

# Send your structures to DiscoveryGate®

## See where they take you

Thanks to an innovative new linking capability from Elsevier MDL, there's even more reason for life sciences companies to make the online DiscoveryGate® content service ([www.discoverygate.com](http://www.discoverygate.com)) their first stop for scientific information and the answers to discovery questions.

Researchers can use the new linking capability to transfer chemical structures from in-house or third party applications (such as an inventory management system or electronic laboratory notebook) directly to DiscoveryGate via a single click in the application. With a DiscoveryGate license in place, researchers can immediately search for transferred compounds on the DiscoveryGate platform, accelerating synthesis planning and decision-making.

### Easy to implement

To implement the linking, Elsevier MDL supplies IT specialists with the software components and documentation to expose a hyperlink in custom applications built on COM, .NET, Java or HTML technology. The molecules are communicated as MDL® Chime Strings with searches conducted over the MDL® Compound Index (which currently indexes 19 diverse databases).

Once the software is installed, scientists can transfer structures of interest as direct queries to DiscoveryGate.

The system runs the following types of structure searches: automatic, exact, substructure search, isomers, tautomers and salts. The automatic search strategy looks for records that match a query using the following combination of search types, moving from a particular to a more general set of search criteria to gradually widen the search until the system finds a hit.

*Transfer chemical structures from in-house or third party applications directly to DiscoveryGate via a single click in the application.*

- 1. Related compounds search:** Searches for related compounds with no additional substitution.
- 2. Exact match search:** Searches for substances that match the structural query exactly.
- 3. Include isomers search:** Searches for all stereoisomers (all *R* and *S* configurations, all *E* and *Z* configurations, and so on).
- 4. Include tautomers search:** Searches for all tautomers, and also for structures with different charges and different isotopes.
- 5. Include salts search:** Searches for substances that include different salts.
- 6. Substructure search:** Searches for substances that contain the query wholly embedded within them.
- 7. Similarity search:** Searches for substances that are structurally similar to the query.

The search workflow also enables researchers to obtain electronic versions of primary literature articles, provided the articles are available in electronic format and the researchers hold the appropriate access rights.

The screenshot shows the MDL Base 1.0 R2 application window. The main area displays the chemical structure of Taxol. To the right, a table lists the following information:

CDBRegNo	139
Molecule Name	Taxol
Corporate ID	MUSE33300371
Molecular weight	853.93

Below the table, there is a section titled "Find Related Data in DiscoveryGate" which includes a search input field containing "sss" and a button labeled "search in DiscoveryGate".

Figure 1: Result screen from search in corporate application in MDL Base environment



Figure 2: Database View of Compound Index results

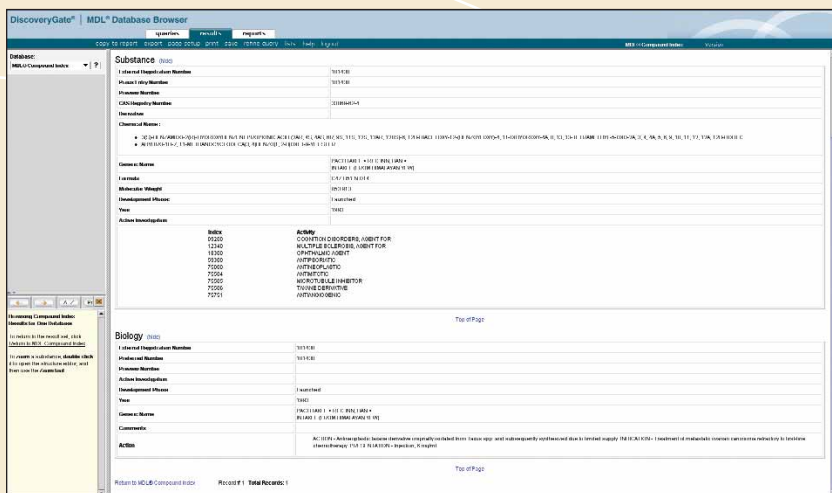


Figure 3: Detail view of pharmacology information for the compound of interest

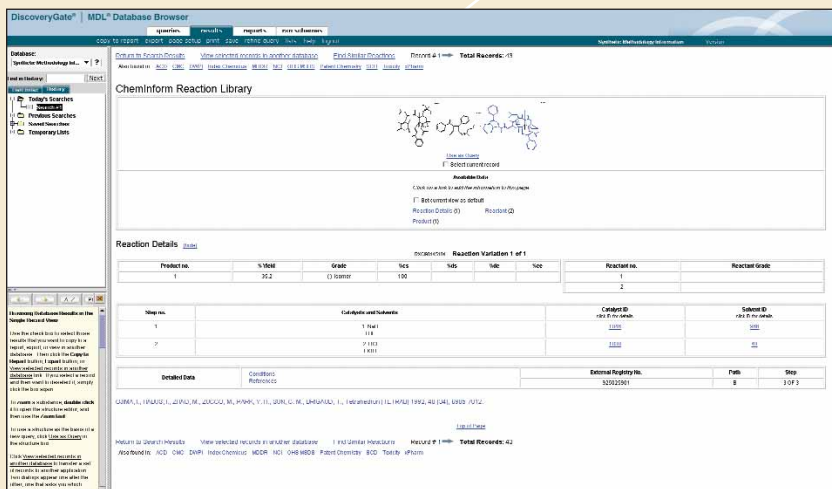


Figure 4: "Also found in" links alert researchers to other data sources containing relevant information pertaining to compounds of interest

## Finding related commercial information

The following workflow assumes that a scientist has searched a corporate database using an MDL® Base application.

1. While working in this application, the scientist finds the Taxol structure illustrated in Figure 1.
2. The scientist can select a search type (e.g., in this case, a substructure search) and transfer the structure to DiscoveryGate with a single click. Following DiscoveryGate authentication, the system searches for the compound of interest in the Compound Index with no further input required from the scientist.
3. The scientist can look at the search results using the Database View shown in Figure 2, which shows other data sources for the related structures located in the search.
4. The scientist can now find additional information on the compound by exploring other available databases (provided the necessary access rights are in place). For example, the MDL® Drug Data Report database (produced by Elsevier MDL and Prous Science) provides information on the pharmacological effects of the compound, as shown in Figure 3. Likewise, the MDL synthetic methodology databases provide useful details on the preparation of the compound.
5. The "Also found in" link directs the scientist to other data sources enabling further exploration of similar compounds or related commercial data that can assist in synthesis planning and decision making. See Figure 4.

With minimal application development effort, IT specialists can enable researchers to quickly and easily supplement their in-house data with related commercial information found on DiscoveryGate. This new linking capability can significantly reduce the risk of researchers missing critical information, especially when they are unsure which databases to search.

For more information on accelerating discovery research by implementing this innovative linking functionality, contact your Elsevier MDL Account Manager or submit a request for information at [www.mdl.com](http://www.mdl.com).

Share your company's experiences with MDL solutions. Submit an article idea at [www.mdl.com/news](http://www.mdl.com/news).



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