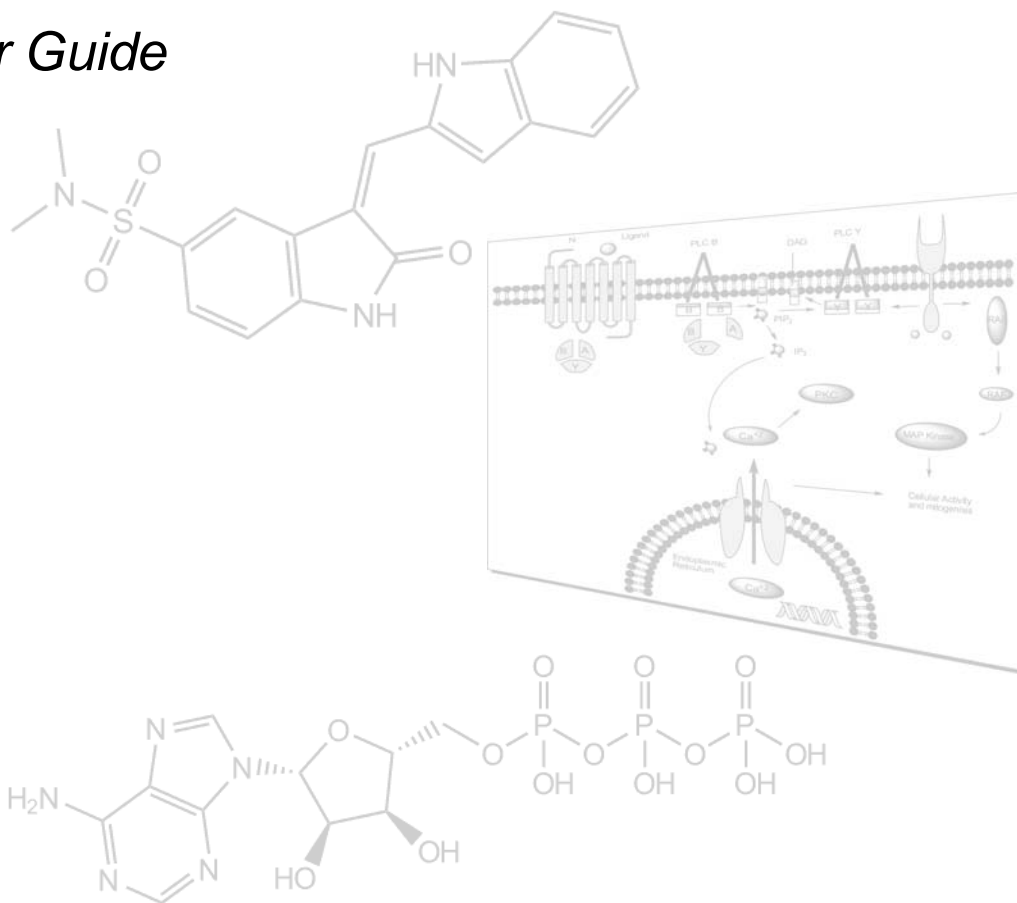


Drug Degradation

*Chem & Bio Office Enterprise 2008
Decision Support Platform
Enterprise 10*

User Guide



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Drug Degradation

About this Guide

Welcome to the Drug Degradation User and Administrator Guide. Inside this guide, you will find a full description Drug Degradation, its features, and complete instructions on how to use them. This guide is available in print, CHM, and Web-based format.

Overview

CambridgeSoft's Drug Degradation system lets you manage records for reagents that degrade over time. You can keep track of products, reactions, and the environments in which the degradation reactions take place. Using the ChemOffice Webserver, you can also look up records from other Drug Degradation users.

Logging in

Before using Drug Degradation, you must first log in. After you log in, you will see the CambridgeSoft ChemOffice Enterprise main Web page. On this page is a menu of applications to which you are subscribed¹, including Drug Degradation.

1. Enter `http://<servername>/` into your web browser where `<servername>` is the

1. Links are displayed only for the applications to which you are subscribed.

name of your webserver. The ChemOffice WebServer Global Login page appears.

NOTE: To find the name of your webserver, see your system administrator.

2. At the login screen, enter your username and password and click the **Log In** button. The CambridgeSoft ChemOffice Enterprise main Web page appears.
3. Under Drug Degradation, click the **Main Page** link.

The CambridgeSoft Drug Degradation Enterprise page appears.

Searching for Compounds

Typically, to view or modify a compound record, you will first need to search for it in the Drug Degradation database.

You can search for compounds using a variety of criteria: the compound name, various chemical properties, or even a drawing of all or part of the structure.

1. On the CambridgeSoft Drug Degradation Enterprise page, click the **Search** link. The Drug Degradation Parent Compound Search page appears.
2. Enter search criteria as desired. The criteria you can enter are defined below:

Parent. Using the ChemDraw plugin, draw a parent structure for which to search and select the appropriate option in the **SearchType** drop-down list.

Formula. Enter the chemical formula.

Molecular weight. Enter the molecular weight.

Functional Group. Select a functional group from the dropdown list.

Conditions. Select a degradation condition.

Salt. Select a salt or salt type from the dropdown list.

Generic name. Enter a generic name, if any, for the compound.

Trade name. Enter a trade name, if any, for the compound.

Common/Other name. Enter a another name, if any, for the compound.

Compound ID. Enter the ID, if any, for the compound.

Degradant. Draw a degradant structure for which to search. Then select the appropriate option in the **SearchType** dropdown list.

3. Click the **Search** button. The results are shown in list view.

Parent Compound Record Data

You can add or edit parent compound records in the Drug Degradation database. Also, if you have DocManager installed, you can link to stored documents.

Adding a Parent Compound

Using the ChemDraw Toolbar, you can add new parent compound structures through a ChemOffice Webserver form.

To add a new parent compound:

1. In the CambridgeSoft Drug Degradation Enterprise Web page, click **Add Parent Compound**.

The Add Parent Compound page appears.

2. Using the ChemDraw Toolbar, draw the parent compound.

3. Enter additional information in the appropriate fields. The fields are described below:

- Generic Name
- Trade Name
- Common/Other Name
- Compound Number

4. If this is a salt, check the appropriate checkbox.

NOTE: Only the structure drawing is required. Steps 3 and 4 are optional.

5. Click the **Add Record** button.

Editing a Parent Compound

To edit a compound, you first search for it in the database and then edit it as desired.

1. In the CambridgeSoft Drug Degradation Enterprise main page, click **Search**.
2. In the Parent Compound Search page, enter the criteria for the compound you want to edit.
3. Click the **Search** button.
4. In the search results, click the **Show Details** button for the compound you want to edit.
5. In the Parent Compound Details screen, click the **Edit Record** button.
6. Edit the parent compound data as desired.
7. Click the **Update** button.

Linking to Parent Compound Records

If you have Document Manager installed and Drug Degradation is configured to integrate with DocManager, you can add document links to parent compound records. The Add Doc

Link button will appear at the bottom of the parent compound records. See your system administrator for more configuration details.

NOTE: Links to the documents you can add are limited to the documents in the Document Manager database.

To add a link to your parent compound record:

1. Search for the record to which you want to link a document.
2. In the search results, locate the compound you want and click its corresponding **Show Details** button.
3. Click the **Add Doc Link** button. The Documentation Manager Search window appears.

A document Manager search window appears.

4. Enter criteria to search for the document that you want to link to the compound. For more information about searching for documents in DocManager, see the DocManager user's guide.
5. Click the **Search** button.
6. In the search results, click **Add Doc Link** next to the appropriate document. The link is added to the parent compound record.

Adding an Experiment

Degradation experiment data is specific to each parent compound. Therefore, after you add or search for a parent compound, you can add an experiment to it.

To add degradation experiment data:

1. Do one of the following:
 - To add an experiment to a parent compound record that you just added, click **Add an Experiment to this Parent Com-**

pound. in the Parent Compound Details page.

- To add an experiment to a compound you found in a search, click its corresponding **Show Details** button and click **Add an Experiment to this Parent Compound.** The Add Degradation Experiment page appears.
2. Select a degradation condition from the **degradation conditions** dropdown list.

NOTE: If your degradation condition is not listed, see your system administrator or the Drug Degradation Administrator's Guide.

3. Enter appropriate information in the other fields.
4. Click the **Add Record** button. A link with the conditions name is added to the record.

Experimental Details

Viewing Experimental Details

1. Search for the record for which you want to view details.
2. In the search results, locate the record you want and click its corresponding **Show Details** button.
3. Under **View an existing experiment**, select the experiment you want to view. The Degradation Experiment Details page appears.

While viewing experimental details, you can edit the record and add information to the experiment, such as degradants and mechanisms.

Editing the experimental record

To edit an experiment record:

1. Click the **Edit Record** button or the **Edit Experiment** link.
2. Enter the appropriate information.
3. Click the **Update** button.

The new information is reflected in the Degradation Experimental Details Page.

Adding a degradant

To add a degradant to an experiment record:

1. In the Degradation Experiment Details page, click **Add a Degradant to this experiment**.

The Add Degradant Compound page appears.

2. Using the ChemDraw toolbar, draw the degradant in the structure window.
3. Enter additional information as needed.
4. Click the **Add Record** button. The degradant is added to the experiment record.
5. Complete the form again to add another degradant compound or click one of the following to exit the page:

- The **Main Menu** button
- The **Return to Experiment Details** link
- The **Return to main page** link

Editing a degradant

1. In the Degradation Experiment Details page, click the corresponding **Edit Degradant** link for the degradant you want

to edit. The Edit Degradant Compound page appears.

2. Modify the degradant text fields or drawing as desired.
3. Click the **Update Record** button. The Degradant Compound Details page appears, displaying the updated degradant record.
4. Click the **Return to Experiment** button to view the experiment.

Adding a mechanism

1. In the Degradation Experiment Details page, click the **Add Mechanism** link for the degradation to which to add a mechanism. The Add Degradation Mechanism page appears.
2. Using the ChemDraw toolbar, draw the mechanism in the drawing field.
3. Click the **Add Record** button.

Viewing a Mechanism

To view a mechanism that has been added to an experiment:

1. Go to the Degradation Experiment Details page.
2. Under Degradants in this experiment, click the **View Mechanism** link for the desired degradant.

Managing Lists

Managing Conditions and Salts Lists

Users with the appropriate privileges can populate lists of conditions and salts through the Drug Degradation interface. These lists appear in the conditions and salt options when users fill out the record submission forms.

Managing Conditions Lists

The conditions lists appear in experiment submission forms. These forms let users select a degradation condition for an experiment.

Adding a New Condition

To add a new condition to the list:

1. In the CambridgeSoft Drug Degradation Enterprise page, click the **Manage Experimental Conditions List** link. The Manage Degradation Condition List appears.
2. Enter the name of a degradation condition in the textbox.
3. Click **Add Record**.
4. Click the **Main Menu** button to return to the CambridgeSoft Drug Degradation Enterprise page.

Editing an existing Condition

To edit a condition already in the conditions list:

1. In the CambridgeSoft Drug Degradation Enterprise page, click the **Manage Experimental Conditions List** link. The Manage Degradation Condition List appears.

2. Click the corresponding **Change Text** button for the condition you want to edit. The Change Degradation Condition Text page appears.
3. Enter a new name for the condition.
4. Click **Update**.

Deleting a Condition from the List

You can delete only those conditions you added to the list.

To delete a condition from the list:

1. In the CambridgeSoft Drug Degradation Enterprise page, click the **Manage Experimental Conditions List** link. The Manage Degradation Condition List appears.
2. Click the corresponding **Delete Condition** button for the condition you want to delete.
3. You are asked to confirm your decision to delete the condition. Click the **Delete** button.

Managing Salts Lists

The salt lists appear in parent record submission forms. These forms allow users to select salts to be associated with parent compounds.

To add to or edit the salt lists, do one of the following:

- Click **Manage salt list** in the CambridgeSoft Drug Degradation Enterprise page.
- Click **Add/Edit Salts** in the ChemOffice Webserver global login page.

The Manage Parent Salt List page appears.

Adding a New Salt

To add a new salt to the list:

1. Enter a salt code and salt name in the appropriate textboxes.

NOTE: Salt codes must be unique and be two characters long.

2. Click **Add Record**.

The salt you added appears in the salt list with its corresponding salt code shown in parentheses.

Editing an existing Salt

To edit a salt already in the salt list:

1. In the Manage Parent Salt List page, click the name of the salt you want to edit. The salt name becomes highlighted.
2. Click the **Edit Record** button. A page allowing you to edit the salt name appears.
3. Enter a new salt name in the text box.
4. Click the **Update** button.

Managing Functional Groups

Adding Functional groups

1. In the CambridgeSoft Drug Degradation Enterprise page, click the **Manage functional group list** link.

2. In the New functional group text box, enter the formula or name for the functional group. (examples: “CH3”, “Acetyl”)
3. Click the **Add Record** button.

Deleting functional groups

You can delete only those functional groups you have added to the list.

To delete a functional group:

1. In the CambridgeSoft Drug Degradation Enterprise page, click the **Manage functional group list** link.
2. In the functional group list, select the **Delete Functional Group** link for the group you want to delete.
3. Click the corresponding **Delete functional group** link for the functional group to delete. When you are prompted to verify that you want to delete the functional group.

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