What’s New?

Useful tips for using:

- DiscoveryGate Login page
- DiscoveryGate Homepage
- MDL Database Browser
When you open DiscoveryGate you may be required to provide
   Username
   Password
   Company ID

You will receive these credentials from your DiscoveryGate Administrator. Not all sites use login credentials.

Where login credentials are required you will be asked to provide a new password of your own choosing.

You will only need to enter your Company ID the first time you login.
The DiscoveryGate Homepage – “Home”

Logging on to DiscoveryGate opens the Discovery Gate Homepage
1. Quick Start Guide – find basic information about using the system
   - How to do searches
   - How to personalize the homepage
   - Where to look for software installation
   - How to do Administrator’s tasks

2. Your Setting’s tab
   - Go here to personalize the homepage and change system settings

3. Company Settings tab
   - This page only available to DiscoveryGate Administrators
   - Create users, reset passwords
   - Customize server configurations for LinkFinderPlus and 3rd Party Applications
   - Maintain your company gatelets on the homepage

4. Support tab
   - System requirements
   - Online documentation
   - Report defects
Two New Gatelets on this page:

1. Database Browser Settings
   - Use drop down menu to choose which database will be active when you open the Database Browser
   - Use radio buttons to configure display options for Compound Index search results

2. Autoupdate Configurations
   - When enabled, DiscoveryGate will automatically update Database Browser to most recent version
   - Your site Administrator may over-ride autoupdates
Click any application and start searching DiscoveryGate!

- **MDL® Database Browser**
  Query an *individual* database: synthesis, bioactivity, physical property, metabolism, toxicity or sourcing.

- **LinkFinderPlus**
  Link to over 20,000 journal titles and patent archives.

- **Integrated Major Reference Works**
  Review synthetic methods and learn about their scope and limitations.

- **xPharm**
  Query and browse therapeutic agents, targets, disorders and principles in the xPharm pharmacological reference database.

*Remove descriptive text*
1. **Pull Down Database Menu**  
   Change from one database to another by selecting from this list of available sources.

2. **Save Form**  
   Use the default form supplied for every database. Or, if your DiscoveryGate environment can be personalized, edit the form and save your new form for future sessions. Only one saved form is possible per database.

3. **Query Highlighting**  
   Tick this checkbox to enable substructure queries to be highlighted in blue within retrieved chemical structures.
1. **MDL Compound Index is now searched with MDL Database Browser**

The Compound Locator searching application has been removed from DiscoveryGate. To carry out searches over the Compound Index you can select it from the list of available databases in Database Browser.
1. **Grid View**
   The grid view displays Compound Index results as a matrix containing 12 hits per page.

**Database View**
(Shown on the next page), the Database View lists structures with links to databases containing data for those structures.

**Properties View**
(Shown on the second following page), the Properties View lists structures and shows the corresponding property categories for the databases where the structures are found.
MDL Database Browser – “Results”

Display options unique to Compound Index Search Results
Choose default display setting on “Your Settings” tab of DiscoveryGate Homepage.

1. **Grid View**
(Shown on previous page) the grid view displays Compound Index results as a matrix containing 12 hits per page.

**Database View**
Database View lists structures with corresponding indexed databases containing data for those structures. Click on row identifier for summary of data from all databases.

**Properties View**
(Shown on the following page), the Properties View lists structures and shows the corresponding properties categories for the databases in which the structures are found.
Display options unique to Compound Index Search Results
Choose default display setting on “Your Settings” tab of DiscoveryGate Homepage.

1. **Grid View**
(Shown on two pages prior) the grid view displays Compound Index results as a matrix containing 12 hits per page.

**Database View**
(Shown on previous page), Database View lists structures with corresponding indexed databases containing data for those structures.

**Properties View**
The Properties View lists structures and shows the corresponding properties categories for the databases in which the structures are found. Click on row identifier for summary of data from all databases.
MDL Database Browser – “Results”

More about the list of available databases.

**Databases not Indexed**
- CrossFire Beilstein
- CrossFire Gmelin

**MDL Compound Index**

**Indexed Databases**
- All databases appearing below the MDL Compound Index on this drop down menu are indexed.
- Indexed databases are seen in as “Also Found In” links on Database Browser results pages.

**Note:** Bioactivity Databases and Patent Information are headings and cannot be selected as searchable content. All other menu items are selectable.
1. Browsing results
   To reduce time waiting for display of search results, hits are retrieved in sets of 12. To see the next 12 hits click on “Next”.

2. Get Count
   Click on “Get Count” to retrieve entire hit set. When this is done the number of hits in the full hitset will be displayed (see next page).

Note:
The “Get Count” operation is not present for results from CrossFire databases or results from any of the Synthetic Methodology databases. Full search results are displayed directly from searches of these sources.
1. After “Get Count” is done
   Total number of records in full hitset is displayed.

2. Browsing records
   After “Get Count” is done, additional page selection and a “Next 10” option is available.

Note:
The “Get Count” operation is not present for results from CrossFire databases or results from any of the Synthetic Methodology database. Full search results are displayed directly from searches of these sources.
MDL Database Browser – “Results”

*Results page for searches done over Indexed molecule databases.*
*Shown here for MDL Available Chemical Directory.*

1. **Create List**
   To save temporary lists (which persist for the current session, but are lost following log out) click on the “Create List” link.

2. **Create List Dialog**
   A dialog box will appear that allows you to
   - select the records to be included on your list
   - name the list

![Create List](image.png)
Results page for searches done over Indexed molecule databases. Shown here for MDL Available Chemical Directory.

1. **After Create List**
   The temporary list created by the Create List operation is now shown in the history tree.

   This list will persist for the current DiscoveryGate session (i.e. until you log out from DiscoveryGate).

2. **Save tab**
   Click on the Save tab if you want to permanently save a list (see next page).
Results page for searches done over Indexed molecule databases.
Shown here for MDL Available Chemical Directory.

1. **Saving Lists**
   Clicking on the Save tab allows you to give your list a name and permanently save this list.

2. **Saved Lists**
   Saved lists appear in the Results History pane (see next page).
MDL Database Browser – “Results”

Results page for searches done over Indexed molecule databases. Shown here for MDL Available Chemical Directory.

1. **Saved Lists**
   Saved lists appear in the Results History pane under the heading Saved Searches. **Note:** All search results in the Results History pane may be deleted or renamed by right clicking on the entry name and choosing “delete” or “rename”.

2. **Lists tab**
   Clicking on Lists tab displays a dialog box for list operations.

3. **Lists dialog box**
   - Export list to your desktop and import later to the same database.
   - Import lists
   - Combine lists (see next page)
Combine Lists Dialog
The dialog box elicited by choosing the Combine Lists option allows you to choose any two of the temporary lists and combine them using AND, OR or NOT operators, and give the resulting combined list a name.

Clicking the “Apply” option will carry out the combination and display this combined result.

The combined list will appear under the Temporary Lists tree.
1. **View Selected Records**
   This link allows you to take selected Records from the current list in the Current database and view them in another database.
   - You may move to another Database Browser database
   - You may move to another database using a different application (such as MDL ISIS or CrossFire Commander) if you have such applications available.

2. **Details link**
   Click on the “Details” link to view specific data associated with structures in the Grid display.
1. **Also Found In links**

The Details page for a record in MDL Available Chemicals Directory is shown here.

*Also Found In* links are active links records for the structure on display that are registered to other indexed databases.

In this case, the compound on display is registered to 12 other indexed databases. Clicking on any of these links displays the data for relevant records in that database.

See next page for display evoked by clicking on the “Toxicity” Link.
Also Found In links exploit the power of indexed content. Here you see toxicity data associated with a structure retrieved from a search of MDL Available Chemicals directory (see previous page). No additional searches are required.

1. **Return to “Database”**
   Click this link to return to the original search results (in this case the results retrieved from MDL Available Chemicals Directory).