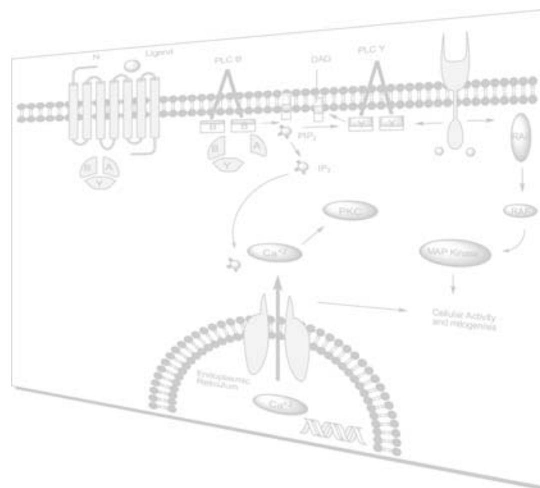
Registration Enterprise 10.0

Chem & Bio Office Enterprise 2008
Decision Support Platform
Enterprise 10

User Guide



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Registration Enterprise 10.0

About this Guide

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

Overview

Registration Enterprise is a ChemOffice Enterprise application that allows you to track and characterize the compounds and batches procured or synthesized by the chemical laboratories. It ensures the uniqueness of the compounds by assigning unique IDs to the compounds and providing provisions for automatic duplicate checking.

The unique IDs that are assigned by Registration Enterprise to the compounds are known as Registration numbers. Registration numbers are drawn sequentially from a table. If a compound is removed from the database, its registration number is not re-used. Administrators define how registry numbers are structured. The default is: Prefix-Sequence, but the numbers can have different delimiters, contain a suffix, etc.

For Example: AB-003255; CST-88475

The compounds can also be identified by their names and structures, but identifying them by their Registration ID is more useful because chemical names can be cumbersome and a compound can have multiple names. Similarly, chemical structures can be unique, but they cannot be verbalized and included easily in the written reports.

Benefits

- Uses Oracle's robust data model to manage chemical products and their properties.
- Checks for uniqueness during registration and will register duplicates as batches of existing substance.
- User administration and data entry are done through simple, easy-to-learn web forms.
- Provides an additional qualifying step before registering the compound.
- Data entry errors, or other human errors can be detected before registering the compound in your company-wide database.
- Highly customizable and easy to use.

Registration Enterprise Workflow

The entire Registration Enterprise workflow can be summarized as follows:

1. Add a compound or batch to the temporary table.
2. Add a salt to a compound.
3. Edit/Review the record if desired.
4. Permanently register the compound record.
5. Add a batch, identifier information, or analytical data to a registered record.

Compounds, when submitted, are initially stored in a temporary table. In order for those compounds to be moved to the permanent table, the compounds must be approved and registered.

The various characteristics of the registration process are as follows:

- Batch and analytical data can only be added to registered compounds.
- Registration numbers are assigned when compounds are moved from the temporary table to the permanent table.
- The application checks for duplicates only when a compound is being registered in the permanent table.

Required Fields

- Required Fields are fields that must be filled in before being allowed to submit a record.
- Required Fields are indicated by a red box enclosing the field and field name. Refer figure below. In the figure the structure field is the required field.

- Required fields on each input form are configurable (see your system administrator for more details).

Registration Enterprise Home Page

To access the home page of Registration Enterprise:

1. Enter username and password in the ChemOffice Enterprise global login page.
2. Click **Main Menu** in the **Registration Enterprise** section in the home page of ChemOffice Enterprise. The home page of Registration Enterprise appears:

NOTE: Registration Enterprise uses Global Login. If you are already logged in and you click the Registration Enterprise link, you will be sent directly to the application.

You can perform the following tasks in this page:

- Add a new compound, batch, or container to the temporary table
- Search the temporary table
- Register a record and add identifier or analytical data to the registered record
- Search Registration Enterprise for a registered record
- View analytics spreadsheet
- Perform administration tasks

Compounds, Batches, and Containers

When a compound or batch is added to Registration Enterprise, it is first added to a temporary table in the database. To add the compound or batch permanently to the database, you need to register it in Registration Enterprise.

In addition to tracking compounds and batches, Registration Enterprise also allows you to create containers in Inventory Enterprise. To create containers using Registration Enterprise, you need to integrate Registration Enterprise with Inventory Enterprise by modifying the .ini settings.

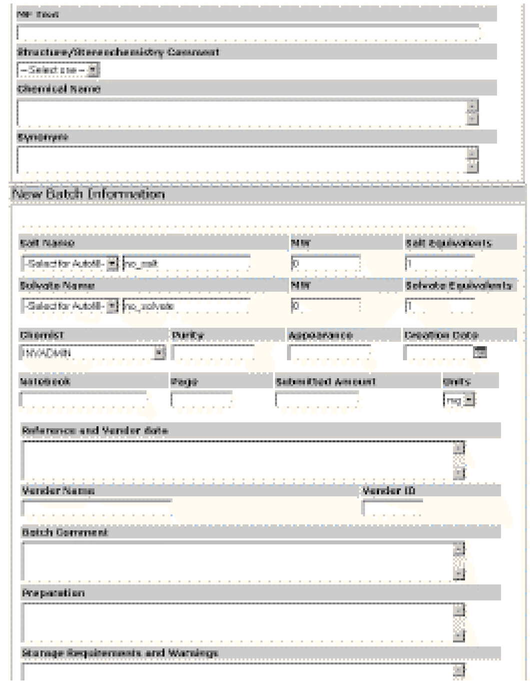
Adding a Compound

A compound is a single and pure chemical substance that can be used by the chemical and pharmaceutical research centers in their experiments and researches. In Registration Enterprise, you can store information about the compound as well as the vendor of the compound.

When you add a compound to Registration Enterprise, the compound is added to a temporary table in the database. This allows you to ensure that the compound information is accurate and complete before it is being added to a permanent table and registered into Registration Enterprise

To add a compound:

1. Click **Add Compound** within the **Add to Temporary** section in the Registration Enterprise home page. The **New Compound Submission Form** appears:



NOTE: You can also access the New Compound Submission Form by clicking the Compound link within the Registration Enterprise section in the home page of ChemOffice Enterprise.

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2. Specify the required information in the **New Compound Submission Form**.

NOTE: For more information about the fields in the New Compound Submission form, see *"Form Fields" on page 34*

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3. Click **Add Record**. A dialog box confirming the addition of compound to the temporary database table appears.

4. Click **OK**. The **New Compound Submission Form** reappears.

NOTE: For more information about registering a compound into Registration Enterprise and associating a registration number with it, see *"Registering a Temporary Record" on page 9*

Adding a Salt to a Compound

The **Add Salt** link within the **Add to Temporary** section allows you to add a salt to a compound and store it in a temporary table in the Registration Enterprise database.

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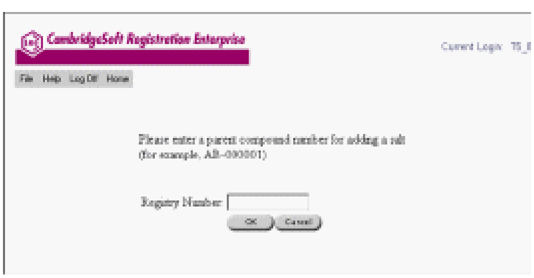
*NOTE: The Add Salt link appears within the Add to Temporary section, in the home page of Registration Enterprise when **BATCH_LEVEL** is set to **SALT** in the cfserver.ini file.*

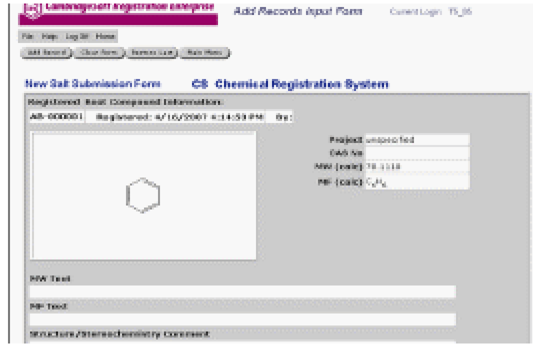
To add a salt to a compound:

1. Click **Add Salt** within the **Add To Temporary** section in the Registration Enterprise database. The following window appears:



2. Enter a parent compound number in the **Registry Number** text box.

3. Click **OK**. The **Add Records Input Form** page appears:



4. Scroll down and select a salt in the **New Compound Salt Information** section.

NOTE: The salts appearing in the drop down list are those, which are stored in the Salts table. For more information, please see *"Salts" on page 21*.

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5. Click **Add Record**. A success message appears.
6. Click **OK** to add the salt.

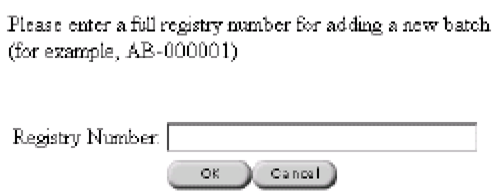
Adding a Batch or Lot

In Registration Enterprise, you can add batch or lot information for a compound. This allows you to maintain different records for the compounds that are similar but have slightly different properties. For example, you can create batch records for the compounds that are similar but contain different impurities, behave differently in tests, or are procured from the different suppliers.

You can add batch information for a compound only if the compound is registered in Registration Enterprise and has a Registration number associated with it. When you associate a batch record with a registered compound, a unique batch number is assigned to the batch record and the batch record is added to the temporary table. When the batch record is registered, the batch number is suffixed to the Registry number of the compound, with which the batch is associated. For more information about registering batch records and temporary compounds, see *"Registering a Temporary Record" on page 9*

To associate a batch with a registered compound:

1. Click **Add Batch** in the **Add to Temporary** section in the Registration Enterprise home page. The following page appears:



NOTE: You can also access this page by clicking the Batch link within the Registration Enterprise section in the home page of ChemOffice Enterprise.

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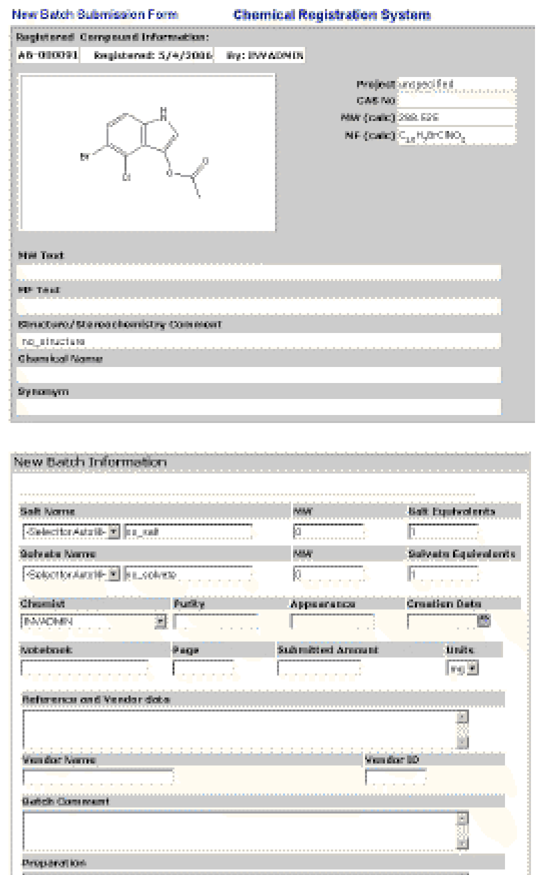
2. Enter the registration number of the compound with which the batch is to be associated in the **Registry Number** text box.

3. Click **OK**. The **New Batch Submission Form** containing the information of the compound appears:



4. Specify the required information in the **New Batch Submission Form**.

NOTE: For more information about fields in the New Batch Submission form, see "Form Fields" on page 34

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5. Click **Add Record**. A dialog box confirming the addition of batch to the temporary table appears.

6. Click **OK**. The **New Batch Submission Form** reappears.

Adding a Container

A container is a physical entity that is capable of storing chemical substances. You can store a complex mixture of chemical substances in a container, but the chemical structure of the container should be unique. The various types of containers, which you can create include bottle, vial, tube, cylinder, and box.

In Registration Enterprise, containers can be created only for the registered compounds. If you do not have appropriate privileges to create containers using Registration Enterprise, grant the appropriate privileges.

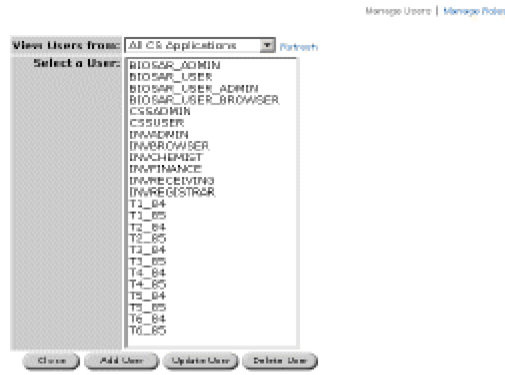
NOTE: You can create container using Registration Enterprise only if Registration Enterprise is integrated with Inventory Enterprise. For this, you need to modify the .ini settings.

Granting Privileges

To add a container from Registration Enterprise, you need to grant appropriate privileges to the currently logged in user.

To grant privileges:

1. Log in to ChemOffice Enterprise as an administrator user. The home page of ChemOffice Enterprise appears.
2. Click **Manage Users** in the **Manage Security** section. The **Manage Users** window appears:



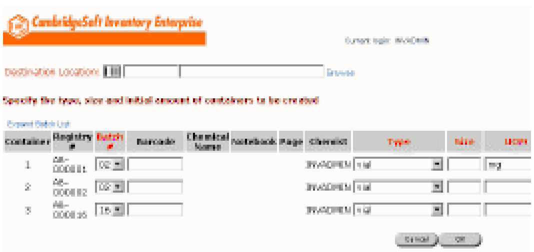
3. Select **Chemical Registration** from the **View Users** from drop-down list and click **Refresh**.
4. Select the currently logged-in user in the **Select a User** list.
5. Click **Update User**. The following window appears:

6. Select **INV_ADMIN** from the **Available Roles** list and click **Add** to add it to the **Current Roles** list.
7. Click **OK**.

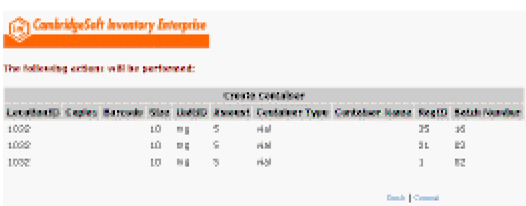
8. Click **Close**.

To add a container using Registration Enterprise:

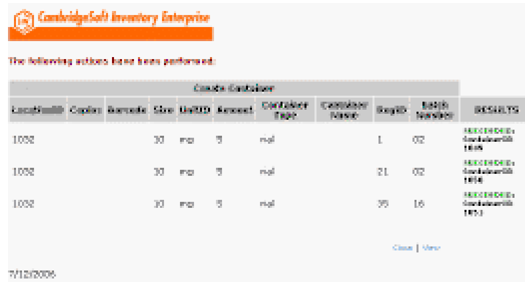
1. Search the registered records for which the containers are to be created.
2. Mark the records for which the containers are to be created in the page containing the search results.
3. Select **Marked Hits --> Send Marked**. The following window appears:



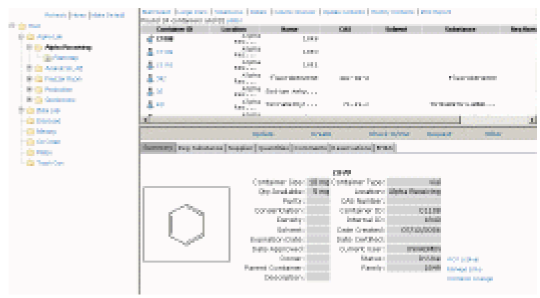
4. Click **Browse** and select the destination location where you want to place the containers in Inventory Enterprise.
5. Specify the type, size, and initial amount of the containers being created.
6. Click **OK**, the following window appears:



7. Click **Commit**. The following window appears:



8. Click **View**. The following window appears:



You can observe that the containers have been created at the desired location in Inventory Enterprise.

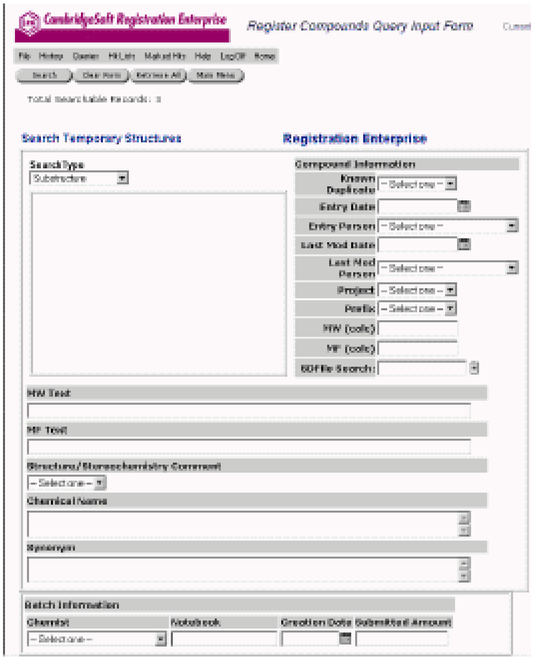
Searching the Temporary Table

As the number of records in the temporary table increases, it becomes more difficult to locate a particular record. The searching feature of Registration Enterprise allows you to easily locate a particular record and view its information.

To search the temporary table for a particular record:

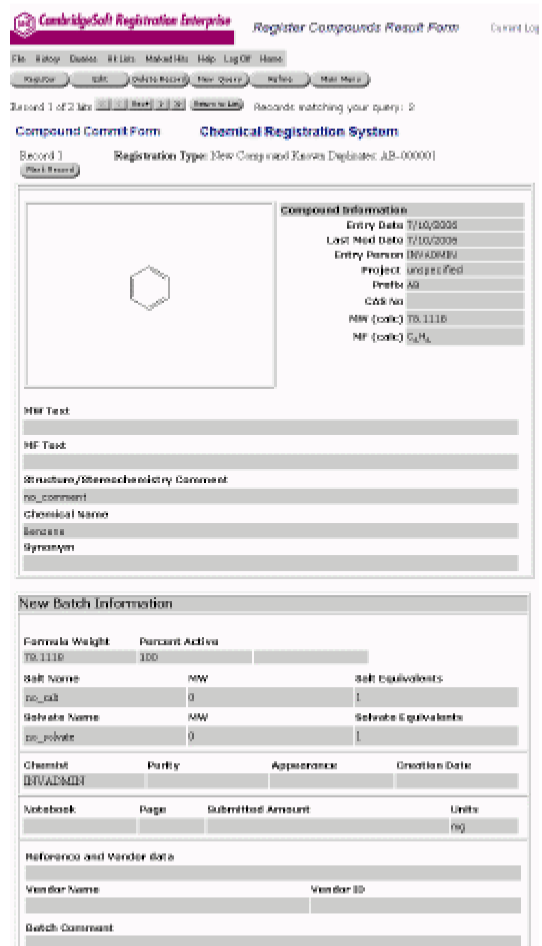
1. Click **Search Temp** in the **Registration** section in the Registration Enterprise home

page. The **Search Temporary Structures** form appears:



NOTE: For information about the fields in the Search Temporary Structures form, see "Form Fields" on page 34

2. Perform one of the following task in the Search Temporary Structures form:
   - Specify the attributes on the basis of which you want to search the record, such as chemical name, molecular formula, weight, or batch information, and click **Search**.
   - Click **Retrieve All** to obtain a list of all the records stored in the temporary table.
3. In the result list, click **Review/Register** corresponding to the desired record. The **Compound Commit Form** containing all the information about the record appears:



In addition to viewing the record information, you can also perform various other actions, such as editing, deleting, or registering the record, in the Compound Commit Form.

Editing Records in Temporary Table

You can edit the records stored in the temporary table before they are registered and inserted into the permanent table in the database.

NOTE: An edit operation cannot be undone.

To edit the records stored in the temporary table:

1. Search the temporary table to locate the record that is to be edited.
2. Click **Review/Register** in the results list, corresponding to the required record. The **Compound Commit Form** appears.
3. Click **Edit**.
4. Make the required changes and click **Update Record** to save the changes.

Deleting Records in Temporary Table

Instead of moving the records stored in the temporary table to the permanent table, you can also delete the records, if required.

NOTE: A delete operation cannot be undone.

To delete a record from the temporary table:

1. Search the temporary table to locate the record that is to be deleted.
2. Click **Review/Register** in the results list, corresponding to the required record. The **Compound Commit Form** appears.
3. Click **Delete Record**. A dialog box asking you to confirm the deletion action appears.
4. Click **OK**.

Registering Records

When a record stored in the temporary table is registered, the record is deleted from the temporary table and moved to the permanent table. After the record is registered, you can add identifier and analytics data to the record to help identify the record easily.

Registering a Temporary Record

When you register a compound record, a unique Registration number is assigned to the compound, and when you register a batch record, the batch number is added to the Registration number previously assigned to the compound. In addition to registering each record individually, Registration Enterprise also allows you to register all the temporary table records, at once.

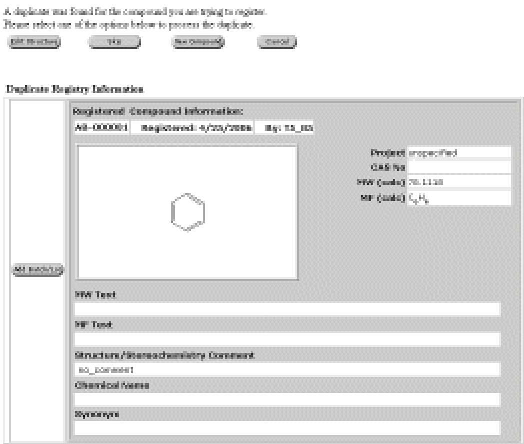
NOTE: The records stored in the permanent table can only be accessed if Row Level Security is not enabled.

Registering a Compound Record

To register a temporary compound record:

1. Search the temporary table to locate the compound record that is to be registered.
2. Click **Review/Register** the results list, corresponding to the required record. The **Compound Commit Form** appears.
3. Click **Register**. A page informing you about the successful registration of the compound record appears. Click **go to full record** if you want to review full details of the registered compound.

If the compound that you are registering already exists in Registration Enterprise, the compound does not get registered and the Duplicates page appears:



You can handle the duplicate compounds by performing one of the following tasks:

- Click **Edit Structure** to edit the structure of the duplicate compound. If the structure of the compound is edited, the compound is no longer similar to the existing compound and it can then be registered into Registration Enterprise.
- Click **Skip** to skip the registration of the compound.
- Click **New Compound** to register the duplicate compound as a new compound and assign it a new Registration ID.
- Click **Cancel** to cancel the registration of the duplicate compound.

NOTE: For information about viewing and deleting duplicates, see *"Managing Duplicates" on page 12*

Registering a Batch Record

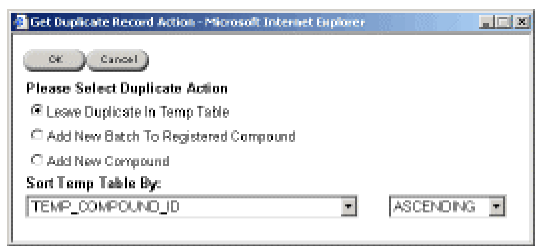
To register the temporary batch records:

1. Search the temporary table to locate the batch record that is to be registered.
2. Click **Review/Register** in the results list, corresponding to the required record. The **New Batch Registry Form** appears.
3. Click **Register**. A page informing you about the successful registration of the batch record appears.

Registering All the Temporary Table Records

To register all the temporary compound and batch records, at once:

1. Click **Review/Register** in the **Registration** section in the Registration Enterprise home page. A page containing all the records stored in the temporary table appears.
2. Click **Register All**. The **Get Duplicate Record Action** dialog box is displayed if the temporary table contains a duplicate compound record:



3. Select one of the following options in the **Get Duplicate Record Action** dialog box:
   - **Leave Duplicate in Temp Table**: Allows you to register the records other than the duplicate ones.
   - **Add New Batch To Registered Compound**: Allows you to add new batches for the duplicate compounds.
   - **Add New Compound**: Allows you to register duplicate compounds as new compounds in Registration Enterprise.

4. Click **OK**. A dialog box informing you that the records are being processed appears.
5. Click **OK**. A page informing you about the status of the records appears.

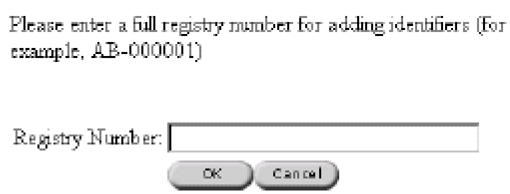
NOTE: For more information about adding identifier and analytics data to a registered record, see "Adding Identifier Information" on page 11 and "Adding Analytics Data" on page 11.

Adding Identifier Information

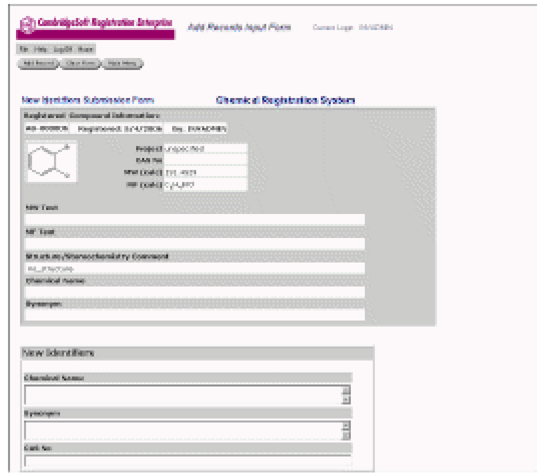
Identifier information includes information about the chemical name, synonym, and CAS number of a compound. This information helps identify a record easily. Identifier information can be added only to the registered compounds.

To add identifier information to a compound record:

1. Click **Add Identifier** in the **Registration** section in the Registration Enterprise home page. The following page appears:



2. Enter the Registration number of the compound to which the identifier information is to be added, in the **Registry Number** text box and click **OK**. The **New Identifiers Submission Form** appears:



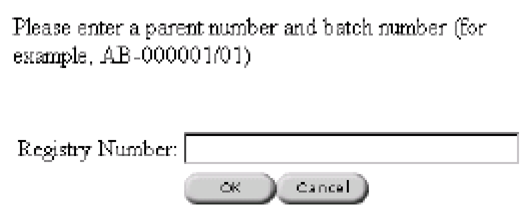
3. Enter the required identifier information in the **New Identifiers** section and click **Add Record**. A dialog box informing you that the identifier is added to the permanent registry table appears.
4. Click **OK**.

Adding Analytics Data

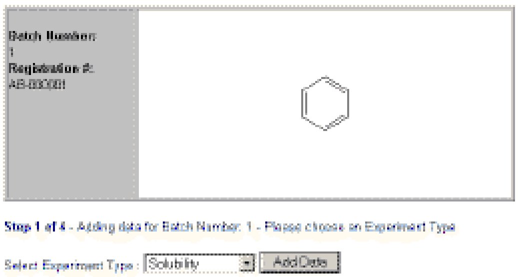
Analytics data includes solubility, optical rotation, and 1H NMR data for a batch record. You can add analytics data to only registered batch records. Like identifier information, analytics data also allows you to identify a record easily.

To add analytics data to a batch record:

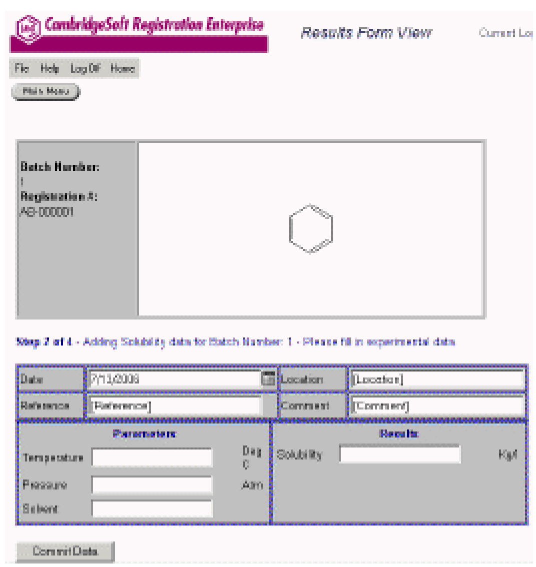
1. Click **Add Analytic Data** in the **Registration** section in the Registration Enterprise home page. The following page appears:



2. Enter the Registry number followed by the batch number for which the analytics data is to be added, in the **Registry Number** text box.
3. Click **OK**. The following page appears:



4. Specify which type of analytics data is to be added by selecting experiment type from the **Select Experiment Type** list box. For more information about experiments, see "Defining New Experiments" on page 23.
5. Click **Add Data**. The following page appears:



6. Provide the required analytic data and click **Commit Data**.

Managing Duplicates

To manage duplicates in Registration Enterprise:

1. Click **View Duplicates** in the **Administration** section in the Registration Enterprise home page. The list of all the duplicates available in Registration Enterprise appears.

NOTE: The View Duplicates link is available only if RLS is enabled. For information about enabling RLS, please see Registration Enterprise Admin guide.

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2. Click **Mark Record** next to the duplicate records that are to be deleted.
3. Click **Delete Marked Records** to delete the marked duplicate records from Registration Enterprise.

Query and Reporting

Queries are used to search the Registration Enterprise database for specific records. A query specifies the field(s) on the basis of which Registration Enterprise is to be searched. Reporting allows you to group records on the basis of the experiment type and view them in a spreadsheet.

Searching Registered Compounds

Registration Enterprise facilitates two types of searches: Compound search and Batch search. The difference between the two searches can be observed in the search results. The result of a Batch search displays all the compounds matching the search criteria along with their batch information whereas the result of a Compound search displays only compound information.

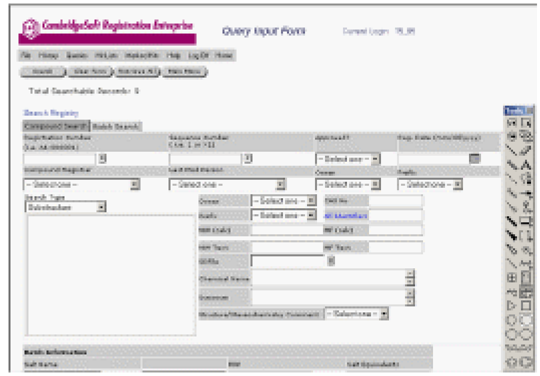
It also allows you to search for substances on the basis of any field. If the Registration Enterprise database contains a large number of records, make your search criteria as specific as possible. This reduces the size of the search result list and allows you to locate the required record easily and quickly. However, try broadening your search criteria if you are not able to locate the required record due to your search criteria.

NOTE: After searching the records, you can mark the records for later review. For information about marking records, please see Marking Records.

Compound Search

To search the registered compounds stored in the permanent table:

1. Click **Search** in the **Query and Reporting** section in the Registration Enterprise home page. The **Query Input Form** page appears:



NOTE: For information about the fields in the Query Input Form, please see *"Form Fields" on page 34**.*

NOTE: The Approved field does not appear by default. You need to make changes in the inv-config.ini file to make the Approved field visible in the Query Input form page. For more information, please consult your system administrator.

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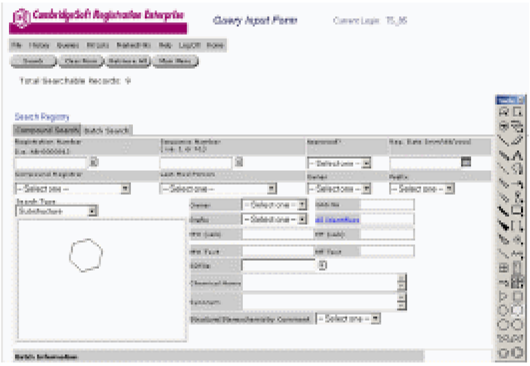
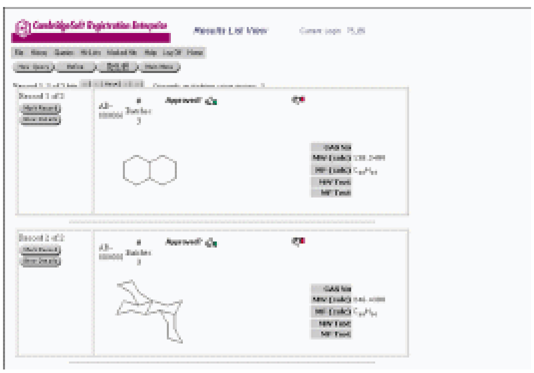
2. Ensure that the **Compound Search** tab is selected.

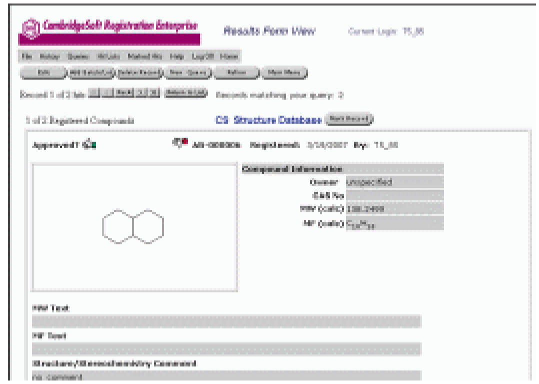
3. Enter the search criteria, as shown in the following figure:



4. Click the **Search** button. The **Results List View** page appears:



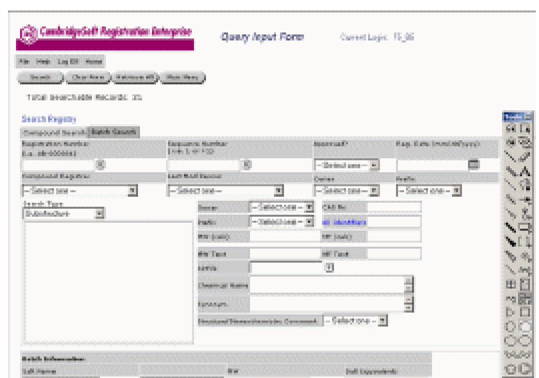
5. Click **Show Details** corresponding to the desired record. The **Results Form View** page appears:



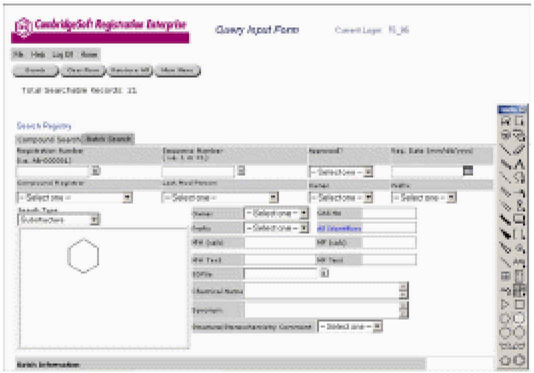
Batch Search

To perform a batch operation:

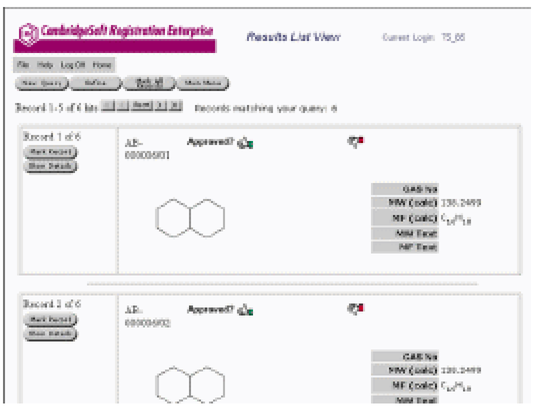
1. Click **Search** in the **Query and Reporting** section in the Registration Enterprise home page. The **Query Input Form** page appears.
2. Click **Batch Search** tab. The following page appears:



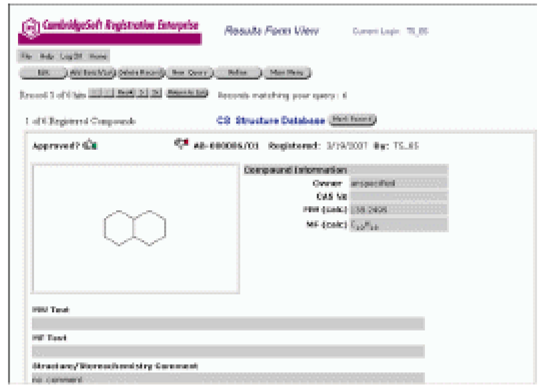
3. Enter the search criteria, as shown in the following figure:



4. Click **Search**. The **Results List View** page appears:



5. Click **Show Details** corresponding to the desired record. The **Results Form View** page appears:



Marking Records

You can mark the records displayed in the search result list so that records can be viewed later, when required. This allows you to view the records without creating a search query for them again. The list of the marked record is client-specific and is saved only on the clients.

In order to mark a record, click **Mark Record** next to the desired record. After marking the records, you can view or unmark the marked records or send the marked records to Inventory Enterprise for creating containers.

Viewing Marked Records

To view the marked records:

1. Click **Search** in the **Query and Reporting** section in the Registration Enterprise home page. The **Query Input Form** appears.

2. Select **Marked Hits-->Show Marked** from the menu bar. All the marked records are displayed.

NOTE: The Marked Hits menu is also available on the page containing the search results.

Unmarking Marked Records

To unmark the marked records:

1. Click **Search** in the **Query and Reporting** section in the Registration Enterprise home page. The **Query Input Form** appears.
2. Select **Marked Hits-->Clear Marked** from the menu bar. This unmark all the marked records.

NOTE: If you want to unmark a particular record, click the Unmark Record button next to the desired record.

Sending Marked Records

To send marked records to Inventory Enterprise:

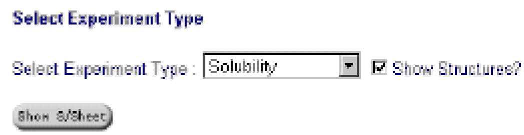
1. Click **Search** in the **Query and Reporting** section in the Registration Enterprise home page. The **Query Input Form** appears.
2. Select **Marked Hits-->Send Marked** from the menu bar. This sends the marked records to Inventory Enterprise and allows you to create new containers. For more information about creating containers in Inventory Enterprise from Registration Enterprise, see "Adding a Container" on page 6.

Viewing Analytics Spreadsheet

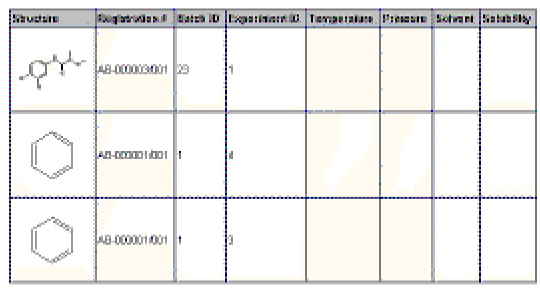
In the analytics spreadsheet, you can view the records grouped on the basis of the experiment type.

To view the analytics spreadsheet:

1. Click **Show Spreadsheet** in the **Query and Reporting** section in the Registration Enterprise home page. The following page appears:



2. Select the required experiment type from the **Select Experiment Type** list box.
3. Click **Show S/Sheet**. The spreadsheet appears:



Administration

Administration tasks can be performed within Registration Enterprise to manage and maintain Registration Enterprise and its users. Only users having appropriate privileges can perform the administration tasks in Registration Enterprise. Various administration tasks that can be performed in Registration Enterprise are:

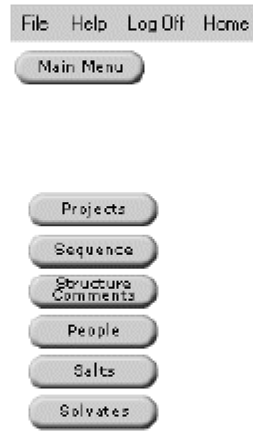
- Managing tables

- Defining new experiments
- Managing users and roles
- Managing analytics tables
- Changing passwords
- Importing SDFiles
- Managing workgroups
- Exporting Registration Enterprise Records to SDFiles

Managing Tables

Managing tables involves adding, editing, or deleting rows from the Registration Enterprise tables. This allows you to add, edit, or delete the pick lists values. Picklists are the drop-down lists that provide you with a list of all the values possible for a field. For example, when you are adding a compound to Registration Enterprise, you are provided with the Project drop-down list. This drop-down list contains all the possible types of projects that can be associated with a compound in Registration Enterprise.

In order to manage tables in Registration Enterprise, click **Manage Tables** in the **Administration** section in the Registration Enterprise home page. The Manage Tables area appears:



In the Manage Tables area, you can manage the following tables:

- Projects
- People
- Sequence
- Salts
- Structure Comments
- Solvates

Projects

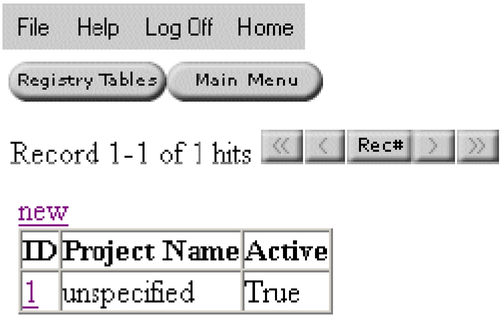
Projects table stores the projects that can be associated with the compounds in Registration Enterprise. This information appears in the Project drop-down list, when the compounds are added to Registration Enterprise. You can perform the following tasks on the Projects table:

- Add a new project
- Edit a project
- Delete a project

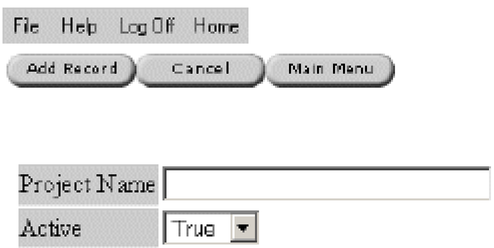
ADDING A NEW PROJECT

To add a new project to the Projects table:

1. Click **Projects**, in the **Manage Tables** area. The Projects table appears:



2. Click **new**. The following page appears:



3. Enter the name of the project in the **Project Name** text box.
4. Select **True** from the **Active** list box if you want the new project to appear in the Project drop-down list.
5. Click **Add Record**. The new project is added to the Projects table.

EDITING A PROJECT

To edit a project in the Projects table:

1. Click **Projects** in the Manage Tables area. The Projects table appears.
2. Click the ID of the project that is to be edited. A page containing the project information in the editable mode appears.
3. Make the required changes and click **Update Record**.

DELETING A PROJECT

To delete a project from the Projects table:

1. Click **Projects** in the **Manage Tables** area. The Projects table appears.
2. Click the ID of the project that is to be deleted.
3. Click **Delete Record**. The specified project is deleted from the Projects table.

NOTE: You cannot delete built-in projects, such as Unspecified, from the Projects table.

Sequence

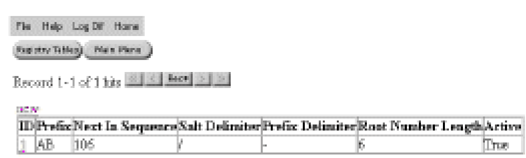
Sequence tables stores prefixes and starting numbers for the Registration numbers of the compounds. This information appears in the Prefix drop-down list, when the compounds are added to Registration Enterprise. You can perform the following tasks on the Sequence table:

- Add a new sequence
- Edit a Sequence table record
- Delete a Sequence table record

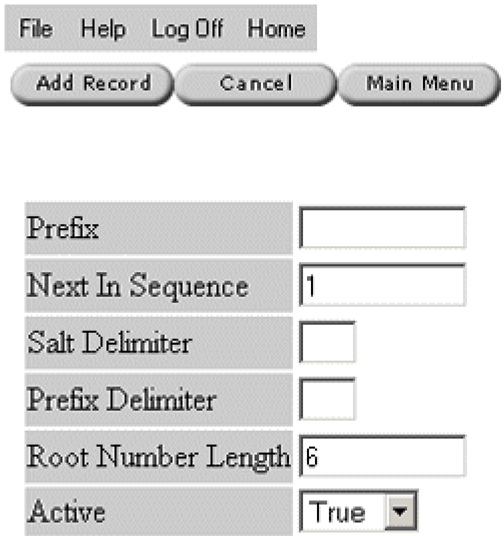
ADDING A NEW SEQUENCE

To add a new prefix and starting number to the Sequence table:

1. Click **Sequence** in the **Manage Tables** area. The **Sequence** table appears:



2. Click **new**. The following page appears:



3. Enter the required information in the **Prefix**, **Next In Sequence**, and **Root Number Length** fields.
4. Select **True** from the **Active** list box if you want the new record to appear in the **Prefix** drop-down list.
5. Click **Add Record**. The new record is added to the **Sequence** table.

EDITING A SEQUENCE

To edit a sequence in the Sequence table:

1. Click **Sequence** in the **Manage Tables** area. The Sequence table appears.
2. Click the ID of the sequence that is to be edited. A page containing the sequence information in the editable mode appears.
3. Make the required changes and click **Update Record**.

DELETING A SEQUENCE

To delete a sequence from the Sequence table:

1. Click **Sequence** button, in the **Manage Tables** area. The Sequence table appears.
2. Click the ID of the sequence that is to be deleted.
3. Click **Delete Record**. The specified sequence is deleted from the Sequence table.

Structure Comments

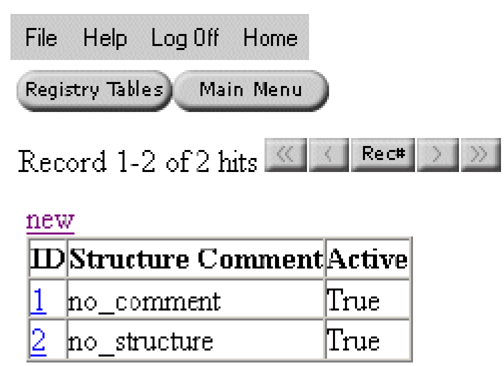
Structure Comments table stores the comments about the structure of the compounds in Registration Enterprise. This information appears in the Structure/Stereochemistry Comment drop-down list, when the compounds are added to Registration Enterprise. You can perform the following tasks on the Structure Comments table:

- Add a new structure comment
- Edit a structure comment
- Delete a structure comment

ADDING A NEW STRUCTURE COMMENT

To add a new structure comment to the Structure Comments table:

1. Click **Structure Comments** in the **Manage Tables** area. The Structure Comments table appears:



2. Click **new**. The following page appears:

3. Enter the comment in the **Structure Comment** text box.
4. Select **True** from the **Active** list box if you want the new structure comment to appear in the Structure/Stereochemistry Comment drop-down list.
5. Click **Add Record**. The new structure comment is added to the **Structure Comment** table.

NOTE: The "no comment" structure comment allows you to add a compound to Registration Enterprise without specifying the structure of the compound, even if the structure is a required field.

EDITING A STRUCTURE COMMENT

To edit a structure comment in the Structure Comments table:

1. Click **Structure Comments** in the **Manage Tables** area. The Structure Comments table appears.
2. Click the ID of the structure comment that is to be edited. A page containing the structure comment information in the editable mode appears.
3. Make the required changes and click **Update Record**.

DELETING A STRUCTURE COMMENT

To delete a structure comment from the Structure Comments table:

1. Click **Structure Comments** in the **Manage Tables** area. The Structure Comments table appears.
2. Click the ID of the structure comment that is to be deleted.
3. Click **Delete Record**.

NOTE: You cannot delete default structure comments, such as no_comment, from the Structure Comments table.

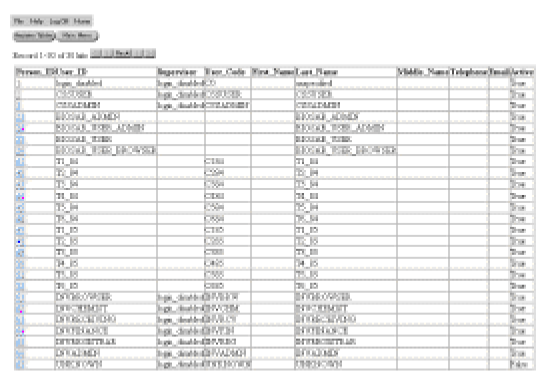
People

People table stores information about the users of the ChemOffice applications. This information appears in the Chemist drop-down list, when the compounds are added to Registration Enterprise.

For more information about adding a new record to the People table, see *“Managing Users and Roles” on page 23*.

To edit a record in the People table:

1. Click **People** in the **Manage Tables** area. The People table appears:



2. Click the ID of the record that is to be edited. The record opens in the editable mode.
3. Make the required changes and click **Update Record**.

NOTE: The login name of a ChemOffice Enterprise user is displayed in the Chemist drop-down list only if the Active field for the user record in the People table is set to True.

NOTE: By default, the last name of the user is displayed as the login name of the user in the Chemist drop-down list.

Salts

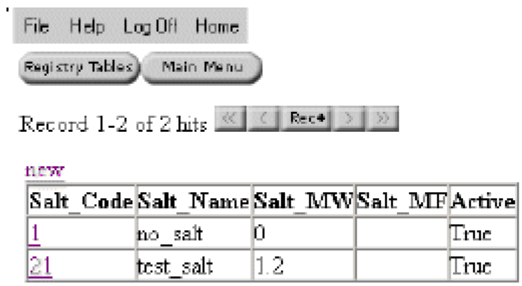
Salts table stores information about the salts that can be associated with the Registration Enterprise compounds. This information appears in the Salt Name drop-down list, when the compounds are added to Registration Enterprise. You can perform the following tasks on the Salts table:

- Add a new salt record
- Edit a salt record
- Delete a salt record

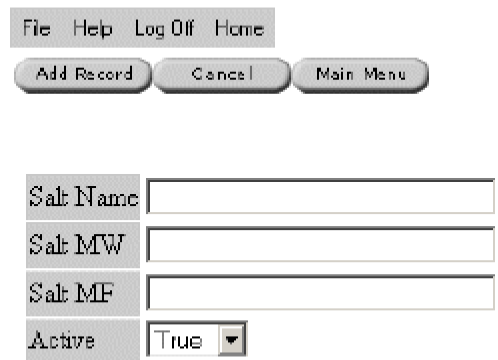
ADDING A NEW SALT RECORD

To add a new salt record to the Salts table:

1. Click **Salts** in the **Manage Tables** area. The Salts table appears:



2. Click **new**. The following page appears:



3. Enter the required information in the **Salt Name** and **Salt MW** fields.
4. Select **True** from the **Active** list box if you want this salt to appear in the Salt Name drop-down list.
5. Click **Add Record**. The new salt is added to the Salts table.

EDITING A SALT RECORD

To edit a record in the Salts table:

1. Click **Salts** in the **Manage Tables** area. The Salts table appears.
2. Click the ID of the record that is to be edited. The record opens in the editable mode.
3. Make the required changes and click **Update Record**.

DELETING A SALT RECORD

To delete a record from the Salts table:

1. Click **Salts** in the **Manage Tables** area. A page containing the Salts table appears.
2. Click the ID of the record that is to be deleted.
3. Click **Delete Record**.

NOTE: You cannot delete the default salts, such as no_salt, from the Salts table.

Solvates

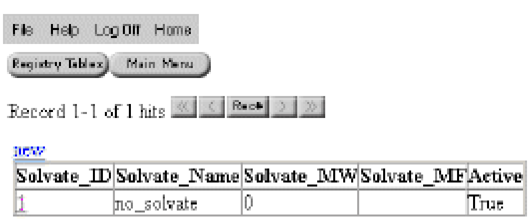
Solvates table stores information about the solvates that can be used for solvating Registration Enterprise compounds. This information appears in the Solvate Name drop-down list, when the compounds are added to Registration Enterprise. You can perform the following tasks on the Solvates table:

- Add a new solvate record
- Edit a solvate record
- Delete a solvate record

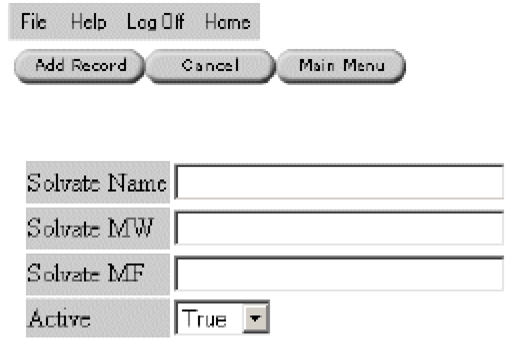
ADDING A NEW SOLVATE RECORD

To add a new solvate record:

1. Click **Solvates** in the **Manage Tables** area. The Solvates table appears:



2. Click **new**. The following page appears:



3. Enter the required information in the **Solvate Name** and **Solvate MW** fields.
4. Select **True** from the **Active** list box if you want the new solvate to appear in the Solvate Name drop-down list.
5. Click **Add Record**. The new solvate is added to the Solvates table.

EDITING A SOLVATE RECORD

To edit a record in the Solvates table:

1. Click **Solvates** in the **Manage Tables** area. The Solvates table appears.
2. Click the ID of the record that is to be edited. The record opens in the editable mode.
3. Make the required changes and click **Update Record**.

DELETING A SOLVATE RECORD

To delete a record from the Solvates table:

1. Click **Solvates** in the **Manage Tables** area. The Solvates table appears.
2. Click the ID of the record that is to be deleted.

3. Click **Delete Record**.

NOTE: You cannot delete the default solvates, such as no_solvate, from the Solvates table.

Managing Users and Roles

You can manage users and roles for Registration Enterprise only if you have sufficient privileges. The links for managing users and roles for Registration Enterprise are available within the interface of the Registration Enterprise application as well as on the home page of ChemOffice Enterprise.

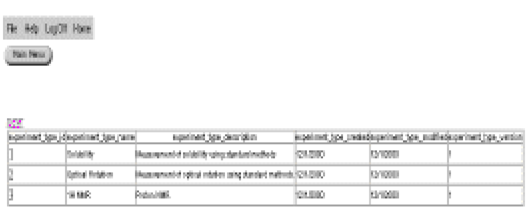
NOTE: You can also manage users and roles for the other ChemOffice applications, such as Inventory Enterprise and BioSAR, from the Registration Enterprise interface.

Defining New Experiments

You can store information about the different tests performed on the compounds by defining experiments in Registration Enterprise.

To define a new experiment:

1. Click **New Experiment** in the **Administration** section in the Registration Enterprise home page. The following page containing all the experiments defined in Registration Enterprise appears:



2. Click **new**. The following page appears:

3. Enter the required information and click **Add Record**.

To edit the information in an experiment, see "**Editing an Experiment**" in *"Experiment Type" on page 24*.

Changing Passwords

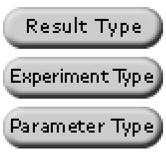
To change your password:

1. Click **Change Password** in the **Administration** section in the Registration Enterprise home page. The following page appears:

2. Enter the new password in the **New Password** and **Confirm New Password** text boxes.
3. Click **OK**.

Managing Analytics Tables

In Registration Enterprise, different types of analytics data is stored in different analytics tables. In order to manage these analytics tables, click the Manage Analytics link within the Administration section in the Registration Enterprise home page. The Analytics Table management area appears:



Experiment Type

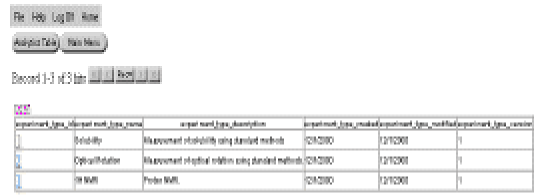
You can perform the following tasks on the Experiments Types table:

- Add a new experiment
- Edit an experiment
- Delete an experiment

ADDING A NEW EXPERIMENT

To add a new experiment to the Experiments Type table:

1. Click **Experiments Type** in the Analytics Table management area. The following page containing the Experiment Type table appears:



NOTE: For information about accessing the Analytics Table management area, see *"Managing Analytics Tables" on page 23**.*

2. Click **new**. The following page appears:

3. Enter the required information and click **Add Record**.

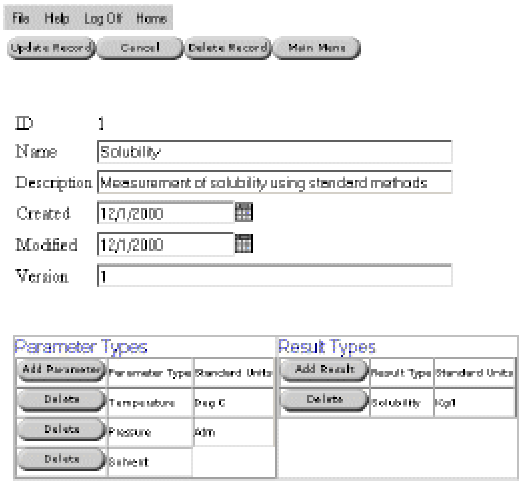
EDITING AN EXPERIMENT

You can add or delete parameters and result types associated with an experiment by editing it. To edit an experiment:

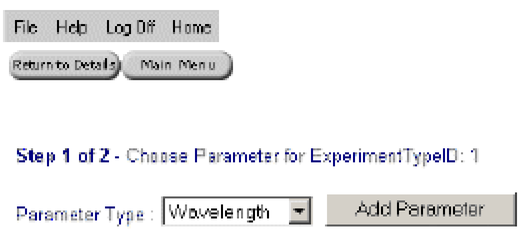
1. Click **Experiments Type** in the Analytics Table management area. A page containing the Experiment Type table appears.

NOTE: For information about accessing the Analytics Table management area, see *"Managing Analytics Tables" on page 23**.*

2. Click the ID of the record that is to be edited. The following page containing the record in the editable mode appears:

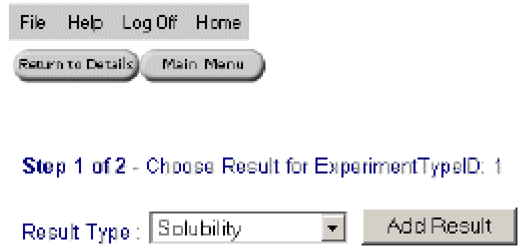


3. Perform the following tasks if you want to add a new parameter to the experiment:
   - Click **Add Parameter**. The following page appears:



   - Select the required parameter type from the **Parameter Type** list box and click **Add Parameter**.

4. Perform the following tasks if you want to add a new result type to the experiment:
   - Click **Add Result**. The following page appears:



   - Select the required result type from the **Result Type** list box and click **Add Result**.

5. Click **Delete** next to a parameter or result type if you want to delete the parameter or result type.
6. Make changes to other information, such as name and description, if required.
7. Click **Update Record**.

DELETING AN EXPERIMENT

To delete an experiment:

1. Click **Experiments Type** in the Analytics Table management area. A page containing the Experiment Type table appears.

NOTE: For information about accessing the Analytics Table management area, see "Managing Analytics Tables" on page 23.

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2. Click the ID of the record that is to be deleted.
3. Click **Delete Record**. A dialog box asking you to confirm the deletion action appears.
4. Click **OK**.

Parameter Type

You can perform the following tasks on the Parameter Type table:

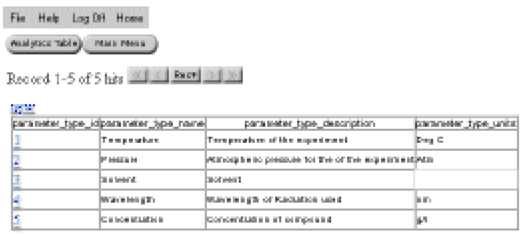
- Add a new parameter

- Edit a parameter
- Delete a parameter

ADDING A NEW PARAMETER

To add a new parameter:

1. Click **Parameter Type** in the Analytics Table management area. The following page containing the Parameter Type table appears:



NOTE: For information about accessing the Analytics Table management area, see "Managing Analytics Tables" on page 23.

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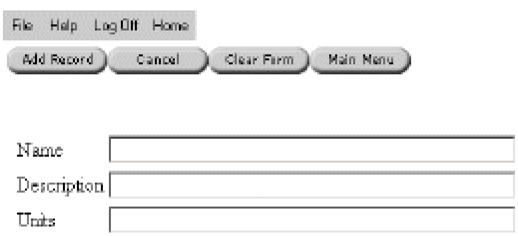
2. Click **new**. The following page appears:



3. Enter the required information, such as name, description, and unit for the new parameter and click **Add Record**.

EDITING A PARAMETER

To edit a parameter:

1. Click **Parameter Type** in the Analytics Table management area. A page containing the Parameter Type table appears.

NOTE: For information about accessing the Analytics Table management area, see "Managing Analytics Tables" on page 23.

---

2. Click the ID of the record that is to be edited. The parameter record opens in the editable mode.
3. Make the required changes and click **Update Record**.

DELETING A PARAMETER

To delete a parameter from the Parameter Type table:

1. Click **Parameter Type** in the Analytics Table management area. A page containing the Parameter Type table appears.

NOTE: For information about accessing the Analytics Table management area, see "Managing Analytics Tables" on page 23.

---

2. Click the ID of the record that is to be deleted.
3. Click **Delete Record**. A dialog box asking you to confirm the deletion action appears.
4. Click **OK**.

Result Type

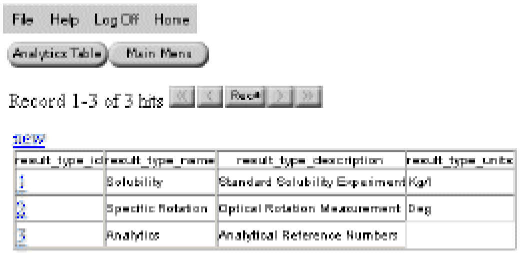
You can perform the following tasks on the Result Type table:

- Add a new result type
- Edit a result type
- Delete a result type

ADDING A NEW RESULT TYPE

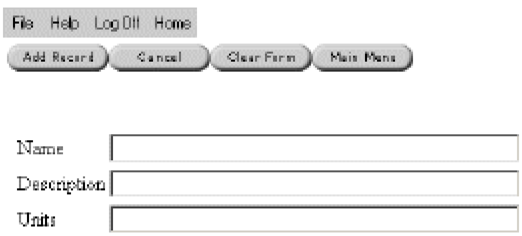
To add a new result type:

1. Click **Result Type** in the Analytics Table management area. The following page containing the Result Type table appears:



result_type_id	result_type_name	result_type_description	result_type_units
1	Solubility	Standard Solubility Experiment	Kg/l
2	Specific Rotation	Optical Rotation Measurement	Deg
3	Analytics	Analytical Reference Numbers	

2. Click **new**. The following page appears:



3. Enter the required information, such as name, description, and unit for the new result type and click **Add Record**.

EDITING A RESULT TYPE

To edit a result type:

1. Click **Result Type** in the Analytics Table management area. A page containing the Result Type table appears.

NOTE: For information about accessing the Analytics Table management area, see "Managing Analytics Tables" on page 23.

---

2. Click the ID of the result type that is to be edited. The result type record opens in the editable mode.
3. Make the required changes and click **Update Record**.

DELETING A RESULT TYPE

To delete a result type from the Result Type table:

1. Click **Result Type** in the Analytics Table management area. A page containing the Result Type table appears.

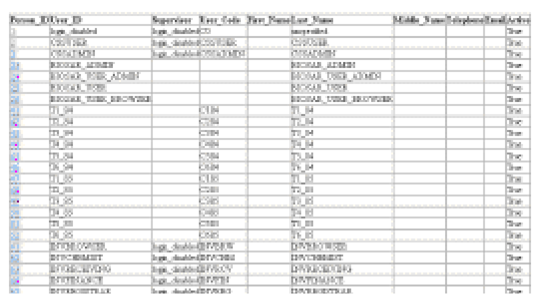
NOTE: For information about accessing the Analytics Table management area, see "Managing Analytics Tables" on page 23.

---

2. Click the ID of the result type that is to be deleted.
3. Click **Delete Record**. A dialog box asking you to confirm the deletion action appears.
4. Click **OK**.

Managing Workgroups

Workgroups refer to the users of the ChemOffice applications. The People table stores the information about the users of the ChemOffice applications. In order to manage workgroups in Registration Enterprise, click the Manage Workgroups link within the Administration section in the Registration Enterprise home page. The following page containing the People table appears:



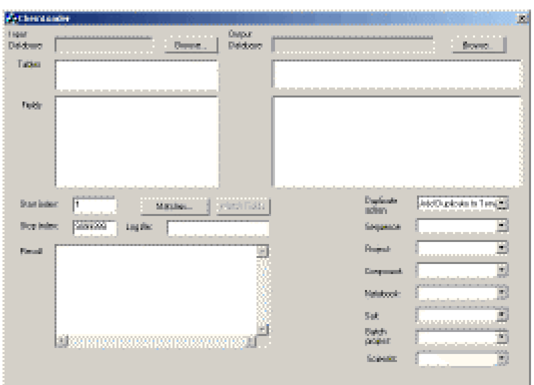
For information about adding or editing the workgroups or users, see "People" on page 20.

Importing SDFiles

SDFile are used to store structure information of the compounds. You can import a SDFile into Registration Enterprise to store the compounds contained in the SDFile in Registration Enterprise. This prevents you from entering the compound records manually into Registration Enterprise.

You can import a SDFile into Registration Enterprise using ChemLoader. To import a SDFile into Registration Enterprise using ChemLoader:

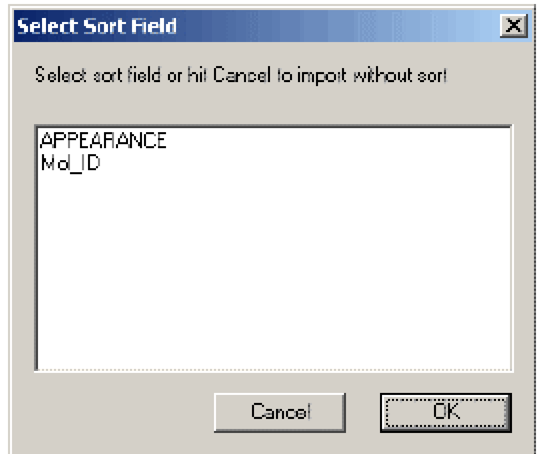
1. Import the SDFile into the ChemFinder database.
2. Browse to the following location: **<webroot>\Inetpub\wwwroot\ChemOffice\chem_reg\ChemLoader_Client**.
3. Double click **ChemLoader.exe** to open ChemLoader. The following page appears:



NOTE: If ChemLoader.exe is not available on your machine, please see your system administrator.

---

4. Specify input and output databases.
5. Match fields in the input and output databases.
6. Specify import options.
7. Click **Import**. The **Select Sort Field** dialog box appears:

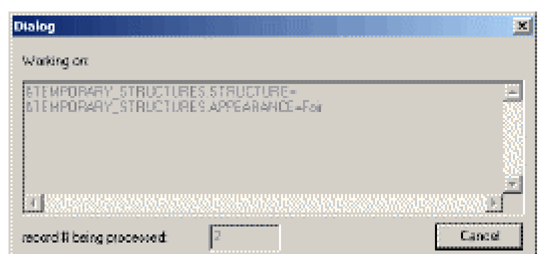


8. Select the field on the basis of which the imported records are to be sorted.

NOTE: The records can be imported without specifying a sort field also.

---

9. Click **OK**. The following page showing the progress of the import process appears:



NOTE: You can terminate the import process in between by clicking the Cancel button. When you do so, the import process stops, but the *records that have already been imported, by ChemLoader, remain there in Registration Enterprise.*

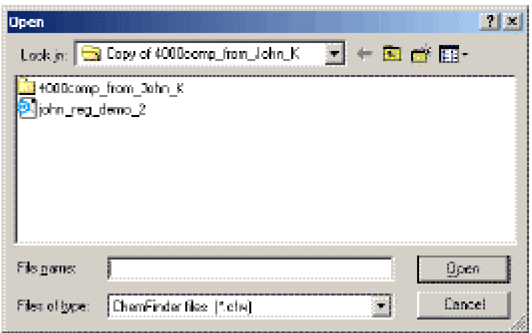
---

10. Click **Close** to close ChemLoader when the import process finishes.

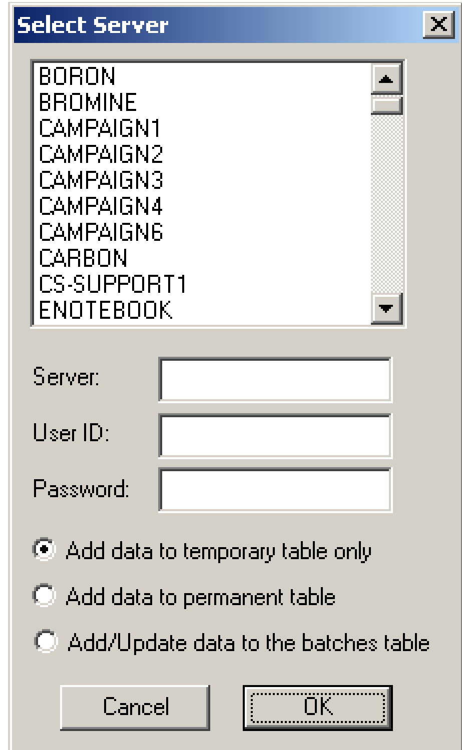
Specifying Input and Output Databases

To specify input and output databases:

1. Click **Browse** next to the **Input Database** field. The **Open** dialog box appears:



2. Browse to the location of the desired ChemFinder database in the **Look In** field.
3. Select the database and click **Open**. This populates the **Input Database** field with the input database and **Tables** field with the database tables. The fields of a table can be viewed in the **Fields** field by clicking the table.
4. Click **Browse** next to the **Output Database** field. The **Select Server** dialog box appears:



5. Specify the output server either by:
   - Selecting a server from the list of servers, or
   - Entering the server name in the Server text box.
6. Enter the user ID and password with which you have logged into Registration Enterprise in the **User ID** and **Password** text boxes.
7. Select one of the following options:
   - Add data to temporary table only: Imports data to the temporary table.
   - Add data to permanent table: Imports data to the permanent table.

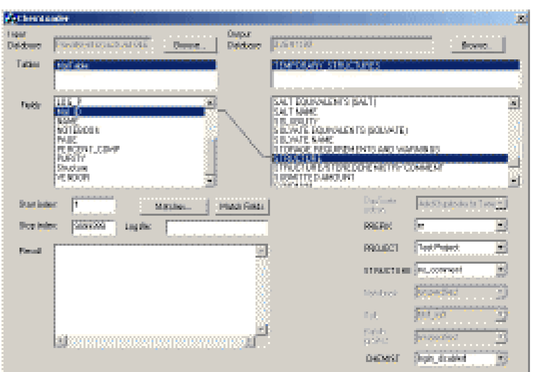
- Add/Update data to the batches table: Imports data to the batches table or updates the data.

8. Click **OK**. This populates the **Output Database** field with the output database and **Tables** field with the database tables. The fields of a table can be viewed in the **Fields** field by clicking the table.

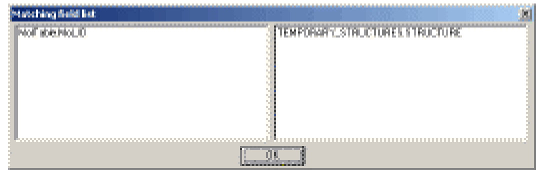
Matching Fields

To match fields in the input and output databases:

1. Select the input and output tables containing the fields that are to be matched. The fields of the selected tables are displayed in the input and output **Fields** field.
2. Select the fields that are to be matched.
3. Click **Match Fields**. The selected fields are matched with each other, as shown in the following figure:



4. Repeat steps 1, 2 and 3 to match other fields, if required.
5. Click **Matches-->View** to view the matches. A list of the matching field appears:



6. Click **OK** to close the list of the matching fields.

Specifying Import Options

To specify import options:

1. Enter the record number from which the import process is to be started, in the **Start Index** text box.
2. Enter the record number at which the import process is to be terminated, in the **Stop Index** text box.
3. Enter the location of log file in the **Log File** text box, if you want to log the import process.
4. Select desired duplicate action, sequence, project, compound, notebook, salt, batch project, and scientist from the respective list boxes

Exporting Records to SDFiles

To export the records stored in Registration Enterprise to SDFiles:

1. Search the temporary or registered records that are to be exported. For information about searching temporary records and registered records, see “Searching the Temporary Table” on page 7 and “Searching Registered Compounds” on page 12.
2. Click **File**>**Export Hits**. The Export Hits window appears.

3. Select one of the following options to specify the format in which the records are to be exported:
   - Flat SDFile: Stores batch information of the compounds in the separate fields, if the records that are being exported include batch records also. This increases the size of the SDFile.
   - Nested SDFile: Stores batch information of the compounds by nesting the information, instead of creating separate fields, if the records that are being exported include batch records also. This reduces the size of the SDFile.
4. Specify the template that is to be used for exporting records.
5. Click **OK**. A page displaying the progress of the export process appears.
6. Click **Click to Download**, which is displayed when the export process finishes, to download and save the SDFile at the desired location.

NOTE: You can also export the RDFiles using the preceding steps. For this, you need to select the RDFile option, which is available in the Export Hits window only if the ALLOW_RDFILE_EXPORT parameter is set to 1 in the cfserver.ini configuration file.

Optional Features

The optional features of Registration Enterprise, such as Row Level Security, salt and solvate recognition, and customizable fields are disabled, by default. Please see your system administrator if you want to use the optional features of Registration Enterprise.

Row Level Security

Overview

Row Level Security (RLS) is implemented over the standard Oracle roles in Registration Enterprise. The purpose of using roles in Registration Enterprise is to restrict access to the elements of the interface and data. For example, User A has access to one set of user interface elements, such as buttons and menus, while User B is limited to a subset of those available to A. In addition, roles limit what a user can do with the data. For example, User A can register data and edit that data but User B can only register.

RLS implements an additional layer of security to Registration Enterprise, which is project based. Each compound, when registered, is assigned to a project. If RLS is implemented, users can only see and manipulate data associated with the projects they are a part of. For example, in a system without RLS implemented, User A can see all compounds in the registry, as does User B. However, in a system with RLS implemented, User A is associated with a particular project, and is only able to see compounds that are linked to that project.

The implementation of RLS in Registration Enterprise affects the following:

- User interface
- Linkage of the projects with people
- Unspecified projects
- Duplication of the compounds

User Interface

The home page of Registration Enterprise displays the total number of registered records available in Registration Enterprise. With RLS implemented, this value reflects only the records a user can see, not the total records in Registration Enterprise.

Similarly, with RLS implemented, the Project drop-down list shows only those projects that the user is linked to. Therefore, user can only access the compounds associated with the projects for which the user has rights.

Linkage of Projects With People

When a project is created in Registration Enterprise all the Registration Enterprise users are given permissions to access that project. However, when RLS is implemented some of the users are denied access to the project. In this case, the project information is not modified or deleted, only the restricted users are not allowed to access the compounds in the project.

Unspecified Project

Unspecified project is assigned to the records that do not have a valid Project ID associated with them. The records associated with the unspecified project are stored in the Temporary table and the unspecified project is assigned to the administrator. This allows administrator to check the Temporary table for these types of records and assign them a valid Project ID.

Duplicate Checking

If RLS is enabled, you can register a compound even if the compound exists already in Registration Enterprise, but not in the project associated with the compound. The Duplicate window does not appear in this case, however, being a duplicate the compound is stored in the Duplicates table. On the other hand, you cannot register the compound if the compound is duplicated in the project associated with it. In this case the Duplicate window appears.

VIEWING SYSTEM DUPLICATES

To view the list of the duplicates in Registration Enterprise, click the View Duplicates button, which is displayed in the Registration Enterprise home page if the user has sufficient privileges. The list of the duplicates is displayed in the standard ChemOffice Enterprise List/Display View and the Registration numbers of the duplicated records are highlighted in Red, in the list.

Every time a duplicate is added to Registration Enterprise, two entries are made for it in the Duplicate table. That is, if Compound A is registered as the duplicate of Compound B, then following entries are made in the Duplicates Table:

- Compound A -> Compound B
- Compound B -> Compound A

Therefore, when duplicates are checked users see both sides of the picture: A is a duplicate of B and conversely B is a duplicate of A.

DELETING A DUPLICATE

If a duplicate record is deleted, it is removed from the Duplicates Table.

NOTE: For details regarding activation of RLS, please see the Registration System Admin Guide or your system administrator.

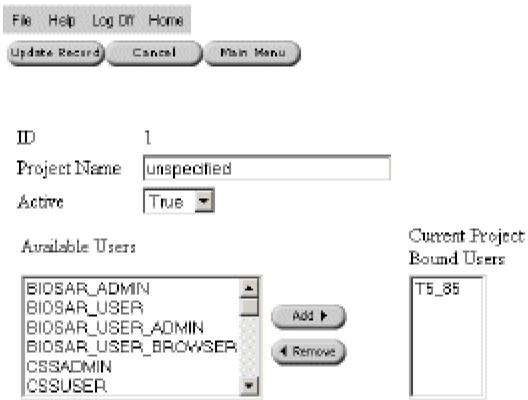
Assigning Users to Projects (for RLS)

You can associate users with a project only if RLS is enabled. For information about enabling RLS in Registration Enterprise, please see Registration Enterprise Admin Guide.

To associate users with a project:

1. Click **Manage Tables** in the **Administration** section in the Registration Enterprise home page. The **Manage Tables** page appears.
2. Click **Projects**. The Projects table appears.

3. Click the ID corresponding to the required project. The following page appears:



4. Select the required user in the **Available Users** list box and click **Add**. This adds the selected user to the **Current Project Bound Users** list box. Repeat this step for the all the users that are to be associated with the project.
5. Click **Update Record**.

Salt and Solvate Recognition

Both compound level and batch level records have salt and solvate information associated with them. The different ways in which the salt and solvate information can be recorded are:

• Populating the batch level record with salt and solvate information in the compound level record, and allowing the equivalents to be changed at the batch level. This is the default way of recording the salt and solvate information.

• Keeping the salt and solvate information in the compound and batch level records completely separate.

For information about using these ways for recording salt and solvate information, please see your system administrator.

Customizable Fields

Registration Enterprise contains some fields that can be customized according to the requirements. You can customize the name, data type, and display type for these fields. The customizable fields for the compound records are:

- 4 text fields
- 4 integer fields
- 4 real number fields
- 4 date fields

The customizable fields for the batch records are:

- 6 integer fields
- 6 real number fields
- 6 date fields

By default, the customizable fields are hidden. For information about making the customizable fields visible to the users and customizing them, please see your system administrator or Registration Enterprise Admin Guide.

Integrating ChemScript

Here we describe how to integrate ChemScript with Registration Enterprise. ChemScript is a chemical programming environment that is integrated with the ChemOffice Enterprise applications. Using ChemScript, you can create your own chemistry business rules and execute those rules on scientific data in batch mode. ChemScript is based on the non-proprietary scripting language Python, which provides clear syntax, object-oriented programming, dynamic data typing, and high performance across a broad range of operating systems including Windows, UNIX, and Linux.

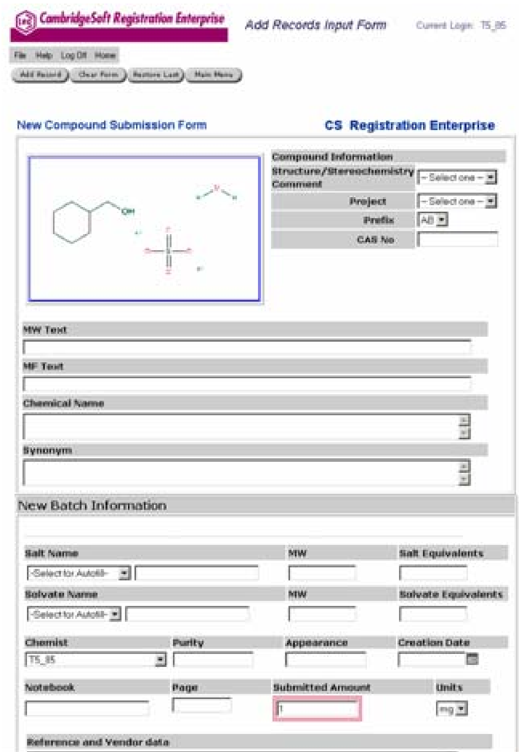
Getting started with ChemScript

To use the ChemScript files, follow the installation guide of ChemScript Integration section to have it installed and configured.

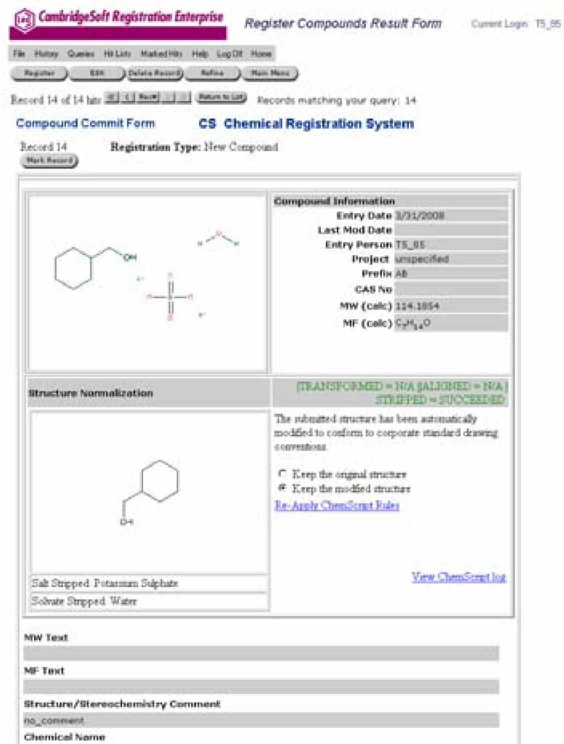
Using ChemScript

Add Compound screen

Enter structure as a combination of base structure, salts and solvates.



Review the newly added compound:



Form Fields

The following is a complete list of default fields found in the Registration Enterprise forms.

NOTE: The System Administrator can add fields to this list or alter the list, if required.

Compound Attributes

- CAS Number
- Chemical Name
- Compound Registrar
- Identifiers
- Known Duplicates

- Molecular Formula
- Molecular Weight
- Prefix
- Project
- Registration Date
- Registration Number
- Sequence Number
- Substructure
- Synonym

Batch Attributes

- Appearance
- Batch Comment
- Creation Date
- Entry Date
- Entry Person
- Formula Weight
- Notebook
- Page
- Percent Active
- Physical & Analytical Information
- Preparation
- Purity
- References and Vendors
- Salt Name
- Solvate Name
- Storage Requirements & Warnings
- Structure/Stereochemistry Comments
- Submitted Amount
- Other Attributes
- Chemist
- Last Mod Date
- Last Mod Person
- Units

NOTE: For more information about the preceding fields, please refer to the HTML help of Registration Enterprise.

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