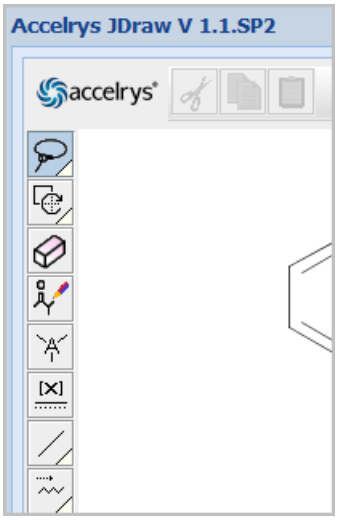
User Guide for the All New DiscoveryGate

The All New DiscoveryGate enables you to search for over millions of structures by typing in a string or number, drawing a structure, importing a file, or selecting a catalog. This Guide covers the following topics:

Initial Setup - Java and Certificate

The All New DiscoveryGate allows you to create and edit visual representations of molecules because it integrates with the Accelrys JDraw Applet. For information about Accelrys JDraw Applet, see `http://accelrys.com/products/informatics/cheminformatics/draw/`



Note: Reactions are not supported, even if JDraw allows reactions to be drawn.

To query DiscoveryGate by drawing a structure, your computer needs both a browser and an installation of the Java Runtime Environment (JRE). If your computer does not have a JRE, a message indicates that it is missing. The JRE installer is available for Windows, Macintosh, Linux, and Solaris at **`http://www.oracle.com/technetwork/java/javase/downloads/index.html`**

If you are running Windows 7, install the "**`Windows`**" JRE, which is 32-bit, instead of the "**`Windows x64`**" JRE because the default Internet Explorer is currently 32-bit, even on 64-bit Windows 7.

Accelrys JDraw Applet was formerly know as Symyx JDraw Applet. Therefore, you might see a message asking if you accept the certificate from Symyx Technologies, Inc. for the JDrawRenderer.

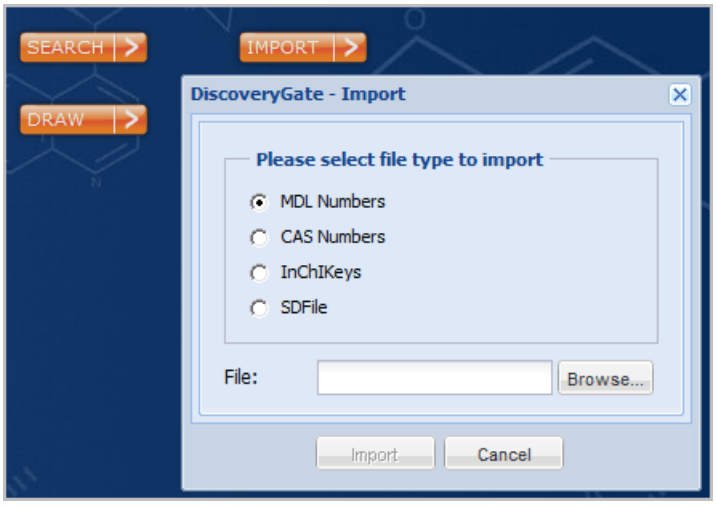
Free Searching

The All New DiscoveryGate provides free searching. Without purchasing a subscription, registering, or logging in you can:

- Search for Structures in any of four ways.
  - By identifier (compound name, MDL number, CAS number, or catalog number). Type the first alphanumeric characters and select from the dynamic list.

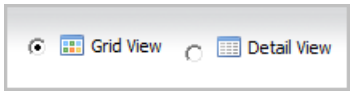
  - By drawing the structure
  - By pasting the InChIKey

  - By importing a hit list file with MDL Numbers, CAS Numbers (Chemical Abstracts Service registry), InChiKeys, or an SDFile. Importing a hit list allows you to continue a previous session (see Export Hits, which requires logging in). The search results from the previous session become the starting point for the current session.

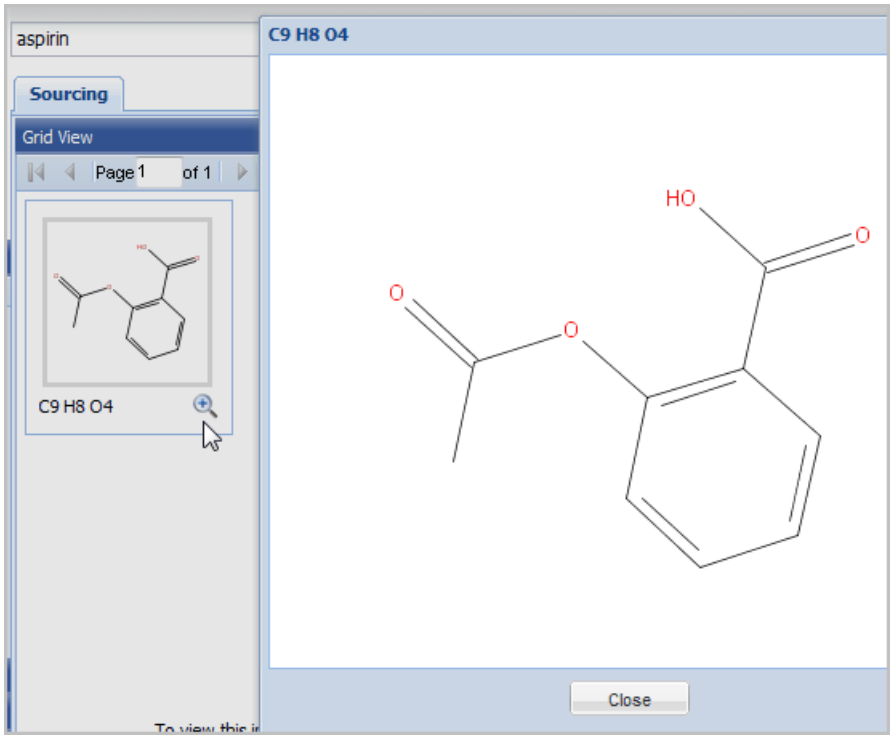


Note: There is an exact 1-to-1 correspondence between a compound and its MDL Number. Other identifier types are not guaranteed to be unique. The size limit for an SDFile is 500 structures.

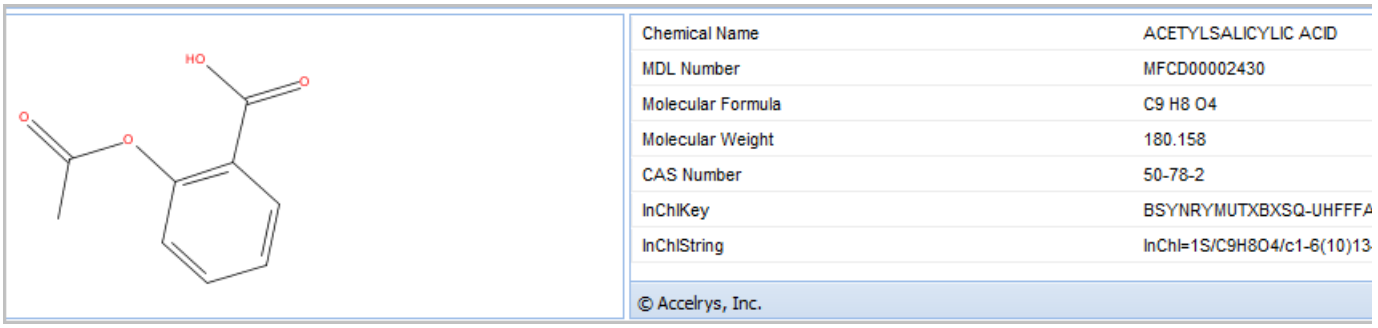
- See the results in Grid View (multiple compounds) or Detail View (one compound with rows of specific data).



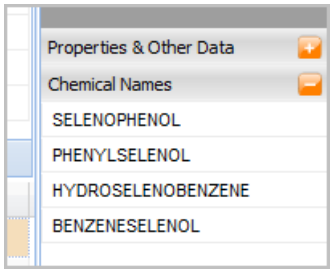
- To enlarge a molecule in the Grid View, click the magnifying glass icon.



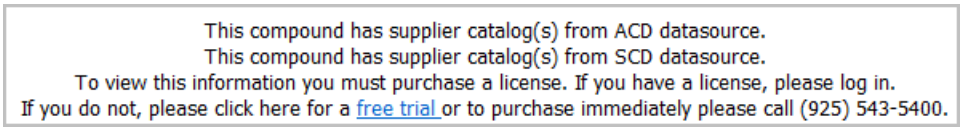
- To switch from Grid View to Detail View of one specific compound, click that compound. The Detail View shows the "top-level information", such as the structure, chemical name, MDL number, Molecular Formula, Molecular Weight, CAS Number, InChIKey and InChIString



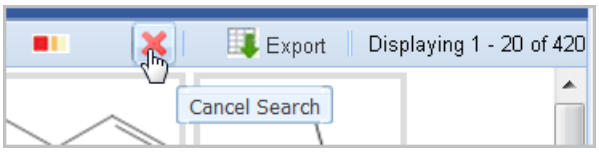
- To see synonyms for the molecule, click **`Chemical Names`**.



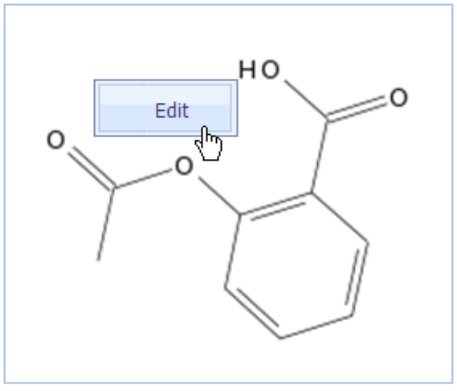
- See whether supplier catalogs in ACD and SCD are associated with the compound



- Initial results display without having to wait for the entire query to complete. If the query is taking too long, you can cancel it by clicking the red **X**.



- To edit the structure, right-click and click Edit.



- Some molecules have a ChemADVISOR MSDS Summary Sheet, which is available at **`Health & Safety`**.

User Registration

As soon as you register as a user and log in, you can: Filter Settings for all searches globally, request access to the Users' Forum, which provides a means of Support and assistance among the user community, and use additional features for registered users as they become available.

Subscriptions

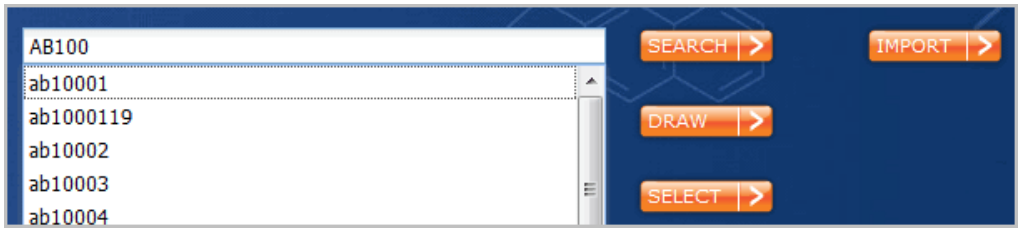
Paid subscriptions expand your capabilities:

- Search for Structures with the complete set of features, including Catalog Retrieval
- Filter Hits
- View Hits and Export Hits with the complete set of features
- Export Hits for use in later sessions
- Use the Shopping Cart and export its information

Search for Structures

To search for structures (compounds) in ACD (Available Chemical Directory) and/or SCD (Screening Compounds Directory), type or paste any of the following:

- compound name
- InchIKey
- CAS number
- MDL number
- Catalog number

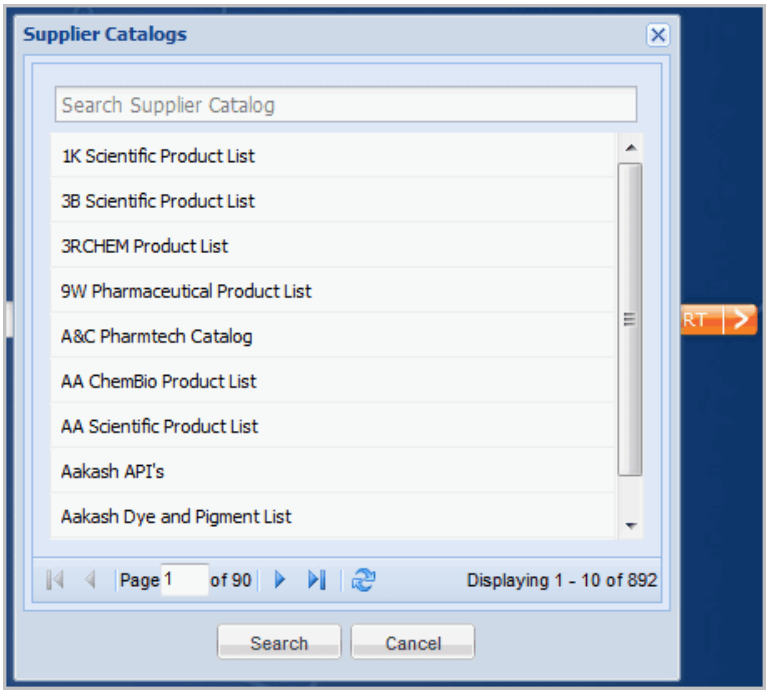


or click **Draw** to draw a structure

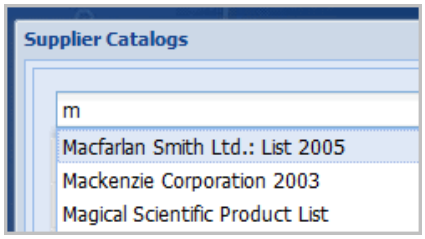
or click Catalog Retrieval **SELECT**, which is illustrated in the following.

Catalog Retrieval

When you click Catalog Retrieval **SELECT**, the Supplier Catalogs dialog appears.

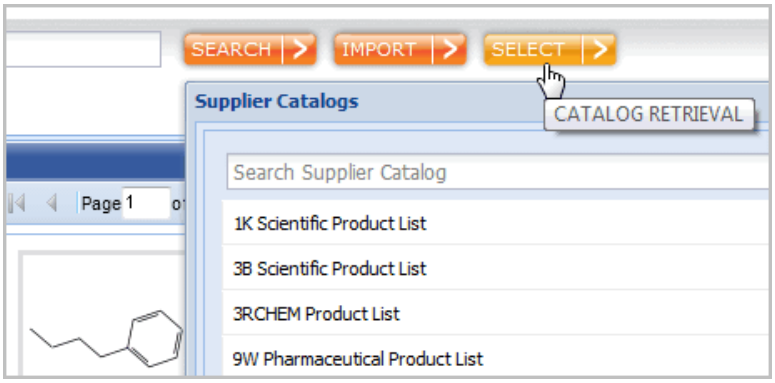


TIP: To get to the supplier catalogs that begin with a particular letter, type that letter:



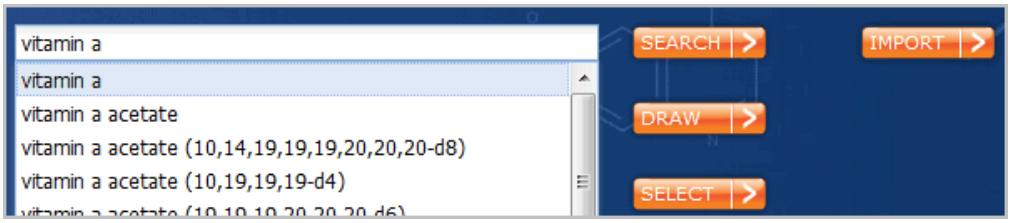
To further narrow the search, continue typing letters.

You can also access Catalog Retrieval from the **SELECT** button on any page of search results.



Name Search

When you type in the name, the All New DiscoveryGate prompts you with choices from the full compound index.



If you draw a structure, you can search for that **Exact** structure, or for structures that contain your drawing as a **Substructure**.

The hits contain sourcing information and are listed alphabetically by **Supplier Catalog**.

Supplier Catalog	Catalog Number	Size	Price	Purity	$/Gram	
ABCR GmbH Product List	AB113303-0100.00-GRM	100 G	EUR 11.80	99 %	0.149	Add to Cart
ABCR GmbH Product List	AB113303	2.5 KG	EUR 62.50	99 %	0.032	Add to Cart
ABCR GmbH Product List	AB113303-0500.00-GRM	500 G	EUR 22.50	99 %	0.057	Add to Cart
Acros Organics	15818-5000	500 G	USD 33.90	99 %	0.068	Add to Cart
Acros Organics	15818-0500	50 G	USD 18.30	99 %	0.366	Add to Cart
Acros Organics	15818-0025	2.5 KG	USD 105.00	99 %	0.042	Add to Cart
Advanced Tech Ind. 2007	3530522					Add to Cart
Advanced Tech Ind. 2007	1003109	100 G	USD 12.00	99 %	0.120	Add to Cart
AK Scientific Catalog	H740-POA					Add to Cart
AKOS 2007	BBS-00003798					Add to Cart
Aldrich Chemical Co.	239631-50G	50 G	USD 42.10	99 %	0.842	Add to Cart
Aldrich Chemical Co.	239631-1G	1 G	USD 21.20	99 %	21.200	Add to Cart

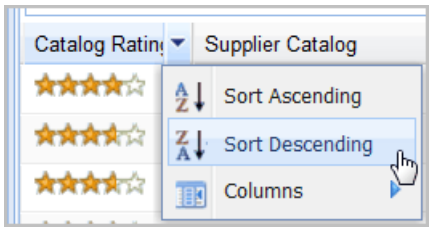
You can sort the hit list by **`Catalog Rating`**, **`Catalog Number`**, **`Size`**, **`Purity`**, or **`$/Gram`**. For easy price comparison, the **`$/Gram`** column automatically converts international currencies, such as Common Market euro, Japanese yen, Chinese yuan, and British pound.

Sigma Biochemicals	A5376-250G	250 G	USD 25.20	99 %	0.101
Wako Pure Chemical Product List	019-10265	500 G	JPY 4600	99 %	0.101
TCI UK Chemicals Catalog	A2262	500 G	GBP 35.15	98 %	0.104
TCI Europe	A2262	500 G	EUR 42.15	98 %	0.106
Fluka Chemie AG	01459-250G	250 G	USD 29.10	99 %	0.116

Catalog Ratings

Catalogs can have ratings:

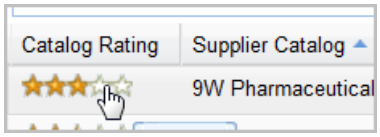
You can sort by **`Catalog Rating`**:



Rating a catalog

If you have experienced ordering from a specific catalog, you are welcome to provide a rating for that catalog.

1. Click in the stars area to open the Ratings dialog:



2. Click the down-arrow for **`Rate This Supplier`**.

Click the star rating you want for each row, check the confirmation that you have purchased from this catalog, and click **Save**.:

Filter Settings for all searches globally

On the **Filter Settings** tab, you can select:

- whether to filter on **All (ACD and SCD)**, **Building Blocks & Reagents (ACD)**, or **Screening (SCD)**. For example, if you select **Screening (SCD)**, **Building Blocks & Reagents (ACD)** is filtered out, and you must have a license to **Screening (SCD)** to see the hits.
- which **Supplier Catalogs** belong to your **Preferred Supplier Catalogs**. To have the list of hits for any search reflect your choice of preferred suppliers, check **Filter on preferred supplier catalogs while searching**. To create (or view) a list of preferred suppliers, click **Create Preferred Supplier Catalogs**.

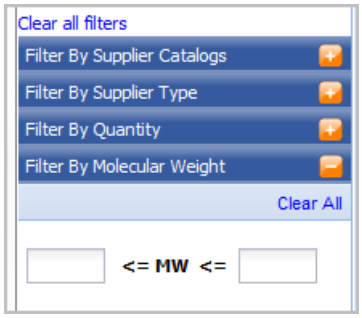
- To create (or view) a list of excluded suppliers, click **Create Excluded Supplier Catalogs**. The same company can be both the Preferred and Excluded lists because at any time you can apply either one (but never both). See Filter Hits.

To save your User Settings, click **Save**. Then click **Close**.

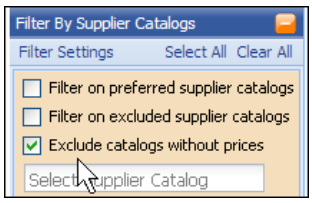
Filter Hits

This section applies to hits for a particular search. To establish general preferences, see “Filter Settings for all searches globally” on page 12.

To set filters that limit the amount of results (“hits”) for a query, you can set **Filter by Supplier Catalogs**, **Filter by Supplier Type**, **Filter By Quantity**, or **Filter By Molecular Weight**.

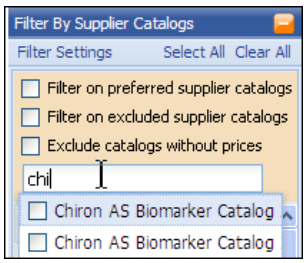


- To configure a filter, click the + sign.

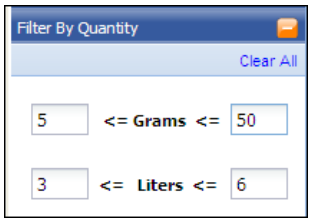


- To see hits only from preferred supplier catalogs, check **Filter on preferred supplier catalogs list**
- If you want to focus on pricing, check **Exclude catalogs without prices**

- To select the name of supplier, in the **`Select Supplier Catalog`** field, type three letters and select a name



- To **`Filter By Quantity`**, click **`+`** and set the values you want

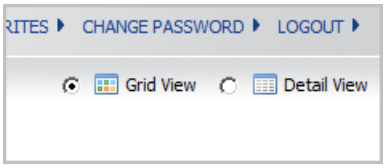


To activate your Filters, click **`Apply`**

To reset all the “filter” areas to their default state, click **Clear all filters**.

View Hits

To browse search results (“hits”) as structures, use the **Grid** view.

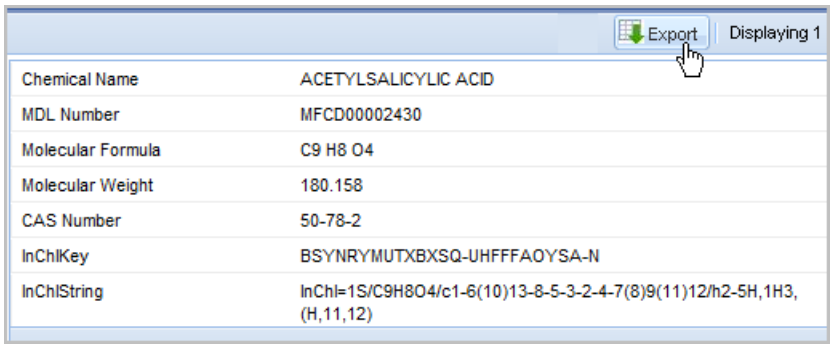


To see Catalog Number and Package Size, click **Detail View**, which also gives you access to **Properties and Other Data**, **Chemical Names**, and **Distributor Address**.

Export Hits

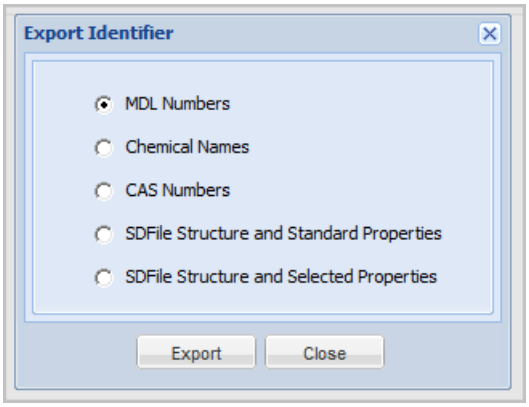
Exporting your search results (“hits”) to a file is useful because these results can be imported as a starting point for another session or another user.

1. Click **Export**.



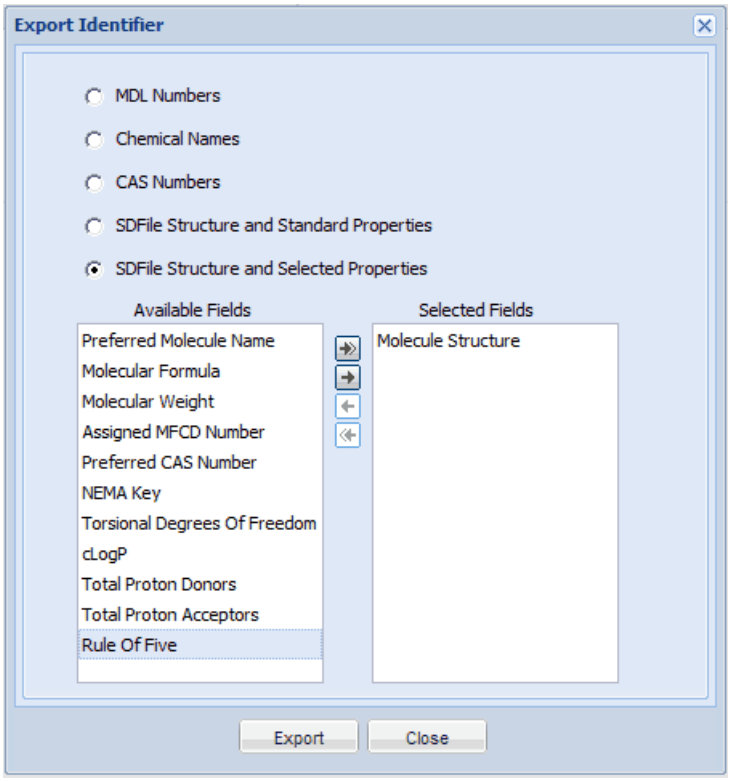
2. Select the type of identifier to export: **MDL Numbers**, **CAS Numbers**, **Chemical Names**, **SDFile Structure and *Standard* Properties**, or **SDFile Structure and *Selected* Properties**.

   There is an exact 1-to-1 correspondence between a compound and its MDL Number. Other identifier types are not guaranteed to be unique. (Note: The SDFile property called NEMA key is almost always unique.)



Note: The size limit for an SDFile is 500 structures, so you might see a message that says "Results contains more than 500 Molecules. Only first 500 will be exported."

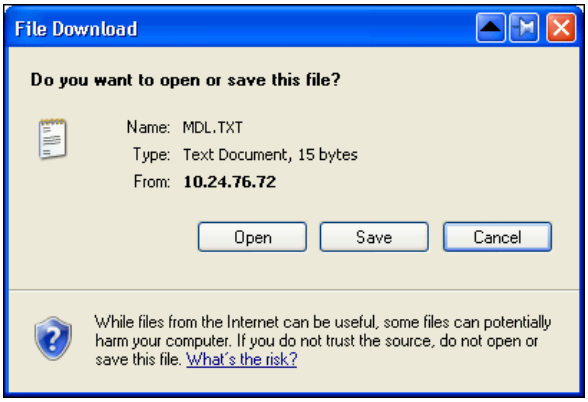
3. If you select **`SDFile Structure and Selected Properties`**, you can pick which properties to export.



Note: **`Molecule Structure`** is a required field and cannot be removed from the list.

4. Click **`Export`**.

5. Click **Save**.



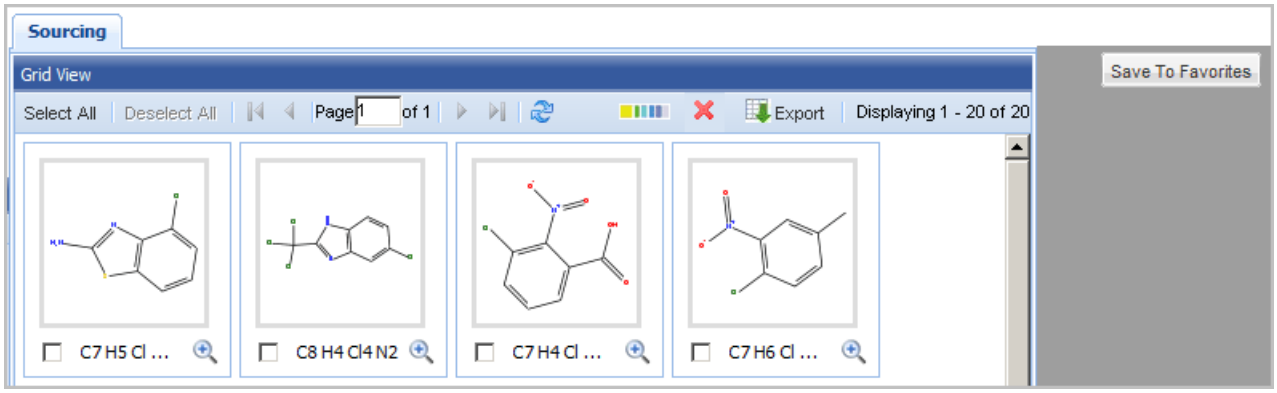
You are then prompted to open the exported file. The default names are:

- `MDL.txt` for the MDL IDs, such as MFCD00002430
- `CHEMICAL_NAMES.txt` for chemical names, such as ACETYLSALICYLIC ACID
- `CAS.txt` for CAS (Chemical Abstracts Service registry) numbers, such as 108-37-2
- `SDF.sdf` for SDFiles, which contain one or more molfiles
- `SDF_STANDARD_PROPERTIES.sdf` for SDFiles with standard properties
- `SDF_SELECTED_PROPERTIES` for SDFiles with the properties you select

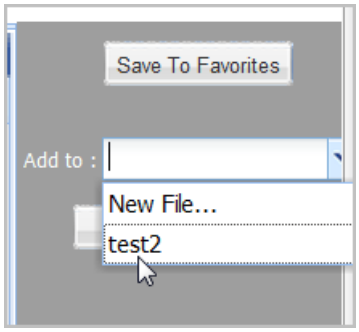
Favorites (Saved Search Result Sets)

You can save the result set a molecule search as a Favorite, which provides quick access to both the query and its hits. You can save a Favorite from both the Grid view and the Detail view.

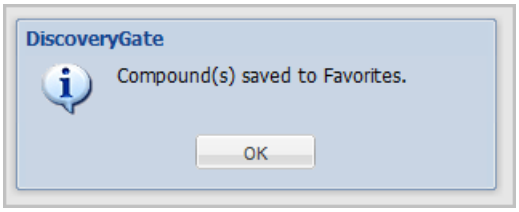
1. Check the box for one or more of the hits or click “Select All”.



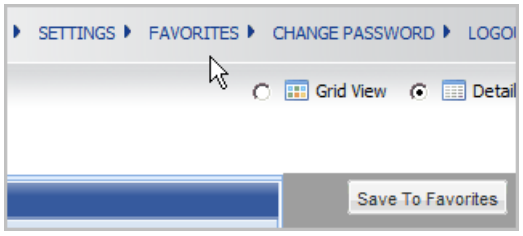
2. Click **`Save To Favorites`** and either save to a new list (or append this list to an existing list).



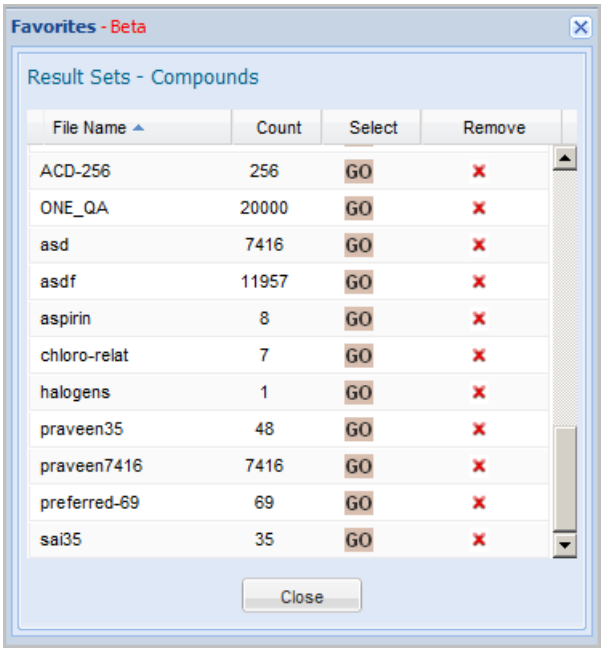
3. See the confirmation.



Whenever you want, you can return to your saved lists by clicking **FAVORITES**.



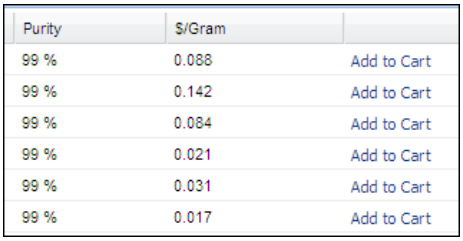
You can see the “Count” of hits for each Favorite, “Go” to a saved favorite to view its query and hits, rename the Favorite, or remove it.



Shopping Cart

The list of items in your Shopping Cart can be viewed and saved to a file that can be used to procure items from suppliers.

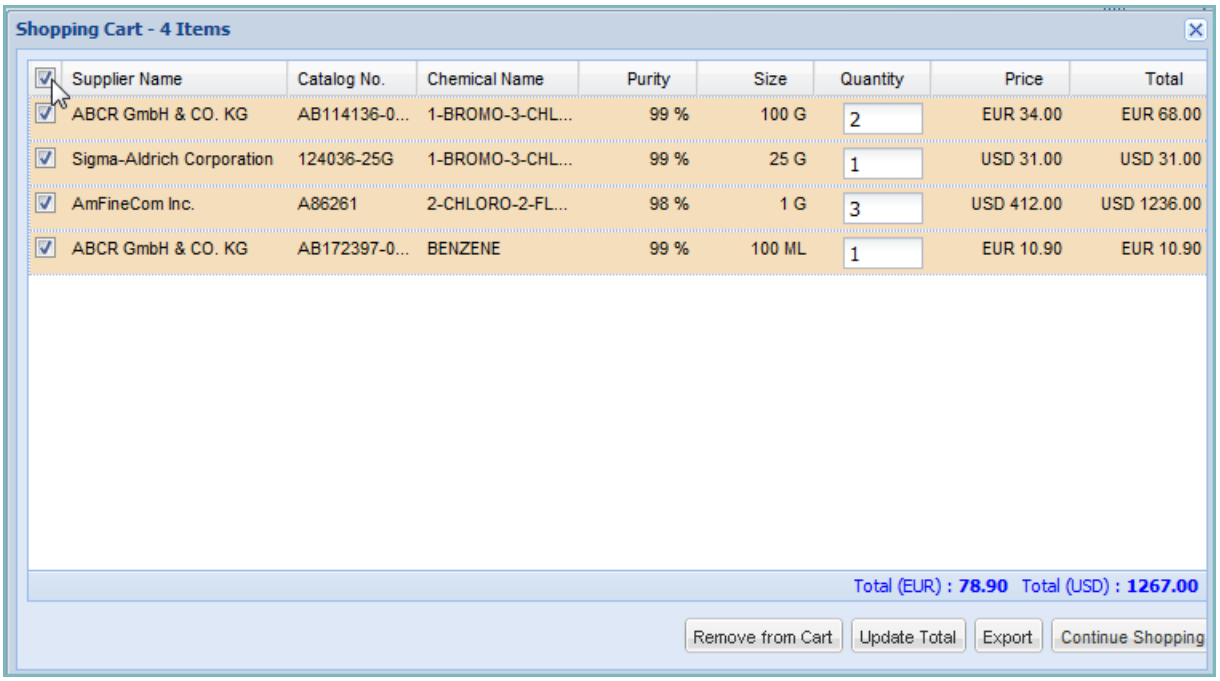
To add an item to the Shopping Cart, click **`Add to Cart`** while viewing in the search results in the **`Detail View`**.



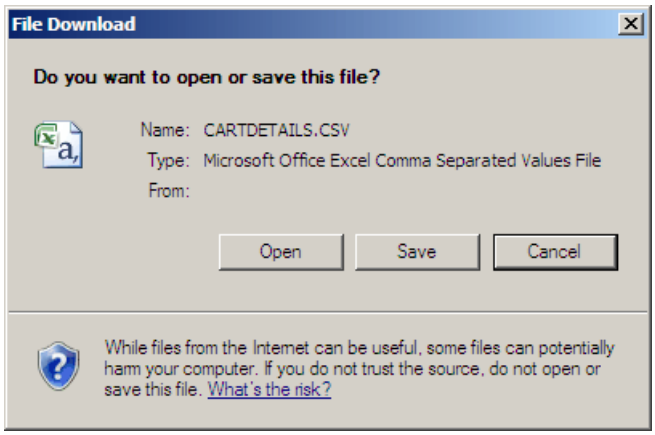
Purity	$/Gram	
99 %	0.088	Add to Cart
99 %	0.142	Add to Cart
99 %	0.084	Add to Cart
99 %	0.021	Add to Cart
99 %	0.031	Add to Cart
99 %	0.017	Add to Cart

The shopping cart icon in the top right indicates how many items it contains.

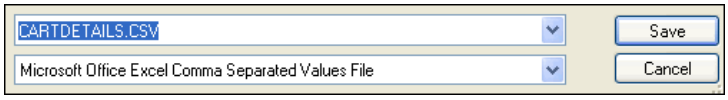
To see the items in the Shopping Cart, click the icon. In the table, the `Total` column represents `Price` multiplied by `Quantity`. There is also a total for each currency, such as USD and EUR. The top checkbox selects (or unselects) all the rows.



To save the list of items as a comma-delimited text file, click **Export**.



In the File Download dialog, click **Save** and navigate to where you want to save the file.



In Microsoft Excel, the contents of the .csv file look similar to the following:

Chemical Name	Mol. Form	MDL Num	Molecular We	CAS	Properties	Supplier	Catalog N
1-BROMO-3-CHL	C6 H4 Br C	MFCD0000	191.4550018	108-37-2		ABCR Gmb	AB114136
1-BROMO-3-CHL	C6 H4 Br C	MFCD0000	191.4550018	108-37-2		Sigma-Ald	124036-25
2-CHLORO-2-FLU	C9 H4 Cl F	MFCD0497	258.572998			AmFineCo	A86261
BENZENE	C6 H6	MFCD0000	78.11340332	71-43-2		ABCR Gmb	AB172397

and the fields typically include: `Chemical Name, Mol. Formula, MDL Number, Molecular Weight, CAS Number, Properties and Other Data, Supplier, Catalog Number, Quantity, Package Size, Unit, Purity, Currency, Price, Normalized Price, Data Source Name, Supplier Headquarters`

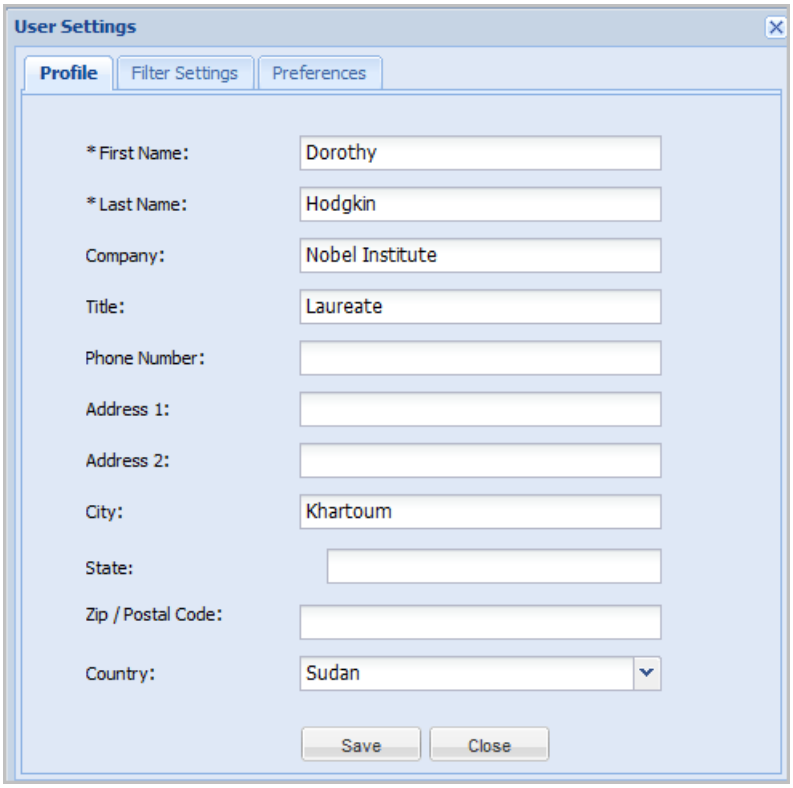
In a text editor, the contents of the .csv file have the field names in the first line, and then a line for each hit.

Note: Accelrys provides products that will also display the structures exported from the Shopping Cart. See "For Users of Isentris for Excel and ISIS for Excel" on page 23.

Set User Preferences

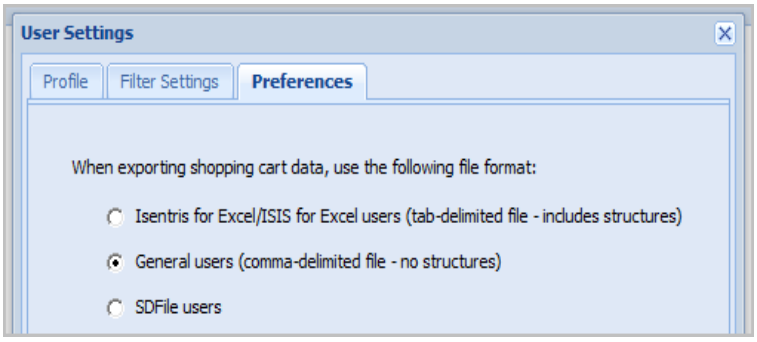
To set your preferences, click **`Settings`**.

- On the **`Profile`** tab, enter your first name and last name. Optionally, you can provide the DiscoveryGate team with your phone number and/or address.



For Users of Isentris for Excel and ISIS for Excel

If you are using Isentris for Excel (or ISIS for Excel), use the **`Preferences`** tab to ensure that when you export your Shopping Cart, structures are also exported to spreadsheet display. See also “Shopping Cart” on page 20.



60-Minute Sessions

Each time you send a query to the server, your current session is renewed for 60 minutes.

Note: The time spent drawing a query does not renew the session. Therefore, if you spend 61 minutes drawing a molecule, when you try to run the query, a message will tell you to log in. When you log in, a completely new session begins, and you would have to re-draw the molecule.

This concludes the October 2012 edition of the User Guide for the All New DiscoveryGate.