase their water solubility. "Salt Form" refers to whether the sample used is a salt and what the counter ion is if it is a salt. Compounds prepared with no counter ions are called "Salt Free"

Score

A valuation measure specific to the report. For expressions it is the **p value** of the measurements (i.e. the log ratio and its standard error).

Selected Record

A table row on one of the Chemogenomic Report panels. The value of all table cells within a given row are directly associated. For example, the name and molecular structure of a specific compound used in a given experiment.

Search and List Area

Comprehensive tools to define very specific database queries and manage generated lists that are relevant to your research.

Sequence

The nucleotide sequence of the gene or the amino acid sequence of the gene product.

Signature

A Signature is a pattern of gene expression weights for a small set of genes that can be used to classify a set of common experiments reliably compared to the experiment population, or a defined set of control experiments.

Signatures can be used to find compounds that are similar to the query compound, more reliably than by using the full gene expression pattern. The content of a signature can also be used to provide understanding of key genes that are used to describe the characteristics of the experiments in the set.

SMILES

(Simplified Molecular Input Line Entry Specification) A systematic string representation of a compound where the hydrogen atoms are omitted.

For example, cco = ethanol.

SP

Scalar Product. The score metric used for the SVM signature algorithm. The sum of the weighted expression values plus the bias term.

SPS

Signature projection score. The score metric used for the TRANK signature algorithm. This is the similarity metric for the signature compared to the best score for that signature. For more information see **DrugMatrix Calculations** in the online **HELP** files.

Standard Deviation of Log Ratio

The standard deviation of the log ratio (based on the pairwise log ratios of compound treated vs control for all arrays in an experiment).

Standard Error

The standard deviation/square root of the number of observations.

SVM

The support vector machine is a machine learning algorithm that is designed to build classifiers by finding the hyperplane that optimally separates the two classes.

Synonyms

Other names for the query item.

Tanimoto

A standard industry method of determining the similarity between two compounds based on their structure.

Time Course

This is a chart of gene expression changes for the experimental compound where the dose is fixed and the time periods are varying.

TRANK

The t-rank algorithm computes the score for each variable using a modified z-score. See **Drug-Matrix Calculations** in the online **HELP** files for formula details.

Appendix - Chemical Ontology

Product Class

Analgesics
Anti-cancers
Anti-infectives
Anti-inflammatories
Autonomic Nervous System (ANS)
Biochemicals
Biologicals
Cardiovasculars
Central Nervous System (CNS)
Chelators / Heavy Metals
Diagnostics / Pharmaceutical Aid
Endocrine / Metabolic
Gastrointestinal and Genitourinary
Hematologic
Immune Response / Immunomodulators
Neuromuscular Disorders
Other Human Use
Peripheral Nervous System (PNS)
Respiratory
Toxicants
Vitamins / Nutrients

Therapeutic Class

- Acne Preparations
- Analgesics
 - Analgesics, Non-Opioid
 - Analgesics, Opioid
 - Analgesics, Topical
- Anorexiant
- Anti-Inflammatories
- Antiallergics
- Antianginals
- Antiarrhythmic
- Antibacterials
 - Antibacterials, Systemic
 - Antibacterials, Topical
- Antidepressants
- Antidiabetic Agents
- Antidotes
- Antiemetics
- Antiepileptics / Anticonvulsants
- Antifungals
 - Antifungals, Systemic
 - Antifungals, Topical
- Antihistamines
- Antihypertensives
- Antimigraines
- Antineoplastics
- Antiparasitics
- Antiplatelets
- Antipsychotics
- Antirheumatics
- Antitussives
- Antiulcers
- Antivirals
 - Antivirals, Systemic
 - Antivirals, Topical
- Anxiolytics
- Astringents
- Bronchodilators
- Cerebral Vascular Disorders
- Chelating Agents

Chemoprophylactics / Preventives / Protectives
Coagulation Disorders
Congestive Heart Failure
Contraceptives
Corticosteroids
 Corticosteroids, Topical
Disinfectants
Diuretics
Drug Dependence Therapy
General Anesthetics
 General Anesthetics, Inhaled
 General Anesthetics, Intravenous
Glaucoma Agents
Gonadal Hormone Disorders
Gout-Related Agents
Hypolipidemics
Immunomodulants
Immunosuppressants
Laxatives
Local Anesthetics
Movement Disorders
Nonsteroidal Anti-Inflammatories (NSAIDs)
Pancreatic Hormone Disorders
Parasympatholytics
Parasympathomimetics
Pituitary Hormone Disorders
Prokinetic Agents
Psoralens
Sedatives/Hypnotics
Skeletal Muscle Relaxants
Smooth Muscle Stimulants
Spasmolytics
Stimulants
Sympatholytics
Sympathomimetics
Thyroid Hormone Disorders
Vasodilators
Vitamins / Minerals / Nutrients

Mechanism

- Block G-protein coupled signal transduction
- Block channel gating
- Block neural transmission
- Derepress G-protein-coupled tyrosine kinase activity
- Derepress gene transcription
- Destroy cell membrane integrity
- Incorporate into DNA/RNA/Protein
- Increase/prolong neural transmission
- Induce free oxygen radical associated tissue and DNA damage
- Inhibit
 - Inhibit DNA synthesis, repair, and function
 - Inhibit bacterial DNA synthesis
 - Inhibit bacterial protein synthesis
 - Inhibit cholesterol biosynthesis
 - Inhibit fungal cell membrane biosynthesis
 - Inhibit mitochondrial function
 - Inhibit mitosis
 - Inhibit precursor synthesis
 - Inhibit prostaglandin and thromboxane biosynthesis
 - Inhibit protein synthesis
 - Inhibit steroid biosynthesis
 - Inhibit viral DNA synthesis
 - Inhibits bacterial cell wall biosynthesis
- Interfere glucose metabolism
- Interferes with Cell-Cell signaling
- Modulate G-protein coupled signal transduction
- Modulate channel gating
- Modulate gene transcription
- Repress gene transcription
- Scavenges hydrogen peroxide and free radicals
- Stimulate/prolong G-protein coupled signal transduction

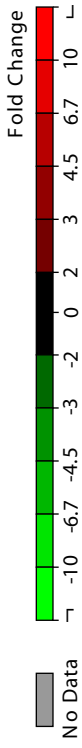
Mode Class

- Channel /Receptor ligand mimic
- Channel Blocker
 - Channel Blocker, Non-selective
 - Channel Blocker, selective
- Channel Modulator
- Distorts /blocks macromolecular scaffold function
- Distorts /blocks macromolecular synthesis scaffold
- Endogenous Enzyme Substrate
- Endogenous Receptor Ligand
- Enzyme Inhibitor
 - Enzyme Inhibitor, Non-selective
 - Enzyme Inhibitor, selective
- Enzyme substrate mimic
- Receptor Agonist
 - Receptor Agonist, Non-selective
 - Receptor Agonist, selective
- Receptor Ligand Antagonist
 - Receptor Ligand Antagonist, Non-selective
 - Receptor Ligand Antagonist, Selective
- Receptor Partial Agonist

Known Toxicity

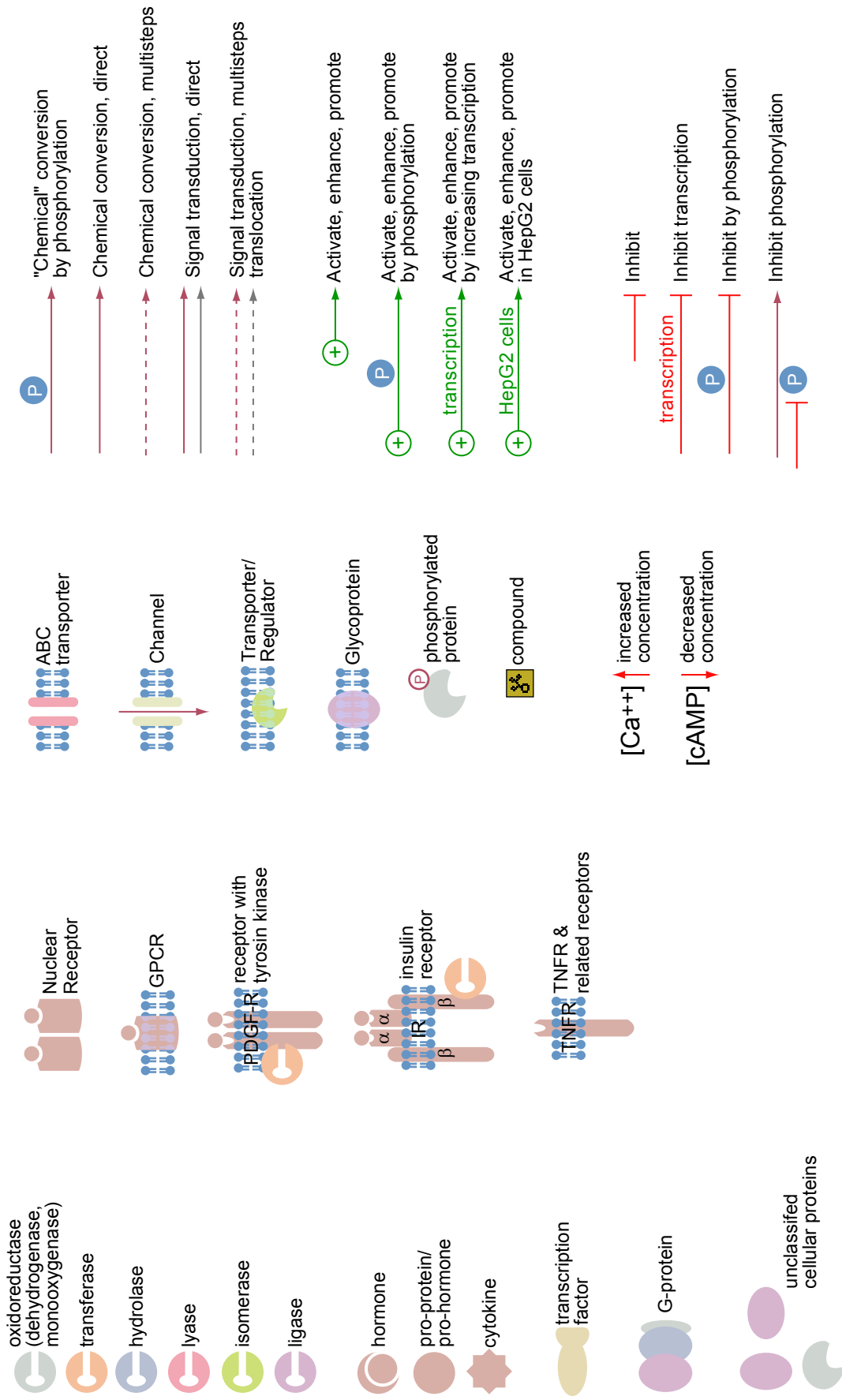
Bone Marrow Toxicity
Carcinogenicity
Cardiovascular Toxicity
Death
Embryotoxicity
Endocrine/Metabolic Toxicity
Gastrointestinal Toxicity
Genitourinary System Toxicity
Halocarbon toxicant
Hematotoxicity
Hepatotoxicity
Hypotensive Shock
Immune System Toxicity
Mental Health Disorders
Mitochondrial poison
Mutagenicity
Nephrotoxicity
Neurotoxicity
Organometallic Toxicant
Poisoning
Polyaromatic toxicants
Respiratory Toxicity
Rupture of Uterus
Sexual Dysfunction & Infertility
Teratogen
Toxicology Control
Toxicology control
Toxicology standard
Tumor Lysis Syndrome
kidney toxicant
liver toxicant

DrugMatrix Pathway Legend



Pathways concerns functions of proteins not genes *per se*.

Unless otherwise noted, the processes and transformations depicted in DM pathways are relevant to rodents and humans.



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Numerics

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A

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