

DiscoveryGate[®] Installation and Configuration

Last updated on:

28 February 2007

For latest version:

Go to www.discoverygate.com, and log in. Click on the **Support** tab. Then click the **Knowledge Base** link, and click **DiscoveryGate Installation Manual** to open the PDF.

March 2007

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Overview

This guide explains how to install and configure DiscoveryGate® on Intel and Intel-compatible computers that run the Microsoft Windows client operating system.

This guide also explains how to install DiscoveryGate® on Macintosh computers.

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What is DiscoveryGate?

DiscoveryGate is a Web-based application that integrates, indexes, and links scientific information. It provides scientists immediate access to compounds and related data, reactions, original journal articles and patents from a Web browser on their desktop.

Using This Installation Guide

This section explains:

- The audience
- Prerequisite knowledge
- Documentation conventions and symbols

Audience for this guide

This guide is for people who install, configure, and administer DiscoveryGate at your site, such as:

- System administrators
- DiscoveryGate site administrators
- Database administrators



Caution: Elsevier MDL recommends that you do not make this guide available to users. If you distribute the guide to your users, this could compromise DiscoveryGate and MDL Hop-Into security.

Prerequisite knowledge

This guide assumes that you are familiar with:

- Microsoft Windows operating systems
- Microsoft Windows system administration
- Macintosh operating systems
- Macintosh system administration

Document conventions and special symbols

Table 1 Documentation conventions and symbols used in this guide

Convention or Symbol	Example
File listings and commands that form separate paragraphs in the guide use a fixed-width font to contrast with the text of the guide.	<code>DiscoveryGate.exe</code>
Examples that show your dialog with a program use fixed-width regular type for program prompts and other output, and bold type for your input.	<code><default rootdir="D:\mdlweb\21"></code>
Examples of commands use italic type to represent input that is variable.	<code>TABLESPACE <i>your_tablespace</i></code>
Examples of commands and other items that users choose graphically when interacting with DiscoveryGate are shown in bold font. The greater than sign (>) indicates a cascading menu.	Start > Programs > Accessories > Windows Explorer
This symbol denotes a carriage return. Press the appropriate key (for example, Enter or Return) on your keyboard.	↵
In dialog with a program, users must end each line with a carriage return. This guide does not show carriage returns unless a carriage return is the only user input.	
This symbol indicates that a single Microsoft Windows command or a single line in a file is continued on the next line.	^
Command prompt for Microsoft Windows operating systems. Microsoft Windows displays the path to the current folder followed by a greater than sign.	>
Command prompt for Microsoft Windows operating systems when a command is continued to the next line.	More?

Installing and Configuring DiscoveryGate

This chapter provides information that is necessary to correctly install and configure DiscoveryGate at your site.



Tip: Most of the information in this chapter explains how to install DiscoveryGate, or update your DiscoveryGate installation, on Microsoft Windows computers. For information about installing the DiscoveryGate client on Macintosh computers, you can skip the first several sections. Proceed to [“Installing DiscoveryGate on Macintosh clients”](#) on page 21.

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Before You Install DiscoveryGate

The list that follows explains the requirements that you must meet in order to install DiscoveryGate at your site.

- Verify that your hardware and software meets the system requirements.**
For the most current hardware and software requirements, go to discoverygate.com and click **System Requirements** at the bottom of the page.
- Verify that Internet Explorer works.**
You access the following DiscoveryGate Web sites through Internet Explorer (on PCs) or through Safari (on Macintoshes):
 - For commercial customers: www.discoverygate.com
 - For academic customers: gateway.discoverygate.com
- Verify the active version of JRE at your site.**
For more information, see “[Verifying the Active Version of Java 2 Runtime Environment](#)” on [page 11](#).
- Verify that the Java Plug-in that you are using is set to Default on each end-user computer.**
See “[Determine the default version of JRE at your site](#)” on [page 11](#) for more information.
- Verify that you have at least read-access to the folder that contains the DiscoveryGate executable file.**
- Verify that you are logged on to the computer as Administrator.**

Verifying the Active Version of Java 2 Runtime Environment



Note: This version of DiscoveryGate requires that Java 2 Runtime Environment (JRE) 1.4.2_06 or 1.5.0 is set as the active JRE at your site. Elsevier MDL supports version 1.4.2_06 or 1.5.0. Versions lower than 1.4.2_06 have a known security risk that is fixed in version 1.4.2_06.

The current DiscoveryGate installer determines whether JRE is installed on the client computer:

- If the installer detects *no* JRE installed, it will install version 1.4.2_06, which will be set as the active JRE.
- If the installer detects an *older* version of JRE (for example, JRE 1.4.2_04 or lower), the installer will install version 1.4.2_06 and set this version as the active JRE.
- If the installer detects a *newer* version of JRE (for example, JRE 1.5.0) the installer will *not* install version 1.4.2_06. The newer version will remain the active JRE.

If you have JRE installed on the client computer, Elsevier MDL recommends that you determine which version you have installed. If you have applications that only run on a version older than JRE 1.4.2_06, you might need to update your environment before you install DiscoveryGate.

Determine the default version of JRE at your site

1. Verify that the default Java Plug-in is used as the default in Microsoft Internet Explorer:

If you are using JRE 1.4.2_06, follow this procedure:

- a. On the Control Panel, double-click **Java Plug-in** to launch the **Java Plug-in Control Panel**.
- b. Click the **Advanced** tab.
- c. Verify that **Use Java Plug-in Default** displays in the Java Runtime Environment drop-down box.
- d. If you changed the selection to **Use Java Plug-in Default** in Step 1c, click **Apply**.



Note: You will need to restart Internet Explorer to enable the default setting before completing this section.

- e. Click the **Browser** tab.
- f. Verify that Microsoft Internet Explorer checkbox is checked.
- g. Close the **Java Plug-in Control Panel** window.

If you are using JRE 1.5.0, follow this procedure:

- a. Open the Control panel, double-click the Java icon.
- b. Click **Advanced**.
- c. Expand **<APPLET> tag support**.
- d. Put a checkmark next to **Internet Explorer**.
- e. Click **OK**.

2. Open Internet Explorer.

3. Select **Tools > Sun Java Console**.
4. The default version is noted at the top of the screen.
5. Close the **Sun Java Console**.
6. Close Internet Explorer.



Note: If Java Plug-in 1.4.2_06 or 1.5.0 is not the default version, or if JRE 1.4.2_06 or 1.5.0 is not yet installed, you might need to update your environment before proceeding with the DiscoveryGate installation.

Save the DiscoveryGate Installation Package to Your Computer

Before you install DiscoveryGate, verify that you have your username, password, and company ID available. If you are installing DiscoveryGate for this first time, you should have received this information in an email from your DiscoveryGate administrator. If you are upgrading DiscoveryGate, the username, password, and company ID that you used for your previous version will apply to this upgrade.



Note: If you have already saved the DiscoveryGate installer to a folder on your computer, you can skip this step. Proceed to [“Start the Installer” on page 14](#).

Permissions required: Log on as a member of the Administrators group. Must have Full Control privileges on the computer on which DiscoveryGate is installed.

Log in to the DiscoveryGate Web site

1. Open Internet Explorer and enter the appropriate URL.
 - For corporate users, enter:
www.discoverygate.com
 - For academic users, enter:
gateway.discoverygate.com
2. In the left pane of the DiscoveryGate Web site home page, enter your username and password.



Tip: If you are installing for the first time, or if you did not select to remember your company ID, you will also need to enter that number.

3. Click **Go**.



Note: The procedure for saving the DiscoveryGate installer differs depending on whether you are installing the current version of DiscoveryGate for the first time on your computer, or accessing the installer after you have already installed the current version on your computer:

Installing the current version of DiscoveryGate for the first time on your computer

After you click **Go**, the Download DiscoveryGate Web page appears. Follow the instructions on the screen to install the current version of DiscoveryGate or the first time on your computer.

Reinstalling the current version of DiscoveryGate on your computer



Tip: Perform this task if you need to reinstall the current version DiscoveryGate and no longer have the installer saved on your computer.

1. After you click **Go**, you see the Home page of the DiscoveryGate application.
2. Select your **Settings** tab in the upper right corner of the screen.
3. On your Profile screen, scroll down until you see the **Software Download** section.
4. Click the link **Click to install software**. You see the DiscoveryGate Software Download Center Web page.
5. Follow the instructions on the screen to save the DiscoveryGate executable (.exe) file to a folder on your computer or network.

Start the Installer



Note: Before you launch the DiscoveryGate installer, you must close all open applications, including Internet Explorer. After you start the installer, you might be prompted to close any open Internet Explorer windows, even though you have already done so. In this case, you might need to kill Internet Explorer processes that are still running. Perform this task through the Windows Task Manager, on the Processes tab.

1. Open Windows Explorer.
2. Navigate to the folder into which you downloaded the executable file.
3. Double-click the DiscoveryGate executable (.exe) file.
4. Follow the screen prompts to complete the installation of DiscoveryGate.

Installer prompts

To install DiscoveryGate, follow the installer prompts. Click **Next** and **Back** to move through the installation screens. Click **Cancel** to quit the installation. After you click **Install**, the installer begins to write files to your hard drive. After that, you cannot cancel the installation.

If you have manually set the current JRE to something other than default, the installer will install JRE version 1.4.2_06.

After the installation, the installer informs you that the installation was successful. To launch DiscoveryGate, open Internet Explorer and enter the appropriate URL:

- For corporate users, enter:
`www.discoverygate.com`
- For academic users, enter:
`gateway.discoverygate.com`

Configuring DiscoveryGate



Caution: The information in this section is specific to the DiscoveryGate administrator at your site. Providing this information to DiscoveryGate users might compromise the setup and security of DiscoveryGate at your site. Elsevier MDL strongly recommends that you do not share the information in this section with other DiscoveryGate users at your site.

After you complete the installation of DiscoveryGate, you might want to perform some or all of the following tasks. Perform these tasks before you install DiscoveryGate on end-user computers.

- [Configure the DGPreConfig file](#)
- [Change the storage location of the saved searches](#)
- [Disable automatic updates of .jar files](#)
- [Configure access to IMRW](#)

These tasks are explained in the sections that follow.

Configure the DGPreConfig file



Note: This section is optional. If you are installing DiscoveryGate for the first time at your site, or you do not plan to change the settings for MDL Hop-Into at this time, you can skip this section. You can edit the `DGPreConfig.cfg` file at a later time.

If you have a previous installation of DiscoveryGate, you might have edited the `sample.cfg` or the `DGPreConfig.cfg` file that shipped with a previous version of DiscoveryGate. You might have edited this file manually, or by using the MDL Hop-Into Configuration Tool. This file updated the registry keys in the Windows registry for those custom applications.

You can include those custom settings for the current version of DiscoveryGate. The file, `DGPreconfig.cfg`, is installed with DiscoveryGate. The DiscoveryGate installer reads the contents `DGPreconfig.cfg` and enters the configuration information into the Windows registry of the client computer that will run MDL Hop-Into-enabled applications.

Editing the DGPreconfig.cfg file

1. After you have successfully installed DiscoveryGate, open Windows Explorer.
2. Navigate to the folder that contains the file `DGPreConfig.cfg`:


```
C:\MDL\DiscoveryGate\
```
3. Make a backup copy of this file (for example, save this file as `DGPreConfig_original.cfg`).
4. In Windows Explorer, locate the `sample.cfg` file on your computer.


```
C:\MDL\DiscoveryGate\
```
5. Make a backup copy of this file.
6. Open the file `sample.cfg` with a text editor.
7. Copy the custom information in the file.

8. Open the file `DGPreConfig.cfg` with a text editor.
9. Paste the custom information from the file `sample.cfg` into the file `DGPreConfig.cfg`.
10. Close the file `sample.cfg`.
11. Save and close the file `DGPreConfig.cfg`.
12. Place a copy of the file `DGPreConfig.cfg` into the folder that contains the DiscoveryGate executable (.exe) file that was previously downloaded.

When end-users run the installer from this location, the installer will use settings specified in the edited file `DGPreConfig.cfg` and update the registry keys accordingly. The installer will save this file into the folder `C:\MDL\DiscoveryGate\Help` for future use.

Using the automatic configuration

If your end-users have already installed the current version of DiscoveryGate, they can still update the registry keys with the information in the edited `DGPreConfig.cfg` file.

1. Locate the `DGPreConfig.cfg` file:
`C:\MDL\DiscoveryGate\Help`
2. Run the MDL Hop-Into Configuration Tool:
Choose **Start > Programs > DiscoveryGate > Hop-Into Configuration tool**
3. Select the **Automatic Configuration** option.
4. Click **Next**.
5. Navigate to the location of the file `DGPreConfig.cfg`, and select it.
6. Click **Open**.
7. The MDL Hop-Into Configuration Tool reads the specified configuration file, and updates the Windows registry according to the definitions in the configuration file.
 - If the MDL Hop-Into Configuration Tool encounters invalid or missing information in the configuration file, it notifies the end-user, and writes the incorrect XML entries to an error file. You will be prompted to view the error file. Click the **Yes** button to view the file. The end-user must report any error to the administrator. Close the error file to return to the Hop-Into Configuration Tool.
 - If the MDL Hop-Into Configuration Tool did not encounter any error, it confirms that all configuration information has been entered in the Windows registry.
8. To close the MDL Hop-Into Configuration Tool, select the **Cancel** radio button, and click **Yes**.

The automatic configuration error file

If the MDL Hop-Into Configuration Tool encounters an error in the configuration file, it writes the incorrect XML entry into an error file, `AutoConfigError.txt`. The MDL Hop-Into Configuration Tool writes `AutoConfigError.txt` in the temporary directory, as defined by the `%TEMP%` environment variable. If this file already exists, the MDL Hop-Into Configuration Tool overwrites the existing file. If the MDL Hop-Into Configuration Tool does not encounter an error, it does not remove an existing error file.

The error file includes a list of the most common errors encountered in a configuration file. You can refer to this list and Chapter 2, “XML Tags for Hop-Into Configuration” in the document *MDL Hop-Into Administration* (`hopinto_admin.pdf`) to determine the error in your XML entry.

Change the storage location of the saved searches



Tip: If end-users at your site have WRITE permission to the C: drive, *and* you choose not to change the default storage location of saved searches in MDL Database Browser, you can skip this section.

The `dbbinfo.xml` file defines the folder into which saved searches will reside. By default, MDL Database Browser creates the folder `C:\mdlweb\21\Profiles` and subdirectories for each DiscoveryGate user on the computer on which DiscoveryGate is installed. Searches performed in MDL Database Browser are saved as `.xml` files in these directories.



Note: If you are updating an existing version of DiscoveryGate, a new folder under `mdlweb` is not created. The installer uses the existing folder and subfolders does not rename them. If you are a new user, the installer creates a new folder and subfolder under `mdlweb` and names them `21\Profiles`.

At some sites, end-users might not have WRITE permission to the C: drive. In this case, you can edit the `dbbinfo.xml` file to change the storage location of the saved searches.

1. After you have successfully installed DiscoveryGate, locate the file `dbbinfo.xml`. This file is installed in:

```
C:\JRE_folder\lib\ext
```

2. Create a copy of this file, for example `dbbinfo.xml_copy`.
3. Open the original file (`dbbinfo.xml`) with an XML or a text editor.

The contents of the file resembles:

```
<default rootdir="C:\mdlweb\21" old_rootdir="C:\mdlweb"/>
```

The directory 21 may be 20. Consider the directory to be named **2x**.

4. To save the search files into a folder other than the default (for example, `C:\mdlweb\23`), change *only* the `default rootdir` path to the correct location. For example, to change the default directory to `D:\dbb_history`, modify the file as follows:

```
<default rootdir="D:\dbb_history" old_rootdir="C:\mdlweb"/>
```

5. Save the `dbbinfo.xml` file.
6. Verify that the edited file is a valid `.xml` file:
 - a. Open the file in Internet Explorer.
 - b. If prompted, choose Internet Explorer as the program to open the file.

If Internet Explorer does not show error messages, the file is valid.

Disable automatic updates of .jar files



Note: Academic users (those accessing DiscoveryGate through `gateway.discoverygate.com`) cannot disable automatic updates. If you are an academic user, proceed to the section “Configure access to IMRW” on page 19.

By default, the new AutoUpdate feature is *enabled* when you install DiscoveryGate. Each time a user logs on to DiscoveryGate, DiscoveryGate compares the Java component names and signature on the server to those on the client computer. If the signature on the server and client computer are not the same, DiscoveryGate prompts the user to copy the Java components from the server onto the client. These files are installed into:

```
C:\JRE_folder\lib\ext
```

where *JRE_folder* is the directory path of the active version of JRE, for example `C:\Program Files\Java\j2re1.4.2_06`. After all the Java components are copied onto the client, the Browser closes. The user must log into DiscoveryGate again.

DiscoveryGate provides users the ability to disable the AutoUpdate feature. Any user can choose to disable this feature for their own computer. Alternatively, the DiscoveryGate Administer can disable this feature for all DiscoveryGate users at your company.



Tip: If you disable the autoupdate feature in DiscoveryGate, Elsevier MDL recommends that you also disable the autoupdate feature of Java. If you leave the Java autoupdate feature enabled while the DiscoveryGate feature is disabled and Java sends updates, your DiscoveryGate installation will not find the correct .jar files and will not launch.

Disabling AutoUpdate on individual computers

After DiscoveryGate has been successfully installed, users can disable the AutoUpdate feature from their own Settings tab. Instruct users to scroll to the Autoupdate Configuration gatelet. To disable AutoUpdate, instruct users to click the **Disable Autoupdate** radio button and click **Update**.

Users can enable AutoUpdate at any time.

Disabling AutoUpdate on all DiscoveryGate computers



Tip: If the DiscoveryGate site administrator disables AutoUpdate, end-users will not see the AutoUpdate gatelet on their **Settings** tab.

After DiscoveryGate has been successfully installed, the DiscoveryGate site administrator can disable the AutoUpdate feature from the DiscoveryGate Software Download Center. On the DiscoveryGate Software Download Center screen, click the link **Setup user access to autoupdate**. You see the Grant or Deny Access screen. To disable AutoUpdate, click the **Deny Access** radio button and click **Update**.

You can grant access to users at any time.

Configure access to IMRW

The DiscoveryGate installer installs Integrated Major Reference Works (IMRW) during the installation process of DiscoveryGate. You no longer have to install IMRW separately. The IMRW files are installed into C:\MDL\DiscoveryGate.

1. On the computers on which you install DiscoveryGate, open Internet Explorer.
2. In Internet Explorer, choose **Tools > Internet Options**.
3. In the Internet Options window, click the **Security** tab and select the **Internet** icon.
4. Click **Custom Level**.

You see the Security Settings window.

5. Verify that the following ActiveX components are *enabled*:
 - Run ActiveX controls and plug-ins
 - Script ActiveX controls marked safe for scripting
6. Click **OK** to save the changes and close the Security Settings window.
7. Click **OK** to close the Internet Options window.

Installing DiscoveryGate on the End-User Computers



Note: Only a user with Administrator privileges can install DiscoveryGate.

Use the following checklist to prepare to install DiscoveryGate on end-user computers.

- (For Microsoft Windows users only) Verify that the JRE version that you are using is the supported version on each end-user computer.**
See “[Determine the default version of JRE at your site](#)” on page 11 for more information.
- (For Microsoft Windows users only) If you edited the `dbbinfo.xml` file, ensure that you saved it into the same folder that contains the DiscoveryGate executable (.exe) file you previously downloaded.**
- (For Microsoft Windows users only) If you edited the `DGPreConfig.cfg` file, ensure that you saved it into the same folder that contains the DiscoveryGate executable (.exe) file you previously downloaded.**
- Verify that the person installing DiscoveryGate has at least Read&Execute access to the folder that contains the executable file.**
- Verify that the person installing DiscoveryGate is logged on to the computer as Administrator.**
- Verify that the person installing DiscoveryGate has closed all applications, except Internet Explorer (on PCs) or Safari (on Macintoshes).**
- (For Microsoft Windows users only) Inform the person installing DiscoveryGate that the installer is available.**
Provide the person the location of the installer, instruct the person to launch the executable from that folder, and instruct the person to follow the installation prompts.
- Inform the person installing DiscoveryGate to launch the application.**
To launch DiscoveryGate, open Internet Explorer (or Safari) and enter the appropriate URL:
 - For corporate users, enter:
`www.discoverygate.com`
 - For academic users, enter:
`gateway.discoverygate.com`

Installing DiscoveryGate on Macintosh clients

If you are installing DiscoveryGate on a Macintosh client, instruct your end-users to open their browser and navigate to the link `gateway.discoverygate.com`.

The autoupdate functionality of DiscoveryGate installs the `.jar` files onto the computer. There are no other tasks required to install DiscoveryGate on Macintosh client computers.



Tip: If the DiscoveryGate site administrator disables AutoUpdate, end-users will not see the AutoUpdate gatelet on their **Settings** tab.

Enabling AutoUpdate

On the DiscoveryGate Software Download Center screen, click the link **Setup user access to autoupdate**. You see the Grant or Deny Access screen. To enable AutoUpdate, click the **Grant Access** radio button and click **Update**.

You can grant access to users at any time.

Postinstallation Tasks

During the installation process, the DiscoveryGate installer determines which files and add-ins to install. If you run the installer after you have successfully installed DiscoveryGate, you are prompted to choose one of the following tasks:

- Modify the installation
- Repair the installation
- Remove the installation

Modify the installation

You will need to modify your DiscoveryGate installation if:

- You install MDL ISIS/Base after you install DiscoveryGate

If the installer determines that MDL ISIS/Base is not installed, the installer does *not* install the associated add-ins. If you choose to install MDL ISIS/Base *after* you install DiscoveryGate, you must modify the installation of DiscoveryGate.

- You changed your active JRE *and* you have turned off the AutoUpdate feature

To modify the current installation, run the installer. At the prompt, click the **Modify** radio button and click then **Next**. The DiscoveryGate installer reinstalls the original files, and installs the appropriate files for MDL ISIS/Base or installs the `.jar` files into the new active JRE path.



Note: The installer will *not* migrate the history files (with the file `dbbinfo.xml`) or update the registry entries (with the file `DGPreConfig.cfg`) during the modification process.

Repair the installation

If you determine that one or more files have been corrupted at any time during the use of DiscoveryGate, you can repair the installation.

To repair the current installation, un the installer. At the prompt, click the **Repair** radio button and then click **Next**. The DiscoveryGate installer reinstalls the original files, replacing the corrupted files.



Note: The installer will *not* migrate the history files (with the file `dbbinfo.xml`) or update the registry entries (with the file `DGPreConfig.cfg`) during the modification process.

Remove the installation

If you choose to uninstall DiscoveryGate, you can run the installer. At the prompt, click the **Remove** radio button and then click **Next**. The DiscoveryGate installer removes the DiscoveryGate files from your computer.



Note: The Uninstall program does not remove all of the files that are installed. For more information, see [“Uninstalling DiscoveryGate” on page 22](#).

Uninstalling DiscoveryGate



Note: You must log out of all applications, including Internet Explorer, in order to uninstall DiscoveryGate.

To uninstall DiscoveryGate, you have a choice:

- Run the installer and click the **Remove** button as explained in [“Remove the installation” on page 22](#).
- Run the **Add/Remove Programs** tool from the Control Panel.

The uninstall program does not remove all of the files that were installed. Table 2 lists the files that remain on your computer.

Table 2 Files that remain after uninstalling DiscoveryGate

File	Location
Java 2 Runtime Environment files	<i>JRE_folder</i>
<code>rcdll32pp.dll</code>	<i>ISIS/Base_folder</i>
<code>typ32_25.dll</code>	<i>ISIS/Base_folder</i>
<code>dbbinfo.xml</code>	<i>JRE_folder\lib\ext</i>
DiscoveryGate history files	<i>\mdlweb\version_number</i>

Verifying Your DiscoveryGate Installation

This chapter provides information that helps you to verify your DiscoveryGate installation.

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Verifying That JRE 1.4.2_06 or 1.5.0 is the Active Version of JRE

DiscoveryGate runs on JRE 1.4.2_06 or 1.5.0. If you manually set your Java environment to a version lower than 1.4.2_06, and did not click **Yes** during the installation process to have the installer set version 1.4.2_06 as the default, you need to manually change the version of JRE before you can run the current version of DiscoveryGate.

1. Open Internet Explorer.
2. Select **Tools > Sun Java Console**.
3. The default version is noted at the top of the screen.



Tip: If a version of Java Plug-in 1.4.2_05 or lower (or JRE 1.5) displays as the default version, you need to update your environment before performing the DiscoveryGate installation. Perform the steps that follow.

4. Close Internet Explorer.
5. Open the Control Panel.
6. Double-click **Java Plug-in** to launch the **Java Plug-in Control Panel**.
7. Click the **Advanced** tab.
8. Choose **JRE 1.4.2_06 in *drive*:\Program Files\Java\j2re1.4.2_06** from the drop-down list box where *drive* is the drive on which you installed JRE.
9. Click **Apply**.
10. Restart Internet Explorer to enable the new setting.

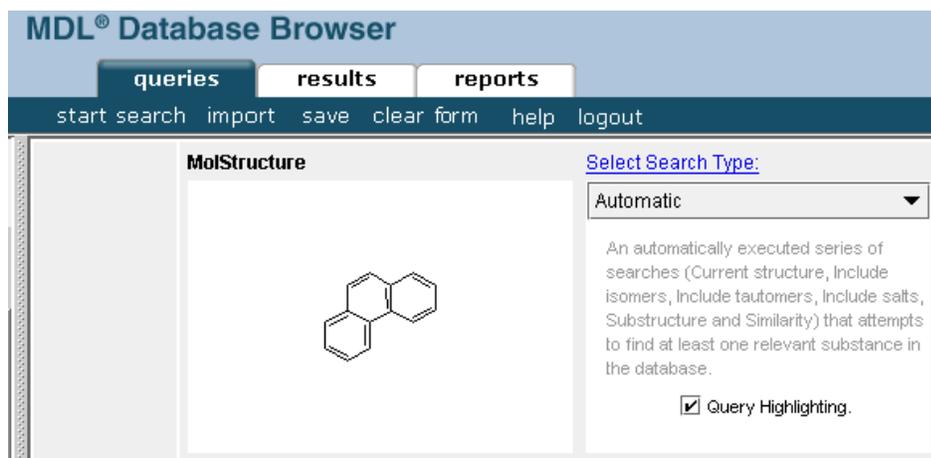
Verifying That You Can Use Hop-In With MDL Database Browser

This section contains procedures that help you to verify that you can use MDL Hop-Into with MDL Database Browser. To perform these procedures, you must first verify that you have enabled the corresponding database with MDL Hop-Into. See the document *MDL Hop-Into Administration* for information about enabling MDL Hop-Into.

Verify that you can search databases using MDL Database Browser

This section explains how to hop in to MDL content databases using MDL Database Browser. You must have access to the content databases in order to hop into them from MDL Database Browser.

1. Verify that you have added the MDL content databases as MDL Hop-Into-enabled applications. See:
 - The section “[Configure the DGPreConfig file](#)” on page 15, or
 - The document *MDL Hop-Into Administration* or MDL Hop-Into Help for more information
2. Log in to DiscoveryGate.
3. Launch MDL Database Browser. To launch MDL Database Browser, start from the Home page and either use QuickSearch or under Applications, click Search Databases.
4. Perform a search in MDL Database Browser. For example, in the MDL Compound Index, perform an Automatic search for Phenanthrene:



The screenshot displays the MDL Database Browser interface. At the top, there are tabs for "queries", "results", and "reports". Below these are navigation links: "start search", "import", "save", "clear form", "help", and "logout". The main content area is titled "MolStructure" and features a chemical structure of Phenanthrene. To the right of the structure is a "Select Search Type:" dropdown menu set to "Automatic". Below the dropdown, a description reads: "An automatically executed series of searches (Current structure, Include isomers, Include tautomers, Include salts, Substructure and Similarity) that attempts to find at least one relevant substance in the database." A checkbox labeled "Query Highlighting" is checked.

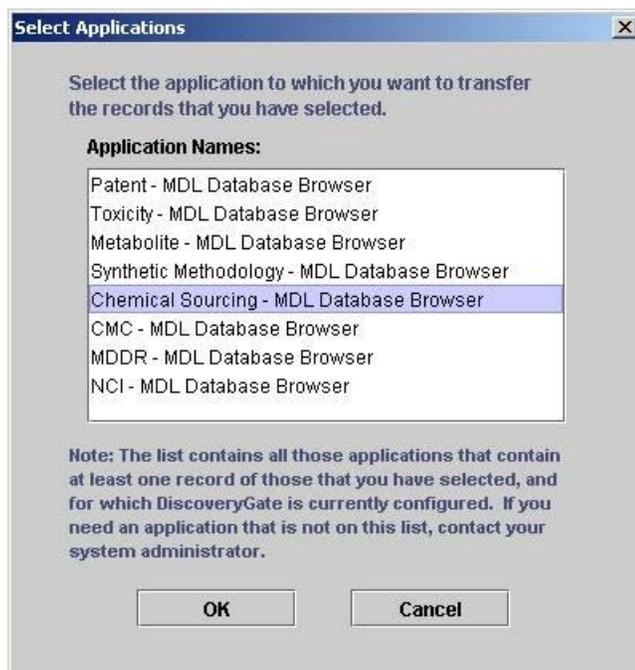
You see the results of your search in MDL Compound Index. The databases listed to the right of the search structure are the MDL Compound Index databases that contain the structure Phenanthrene.

The screenshot displays the DiscoveryGate MDL Database Browser interface. The top navigation bar includes tabs for 'queries', 'results', and 'reports', with 'results' selected. Below the navigation bar are utility links: 'copy to report', 'export', 'page setup', 'print', 'save', 'refine query', 'lists', 'help', and 'logout'. The main interface is divided into several sections:

- Database:** A dropdown menu set to 'MDL® Compound Index'.
- Find in History:** A search input field and a 'Next' button.
- Field Index / History:** A tree view showing search history with categories like 'Today's Searches', 'Previous Searches', 'Saved Searches', and 'Temporary Lists'. 'Search #2' is highlighted.
- View Options:** Links for 'Grid View', 'Database View', and 'Properties View'.
- Action Links:** 'View selected records in another database'.
- Page Controls:** 'Pages: 1' and buttons for 'Select All' and 'Clear All'.
- Search Results:** A table with one row containing a chemical structure of Phenanthrene (SMILES: c1ccc2c(c1)ccc3ccccc23), a checkbox labeled 'Record#1', and a grid of database names: ACD, CCR, CIRX, CSM, DJSM, DWPI, Metabolite, NCI, OHS MSDS, ORGSYN, Pat Chem, REFLIB, SCD, and Toxicity.
- Bottom Section:** Repeats the 'Pages: 1', 'Select All', 'Clear All', and view options.

5. In the results page, click the link **View selected records in another database** at the top of the page.
6. Select the number of records that you want to view. The default setting is **Current Page**.
7. Click **OK**.

- From the **Select Application** drop-down list box, select **Chemical Sourcing - MDL Database Browser**:

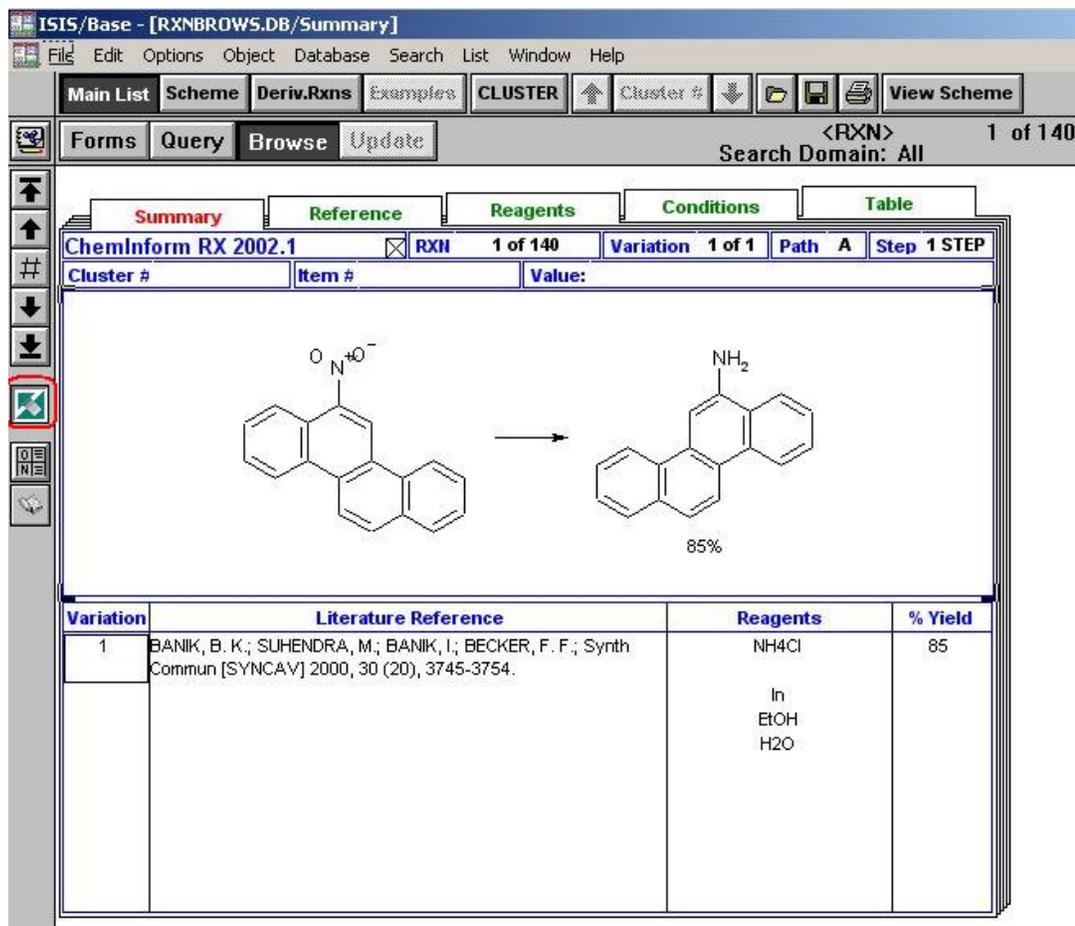


- Click **OK**.
- MDL Database Browser displays records that match your search requirements in the Chemical Sourcing and Logistics database:

Verify that you can hop-into MDL Database Browser from MDL ISIS/Base

This section explains how to hop-into MDL Database Browser from MDL ISIS/Base. Verify that you have installed MDL ISIS/Base before you continue with this section.

1. Log in to MDL ISIS/Base.
2. Perform a search in MDL ISIS/Base.
3. To hop into MDL Database Browser, click the green arrow button  on the left menu bar:



The screenshot shows the MDL ISIS/Base interface. The main window displays a chemical reaction scheme for the reduction of a nitro compound to an amine. The reaction is shown as:

O=[N+]([O-])c1ccc2cc3ccccc3cc2c1>>Nc1ccc2cc3ccccc3cc2c1

The yield is indicated as 85%.

Below the reaction scheme is a table with the following data:

Variation	Literature Reference	Reagents	% Yield
1	BANIK, B. K.; SUHENDRA, M.; BANIK, I.; BECKER, F. F.; Synth Commun [SYNCAV] 2000, 30 (20), 3745-3754.	NH4Cl In EtOH H2O	85

MDL Database Browser launches.



Tip: If you do not have an active session of DiscoveryGate open, you will be prompted for your username, password, and company ID before MDL Database launches. This information is the same as your DiscoveryGate login information.

4. MDL Database Browser displays the results in MDL Compound Index.
5. To view a specific result in a specific database, click the number of the result and then choose a database from the drop-down list in the left pane.

Verify that you can hop-into MDL Database Browser from MDL CrossFire Commander

1. Verify that you have enabled hop-into for MDL CrossFire Commander:
 - a. Open the file `DGPreConfig.cfg` with a text editor (or the file `sample.cfg` if you are a new DiscoveryGate user).
 - b. Scroll through the file until you see this section:

```
<!-- Example to configure MDL Crossfire Commander 7.0          --!>
<configinfoitem targetappname = "MDL Crossfire Commander"
  apptype = "others"
  datasource = "XFG + XFR + XFRA + XFRAE + XFPAT"
  targetexecutable="C:\Program Files\MDL Crossfire Commander 7.0\XfCm.exe"
  function_enabled = "classification" />
```

- c. The `<configinfoitem />` statement should not be preceded with the comment symbols (that is, the `<!--` and `--!>` symbols should be removed from the statement).
 - d. If the statement is uncommented, close the file. Continue to Step 2.
 - e. If the statement *is* commented, remove the comments and save the file.
 - f. Run the Hop-Into Configuration Tool to enable MDL CrossFire Commander.

See the section [“Using the automatic configuration” on page 16](#) for more information. Select the file that you have just edited.

2. Conduct a search in MDL CrossFire Commander (for example, a substructure search for Phenanthrene) and select the structures you want to transfer to MDL Database Browser by selecting the checkbox next to the **Go** button in the Short view. For example:

Substance Identification		Hitset Family	<input checked="" type="checkbox"/> Go	<input checked="" type="checkbox"/>
Beilstein Registry Number	7094			
Beilstein Preferred RN	203-65-6			
CAS Registry Number	203-65-6			
Chemical Name	4 <i>H</i> -benzo[<i>d</i> e]carbazole			
	4,5-epiminophenanthrene			
Autoname	4 <i>H</i> -benzo[<i>d</i> e]carbazole			
Molecular Formula	C ₁₄ H ₉ N			
Molecular Weight	191.23			
Lawson Number	24516			
Type of Substance	heterocyclic			
Constitution ID	19420			
Tautomer ID	40854			
Beilstein Reference	4-20-00-04135, 5-20-08-00352, 6-20			

3. Click the **Go**  button.
4. Select the option **MDL Database Browser**.
5. If multiple compounds have been selected, you will be prompted to hop using RegNo list of the entries. Click **Yes**.

MDL Database Browser launches.

- You are prompted for your username and password before MDL Database Browser can open. This information is the same as your DiscoveryGate login information.



Tip: You are prompted for your username and password each time you transfer hits from MDL CrossFire Commander to MDL Database Browser.

- The hit list compounds are now displayed in MDL Database Browser. For example:

The screenshot displays the MDL Database Browser interface. At the top, the title bar reads "DiscoveryGate® | MDL® Database Browser". Below this is a navigation menu with tabs for "queries", "results" (which is active), "reports", and "rxn schemes". A secondary menu contains options: "copy to report", "export", "page setup", "print", "save", "refine query", "lists", "help", and "logout".

The main content area is divided into several sections:

- Database:** A dropdown menu is set to "CrossFire Beilstein".
- View selected records in another database** and **Create List** links are present.
- Pages: 1** and **Total Records: 1** are displayed, along with **Select All** and **Clear All** buttons.
- A central box shows the record details for **BRN: 7094**, featuring a chemical structure of a tricyclic compound (indole derivative) and links for **Details** and **Synthesize**.
- At the bottom of the record box, there is a checkbox labeled **Record#1**.
- Below the record box, the same pagination information is repeated: **Pages: 1**, **Select All**, **Clear All**, and **Total Records: 1**.

On the left side of the interface, there is a sidebar with a tree view under "History". It includes "Today's Searches" (with "Search #1" and "Search #2"), "Previous Searches", "Saved Searches", and "Temporary Lists".

Hopping into MDL Crossfire Commander from MDL Database Browser

1. Verify that you have enabled hop-into for MDL CrossFire Commander. See [Step 1 on page 29](#) for more information.
2. Follow the steps in the procedure “[Verify that you can search databases using MDL Database Browser](#)” on page 25.
3. Choose either CrossFire Beilstein or CrossFire Gmelin from the drop-down list:

DiscoveryGate® | MDL® Database Browser

queries results reports

copy to report export page setup print

Database: MDL® Compound Index ?

Grid View Database View Properties

View selected records in another database

Pages: 1 [Select All](#) [Clear All](#)

1

ACD
CSM
Metabolite
ORGSYN

4. Your results show in MDL Database Browser, which has connected to MDL CrossFire Beilstein:

start search import save clear query help logout **CrossFire Beilstein**

Database: **CrossFire Beilstein** ?

Find in Field Index: Next

Field Index History

Structure

Easy Data Search

Basic Indexes

Bibliographic Information

Substance Identification

Chemical Properties

Physical Properties

Pharmacological and Eco

Structure

Find this compound and its properties

Substitution as drawn, exclude tautomers

Substitution as drawn, include tautomers

Unlimited substitution on all atoms, exclude tautomers

Allow:

Multi-component substances

Ring closure through substitution

Isotopes Charges Radicals

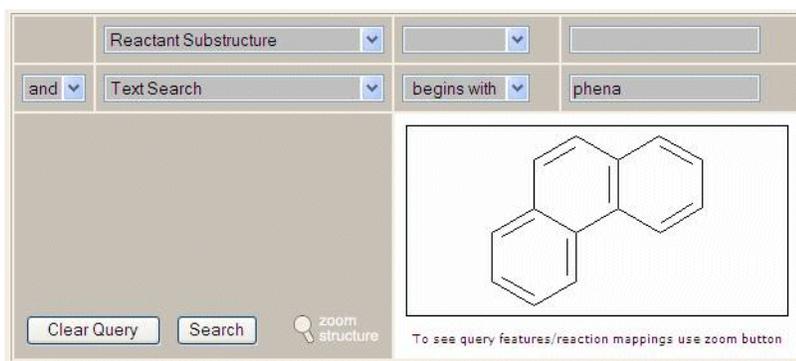
Keep fragments separate

Search Stereoinformation As drawn

Query Highlighting

Verify that you can hop into MDL Database Browser from IMRW

1. Verify that you have added IMRW as an MDL Hop-Into-enabled application. See:
 - The section “[Configure the DGPreConfig file](#)” on page 15, or
 - The document *MDL Hop-Into Administration* or MDL Hop-Into Help for more information
2. Log in to DiscoveryGate.
3. Click the link **Integrated Major Reference Works** to launch IMRW.
4. In IMRW, perform a search. For example, perform a Reactant Substructure search for Phenanthrene:



The screenshot shows a search interface with the following elements:

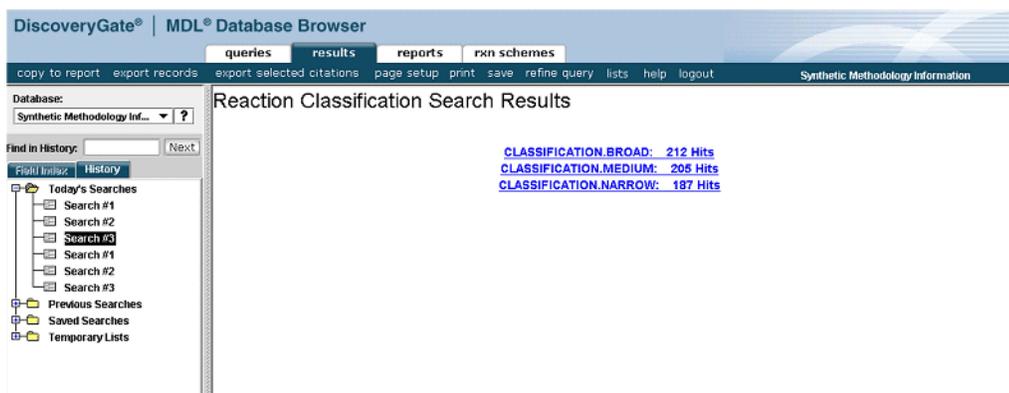
- Search type: **Reactant Substructure** (dropdown menu)
- Operator: **and** (dropdown menu)
- Search method: **Text Search** (dropdown menu)
- Filter: **begins with** (dropdown menu)
- Search term: **phena** (text input)
- Buttons: **Clear Query**, **Search**, and **zoom structure** (with a magnifying glass icon)
- Chemical structure: A skeletal structure of Phenanthrene is displayed in a box.
- Footnote: **To see query features/reaction mappings use zoom button**

- Two hits are returned.
5. From the drop-down listbox for the first hit, select **Synthetic Methodology - MDL Database Browser**:
 6. Click **Go**.
MDL Database Browser launches.
 7. You are prompted for your username and password before MDL Database Browser can open. This information is the same as your DiscoveryGate login information.



Tip: You are prompted for your username and password each time you transfer hits from IMRW to MDL Database Browser.

8. MDL Database Browser displays the Classification Search Results as links in the results pane. To view the results of a specific hit, click the corresponding link.



Changes to the Registry

Table 3 lists the information that the DiscoveryGate installer writes to your registry.

Table 3 Information that the DiscoveryGate installer writes to the registry

Key	Name	Value
HKEY_LOCAL_MACHINE\SOFTWARE\MDL Information Systems, Inc.\DiscoveryGate\version.number	Path	Directory into which you installed DiscoveryGate
HKEY_LOCAL_MACHINE\SOFTWARE\MDL Information Systems, Inc.\ DiscoveryGate\version.number	JARFilesPath	JRE_folder\li b\ext
HKEY_LOCAL_MACHINE\SOFTWARE\MDL Information Systems, Inc.\ DiscoveryGate\version.number	Program Folder	Name of folder into which you install DiscoveryGate
HKEY_LOCAL_MACHINE\SOFTWARE\MDL Information Systems, Inc.\ DiscoveryGate\version.number	Version	Build version of DiscoveryGate
HKEY_LOCAL_MACHINE\SOFTWARE\InfoChem\MRW\ Client	Editor	Location of MDL Draw
HKEY_LOCAL_MACHINE\SOFTWARE\InfoChem\MRW\ Client	Isisbase	Location of MDL ISIS/Base

Table 3 Information that the DiscoveryGate installer writes to the registry (Continued)

Key	Name	Value
HKEY_LOCAL_MACHINE\SOFTWARE\InfoChem\MRW\Client	Isisdraw	Empty
HKEY_LOCAL_MACHINE\SOFTWARE\InfoChem\MRW\Client	OCX	Directory into which DiscoveryGate installs IMRW
HKEY_LOCAL_MACHINE\SOFTWARE\MDL Information Systems, Inc.\Hop-Into	Base Executable	Location of MDL ISIS/Base
HKEY_LOCAL_MACHINE\SOFTWARE\MDL Information Systems, Inc.\Hop-Into	Path	Directory into which DiscoveryGate installs MDL Hop-Into
HKEY_LOCAL_MACHINE\SOFTWARE\MDL Information Systems, Inc.\Hop-Into\1.1 SP2	Path	Directory into which DiscoveryGate installs MDL Hop-Into
HKEY_LOCAL_MACHINE\SOFTWARE\MDL Information Systems, Inc.\Hop-Into\1.1 SP2	Program Folder	Folder into which DiscoveryGate installs MDL Hop-Into
HKEY_LOCAL_MACHINE\SOFTWARE\MDL Information Systems, Inc.\Hop-Into\1.1 SP2	Version	1.1 SP2
HKEY_LOCAL_MACHINE\SOFTWARE\MDL Information Systems, Inc.\Hop-IntoCfg	LeastReuseKey	21
HKEY_LOCAL_MACHINE\SOFTWARE\MDL Information Systems, Inc.\Hop-IntoCfg	NextAppKey	21