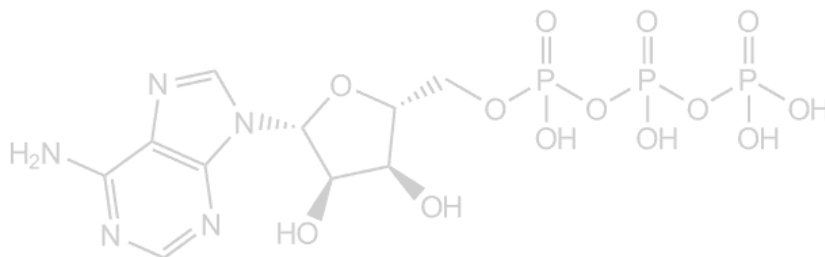
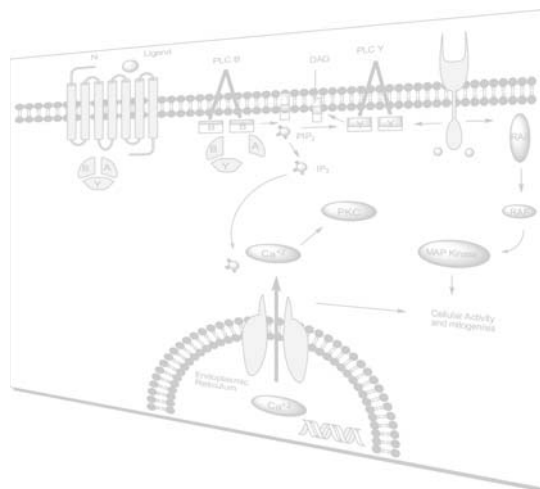
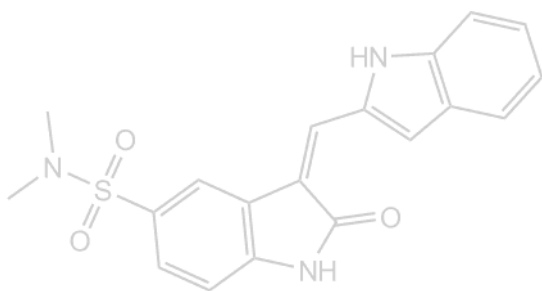


# Registration

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

## *User and Administrator Guide*



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# Contents

<b>Registration Enterprise 10.0 .....</b>	<b>1</b>	<i>Changing Passwords.....</i>	<i>23</i>
About this Guide .....	1	<i>Managing Analytics Tables.....</i>	23
Overview .....	1	Managing Workgroups.....	27
<i>Benefits.....</i>	1	Importing SDFiles .....	28
<i>Registration Enterprise Workflow .....</i>	1	<i>Specifying Input and Output Databases....</i>	29
<i>Required Fields.....</i>	2	<i>Matching Fields .....</i>	30
Adding New Compounds, Batches, and		<i>Specifying Import Options .....</i>	30
Containers .....	2	Exporting Records to SDFiles.....	30
<i>Adding a Compound .....</i>	3	Optional Features .....	31
<i>Adding a Batch or Lot.....</i>	4	<i>Row Level Security.....</i>	31
<i>Adding a Container.....</i>	6	Salt and Solvate Recognition .....	33
Searching and Viewing Records in Tempo-		Customizable Fields .....	33
rary Table .....	7	Integrating ChemScript .....	33
<i>Editing Records in Temporary Table.....</i>	8	Form Fields .....	35
<i>Deleting Records in Temporary Table.....</i>	9	<i>Compound Attributes .....</i>	35
Registering Records .....	9	<i>Batch Attributes.....</i>	35
<i>Registering a Temporary Record.....</i>	9	Roles .....	36
<i>Adding Identifier Information.....</i>	11	Privileges .....	37
<i>Adding Analytics Data .....</i>	11	<b>Administrator Guide.....</b>	<b>45</b>
<i>Managing Duplicates.....</i>	12	Configuration .....	45
Query and Reporting.....	12	<i>Customizable Fields.....</i>	45
<i>Searching Registered Compounds .....</i>	12	<i>CFServer.ini Configuration File.....</i>	46
<i>Marking Records.....</i>	15	<i>Reg.ini Configuration File .....</i>	93
Viewing Analytics Spreadsheet .....	16	Optional Features .....	105
Administration .....	16	<i>Row Level Security (RLS) .....</i>	105
<i>Managing Tables .....</i>	17	<i>Salt and Solvate Recognition .....</i>	106
<i>Managing Users and Roles.....</i>	23		
<i>Defining New Experiments .....</i>	23		



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# Registration Enterprise 10.0

## About this Guide

Welcome to the Registration Enterprise 10.0 User and Administrator Guide. Inside this guide, you will find a full description 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, although 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

## Adding New 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 data-

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.

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.

To add a compound:

1. Click **Add Compound** within the **Add to Temporary** section in the Registration

MR Test			
Structure/ Stereochemistry Comment			
Select size			
Chemical Name			
Synonyms			
New Batch Information			
Salt Name	MR	Salt Equivalents	
Select for Addtl. <input type="checkbox"/> No salt	0	1	
Solvent Name	MR	Solvent Equivalents	
Select for Addtl. <input type="checkbox"/> No solvent	0	1	
Distict	Dilute	Appearance	Reaction Date
IN/ADMIN			
Batch Lot	Page	Submitted Amount	Units
			mg
Reference and Vendor Info			
Vendor Name		Vendor ID	
Batch Comment			
Preparation			
Storage Requirements and Warnings			

*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.*

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](#)*

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](#)*

---

### 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.

---

*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.*

---

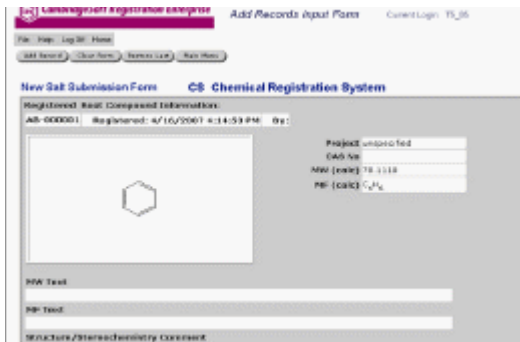
To add a salt to a compound:

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](#).*

---

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](#)

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:

Please enter a full registry number for adding a new batch (for example, AB-000001)

Registry Number:

---

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

---

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](#)*

---

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.

---

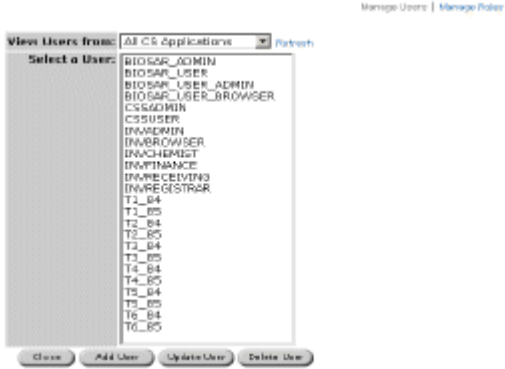

*NOTE: You can create container using Registration Enterprise only if Registration Enterprise is integrated with Inventory Enterprise. For this, you need to modify the .ini settings.*

---

## 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:

Container #	Registry #	Batch #	Barcode	Chemical Name	Notebook Page	Chemical	Type	Size	UOM
1	00000001	00000001		HYDROGEN			mg		
2	00000002	00000002		HYDROGEN			mg		
3	00000003	00000003		HYDROGEN			mg		

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:

LocationID	Copies	Barcode	Size	UOM	Amount	Container Type	Container Name	RegID	Batch/Volume
1002	10	mg	5	ml				35	35
1002	10	mg	5	ml				31	82
1002	10	mg	5	ml				3	82

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

LocationID	Copies	Barcode	Size	UOM	Amount	Container Type	Container Name	RegID	Batch/Volume
1002	10	mg	5	ml				1	02
1002	10	mg	5	ml				21	02
1002	10	mg	5	ml				35	16

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

Container ID	Location	Name	UOM	Subunit	Quantity
1002	1002	HYDROGEN	mg	5	35

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

## Searching and Viewing Records in Temporary Table

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

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](#)*

- 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.
- In the result list, click **Review/Register** corresponding to the desired record. The

**Compound Commit Form** containing all the information about the record appears:

Compound Information	
Entry Date	7/10/2005
Last Mod Date	7/10/2005
Entry Person	INFORMAT
Project	unspecified
Prefix	AG
CAS no	
MW (calc)	78.1116
MF (calc)	C <sub>6</sub> H <sub>6</sub>

New Batch Information			
Formula Weight	Percent Active		
78.1116	100		
Salt Name	MW	Salt Equivalents	
so_salt	0	1	
Solvate Name	MW	Solvate Equivalents	
so_solvate	0	1	
Chemical	Purity	Appearance	Creation Date
INFORMAT			
Notebook	Page	Submitted Amount	Units
			mg
Reference and Vendor data			
Vendor Name		Vendor ID	
Batch Comment			

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 tem-

porary 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:

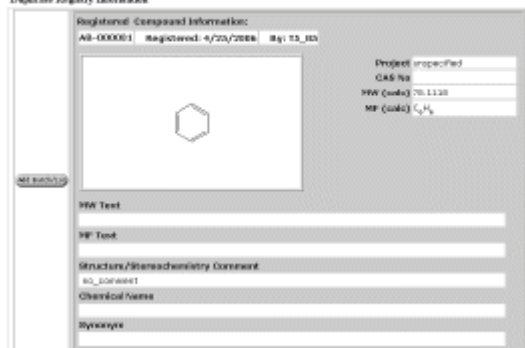
1. Search the temporary table to locate the compound record that is to be registered.
2. Click **Review/Register** the results list, corresponding to the required record. The **Compound Commit Form** appears.
3. Click **Register**. A page informing you about the successful registration of the compound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

A duplicate was found for the compound you are trying to register.  
Please select one of the options below to process the duplicate:

#### Duplicate Registry Information



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](#)*

---

## Registering a Batch Record

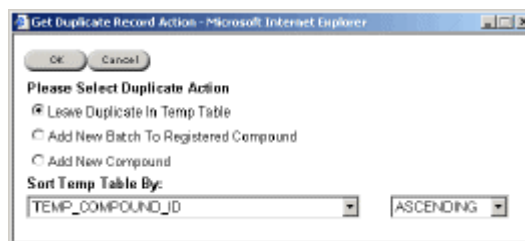
To register the temporary batch records:

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.

- Click **OK**. A dialog box informing you that the records are being processed appears.
- 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](#) and [Adding Analytics Data](#).

---

## 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:

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

Please enter a full registry number for adding identifiers (for example, AB-000001)

Registry Number:

- 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:

- 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.
- Click **OK**.

## Adding Analytics Data

Analytics data includes solubility, optical rotation, and <sup>1</sup>H 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:**

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

Please enter a parent number and batch number (for example, AB-000001/01)

Registry Number:

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

- 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](#).
- Click **Add Data**. The following page appears:

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

## Managing Duplicates

To manage duplicates in Registration Enterprise:

- 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.*

---

- Click **Mark Record** next to the duplicate records that are to be deleted.
- 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](#).*

---



---

*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.*

---

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



- Enter the search criteria, as shown in the following figure:

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

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

## Batch Search

To perform a batch operation:

- Click **Search** in the **Query and Reporting** section in the Registration Enterprise home page. The **Query Input Form** page appears.
- Click **Batch Search** tab. The following page 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](#).

## 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:

#### Select Experiment Type

Select Experiment Type :  ☒ Show Structures?

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

Structure	Supplies #	Batch ID	Experiment ID	Temperature	Pressure	Solvent	Solubility
	AB-000003001	23	1				
	AB-000001001	1	1				
	AB-000001001	1	3				

## 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:

File Help Log Off Home

Registry Tables Main Menu

Record 1-1 of 1 hits << < Rec# > >>

new

ID	Project Name	Active
<u>1</u>	unspecified	True

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

File Help Log Off Home

Add Record Cancel Main Menu

Project Name

Active

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:

File Help Log Off Home

Registry Tables Main Menu

Record 1-1 of 1 hits << < Rec# > >>

new

ID	Prefix	Next In Sequence	Salt Delimiter	Prefix Delimiter	Root Number	Length	Active
1	AB	105	/	-	5		True

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

File	Help	Log Off	Home
Add Record		Cancel	Main Menu
Prefix	<input type="text"/>		
Next In Sequence	<input type="text" value="1"/>		
Salt Delimiter	<input type="text"/>		
Prefix Delimiter	<input type="text"/>		
Root Number Length	<input type="text" value="6"/>		
Active	<input type="text" value="True"/> ▼		

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

#### EDITING A SEQUENCE

##### To edit a sequence in the Sequence table:

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

#### DELETING A SEQUENCE

To delete a sequence from the Sequence table:

- Click **Sequence** button, in the **Manage Tables** area. The Sequence table appears.
- Click the ID of the sequence that is to be deleted.
- 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:

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

File	Help	Log Off	Home
Registry Tables		Main Menu	
Record 1-2 of 2 hits << < Rec# > >>			
<u>new</u>			
ID	Structure Comment	Active	
<a href="#">1</a>	no_comment	True	
<a href="#">2</a>	no_structure	True	

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

- Enter the comment in the **Structure Comment** text box.
- Select **True** from the **Active** list box if you want the new structure comment to appear in the Structure/Stereochemistry Comment drop-down list.
- 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:

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

## DELETING A STRUCTURE COMMENT

To delete a structure comment from the Structure Comments table:

- Click **Structure Comments** in the **Manage Tables** area. The Structure Comments table appears.
- Click the ID of the structure comment that is to be deleted.
- 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](#).

To edit a record in the People table:

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

Person ID	Supervisor	User Code	User Name	Last Name	Middle Name	Telephone	Email/Active
1	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
2	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
3	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
4	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
5	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
6	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
7	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
8	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
9	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
10	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
11	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
12	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
13	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
14	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
15	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
16	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
17	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
18	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
19	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True
20	logn_disabled	logn_disabled	logn_disabled	logn_disabled			True

- Click the ID of the record that is to be edited. The record opens in the editable mode.
- 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:

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

Salt_Code	Salt_Name	Salt_MW	Salt_MF	Active
1	no_salt	0		True
21	test_salt	12		True

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

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

### EDITING A SALT RECORD

To edit a record in the Salts table:

- Click **Salts** in the **Manage Tables** area. The Salts table appears.
- Click the ID of the record that is to be edited. The record opens in the editable mode.
- 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:

Solvate_ID	Solvate_Name	Solvate_MW	Solvate_MF	Active
1	no_solvate	0		True

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

Solvate Name	<input type="text"/>
Solvate MW	<input type="text"/>
Solvate MF	<input type="text"/>
Active	True

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:



experiment_id	experiment_name	experiment_description	experiment_created_date	experiment_created_by
1	Solubility	Measurement of solubility using standard method	12/1/2000	1
2	Optical Rotation	Measurement of optical rotation using standard method	12/1/2000	1
3	1H NMR	Proton NMR	12/1/2000	1

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

*To add parameters types and result types, please add the new experiment type and then edit the new record.*

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

To edit the information in an experiment, see “**Editing an Experiment**” in [Experiment Type](#).

## Changing Passwords

To change your password:

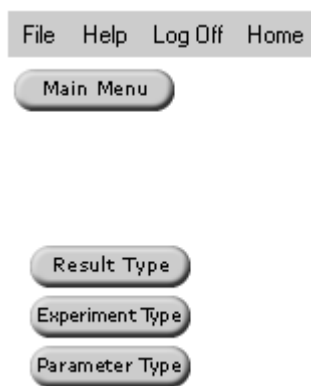
1. Click **Change Password** in the **Administration** section in the Registration Enterprise home page. The following page appears:

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](#).*

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](#).*

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

File Help Log Off Home

Update Record Cancel Delete Record Main Menu

ID: 1

Name: Solubility

Description: Measurement of solubility using standard methods

Created: 12/1/2000

Modified: 12/1/2000

Version: 1

Parameter Types			Result Types		
Add Parameter	Parameter Type	Standard Units	Add Result	Result Type	Standard Units
Delete	Temperature	Deg C	Delete	Solubility	Kg/L
Delete	Pressure	Atm			
Delete	Salinity				

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

File Help Log Off Home

Return to Details Main Menu

Step 1 of 2 - Choose Parameter for ExperimentTypeID: 1

Parameter Type: Wavelength Add Parameter

- Select the required parameter type from the **Parameter Type** list box and click **Add Parameter**.
- Perform the following tasks if you want to add a new result type to the experiment:

- Click **Add Result**. The following page appears:

File Help Log Off Home

Return to Details Main Menu

Step 1 of 2 - Choose Result for ExperimentTypeID: 1

Result Type: Solubility Add Result

- Select the required result type from the **Result Type** list box and click **Add Result**.
- Click **Delete** next to a parameter or result type if you want to delete the parameter or result type.
  - Make changes to other information, such as name and description, if required.
  - Click **Update Record**.

#### DELETING AN EXPERIMENT

To delete an experiment:

- 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](#).*

- Click the ID of the record that is to be deleted.
- Click **Delete Record**. A dialog box asking you to confirm the deletion action appears.
- 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:

parameter_type_id	parameter_type_name	parameter_type_description	parameter_type_unit
1	Temperature	Temperature of the experiment	Deg C
2	Pressure	Atmospheric pressure for the of the experiment	mmHg
3	Weight	Weight of the sample	g
4	Wavelength	Wavelength of Radiation used	nm
5	Concentration	Concentration of the sample	g/L

*NOTE: For information about accessing the Analytics Table management area, see [Managing Analytics Tables](#).*

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

File Help Log Off Home

Add Record Cancel Clear Form Main Menu

Name

Description

Units

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](#).*

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](#).*

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:

File Help Log Off Home

Analytics Table Main Menu

Record 1-3 of 3 hits

**new**

result_type_id	result_type_name	result_type_description	result_type_units
1	Solubility	Standard Solubility Equipment (Karl)	
2	Specific Rotation	Optical Rotation Measurement	Deg
3	Analytics	Analytical Reference Numbers	

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

File Help Log Off Home

Add Record Cancel Clear Form Main Menu

Name

Description

Units

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](#).*

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](#).*

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:

Person ID	Supervisor	First Name	Last Name	Middle Name	Initials	First Name	Last Name	Middle Name	Initials
1	None	John	Doe			John	Doe		
2	1	Jane	Doe			Jane	Doe		
3	1	John	Doe			John	Doe		
4	1	John	Doe			John	Doe		
5	1	John	Doe			John	Doe		
6	1	John	Doe			John	Doe		
7	1	John	Doe			John	Doe		
8	1	John	Doe			John	Doe		
9	1	John	Doe			John	Doe		
10	1	John	Doe			John	Doe		
11	1	John	Doe			John	Doe		
12	1	John	Doe			John	Doe		
13	1	John	Doe			John	Doe		
14	1	John	Doe			John	Doe		
15	1	John	Doe			John	Doe		
16	1	John	Doe			John	Doe		
17	1	John	Doe			John	Doe		
18	1	John	Doe			John	Doe		
19	1	John	Doe			John	Doe		
20	1	John	Doe			John	Doe		
21	1	John	Doe			John	Doe		
22	1	John	Doe			John	Doe		
23	1	John	Doe			John	Doe		
24	1	John	Doe			John	Doe		
25	1	John	Doe			John	Doe		
26	1	John	Doe			John	Doe		
27	1	John	Doe			John	Doe		
28	1	John	Doe			John	Doe		
29	1	John	Doe			John	Doe		
30	1	John	Doe			John	Doe		

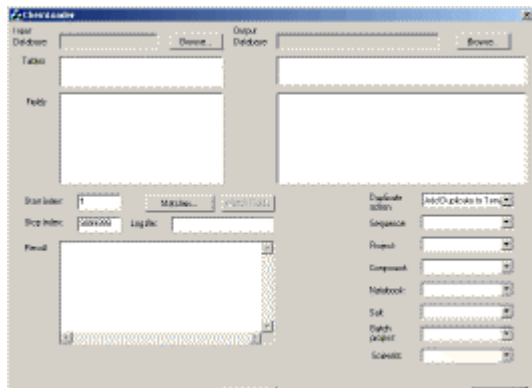
For information about adding or editing the workgroups or users, see [People](#).

## 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:

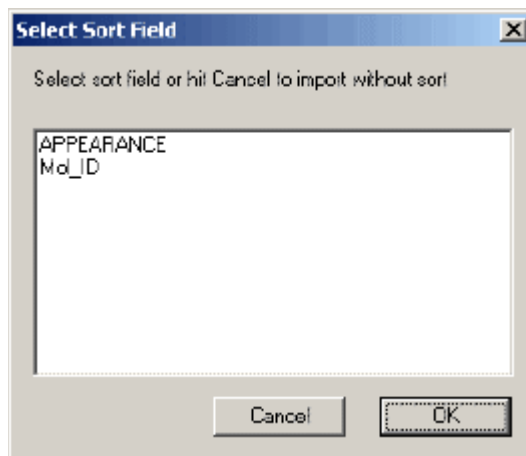
1. Import the SDFile into the ChemFinder database.
2. Browse to the following location:  
<webroot>\Inet-pub\wwwroot\ChemOffice\chem\_reg\ChemLoader\_Client.
3. Double click **ChemLoader.exe** to open ChemLoader. The following page appears:



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

4. Specify input and output databases.

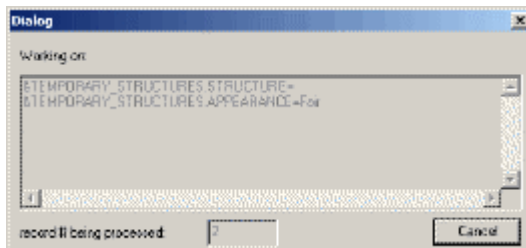
5. Match fields in the input and output databases.
6. Specify import options.
7. Click **Import**. The **Select Sort Field** dialog box appears:



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*

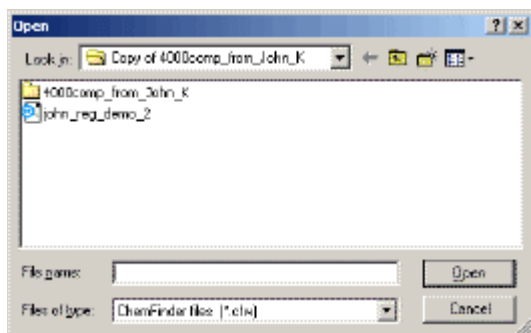
records that have already been imported, by ChemLoader, remain there in Registration Enterprise.

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

## Specifying Input and Output Databases

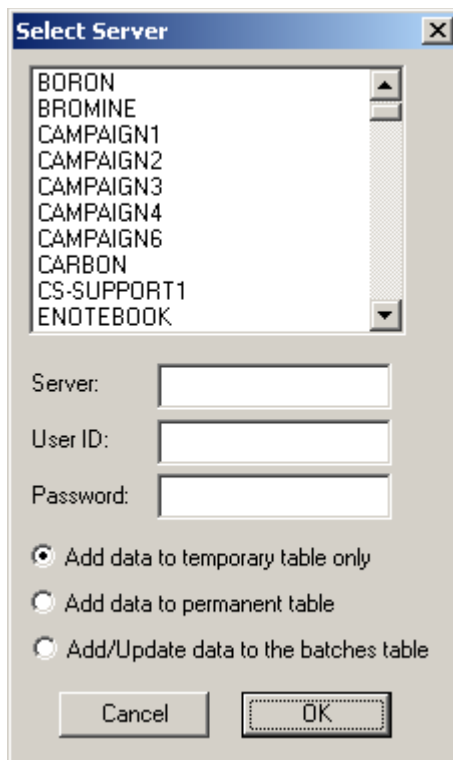
To specify input and output databases:

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



2. Browse to the location of the desired Chem-Finder 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.

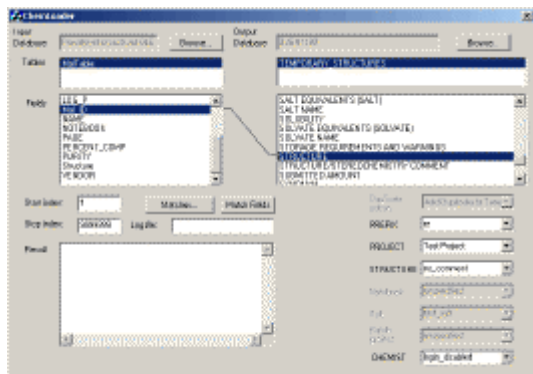


- Add/Update data to the batches table:  
Imports data to the batches table or updates the data.
8. Click **OK**. This populates the **Output Database** field with the output database and **Tables** field with the database tables. The fields of a table can be viewed in the **Fields** field by clicking 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 and Viewing Records in 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 SDFFile: 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 SDFFile.
  - Nested SDFFile: 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 SDFFile.
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 SDFFile at the desired location.

---

*NOTE: You can also export the RDFiles using the preceding steps. For this, you need to select the RDFFile 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.

- Click **Projects**. The Projects table appears.
- Click the ID corresponding to the required project. The following page appears:

File Help Log Off Home

Update Record Cancel Main Menu

ID 1

Project Name unspecified

Active True

Available Users

- BIOSAR\_ADMIN
- BIOSAR\_USER
- BIOSAR\_USER\_ADMIN
- BIOSAR\_USER\_BROWSER
- CSSADMIN
- CSSUSER

Add Remove

Current Project Bound Users

- T5\_85

- 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 all the users that are to be associated with the project.
- 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.
- Populating the batch level record with salt and solvate information in the compound

level record, and allowing all fields to be changed at the batch level.

- 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 to allow users to create their 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.

To integrate ChemScript with Registration Enterprise:

#### 1. Install ChemScript:

- If MS .Net Framework 2.0 is not installed, install MS .Net Framework 2.0 from \\shares\public\Software\Windows\Net Framework\Net Framework 2.0 Shipping.
- Install MS Soap Client from \\shares\Public\Software\Windows\SOAP Installers\SoapToolkit SDK\SoapSDK.exe.
- Install ChemScript 11 (This will install Python 2.5).
- Reboot.
- Apply 9.0SR4 file changes to the server.

---

*NOTE: If SR3 is installed, remove SR3 first.*

---

- Navigate to C:\Inetpub\wwwroot\ChemOffice\chem\_reg\ChemScript\ and copy C:\Inetpub\wwwroot\ChemOffice\chem\_reg\ChemScript\ChemScriptUtils.py to C:\Python25\lib.
- Run any one of the following command:
  - Update\_ChemReg\_DB\_From\_9.0SR3\_to\_9.0SR4.cmd
  - Update\_ChemReg\_DB\_From\_9.0SR2\_to\_9.0SR3.cmd

- Run the command Update\_ChemReg\_DB\_From\_9.0SR3\_to\_9.0SR4.cmd.
2. Install ChemScript web service C:\Inetpub\wwwroot\ChemOffice\Chem\_reg\ChemScript\PyEngine\PyEngine.
  3. Create a virtual directory PyEngine from IIS.
  4. In the IIS properties of PyEngine, choose to run it under .Net 2.0.
  5. Replace the functions search\_func\_vbs.asp, form\_val\_js.js, and Display\_func\_vbs.asp in core with the ones in Chem\_reg.
  6. Open the cfserver.ini file located at: **\\Inetpub\wwwroot\ChemOffice\chem\_reg\config**.
  7. Set the value of MOLECULE\_PROCESS=1 in the GLOBALS section.
  8. Set the value of MOLECULE\_PROCESS\_SCRIPT=C:\Inetpub\wwwroot\ChemOffice\chem\_reg\ChemScript\ChemScriptParent.py.
  9. Browse to C:\Inetpub\wwwroot\ChemOffice\Chem\_Reg\ChemScript\PyEngine\PyEngine\web.config and set the specified values for the following fields:
    - add key="log" value="on"
    - add key="logfolder" value="C:\Inetpub\wwwroot\ChemOffice\chem\_reg\ChemScript\log"
    - add key="logdays" value="30"
    - add key="debug" value="on"
    - add key="pythoncoreversion" value="2.5"

- identity impersonate="true" user-Name="camsoft\_admin" password="cambridgesoft"

10. To manage salt table via chemfinder:

- Open C:\Inet-pub\wwwroot\ChemOffice\chem\_reg\ChemScript\Salts.cfw to add and edit salts in Registration Salts table.
- To add salts to Salts.cfw:
  - Specify salt name and commit.
  - Close the chemfinder form and reopen it.
  - Set salt structure and Active = 1.

---

*NOTE: Be sure to set the value of Active = 1 because the trigger to calculate MF and MW is based on value of this field.*

---

- Save and export as sdf.

---

*NOTE: After adding or editing salts in Salts.cfw, it needs to be exported as Salts.sdf. If an error occurs when exporting, kill process aspnet\_wp.exe from Task Manager.*

---

11. To manage solvate table via chemfinder:

- Open C:\Inet-pub\wwwroot\ChemOffice\chem\_reg\ChemScript\Solvates.cfw to add and edit solvates in Registration Solvates table.

---

*NOTE: After adding or editing solvates in Solvates.cfw, it needs to be exported as Solvates.sdf. If an error occurs when exporting, kill process aspnet\_wp.exe from Task Manager.*

---

## 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.*

---

## Roles

Different users need to perform different tasks using Registration Enterprise. Therefore, while setting up new user accounts, system administrator assigns different roles to different users. Each Registration role is assigned specific privileges, which specify the task that can be performed using the role. For example, BROWSER only has the privilege to view the Registration Enterprise records, however, CHEMICAL\_ADMINISTRATOR is allowed to add, edit, and delete the records, as well. The following table lists the roles available in Registration Enterprise and the Oracle role name associated with each role:

Role Name	Oracle Role Name
BROWSER	BROWSER
CHEMICAL ADMINISTRATOR	CHEMICAL_ADMINISTRATOR
PERFUME CHEMIST	PERFUME_CHEMIST
SUBMITTER	SUBMITTER
SUPERVISING CHEMICAL ADMIN	SUPERVISING_CHEMICAL_ADMIN
SUPERVISING CHEMIST	SUPERVISING_CHEMIST

## Privileges

The following table lists the privileges available in Registration Enterprise along with the roles associated with the privileges:

Privilege	Oracle Privilege Name	Role(s) Associated with Privilege
Add a new experiment to the Experiments table	ADD_ANALYTICS_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN,
Add batch information for a compound in the Temporary table	ADD_BATCH_TEMP	CHEMICAL_ADMINISTRATOR, SUBMITTER, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Add a new batch project to the Batch Projects table	ADD_BATCH_PROJECTS_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Add a new compound to the Temporary table	ADD_COMPOUND_TEMP	CHEMICAL_ADMINISTRATOR, SUBMITTER, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Add a new compound type to the Compound Type table	ADD_COMPOUND_TYPE_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Add analytics data to a batch	ADD_EVAL_DATA	CHEMICAL_ADMINISTRATOR, PERFUME_CHEMIST, SUBMITTER, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Add a new salt to the Salts table	ADD_SALT_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN



<b>Privilege</b>	<b>Oracle Privilege Name</b>	<b>Role(s) Associated with Privilege</b>
Add salt information to a compound that is in the Temporary table	ADD_SALT_TEMP	CHEMICAL_ADMINISTRATOR, SUBMITTER, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Add a new sequence to the Sequence table	ADD_SEQUENCES_TABLE	SUPERVISING_CHEMICAL_ADMIN
Add a new site to the Sites table	ADD_SITES_TABLE	CHEMICAL_ADMINISTRATOR, PERFUME_CHEMIST, SUPERVISING_CHEMICAL_ADMIN
Add a new solvate to the Solvates table	ADD_SOLVATES_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Add identifier to a compound stored in the Temporary table	ADD_IDENTIFIER_TEMP	CHEMICAL_ADMINISTRATOR, SUBMITTER, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Add a new notebook to the Notebooks table	ADD_NOTEBOOKS_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Add a new record to the People table	ADD_PEOPLE_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Add a new project to the Projects table	ADD_PROJECTS_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Add a new utilization to the Utilizations table	ADD_UTILIZATIONS_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Add a new record to the Workgroup table	ADD_WORKGROUP	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST

<b>Privilege</b>	<b>Oracle Privilege Name</b>	<b>Role(s) Associated with Privilege</b>
Delete an experiment from the Experiments table	DELETE_ANALYTICS_TABLES	SUPERVISING_CHEMICAL_ADMIN, PERFUME_CHEMIST
Delete a record from Batch Projects table	DELETE_BATCH_PROJECTS_TABLE	SUPERVISING_CHEMICAL_ADMIN
Delete a batch record from Registration Enterprise	DELETE_BATCH_REG	SUPERVISING_CHEMICAL_ADMIN
Delete a record from the Compound Type table	DELETE_COMPOUND_TYPE_TABLE	SUPERVISING_CHEMICAL_ADMIN
Delete analytics data from a batch	DELETE_EVAL_DATA	SUPERVISING_CHEMICAL_ADMIN
Delete a record from the Notebooks table	DELETE_NOTEBOOKS_TABLE	SUPERVISING_CHEMICAL_ADMIN
Delete a record from the People table	DELETE_PEOPLE_TABLE	SUPERVISING_CHEMICAL_ADMIN
Delete a record from Projects table	DELETE_PROJECTS_TABLE	SUPERVISING_CHEMICAL_ADMIN
Delete a registered compound	DELETE_REG	SUPERVISING_CHEMICAL_ADMIN
Delete a salt from the Salts table	DELETE_SALT_TABLE	SUPERVISING_CHEMICAL_ADMIN
Delete a sequence from the Sequence table	DELETE_SEQUENCES_TABLE	SUPERVISING_CHEMICAL_ADMIN

<b>Privilege</b>	<b>Oracle Privilege Name</b>	<b>Role(s) Associated with Privilege</b>
Delete a site from the Sites table	DELETE_SITES_TABLE	SUPERVISING_CHEMICAL_ADMIN
Delete a solvate from the Solvates table	DELETE_SOLVATES_TABLE	SUPERVISING_CHEMICAL_ADMIN
Delete a compound from the Temporary table	DELETE_TEMP	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Delete a record from the Utilization table	DELETE_UTILIZATIONS_TABLE	SUPERVISING_CHEMICAL_ADMIN
Delete a record from the Workgroup table	DELETE_WORKGROUP	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Edit an experiment in the Experiments table	EDIT_ANALYTICS_TABLES	CHEMICAL_ADMINISTRATOR, PERFUME_CHEMIST, SUPERVISING_CHEMICAL_ADMIN
Edit batch information of a compound	EDIT_BATCH_REG	CHEMICAL_ADMINISTRATOR, SUBMITTER, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Edit a record in the Batch Projects table	EDIT_BATCH_PROJECTS_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Edit a batch record stored in the Temporary table	EDIT_BATCH_TEMP	CHEMICAL_ADMINISTRATOR, SUBMITTER, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Edit a registered compound record	EDIT_COMPOUND_REG	CHEMICAL_ADMINISTRATOR, SUBMITTER, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST

<b>Privilege</b>	<b>Oracle Privilege Name</b>	<b>Role(s) Associated with Privilege</b>
Edit a compound record stored in Temporary table	EDIT_COMPOUND_TEMP	CHEMICAL_ADMINISTRATOR, SUBMITTER, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Edit a record in the Compound Type table	EDIT_COMPOUND_TYPE_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Edit the analytics data	EDIT_EVAL_DATA	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Edit identifier information of a Registered compound	EDIT_IDENTIFIERS_REG	CHEMICAL_ADMINISTRATOR, SUBMITTER, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Edit identifier information for a compound stored in the Temporary table	EDIT_IDENTIFIERS_TEMP	CHEMICAL_ADMINISTRATOR, SUBMITTER, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Edit a notebook record in the Notebooks table	EDIT_NOTEBOOKS_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Edit a people record in the People table	EDIT_PEOPLE_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Edit a project record in the Projects table	EDIT_PROJECTS_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Edit salt information of a registered compound	EDIT_SALT_REG	CHEMICAL_ADMINISTRATOR, SUBMITTER, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Edit a salt record in the Salts table	EDIT_SALT_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN

Privilege	Oracle Privilege Name	Role(s) Associated with Privilege
Edit salt information of a compound stored in the Salts table	EDIT_SALT_TEMP	CHEMICAL_ADMINISTRATOR, SUBMITTER, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Edit a record in the Sequence table	EDIT_SEQUENCES_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Edit a record in the Sites table	EDIT_SITES_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Edit a solvate record in the Solvates table	EDIT_SOLVATES_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Edit a record in the Users table	EDIT_USERS_TABLE	SUPERVISING_CHEMICAL_ADMIN
Edit a record in the Utilizations table	EDIT_UTILIZATIONS_TABLE	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Edit a record in the Workgroup table	EDIT_WORKGROUP	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Manage assignment of people to projects, when RLS is enabled	MANAGE_PEOPLE_PROJECT	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Manage duplicate records, when RLS is enabled	MANAGE_SYSTEM_DUPLICATES	SUPERVISING_CHEMICAL_ADMIN
Register a compound	REGISTER_TEMP	CHEMICAL_ADMINISTRATOR, SUBMITTER, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST

<b>Privilege</b>	<b>Oracle Privilege Name</b>	<b>Role(s) Associated with Privilege</b>
View the analytics spreadsheet	SEARCH_EVAL_DATA	CHEMICAL_ADMINISTRATOR, SUBMITTER, PERFUME_CHEMIST, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Search a compound stored in the Temporary table	SEARCH_TEMP	CHEMICAL_ADMINISTRATOR, SUBMITTER, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Search a registered compound	SEARCH_REG	CHEMICAL_ADMINISTRATOR, SUBMITTER, PERFUME_CHEMIST, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Approve compounds	SET_APPROVED_FLAG	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Mark compounds as quality-checked	SET_QUALITY_CHECK_FLAG	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN, SUPERVISING_SCIENTIST
Disapprove compounds	TOGGLE_APPROVED_FLAG	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN
Unmark compounds as quality-checked	TOGGLE_QUALITY_CHECK_FLAG	CHEMICAL_ADMINISTRATOR, SUPERVISING_CHEMICAL_ADMIN



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# Administrator Guide

## Configuration

### Customizable Fields

The Registration Enterprise has a number of fields which are by default hidden, but are available to be configured if none of the default Registration fields contain necessary information. The following customizable fields exist:

#### For Compound Records

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

#### For Batch Records

- integer fields
- real number fields
- date fields

The name, datatype, and display type can be adjusted for any of the above mentioned fields.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

There are two steps in customizing and displaying a customizable field:

1. Assign field properties to the field listing.

2. Make the field visible to users.

---

*NOTE: If these fields will be used in BioSAR Enterprise, the custom names will need to be updated in schema management for regdb. These fields will not be recognized automatically.*

---

### Assigning Field Properties

Field definitions are found in the Registration Enterprise cfserver.ini file  
(`<webroot>\ChemOffice\chem_reg\config`). The customizable fields follow the following naming convention:

- text fields: `TXT_<TYPE>_FIELD_#`
- integer fields: `INT_<TYPE>_FIELD_#`
- real number fields:  
`REAL_<TYPE>_FIELD_#`
- date fields: `DATE_<TYPE>_FIELD_#`  
where # is a number between 1 and 4 and  
<TYPE> is `COMPD` (for a compound field) or `BATCH` (for a batch field).

### CHANGING THE NAME OF A FIELD

To change the name of a field:

1. Open the CFserver.ini file and scroll down to the section title `Field_Labels` format.
2. Find the appropriate field name in the list. The listing are in the following format:
  - **FIELD\_LABELS#=EXACT FIELD NAME : FIELD LABEL DISPLAY<BR>** The only part of this listing that should be changed is the `FIELD LABEL DISPLAY`.



3. Change the text after the : to the name you would like displayed in the Registration Form for this field.
4. Save your changes.

#### CHANGING THE DISPLAY TYPE OF A FIELD

To change the display type of a field:

1. Open the CFserver.ini file and scroll down to the section title DISPLAY\_TYPES.
2. Find the appropriate field name in the list. The listing are in the following format:

- **DISPLAY\_TYPES#=FieldName ; Input Field : Option [; Display Field : Option]**  
Be sure not to change the text to the left of the = or the FieldName.

For more information about Input Field options, please see “CFServer.ini Configuration File” on page 46.

3. Save your changes.

#### Making the Field Visible

To make a previously hidden field visible:

1. Open the cfserver.ini file and scroll down to the section title "hide fields from GUI and ChemLoader".
2. Find the EXACT FIELD NAME in the GUI\_FIELDS\_TO\_HIDE entries, and delete the name.
3. Save your changes.

---

*NOTE: To see your changes in a Registration Enterprise Field, it is necessary to reset IIS.*

---

For more information about the Cfserver.ini file, please see “CFServer.ini Configuration File” on page 46.

## CFServer.ini Configuration File

The CFServer.ini file, found in the following location:

**<webroot>/ChemOffice/chem\_reg/config** defines parameters that allow the Registration Enterprise application to find necessary information and how to react in certain situations. When editing fields in this file, it is important to be sure what is going to change because many of these settings are necessary for the application to function properly.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### [GLOBALS]

ADJUST\_NETSCAPE  
\_WIDTHS

ADOCONN\_PWDKey  
word

ADOCONN\_UserIDKe  
yword

ADMIN\_REQUIRED

ALLOW\_RDFILE\_EX  
PORT

#### [CS\_SECURITY]

ALLOW\_COOKIE  
E\_LOGIN

COOKIE\_EXPIRE  
S\_MINUTES

CS\_SECURITY\_U  
DL\_PATH

MINIMUM\_REQ  
UIRED\_PRIVILE  
GE

		CDX_CACHING	APPROVED_SCOPE
ALLOW_FLAT_SDFI LE_EXPORT	PRIVILEGE_TAB LE_LIST	DATE_FORMAT	AUTOGENERAT ED_CHEMICAL_ NAME
ALLOW_HITLIST_M ANAGEMENT	STARTUP_LOCA TION	DB_NAMES	BATCH_LEVEL
ALLOW_PUBLIC_HI TLISTS	USE_CS_SECURI TY_APP	DIRECT_KEYWORD _SUPPORT	BATCH_NUMBE R_LENGTH_GUI
ALLOW_PUBLIC_QU ERIES		DISPLAY_GIFS_ONL Y_FORM_IE	BATCH_PROJEC TS_USED
ALLOW_QUERY_MA NAGEMENT	<b>[REGISTRATION]</b>	DISPLAY_GIFS_ONL Y_FORM_NS6	BATCHES_TO_T EMP
ALWAYS_DISPLAY_ ALERTS	ADD_BATCH_FR OM_REG_RESUL TS	DISPLAY_GIFS_ONL Y_FORM_NS	BUILD_SITE_ID
ANIMATED_GIF_PAT H	ADD_IDENTIFIE RS_COMMIT_TA BLE_ORDER	DISPLAY_GIFS_ONL Y_LIST_IE	COMPOUND_TY PES_USED
APP_NAME	ADD_SALT_COM MIT_TABLE_OR DER	DISPLAY_GIFS_ONL Y_LIST_NS	DBA_PWD
APP_TYPE	ALLOW_BATCH _FOR_UNAPPRO VED_CMPD	DISPLAY_GIFS_ONL Y_LIST_NS6	DBA_USERNAM E
BODY_BACKGROUN D	ANALYTICS_US ED	ENCRYPT_PWD	DEFAULT_PREFI X
BRACKET_IN_STRU C_HANDLING	APPROVED_FLA G_USED	ENCRYPT_PWD_KE YS	DELETE_BATCH _TABLE_ORDER

ENCRYPT_PWD_SECTION	DELETE_COMPOUND_TABLE_ORDER	MARKED_HITS_MAX	ORA_SERVICENAME
EXPIRE_HITLIST_HISTORY_DAYS	DELETE_SALT_TABLE_ORDER	MOLSERVER_VERSION	ORA_SQLLDRPATH
EXPIRE_MARKED_HITS_DAYS	DERIVED_FIELDS	MW_ROUND_DIGIT	OUTPUT_AS_GIF_ON_REG
EXPIRE_QUERY_HISTORY_DAYS	DISPLAY_APPKEY	NAV_BAR_WINDOW	PREFIX_DELIMITER
FIELD_SPLIT_CHARACTER	FORMULA_WT_CALC	NAV_BUTTONS_GIF_PATH	PRIMARY_STRWHERE
FLOAT_FORMAT	FULL_COMMIT_TABLE_ORDER	NON_CHEMICAL_SUBMIT	PRIV_TABLE_NAME
FORMAT_FORMULA	GET_MW_FORMULA_METHOD	POST_MARKED_HITS_PAGE	PRODUCER_ID_FIELD
GLOBAL_SEARCH_DBS	IDENTIFIERS_TO_TEMP	POST_MARKED_HITS_TARGET_MENU_NAME	PRODUCER_LOOKUP
GLOBAL_SEARCH_BASE_DB	NEW_BATCH_COMMIT_TABLE_ORDER	POST_MARKED_SENT_TO_PAGE	PROJECT_LEVEL_ROW_SECURITY
HIGHLIGHT_BACKGROUND	NO_STRUCTURE_TEXT	POST_MARKED_SUPPORTED_FORMGROUPS	PROJECTS_NAMED_OWNER
HIGHLIGHT_REQUIRED_FIELDS	NOTEBOOK_LOOKUP	PREFS_FORM_GROUPS	PROJECTS_USED
MAIN_WINDOW	NOTEBOOK_USED	RESIZE_GIFS	REAGENT_BYPASS_DUPLICATES

SEARCH_DEFAULT_PREFS	REAGENT_SEQUENCE	HIT_ANY_CHARGE_HETERO	SHOW_SAR_TABLE
TEMP_DIR_NAME	REAGENTS_TO_TEMP	IDENTITY	SHOW_SEC_TBLES_IN_USR_MGR
TEMP_DIR_PATH	REAGENTS_USED	MATCH_DB_STEREO	SHOW_USER_NOTEBOOKS_ONLY
USE_ANIMATED_GIF	REG_DELIMITER	MATCH_TET_STEREO	SITES_USED
USE_SESSION_RECORD_COUNTS	REG_PWD	RELATIVE_TET_STEREO	SOLVATES_USED
USER_INFO_WINDOW	REG_USERNAME	RXN_HIT_RXN_CENTER	START_BATCH_NUMBER
USERWINDOW-BACKGROUND	ROOT_NUMBER_LENGTH	TAUTOMER	STRUCTURE_COMMENTS_TEXT
<b>[DUPLICATE CHECKING]</b>	SALT_EDITABLE_FOR_REG_SALTS		TABLES_WITH_BASE64_CDX
ABSOLUTE_HITS_REL	SALTS_USED		TABLES_WITH_MOLIDS
EXTRA_FRAGS_OK	SEC_PWD		TEMP_TABLE_QUERY_FORM
EXTRA_FRAGS_OK_IF_RXN	SEC_USERNAME		USE_BATCH_SCIENTIST_AS_REGISTRAR
FRAGS_CAN_OVERLAP	SHOW_NOTEBOOK_USER		USE_GUI_DEFAULTS_IN_API
HIT_ANY_CHARGE_CARBON	SHOW_MF_WITH_SALT_NAME		

USER\_LOOKUP

Default: 1  
Options: 0 | 1

UTILIZATION\_P  
ERMISSIONS\_US  
ED

WORKGROUPS\_  
USED

Entries starting with GUI\_FIELDS\_TO\_HIDE, FIELD\_LABELS, and DISPLAY\_TYPES have standard formats, but the number of entries and values can vary greatly from site to site. These entries make it easy for administrators to define new fields and to control field properties. These entries are specific to the Registration Enterprise cfserver.ini file. For information regarding how to change similar properties in another application, please see the Admin guide for that application or for the Core ChemOffice Enterprise.

### Globals

ADJUST\_NETSCAPE\_WIDTHS

Example: ADJUST\_NETSCAPE\_WIDTHS = 1

Description: Corrects for the differences in widths in Netscape compared to IE. 1 will scale Netscape pages, 0 will not make any changes.

Default: 1

Options: 0 | 1

ADMIN\_REQUIRED

Example: ADMIN\_REQUIRED = 1

Description: Set to True(1) flags the system indicating that username and passwords are required. Editing this value will cause unpredictable behavior.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

ADOCNN\_PWDKEYWORD

Example: ADOCNN\_PWDKeyword = password

Description:

Default: password

Options: **Should not be edited.**

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

ADOCNN\_USERIDKEYWORD

Example: ADOCNN\_UserIDKeyword = user id

Description:

Default: user id

Options: **Should not be edited.**

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of*

*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### ALLOW\_RDFILE\_EXPORT

Example: ALLOW\_RDFILE\_EXPORT = 1

Description: Controls the availability of the RD export option in the Export Hits dialog. It is analogous to ALLOW\_FLAT\_SDFILE\_EXPORT flag. The value, 1 indicates that RD file export is allowed.

Default: 0

Options: 0 | 1

---

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---

#### ALLOW\_FLAT\_SDFILE\_EXPORT

Example:

ALLOW\_FLAT\_SDFILE\_EXPORT = 1

Description: Determines if SDFiles can be exported in flat format. Hits can be exported as SDFiles in either flat or nested. 1 indicates flat SDFile export is allowed. If set to 0, the user will not be given the option, and all SDFiles will be exported in the nested format.

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice*

*Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### ALLOW\_HITLIST\_MANAGEMENT

Example:

ALLOW\_HITLIST\_MANAGEMENT = 1

Description: Determines if hitlist management can be accessed from the application. Hitlist management allows users to add, subtract, create the intersection, and union of hitlists. 1 indicates hitlist management is allowed.

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### ALLOW\_PUBLIC\_HITLISTS

Example: ALLOW\_PUBLIC\_HITLISTS = 1

Description: Determines if saved hitlists can be made public. Making a hitlist public allows all other users of the application to access that hitlist. 1 indicates hitlists can be made public.

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of*

*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### ALLOW\_PUBLIC\_QUERIES

Example: ALLOW\_PUBLIC\_QUERIES = 1

Description: Determines if saved queries can be made public. Making a query public allows all other users of the application to access that query. 1 indicates queries can be made public.

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### ALLOW\_QUERY\_MANAGEMENT

Example:

ALLOW\_QUERY\_MANAGEMENT = 1

Description: Determines if query management can be accessed from the application. Query management allows users save and recover queries. 1 indicates query management is allowed.

Default: 1

Options: 0 | 1

---

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*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### ALWAYS\_DISPLAY\_ALERTS

Example: ALWAYS\_DISPLAY\_ALERTS = 0

Description: Indicates if a user should receive alerts (e.g. compound was registered). 1 turns on all alerts. 0 removes alerts which are not required.

Default: 0

Options: 0 | 1

---

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---

#### ANIMATED\_GIF\_PATH

Example: ANIMATED\_GIF\_PATH = "/cfserverasp/source/graphics/processing\_Ybvl\_Ysh\_grey.gif"

Description: Path to the GIF used for the progress icon. By default, points to the spinning benzene ring. Only useful if USE\_ANIMATED\_GIF=1.

Default: "/cfserverasp/source/graphics/processing\_Ybvl\_Ysh\_grey.gif"

Options: A relative or absolute path.

---

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*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### APP\_NAME

Example: APP\_NAME = chem\_reg

Description: Name of the application displayed in some parts of the user interface.

Default: chem\_reg

Options:

Application Name	APP_NAME value
Sample	sample
Registration System	chem_reg
Inventory Manager	cheminv
Mixture Registration	
BioSAR Browser	biosar_browser
ChemACX	chemacx
Documentation Manager	

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### APP\_TYPE

Example: APP\_TYPE = registration

Description: Tells the system that this is a registration application.

Default: registration

Options: registration

---

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---

#### BODY\_BACKGROUND

Example: BODY\_BACKGROUND = "#FFFFFF"

Description: Indicates the background that should be used for the body section of the page.

Default: "#FFFFFF"

Options: A color (recorded in HEX format) or a relative path to a GIF.

---

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---

#### BRACKET\_IN\_STRUC\_HANDLING

Example:

BRACKET\_IN\_STRUC\_HANDLING = "WARN"



Description: Related to brackets entered in the structure window. Brackets are not recognized as having any chemical significance. WARN indicates the user will be warned if brackets are used, ALLOW ignores the brackets, DISALLOW does not allow the use of brackets in the structure window

Default: WARN

Options: WARN | ALLOW | DISALLOW

---

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---

#### CDX\_CACHING

Example: CDX\_CACHING = false

Description: If set to True, the application will cache cdx files. Registration Enterprise overrides this value internally, so changing the setting will not make a difference in Registration System.

Default: false

Options: true | false

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of*

*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### DATE\_FORMAT

Example: DATE\_FORMAT = 8

Description: Indicates which international date format to use. The choices are:

- 8 - US - mm/dd/yyyy
- 9 - Europe - dd/mm/yyyy
- 10 - Japanese - yyyy/mm/dd

Default: 8

Options: 8 | 9 | 10

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### DB\_NAMES

Example: DB\_NAMES = reg

Description: The name of the directory containing the forms necessary for proper operation of the application. Editing this value may cause unpredictable behavior.

Default: reg

Options: Usually the name of the application. If you would like to enter a list of directories, separate the list with a comma.

Application Name	DB_NAMES value
Sample	sample
Registration Enterprise	reg
Inventory Manager	inv
Mixture Registration	
BioSAR Browser	biosar_browser
ChemACX	chemacx
Documentation Manager	

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### DIRECT\_KEYWORD\_SUPPORT

Example: DIRECT\_KEYWORD\_SUPPORT = true

Description: Takes care of problems in the back end associated with different versions of Oracle. Should be set to false or NONE when the Oracle instance is found on a UNIX

machine, or with Oracle version 7. Otherwise, set to true.

Default: true

Options: true | false | NONE

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### DISPLAY\_GIFS\_ONLY\_FORM\_IE

Example:

DISPLAY\_GIFS\_ONLY\_FORM\_IE = 0

Description: Set to True(1), displays GIFS in Result Form views rather than CDX when a Netscape 6 browser is detected.

Default: 0

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### DISPLAY\_GIFS\_ONLY\_FORM\_NS

Example:

DISPLAY\_GIFS\_ONLY\_FORM\_NS = 0

Description: Set to True(1), displays GIFS in Result Form views rather than CDX when a Netscape browser is detected.

Default: 0

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

DISPLAY\_GIFS\_ONLY\_FORM\_NS6

Example:

DISPLAY\_GIFS\_ONLY\_FORM\_NS6 = 0

Description: Set to True(1), displays GIFs in Result Form views rather than CDX when a Netscape 6 browser is detected.

Default: 0

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

DISPLAY\_GIFS\_ONLY\_LIST\_IE

Example: DISPLAY\_GIFS\_ONLY\_LIST\_IE = "0"

Description: Indicates if GIFs should be used instead of CDX in list view in IE. 1 indicates GIFs should be used.

Default: 0

Options: 1 | 0

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

DISPLAY\_GIFS\_ONLY\_LIST\_NS

Example: DISPLAY\_GIFS\_ONLY\_LIST\_NS = "0"

Description: Indicates if GIFs should be used instead of CDX in list view in Netscape. 1 indicates GIFs should be used.

Default: 0

Options: 1 | 0

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

DISPLAY\_GIFS\_ONLY\_LIST\_NS6

Example: DISPLAY\_GIFS\_ONLY\_LIST\_NS6 = "0"

Description: Indicates if GIFs should be used instead of CDX in list view in Netscape 6. 1 indicates GIFs should be used.

Default: 0

Options: 1 | 0

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

## ENCRYPT\_PWD

Example: ENCRYPT\_PWD = FALSE

Description: When this setting is turned on for the first time, the user names and passwords (listed under the ENCRYPT\_PWD\_KEYS setting) in this file should be entered in plain text ahead of time. When the application is accessed for the first time the passwords will be encrypted and inserted into this INI file as encrypted text. If a password is changed, change all passwords in this INI file back to plain text and restart the application. The passwords will again be encrypted and stored.

Default: FALSE

Options: TRUE | FALSE

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

## ENCRYPT\_PWD\_KEYS

Example: ENCRYPT\_PWD\_KEYS = BIOSAR\_BROWSER\_PWD,SEC\_PWD,DB A\_PWD

Description: A comma delimited list of password settings to be encrypted.

Default:

BIOSAR\_BROWSER\_PWD,SEC\_PWD,DB A\_PWD

Options: The names of password settings in the cfserver.ini file to be encrypted.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

## ENCRYPT\_PWD\_SECTION

Example: ENCRYPT\_PWD\_SECTION = GLOBALS

Description: This setting identifies the heading name that the password settings are found under in the cfserver.ini file.

Default: GLOBALS

Options: The name of a heading in the cfserver.ini file.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

## EXPIRE\_HITLIST\_HISTORY\_DAYS

Example:

EXPIRE\_HITLIST\_HISTORY\_DAYS = 30

Description: The value of this setting is in days. After the number of days specified, hitlist history entries are removed.

Default: 2

Options: An integer indicating a number of days.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### EXPIRE\_QUERY\_HISTORY\_DAYS

Example:

EXPIRE\_QUERY\_HISTORY\_DAYS = 2

Description: The value of this setting is in days. After the number of days specified, queries in the history are removed.

Default: 2

Options: An integer indicating a number of days.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### EXPIRE\_MARKED\_HITS\_DAYS

Example: EXPIRE\_MARKED\_HITS\_DAYS = 365

Description: The value of this setting is in days. After the number of days specified, the marked hitlist is cleared.

Default: 365

Options: An integer indicating a number of days.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### FIELD\_SPLIT\_CHARACTER

Example: FIELD\_SPLIT\_CHARACTER = "|"

Description: Used to indicate the delimiter in lists entered into fields. Most useful for a field like Synonym where more than one synonym might be added at once.

Default: |

Options: Any character

---

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---

#### FLOAT\_FORMAT

Example: FLOAT\_FORMAT = 8

Description: ChemOffice Enterprise now supports international floating number format. US and UK format uses "." as the decimal symbol and "," as the digit grouping symbol,

while most European format uses "," as the decimal symbol, "." as the digit grouping symbol.

If the setting is set to 8, the number will be formatted in US format, if it is set to 9, it will be formatted in European format. The IIS server needs to be consistent with the flag. In other words, if the IIS server is a US system, this flag needs to be set to 8, and the numbers will be in US format. IF the IIS server is a European system, this flag needs to be set to 9, and the numbers will be in European format. The IIS server locale CAN NOT be inconsistent with FLOAT\_FORMAT flag, otherwise there will be malfunctioning.

---

*NOTE: This setting is different from the Date Format. See DATE\_FORMAT for more information*

---

Default: 8

Options: 8 | 9

---

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*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

## FORMAT\_FORMULA

Example: FORMAT\_FORMULA = 1

Description: Indicates if super- and sub- scripts should be used when displaying a molecular formula. 0 removes formatting.

Default: 0

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

## GLOBAL\_SEARCH\_DBS

Example: GLOBAL\_SEARCH\_DBS = reg

Description: An internal setting required for global searching.

Default: reg

Options: The name of an application, or list of applications separated by a comma.

Application Name	DB_NAMES value
Sample	sample
Registration Enterprise	chem_reg
Inventory Manager	cheminv
Mixture Registration	
BioSAR Browser	biosar_browser
ChemACX	chemacx
Documentation Manager	

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

GLOBAL\_SEARCH\_BASE\_DB

Example: GLOBAL\_SEARCH\_BASE\_DB = reg

Description: An internal setting required for global searching.

Default: reg

Options: The name of an application.

Application Name	DB_NAMES value
Sample	sample
Registration Enterprise	chem_reg
Inventory Manager	cheminv
Mixture Registration	
BioSAR Browser	biosar_browser
ChemACX	chemacx
Documentation Manager	

---

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---

HIGHLIGHT\_BACKGROUND

Example: HIGHLIGHT\_BACKGROUND = "border= ""1"" bordercolor= ""#cc0033"""

Description: Color used to make the highlighted border for required fields. Only matters if *HIGHLIGHT\_REQUIRED\_FIELDS=1*.

Default: "border=""1"" bordercolor= ""#cc0033"""

Options: Border size and color (in hex format)

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### HIGHLIGHT\_REQUIRED\_FIELDS

Example:

HIGHLIGHT\_REQUIRED\_FIELDS = 1

Description: 1 indicates required fields (listed in another location in the cfserver.ini) should appear with a border around them in edit mode. 0 indicates no border.

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### MAIN\_WINDOW

Example: MAIN\_WINDOW =  
top.frames["main"]

Description: The frame name for the central frame used internally by javascript. Editing this value may cause unpredictable behavior.

Default: top.frames["main"]

Options: **Should not be edited**

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### MARKED\_HITS\_MAX

Example: MARKED\_HITS\_MAX = "500"

Description: Indicates the maximum number of records that are loaded after a search.

Default: 500

Options: Any integer

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### MOLSERVER\_VERSION

Example: MOLSERVER\_VERSION= "7.1"

Description: Indicates the version of MolServer to be used. Most likely will not need to be changed.

Default: 7.1

Options: NONE

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of*



the application. New versions of the ChemOffice Enterprise use default configurations.

---

#### MW\_ROUND\_DIGIT

Example: MW\_ROUND\_DIGIT = 5

Description: This is to set the rounding of the Molecular Weight. If set to 2 (or other numbers), the MW will be rounded to two digits like 123.45.

Default: 5

Options: Any Integer

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### NAV\_BAR\_WINDOW

Example: NAV\_BAR\_WINDOW = top.frames["navbar"]

Description: The frame name for the top most frame used internally by javascript. Editing this value may cause unpredictable behavior.

Default: top.frames["navbar"]

Options: **Should not be edited**

---

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---

#### NAV\_BUTTONS\_GIF\_PATH

Example: NAV\_BUTTONS\_GIF\_PATH = /chem\_reg/graphics/

Description: Default graphics path

Default: /chem\_reg/graphics/

Options: Absolute or relative path to a directory containing images.

---

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---

#### NON\_CHEMICAL\_SUBMIT

Example: NON\_CHEMICAL\_SUBMIT = "DISALLOW"

Description: Indicates if non chemical information can be used in the structure window. DISALLOW does not allow non-chemical information to be used. ALLOW allows non-chemical information to be entered. PROMPT warns the user that non-chemical information has been entered.

---

*NOTE: The following is true if NON\_CHEMICAL\_SUBMIT is set to ALLOW or PROMPT:*

---

- Searching is not allowed by the non-chemical
- Non-chemical data is viewed in the registry only. The non-chemical information is lost if exported to an SD file&

Default: DISALLOW

Options: PROMPT | ALLOW | DISALLOW

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### POST\_MARKED\_HITS\_PAGE

Example: POST\_MARKED\_HITS\_PAGE = /chem\_reg/sendMarkedHitsToChemInv.asp

Description: Path to page used when user clicks on Send Hits button. Used to Send hits from one application to another (e.g. Send hits from Registration to Inventory - see Registration Enterprise Cfserver.ini for more information).

Default: /chem\_reg/sendMarkedHitsToChemInv.asp

Options: Absolute or relative path to asp file.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### POST\_MARKED\_HITS\_TARGET\_MENU\_NAME

Example:

POST\_MARKED\_HITS\_TARGET\_MENU\_NAME = "to Inventory"

- Description: The text for the menu item (Found in the Marked Hits Menu) when Post Marked Hits is enabled (e.g. when

Send Hits to Inventory Manager) is enabled.

Default: "to Inventory"

Options: Any Text.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### POST\_MARKED\_SEND\_TO\_PAGE

Example:

POST\_MARKED\_SEND\_TO\_PAGE = http://SERVERNAME/cheminv/gui/ImportFromChemReg.asp

Description: Path to page used when user is sent. Used to Send hits from one application to another (e.g. Send hits from Registration to Inventory - see Registration Enterprise Cfserver.ini for more information).

Default: NULL

Options: Absolute or relative path to asp file.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### POST\_MARKED\_SUPPORTED\_FORMGROUPS

Example:

POST\_MARKED\_SUPPORTED\_FORMGR

OUPS =

base\_form\_group,approve\_form\_group

Description: List of formgroups supporting this type of hit export. Used to Send hits from one application to another (e.g. Send hits from Registration to Inventory - see Registration Enterprise Cfserver.ini for more information).

Default:

"base\_form\_group,approve\_form\_group"

Options: Comma delimited list of formgroup names

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

PREFS\_FORM\_GROUPS

Example: PREFS\_FORM\_GROUPS =

base\_form\_group,reg\_ctrbt\_commit\_form\_group

Description: Determines what formgroups will allow display of the preferences dialog box.

Default:

base\_form\_group,reg\_ctrbt\_commit\_form\_group,approve\_form\_group,  
review\_register\_form\_group

Options: Comma delimited list of formgroups

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of*

*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

RESIZE\_GIFS

Example: RESIZE\_GIFS = 1

Description: Resizes GIFs to be the size of the CDX if set to 1. Applies no scaling if set to 0. Only relevant if one of the *DISPLAY\_GIFS\_ONLY\_LIST* settings is set to 1.

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

SEARCH\_DEFAULT\_PREFS

Example: SEARCH\_DEFAULT\_PREFS =

S1:true,S2:true,S3:true,S4:true,S5:true,S6:90,S7:true,S8:true,S9:true,S10:true,S11:false,S12:false,S13:false

Description: Indicates the default search preferences. The following maps the search preference name to its ID in this setting:

MATCH\_TET\_STEREO = PrefsS1

MATCH\_TET\_DB = PrefsS2

HIT\_ANY\_CHARGE\_CARBON = PrefsS3

RXN\_HIT\_RXN\_CENTER = PrefsS4

HIT\_ANY\_CHARGE\_HETERO = PrefsS5

SIM\_SEARCH\_THRESHOLD = PrefsS6

FULL\_STRUCTURE\_SIMILARITY =  
PrefsS7

EXTRA\_FRAGS\_OK = PrefsS8

EXTRA\_FRAGS\_OK\_IF\_RXN = PrefsS9  
FRAGS\_CAN\_OVERLAP = PrefsS10  
IDENTITY = PrefsS11  
RELATIVE\_TET\_STEREO = PrefsS12  
ABSOLUTE\_HITS\_REL = PrefsS13

Therefore S1:true means  
MATCH\_TET\_STEREO is true, and etc.

Default:

S1:true,S2:true,S3:true,S4:true,S5:true,S6:90,S7:true,S8:true,S9:true,S10:true,S11:false,S12:false,S13:false

Options: A comma delimited list of preference ID followed by a colon and either true or false.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

TEMP\_DIR\_NAME

Example: TEMP\_DIR\_NAME = CFWTEMP

Description: The name of the virtual directory which stores temporary files. Editing this value may cause unpredictable behavior.

Default: CFWTEMP

Options: This can be changed to whatever you would like the name of the temp directory to be. The path to the directory is found in TEMP\_DIR\_PATH

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of*

*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

TEMP\_DIR\_PATH

Example: TEMP\_DIR\_PATH = C:\Inet-pub\wwwroot\ChemOffice\cfwtemp

Description: The path to the directory where temporary files are stored. If the installation is not made to the C drive, this must be edited.

Default: C:\Inet-pub\wwwroot\ChemOffice\cfwtemp

Options: This can be changed to wherever you would like the temp directory to exist. The name of the directory is found in TEMP\_DIR\_NAME

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

USE\_ANIMATED\_GIF

Example: USE\_ANIMATED\_GIF = 1

Description: Indicates a GIF should be used for the progress icon.

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of*

*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### USE\_SESSION\_RECORD\_COUNTS

Example:

USE\_SESSION\_RECORD\_COUNTS = 0

Description: Set to 1 when an application is using settings (like RLS in Registration Enterprise) where users are returned record counts according to privileges.

Default: 0

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### USER\_INFO\_WINDOW

Example: USER\_INFO\_WINDOW = top.frames["userinfo"]

Description: The frame name for the left most frame used internally by javascript. Editing this value may cause unpredictable behavior.

Default: top.frames["userinfo"]

Options: **Should not be edited**

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of*

*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### USERWINDOWBACKGROUND

Example: USERWINDOWBACKGROUND = "/cfserverasp/source/graphics/Fine\_Speckled.gif"

Description: Determines the background gif to be used in the left most frame of the window.

Default: "/cfserverasp/source/graphics/Fine\_Speckled.gif"

Options: A hexadecimal number representing a color or path to a GIF.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### Duplicate Checking

##### ABSOLUTE\_HITS\_REL

Example: ABSOLUTE\_HITS\_REL = "1"

Description: Internal setting determining if duplicate checking should take.

---

*NOTE: This is not a preferences setting. This ini settings determines how duplicate checking works.*

---

Default: 1

Options: 0 | 1

##### EXTRA\_FRAGS\_OK

Example: EXTRA\_FRAGS\_OK = "0"

Description: Internal setting determining if duplicate checking should take permit extraneous fragments into account.

This is not a preferences setting. This ini settings determines how duplicate checking works.

Default: 0

Options: 0 | 1

EXTRA\_FRAGS\_OK\_IF\_RXN

Example: EXTRA\_FRAGS\_OK\_IF\_RXN = "0"

Description: Internal setting determining if duplicate checking should take permit extraneous fragments into account when analyzing a reaction.

---

*NOTE: This is not a preferences setting. This ini settings determines how duplicate checking works.*

---

Default: 0

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

FRAGS\_CAN\_OVERLAP

Example: FRAGS\_CAN\_OVERLAP = "0"

Description: Internal setting determining if duplicate checking should take overlapping fragments into account.

---

*NOTE: This is not a preferences setting. This ini settings determines how duplicate checking works.*

---

Default: 0

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

HIT\_ANY\_CHARGE\_CARBON

Example: HIT\_ANY\_CHARGE\_CARBON = "1"

---

*NOTE: Description: Internal setting determining if duplicate checking should take charged carbons into account.*

*This is not a preferences setting. This ini settings determines how duplicate checking works.*

---

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of*

*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

HIT\_ANY\_CHARGE\_HETERO

Example: HIT\_ANY\_CHARGE\_HETERO = "1"

Description: Internal setting determining if duplicate checking should take charged atoms into account.

---

*NOTE: This is not a preferences setting. This ini settings determines how duplicate checking works.*

---

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

IDENTITY

Example: IDENTITY = "1"

---

*NOTE: Description: Internal setting determining if duplicate checking should use identity matching.*

*This is not a preferences setting. This ini settings determines how duplicate checking works.*

---

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

MATCH\_DB\_STEREO

Example: MATCH\_DB\_STEREO = "1"

---

*NOTE: Description: Internal setting determining if duplicate checking should take double bonds into account.*

*This is not a preferences setting. This ini settings determines how duplicate checking works.*

---

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

MATCH\_TET\_STEREO

Example: MATCH\_TET\_STEREO = "1"

---

*NOTE: Description: Internal setting determining if duplicate checking should take tetrahedral stereochemistry into account.*

*This is not a preferences setting. This ini settings determines how duplicate checking works.*

---

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

RELATIVE\_TET\_STEREO

Example: RELATIVE\_TET\_STEREO = "1"

---

*NOTE: Description: Internal setting determining if duplicate checking should take. This is not a preferences setting. This ini settings determines how duplicate checking works.*

---

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

RXN\_HIT\_RXN\_CENTER

Example: RXN\_HIT\_RXN\_CENTER = "1"

---

Description: Internal setting determining if duplicate checking should take the reaction center of a reaction into account.

This is not a preferences setting. This ini settings determines how duplicate checking works.

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

TAUTOMER

Example: TAUTOMER = 0

Description: Internal setting determining if duplicate checking should hit tautomers.

---

*NOTE: This is not a preferences setting. This ini settings determines how duplicate checking works.*

---

Default: 0

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---



## CS\_Security

ALLOW\_COOKIE\_LOGIN

Example: ALLOW\_COOKIE\_LOGIN = 1

Description: Internal setting for disabling/enabling the global login feature.

Default: = 1

Options: **Should not be edited.**

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

COOKIE\_EXPIRES\_MINUTES

Example: COOKIE\_EXPIRES\_MINUTES = 25

Description: Internal setting for disabling/enabling the global login feature. Indicates how long a user should stay logged in after a period of inactivity (in minutes).

Default: = 25

Options: Integer in minutes

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations. COOKIE\_EXPIRES\_MINUTES*

---

Example: COOKIE\_EXPIRES\_MINUTES = 25

Description: Internal setting for disabling/enabling the global login feature. Indicates

how long a user should stay logged in after a period of inactivity (in minutes).

Default: = 25

Options: Integer in minutes

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

CS\_SECURITY\_UDL\_PATH

Example: CS\_SECURITY\_UDL\_PATH = "C:\Inetpub\wwwroot\chemoffice\cs\_security\config\cs\_security.udl"

Description: Internal setting for disabling/enabling the global login feature. Value is the path to the cs\_security udl file.

Default: C:\Inetpub\wwwroot\chemoffice\cs\_security\config\cs\_security.udl

Options: Relative or absolute path to the cs\_security.udl file.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

MINIMUM\_REQUIRED\_PRIVILEGE

Example:

MINIMUM\_REQUIRED\_PRIVILEGE = "SEARCH\_REG"

Description: Internal setting for disabling/enabling the global login feature.

Default: SEARCH\_REG

Options: **Should not be edited.**

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### PRIVILEGE\_TABLE\_LIST

Example: PRIVILEGE\_TABLE\_LIST = "CS\_SECURITY\_PRIVILEGES,CHEM\_REG\_PRIVILEGES"

Description: Internal setting for disabling/enabling the global login feature.

Default:

CS\_SECURITY\_PRIVILEGES,CHEM\_REG\_PRIVILEGES

Options: **Should not be edited.**

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### STARTUP\_LOCATION

Example: STARTUP\_LOCATION = "/chem\_reg/reg/mainpage.asp?dbname=reg&form-group=base\_form\_group&timer="

Description: Internal setting for disabling/enabling the global login feature.

Default: ="/chem\_reg/reg/mainpage.asp?dbname=reg&form-group=base\_form\_group&timer="

Options: **Should not be edited.**

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### USE\_CS\_SECURITY\_APP

Example: USE\_CS\_SECURITY\_APP = 1

Description: Internal setting for disabling/enabling the global login feature.

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

### Registration

#### ADD\_BATCH\_FROM\_REG\_RESULTS

Example:

ADD\_BATCH\_FROM\_REG\_RESULTS = 1

Description: When set to 1, allows a user to add a batch to a compound directly from the record. An Add Batch button appears in the record.

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

ADD\_IDENTIFIERS\_COMMIT\_TABLE\_ORDER

Example:

ADD\_IDENTIFIERS\_COMMIT\_TABLE\_ORDER = Alt\_ids

Description: This is the sequence of INSERTS the Registration Enterprise makes when committing IDENTIFIERS to its permanent table space. Changing these values will result in unpredictable behavior.

Default: Alt\_ids

Options: **Should not be edited.**

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

ADD\_SALT\_COMMIT\_TABLE\_ORDER

Example:

ADD\_SALT\_COMMIT\_TABLE\_ORDER = Compound\_Salt,Batches,Alt\_ids

Description: This is the sequence of INSERTS the Registration Enterprise makes when committing SALTS to its permanent table space.

Changing these values will result in unpredictable behavior.

Default: Compound\_Salt,Batches,Alt\_ids

Options: **Should not be edited.**

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

ALLOW\_BATCH\_FOR\_UNAPPROVED\_CMPD

Example:

ALLOW\_BATCH\_FOR\_UNAPPROVED\_CMPD = 1

Description: If it is set to 1, compounds will need to be approved before adding a second batch.

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

ANALYTICS\_USED

Example: ANALYTICS\_USED = 1

Description: Set to True (1), the Analytics tools are used by the system and appear in the user interface.

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### APPROVED\_FLAG\_USED

Example: APPROVED\_FLAG\_USED = 1

Description: This is for post registration approval. Set to True(1), displays a Approved button in the main page and also allows for approval in details view for a registered compound QUALITY\_CHECKED\_FLAG\_USED = 0

Set to 1 to turn on quality checked parameter. The approval flag is used for the workflow of approve a compound/batch. Basically before or after a compound is registered, admin (or whoever) can choose to have the option of approve and disapprove the compound. From GUI side, there will be check box to approve/disapprove on the edit/register form, then it will show a thumb up/down on the result list/form.

Default: 0

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### APPROVED\_SCOPE

Example: APPROVED\_SCOPE = COMPOUND

Description: Set to COMPOUND means that only the compound needs approval.

Set to BATCH means that each batch needs to be approved - not recommended

Set to BATCH means that only the batch needs quality check after approval to close the record. - not recommended.

Default: COMPOUND

Options: COMPOUND | BATCH

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### AUTOGENERATED\_CHEMICAL\_NAME

Example:

AUTOGENERATED\_CHEMICAL\_NAME = 0

Description: Indicates if the application should automatically generate a name for the compound according to the structure entered.

Default: 0

Options: 0 | 1

---

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---

## BATCH\_LEVEL

Example: BATCH\_LEVEL = COMPOUND

Description: Determines whether salts and solvents will exhibit properties of a batches record or will these be interpreted as parent compounds of a record. This field also determines if duplicate checking should take salt definitions into account. When the value of BATCH\_LEVEL is set to SALT, Registration Enterprise exhibits the following behavior when a user tries to register a new compound as a salt:

- If the salt is already present in the database, the duplicate page of that particular salt opens up and provides the option for adding a new batch.
- If the salt is not present in the database, the duplicate page of the parent compound opens up and provides the option for adding a new salt.

Default: COMPOUND

Options: COMPOUND | SALT

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

## BATCH\_NUMBER\_LENGTH\_GUI

Example:

BATCH\_NUMBER\_LENGTH\_GUI = 2

Description: Displays number with preceding zero, e.g. 01.

Default: 1

Options: Any integer

---

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---

## BATCH\_PROJECTS\_USED

Example: BATCH\_PROJECTS\_USED = 1

Description: Set to True(1), displays a Projects dropdown at the batch level. Adds a Projects button to the manage reg tables interface.

Default: 0

Options: 0 | 1

---

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---

## BATCHES\_TO\_TEMP

Example: BATCHES\_TO\_TEMP = 1

Description: If set to, 0 batches are added directly to permanent table.

Default: 1

Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of*

*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### BUILD\_SITE\_ID

Example: BUILD\_SITE\_ID = NULL

Description:

Default: NULL

Options:

---

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---

#### COMPOUND\_TYPES\_USED

Example: COMPOUND\_TYPES\_USED = 1

Description: Set to True (1), compound types are used by the system and displayed as Structure Comments in the user interface. Set to False(0), Compound Type (structure comment) lists are not displayed in the user interface, and all compound\_type entries are set to 1 (unspecified). If turned to False the item COMPOUND\_TYPE should be added to the GUI\_FIELDS\_TO\_HIDE section of this ini file so this field doesn't appear in chemloader.

Default: 1

Options: 0 | 1

---

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---

*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### DBA\_PWD

Example: DBA\_PWD = MANAGER

Description: The password that can be used for accessing limited dba functions for users with permissions allowing adding users/roles.

Default: MANAGER

Options: A DBA password with correct permissions.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### DBA\_USERNAME

Example: DBA\_USERNAME = SYSTEM

Description: The username that can be used for accessing limited dba functions for users with permissions allowing adding users/roles.

Default: SYSTEM

Options: A DBA username with correct permissions.

---

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---

#### DEFAULT\_PREFIX

Example: DEFAULT\_PREFIX = AB

Description: Determines which prefix is the default in the prefix dropdown list.

Default: = AB

Options: One of the prefixes in the prefix table in Registration.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### DELETE\_BATCH\_TABLE\_ORDER

Example:

DELETE\_BATCH\_TABLE\_ORDER =  
Batches,Reg\_Approved,Reg\_Quality\_Checked

Description: This is the sequence of DELETES the Registration System makes when deleting BATCHES from its permanent table space. Changing these values will result in unpredictable behavior.

Default:

Batches,Reg\_Approved,Reg\_Quality\_Checked

Options: **Should not be edited.**

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### DELETE\_COMPOUND\_TABLE\_ORDER

Example:

DELETE\_COMPOUND\_TABLE\_ORDER =  
ALT\_IDS,Batches,Reg\_Numbers,Compound\_Salt,Reg\_Approved,

Reg\_Quality\_Checked,Structures,Compound\_Project,Compound\_molecule

Description: This is the sequence of DELETES the Registration Enterprise makes when deleting compounds from its permanent table space. Changing these values will result in unpredictable behavior.

Default:

Cmpd\_Mol\_Utilizations,ALT\_IDS,Batches,Reg\_Numbers,Compound\_Salt,Reg\_Approved,Reg\_Quality\_Checked,Structures,Compound\_Project,Compound\_molecule,Duplicates

Options: **Should not be edited.**

---

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---

#### DELETE\_SALT\_TABLE\_ORDER

Example: DELETE\_SALT\_TABLE\_ORDER =

ALT\_IDS,Batches,Reg\_Numbers,Compound\_Salt,Reg\_Approved,Reg\_Quality\_Checked

Description: This is the sequence of DELETES the Registration Enterprise makes when deleting SALTS from its permanent table space. Changing these values will result in unpredictable behavior.

Default:

ALT\_IDS,Batches,Reg\_Numbers,Compound\_Salt,Reg\_Approved,Reg\_Quality\_Checked

Options: **Should not be edited.**

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### DERIVED\_FIELDS

Example: DERIVED\_FIELDS = FORMULA,MW,FORMULA2,MW2,ENTRY\_PERSON,ENTRY\_DATE,FORMULA\_WEIGHT,PERCENT\_ACTIVE,CHIRAL,CLOGP,H\_BOND\_ACCEPTORS,H\_BOND\_DONORS

Description: Determines which fields in the add\_compound and add\_batch form should be hidden from user input because it is populated by the business tier.

Default: FORMULA,MW,FORMULA2,MW2,ENTRY\_PERSON,ENTRY\_DATE,FORMULA\_WEIGHT,PERCENT\_ACTIVE,CHIRAL,CLOGP,H\_BOND\_ACCEPTORS,H\_BOND\_DONORS,CHEM\_NAME\_AUTOG

Options: Comma delimited list of fields

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of*

*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### DISPLAY\_APPKEY

Example: DISPLAY\_APPKEY = Chem Reg

Description: The name of the application which is displayed in the login screen in certain customized sites.

Default: Chem Reg

Options: Any Text

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### FORMULA\_WT\_CALC

Example: FORMULA\_WT\_CALC = SALTS\_AND\_SOLVATES

Description: Determines which values to use in calculating the formula weights.

Default: SALTS\_AND\_SOLVATES

Options: SALTS\_AND\_SOLVATES | SALTS | SOLVATES

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### FULL\_COMMIT\_TABLE\_ORDER



Example: FULL\_COMMIT\_TABLE\_ORDER =

Compound\_Molecule,Reg\_Numbers,Compound\_Salt, Structures,Batches,Alt\_ids,Compound\_Project

Description: This is the sequence of INSERTS the Registration Enterprise makes when committing data to its permanent table space. Changing these values will result in unpredictable behavior.

Default: Compound\_Molecule, Compound\_Project, Reg\_Numbers,Compound\_Salt,Structures,Batches,Alt\_ids, Cmpd\_Mol\_Utilizations  
Options: Should not be edited.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

GET\_MW\_FORMULA\_METHOD

Example: GET\_MW\_FORMULA\_METHOD = PLSQL

Description: Indicates how the molecular weight and molecular formula are searched. The options are as follows:

- PLSQL - retrieves mw and formula using the fastindexaccess procedure
- STANDARD - uses the Oracle Cartridge functions
- JOIN - uses a direct join to the cartridge tables. This option requires a dba grant select on these tables either to public or to individual roles. The tables are in the following format:

- *Molweight:* <SchemaName>\_<index\_name>\_W  
For example - Regdb\_mx\_W in the Molecular Weight table for the regdb schema where the index table is mx.
- *Molecular Formula:* <SchemaName>\_<index\_name>\_A  
For example - Regdb\_mx\_A in the Molecular Formula table for the regdb schema where the index table is mx.
- CDCONTROL - the mw is calculated by the ChemDraw ActiveX control at the point the structure is submitted.

The CDONTROL is not superior to PLSQL as either options have minimum impact on the speed and the performance.

The PLSQL option requires no additional changes to the database and will improve searching speed (over the STANDARD option with CS Oracle Cartridge version 2.1) by an average of 5 times.

Default: PLSQL

Options: PLSQL | STANDARD | JOIN

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

GUI\_FIELDS\_TO\_HIDE

Example: GUI\_FIELDS\_TO\_HIDE = SPECTRUM\_ID,CHIRAL,CLOGP,H\_BOND\_DONORS,H\_BOND\_ACCEPTORS, Collaborator\_ID,FEMA\_GRAS\_NUMBER,R NO\_NUMBER,GROUP\_CODE,ADD\_LINES

Description: The GUI\_FIELDS\_TO\_HIDE entries list all of the fields to hide in the user interface and chemloader. All of the GUI\_FIELDS\_TO\_HIDE entries are interpreted the same so fields can be added or removed from any of the lists and the result will be the same. The fields listed must be the exact field name or the field will not be hidden.  
Default: N/A  
Options: Comma delimited list of field names.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### IDENTIFIERS\_TO\_TEMP

Example: IDENTIFIERS\_TO\_TEMP = 0  
Description: If set to False (0), new identifiers are automatically added to the permanent, Identifiers table. If set to True (1), new Identifiers must be individually reviewed and registered.  
Default: 0  
Options: 0 | 1

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### NEW\_BATCH\_COMMIT\_TABLE\_ORDER

Example:  
NEW\_BATCH\_COMMIT\_TABLE\_ORDER = Batches  
Description: This is the sequence of INSERTS the Registration System makes when committing BATCHES to its permanent table space. Changing these values will result in unpredictable behavior.  
Default: Batches,Alt\_IDs  
Options: **Should not be edited.**

---

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---

#### NO\_STRUCTURE\_TEXT

Example: NO\_STRUCTURE\_TEXT = no\_structure  
Description: This is the text in the Structure Comments table that indicates no structure is to be submitted. This value, when chosen from the add\_compound screen, will allow overriding of the structure requirement.  
Default: no\_structure  
Options: Any text

---

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---

#### NOTEBOOK\_LOOKUP

Example:

USE\_BATCH\_SCIENTIST\_AS\_REGISTRAR = 0

Description: Set to 1 (true) makes the Notebook drop-down menu visible. Set to 0 (false), and the NOTEBOOK field becomes free text.

Default: = 0

Options: 0 | 1

---

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---

#### NOTEBOOK\_USED

Example: NOTEBOOK\_USED = 1

Description: If set to '1', notebooks are used by the system and displayed in the user interface. If set to False(0), notebook lists are not displayed in the user interface, and all notebook entries are set to 1 (unspecified).

Default: 1

Options: 0 | 1

---

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---

#### ORA\_SERVICENAME

Example: ORA\_SERVICENAME = SERVER1

Description: The oracle net 8 service name where the regdb schema resides.

Default: YOUR ORACLE SERVICE NAME

Options: The name of the Oracle service.

---

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---

#### ORA\_SQLLDRPATH

Example: ORA\_SQLLDRPATH = sqlldr.exe

Description: The path to the oracle sqlldr executable. This may need to be set to a full path name.

Default: sqlldr.exe

Options: Relative or absolute path to the sqlldr executable.

---

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---

#### OUTPUT\_AS\_GIF\_ON\_REG

Example: OUTPUT\_AS\_GIF\_ON\_REG = 1

Description: If set to True (1), the Registration Enterprise will output a GIF and a CDX file for the compound when it is registered.

Default: 0

Options: 0 | 1

---

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---

#### PRE\_REGISTER\_APPROVED\_FLAG

Example:

PRE\_REGISTER\_APPROVED\_FLAG = 0

Description: This is for pre-registration approval. Set to 1, the compounds in temp table needs to be pre-approved before registered to permanent table, an Approve button will be shown in the detail view and thumb-up and thumb-down images show the status of the approval.

The approval flag is used for the workflow of approve a compound/batch. Basically before or after a compound is registered, admin (or whoever) can choose to have the option of approve and disapprove the compound. From GUI side, there will be check box to approve/disapprove on the edit/register form, then it will show a thumb up/down on the result list/form.

Default: 0

Options: 0 | 1

---

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---

#### PREFIX\_DELIMITER

Example: PREFIX\_DELIMITER = -

Description: This is the DELIMITER between the Registry Number and the SALT name when Batch\_Level = Salts. For instance: R-1111/Br where 'R' is the Prefix, 1111 is the Registry Number, and Br is the Salt name.

Default: = -

Options: Any character

---

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---

#### PRIMARY\_STRWHERE

Example: PRIMARY\_STRWHERE = COMPOUND\_ONLY

Description: This is primarily a setting to enable Row Level Security (RLS). The default is COMPOUND\_ONLY. This should be changed to COMPOUND\_PROJECT for RLS.

Default: COMPOUND\_ONLY

Options: COMPOUND\_ONLY | COMPOUND\_PROJECT

---

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---

#### PRIV\_TABLE\_NAME

Example: PRIV\_TABLE\_NAME =  
Chem\_Reg\_Privileges

Description: The table name in the cs\_security schema that stores the flags for the privileges that toggle buttons in the user interface.

Default: Chem\_Reg\_Privileges

Options: Table name

---

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---

#### PRODUCER\_ID\_FIELD

Example: PRODUCER\_ID\_FIELD = NULL

Description: A producer is basically a chemist whoever produced the compound. If the PRODUCER\_LOOKUP is set to 1, this field needs to be set to one of the custom fields that is numeric, storing producer ID. The PRODUCER\_ID\_FIELD is one of the customizable number field in BATCHES table, for example INT\_BATCH\_FIELD\_1, then GUI will have an extra field "producer" and do the look up from PEOPLE table for you.

Default: NULL

Options: NULL or the name of one of the custom registration fields.

---

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*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### PRODUCER\_LOOKUP

Example: PRODUCER\_LOOKUP = 0

Description: A producer is basically a chemist whoever produced the compound. To use this settings, turn PRODUCER\_LOOKUP = 1. This setting indicates if Producers should be assigned to compounds as well as scientists.

Default: 0

Options: 0 | 1

---

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---

#### PROJECT\_LEVEL\_ROW\_SECURITY

Example:

PROJECT\_LEVEL\_ROW\_SECURITY = 0

Description: This is primarily a setting to enable Row Level Security (RLS). This should be changed to 1 for RLS.

Default: = 0

Options: 0 | 1

---

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*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### PROJECTS\_NAMED\_OWNER

Example: PROJECTS\_NAMED\_OWNER = 1

Description: Set to True(1), displays "OWNER" rather than "PROJECT" in all places within the user interface. Adds a OWNERS button to the manage reg tables interface in place of the PROJECTS button. This should be set this way if BATCH\_PROJECTS is set tot 1 so there is a clear distinction between the two types projects.

Default: = 0

Options: 0 | 1

---

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---

#### PROJECTS\_USED

Example: PROJECTS\_USED = 1

Description: If set to True (1), Projects are used by the system and displayed in the user interface.

Projects lists are not displayed in the user interface, and all project entries are set to 1 (unspecified)

PROJECTS\_NAMED\_OWNER=0.

Default: 1

Options: 0 | 1

---

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---

#### ROOT\_NUMBER\_LENGTH

Example: ROOT\_NUMBER\_LENGTH = 6

Description: This is the total length of the Registry Number. The Registration Enterprise will 0-pad Registry Numbers to the total length, so all Registry Numbers have the same length. For instance, set to 6, the Registry Number '1111', becomes '001111'.

Default: = 6

Options: Any integer

---

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---

#### REAGENT\_BYPASS\_DUPLICATES

Example:

REAGENT\_BYPASS\_DUPLICATES = 0

Description: When set to 1 this allows use of the reagent input form to add data directly to the registry adding new compounds as duplicates are found.

Default: 0

Options: 0 | 1

---

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---

#### REAGENT\_SEQUENCE

Example: REAGENT\_SEQUENCE = AB

Description: If REAGENTS\_USED = 1 then setting the REAGENT\_SEQUENCE to a valid prefix sets the sequence used for commuting reagents.

Default: AB

Options: Any number of characters.

---

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---

#### REAGENTS\_TO\_TEMP

Example: REAGENTS\_TO\_TEMP = 1

Description: If set to, 0 reagents are added directly to permanent table.

Default: 1

Options: 0 | 1

---

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*Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### REAGENTS\_USED

Example: REAGENTS\_USED = 0

Description: Set to True (1), a reagents button appears on the Main page which takes you to a simpler add compound input form which only has date entry fields for fields relevant to the compound.

Default: 0

Options: 0 | 1

---

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---

#### REG\_DELIMITER

Example: REG\_DELIMITER = /

Description: This is the DELIMITER between the Registry Number and the SALT name when Batch\_Level = Salts. For instance: R-1111/Br where 'R' is the Prefix, 1111 is the Registry Number, and Br is the Salt name.

Default: = /

Options: Any character

---

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the application. New versions of the ChemOffice Enterprise use default configurations.

---

#### REG\_PWD

Example: REG\_PWD = ORACLE

Description: The regdb schema password.

Default: ORACLE

Options: The Registration schema password.

---

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---

#### REG\_USERNAME

Example: REG\_USERNAME = REGDB

Description: The regdb schema owner.

Default: REGDB

Options: The Registration schema username.

---

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---

#### SALT\_EDITABLE\_FOR\_REG\_SALTS

Example:

SALT\_EDITABLE\_FOR\_REG\_SALTS = 0

Description: Set to True (1) allows editing of batch level salt\_name, MW. When set to (0),

the salt name and molecular weight are populated based on the salt choose for the compound. Only relevant if BATCH\_LEVEL = SALT.

Default: 0

Options: 0 | 1

---

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---

#### SALTS\_USED

Example: SALTS\_USED = 1

Description: If set to True (1), salts are used by the system and displayed in the user interface. If set to False(0), salt list are not displayed in the user interface, and all salt entries are set to 1 (no\_salt).

Default: 1

Options: 0 | 1

---

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---

#### SEC\_PWD

Example: SEC\_PWD = ORACLE

Description: The CS\_Security schema password.

Default: ORACLE



Options: A password for the CS\_Security schema.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### SEC\_USERNAME

Example: SEC\_USERNAME =  
CS\_SECURITY

Description: The CS\_Security schema owner.

Default: CS\_SECURITY

Options: A username for the CS\_Security schema.

---

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---

#### SHOW\_NOTEBOOK\_USER

Example: SHOW\_NOTEBOOK\_USER = 0

Description: Set to 1 (true), the Notebook dropdown shows the name of the user in the notebook item. This is only for Notebooks where (Active= 1). Set to 0 (false), the Notebook dropdown shows all Active Notebooks with only the notebook name in the item. This option is only relevant if NOTEBOOK\_LOOKUP is True (1).

Default: = 0

Options: 0 | 1

---

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---

#### SHOW\_MF\_WITH\_SALT\_NAME

Example: SHOW\_MF\_WITH\_SALT\_NAME = 0

Description: When set to 1, salt listboxes display both the salt name and molecular formula.

Default: 0

Options: 0 | 1

---

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---

#### SHOW\_SAR\_TABLE

Example: SHOW\_SAR\_TABLE = 1

Description: Set to True (1), the SAR Table connection with BioAssay HTS is active and a SAR Table button appears when you retrieve results on permanent table searches.

Default: 0

Options: 0 | 1

---

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*Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### SHOW\_SEC\_TBLES\_IN\_USR\_MGR

Example:

SHOW\_SEC\_TBLES\_IN\_USR\_MGR = 0

Description: If set to False (0), the peoples table is accessible through the Manage Users button. If set to True(1), makes the peoples table accessible though the Manage Registry Tables button.

- Default: 0

Options: 0 | 1

---

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---

#### SHOW\_USER\_NOTEBOOKS\_ONLY

Example:

SHOW\_USER\_NOTEBOOKS\_ONLY = 0

Description: Set to 1 (true), the Notebook dropdown shows only those notebooks for the particular user which are Active (Active= 1). Set to 0 (false), the Notebook dropdown shows all Active Notebooks.

This option is only relevant if NOTEBOOK\_LOOKUP is True (=1).

Default: = 0

Options: 0 | 1

---

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---

#### SITES\_USED

Example: SITES\_USED = 0

Description: If set to 1, the sites button is displayed so that the sites table in cs\_securiy can be populated. A button appears when you choose manage registry tables.

Default: 0

Options: 0 | 1

---

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---

#### SOLVATES\_USED

Example: SOLVATES\_USED = 1

Description: Set to True(1), displays a SOLVATES drop down in the user interface and adds a Solvates button to the manage reg tables interface.

Default: 1

Options: 0 | 1

---

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---

#### START\_BATCH\_NUMBER

Example: START\_BATCH\_NUMBER = 1

Description: The initial Batch Number. Typically set to either '1' or '0'. The first Batch for each Registered Compound is assigned this number.

Default: = 1

Options: Any integer

---

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---

#### STRUCTURE\_COMMENTS\_TEXT

Example:

STRUCTURE\_COMMENTS\_TEXT = 0

Description: Set to True(1) shows a text field for entering

Compound\_Molecule.Structure\_Comments\_txt data. If turned to true the item

STRUCTURE\_COMMENTS\_TXT should be removed from the GUI\_FIELDS\_TO\_HIDE section of this ini file so this field appears in chemloader.

Default: 0

Options: 0 | 1

---

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---

#### TABLES\_WITH\_BASE64\_CDX

Example: TABLES\_WITH\_BASE64\_CDX = STRUCTURES,TEMPORARY\_STRUCTURES

Description: This setting tells the registration enterprise what tables Base64\_CDX fields that must be updated when a structure is edited. Editing this value will result in unpredictable behavior.

Default: STRUCTURES,TEMPORARY\_STRUCTURES

Options: **Should not be edited.**

---

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---

#### TABLES\_WITH\_MOLIDS

Example: TABLES\_WITH\_MOLIDS =

REG\_NUMBERS,BATCHES,STRUCTURES,COMPOUND\_MOLECULE,COMPOUND\_SALT

Description: This setting tells the registration Enterprise what tables contain mol\_ids that must be updated when a compound record, previously in a no structure state, is updated with a structure. Editing this value will result in unpredictable behavior.

Default:

REG\_NUMBERS,BATCHES,STRUCTURES,COMPOUND\_MOLECULE,COMPOUND\_SALT

Options: **Should not be edited.**

---

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---

TEMP\_TABLE\_QUERY\_FORM

Example: TEMP\_TABLE\_QUERY\_FORM = SUMMARY

Description: Indicates the types of searchable fields in the temporary search form. There are two kinds of searchable fields in temporary search form. SUMMARY only displays the most common fields on the temporary search form, DETAIL displays all the searchable fields on the temporary search form.

Default: SUMMARY

Options: SUMMARY | DETAIL

---

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*the application. New versions of the ChemOffice Enterprise use default configurations.*

---

USE\_BATCH\_SCIENTIST\_AS\_REGISTRAR

Example:

USE\_BATCH\_SCIENTIST\_AS\_REGISTRAR = 0

Description: By default (0) when a compound is registered through Chemloader, the person logged in is set as the registrar of the batch and the compound. However there may be cases where data is entered by a user that has nothing to do with the registration and the chemist associated with the batch would be the registrar. In this case, this should be set to 1.

Default: = 0

Options: 0 | 1

---

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---

USE\_GUI\_DEFAULTS\_IN\_API

Example: USE\_GUI\_DEFAULTS\_IN\_API = 0

Description: Set to True (1), takes the defaults from the cfserver.ini and applies them when posting from ChemLoader or other apps using the Registration Enterprise API.

Default: 0

Options: 0 | 1

---

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---

#### USER\_LOOKUP

Example: USER\_LOOKUP = 0

Description: Indicates if the user lookup feature should be used. The user lookup feature will provide a drop-down with user codes (from the peoples table). Choosing one will then populate the chemist field with the actual person.

Default: 0

Options: 0 | 1

---

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---

#### UTILIZATION\_PERMISSIONS\_USED

Example:

UTILIZATION\_PERMISSIONS\_USED = 0

Description: When set to 0 the Utilizations button appears. If set to 1 Utilizations button appears in the manage registry tables form. Utilizations are yes/no questions tied to the batches table. All Utilizations must be defined by the site because this is not a default feature.

Default: 0

Options: 0 | 1

---

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---

#### WORKGROUPS\_USED

Example: WORKGROUPS\_USED = 1

Description: Set to True (1), WORKGROUPS are used by the system and a workgroups button appears on the main form. Workgroups are managed by setting the supervisor id of individual users to their supervisor's person id. The workgroup settings impact what records can be edited by the logged in user.

Default: 1

Options: 0 | 1

---

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---

#### DISPLAY\_TYPES

Example: DISPLAY\_TYPES1 =  
AMOUNT;TEXT:5

Description: The DISPLAY\_TYPES entries define the appearance of and validate option for fields. For example, in the example above, the field AMOUNT will appear to users in an

input form as a text box and before being submitted will be verified to be a positive float. We do not recommend changing the field-names or adding/removing any of the items in the list. If you see NOT CONFIGURABLE next to the field this means it is not configurable.

The general format is - **FieldName;Input Field:Option[; Display Field : Option]**

**Display Field:Option** is optional. It is used only when the display field has some sort of formatting consideration. It is really used when the display type is different from Input Field Type. If not specified, same Field Type will be used for display. For example, CHECKBOX:GIF, FORMULA:24, HYPERLINK:FULL, HYPERLINK:FILE and HYPERLINK:LINK are the only valid options.

---

*NOTE: Input Field covers search mode, add record and edit mode. Validation will occur in all modes.*

---

Compatible Input Field Types:

- Text
- Checkbox
- TextArea
- Picklist
- Hyperlink

Compatible Display Field Types:

- If not specified, same as Input Field Type. This is default.
- Checkbox
- Hyperlink
- Formula - formats formula using superscripts and subscripts as long as

FORMAT\_FORMULA=1 in cfserver.ini file.

Display Field is really used when the display type changes. For example, CHECKBOX:GIF and HYPERLINK:FULL or HYPERLINK:FILE or HYPERLINK:LINK

For all Field Types, the options for validation are:

Validate Option	Interpretation
1	Valid Integer
2	Float
3	Positive Integer
5	Positive Float
8	Data mm/dd/yyyy
21	CAS Number
22	not empty
24	Formula

When Input Field Type is Checkbox, same validation options are available. When Display Field Type is Checkbox, the options are:

CheckBox Option	Interpretation
0	Shows raw value

GIF Shows a gif with an X for values of "" or 0 and a check for values of "1"

FILE Displays path of the system's file.

When Input or Display Field Type is Hyperlink, the options are:

---

*NOTE: Supports to access local system files. Also supports to access LAN connected system's file.*

---

Hyperlink Option	Interpretation
FULL	Displays full value in field as link text. Add http:// if missing
	<hr/> <i>NOTE: Supports to access absolute and relative path of web address.</i> <hr/>
LINK	Displays the work link as the link text. Adds http:// if missing
	<hr/> <i>NOTE: Supports to access absolute and relative path of web address.</i> <hr/>

Alternatively the format of HYPER-LINK:Link\_Type[Link\_Name] can also be used:

- Link\_Type is the type of the link (e.g. http, mailto, file, https, ftp)
- Link\_Name is optional. It is the name that should be displayed for the link. If not specified, the full link is displayed.

The following shortcuts can also be used instead of the Link\_Type|Link\_Name format: When Input Field Type is Text or Picklist, a default value can be added. To indicate a default value, add a "!" after **Input-Type:Option**. This will input that value when in add mode or set the Picklist to that value. Valid for Text and Picklist only.

When Input Field Type is Picklist, picklist items must be separated by pipes (i.e. "|"). Default values are added after the last item in the pick list. It is also an option to add **:VALID-DATE:myScript(this)** where myScript(this) is a valid script in app\_js.js to add script validation for add mode.

Default: N/A

Options: FieldName ; Input Field : Option [;  
Display Field : Option]

---

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---

## FIELD\_LABELS

Example: FIELD\_LABELS1 =  
AMOUNT:Submitted Amount

Description: The FIELD\_LABELS entries list actual field names coupled with the name that should be used in the user interface. For example, in the example above, the field name in the database is AMOUNT, but the user will see the field labeled Submitted Amount.

The syntax for these entries is: EXACT FIELD NAME:FIELD LABEL DISPLAY

It is important not to edit the FIELD NAME, only the FIELD LABEL.

Default: N/A

Options: EXACT FIELD NAME:FIELD LABEL DISPLAY

---

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---

## GUI\_FIELDS\_TO\_HIDE

Example: GUI\_FIELDS\_TO\_HIDE =  
SPECTRUM\_ID,CHIRAL,CLOGP,H\_BOND  
\_DONORS,H\_BOND\_ACCEPTORS,  
Collaborator\_ID,FEMA\_GRAS\_NUMBER,R  
NO\_NUMBER,GROUP\_CODE,ADD\_LINES

Description: The GUI\_FIELDS\_TO\_HIDE entries list all of the fields to hide in the user interface and chemloader. All of the GUI\_FIELDS\_TO\_HIDE entries are interpreted the same so fields can be added or removed from any of the lists and the result will be the same. The fields listed must be the exact field name or the field will not be hidden.

Default: N/A

Options: Comma delimited list of field names.

---

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## Reg.ini Configuration File

The Reg.ini file, found in the following location: <webroot>/ChemOffice/chem\_reg/config defines many parameters that allow the Registration Enterprise application to function properly, including the definitions of formgroups (which define all forms) in the application. Most of this file should not be edited since editing this file in the wrong place could cause



major problems when running the Reg System application.

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*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

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#### [GLOBALS] Table Group Definitions

ABOUT\_WINDOW

[BASE\_TABLE\_GROUP]

ADO\_CONNECTION\_NAMES

[REG\_COMMIT\_TABLE\_GROUP]

CHEM\_CONNECTION\_NAMES

[TEMP\_TABLE\_GROUP]

DB\_RECORD\_COUNT

DB\_TYPE ChemFinder Connection Definitions

DISPLAY\_NAME

[REG\_STRUC\_CFW\_FORM]

FIELD\_MAP\_GROUPS

[REGREG\_CFW\_FORM]

FORM\_GROUPS [REG\_CFW\_FORM]

INI\_VERSION [REGTEMP\_CFW\_FORM]

MAIN\_PAGE

MAXHITS

REG\_VERSION

SUBFORM\_VIEW\_NAMES

TABLE\_ALIASES

TABLE\_GROUPS

ADO Connection Definitions

[ BASE\_CONNECTION ]

CONN\_TYPE

CONNECTION\_PASSWORD

CONNECTION\_STRING

CONNECTION\_TIMEOUT

CONNECTION\_USERNAME

COMMAND\_TIMEOUT

DBMS

PWD\_KEYWORD

USERID\_KEYWORD

Form Group definitions are also found in the Reg.ini file, in additions to the settings above. For an example of changing settings in this file to change which fields are required in a form, please see Changing Required Fields.

#### CHANGING REQUIRED FIELDS

Required fields appear in forms with a red box around them. It is necessary to enter something into required fields before the record can be submitted. Which fields are required can be changed. Doing this in the Registration Enterprise input forms is often a request of frequent users.

Which fields will be required is controlled in the Reg.ini file. In each Formgroup definition, there is a key called **REQUIRED\_FIELDS**. All fields in that formgroup which are required are included in a comma delimited list in the **REQUIRED\_FIELDS** key. If the fieldname is in this list, the field will be required.

#### EXAMPLE

For example, the following is a copy of the required\_fields entry in the REG\_CTRBT\_FORM\_GROUP:

```
REQUIRED_FIELDS=Temporary_Structures.Structure:Structure,
Temporary_Structures.Salt_Equivalents;2:Salt_Equivalents,Temporary_Structures.Solvate_Equivalents;2:Solvate_Equivalents,Temporary_Structures.Compound_Type;1:Structure Com-
```

```
ment,Temporary_Structures.Sequence_ID;1:Prefix,
Temporary_Structures.Notebook_Number;1:Notebook,
Temporary_Structures.Notebook_Page;0:Page,Temporary_Structures.Project_ID;1:Project,
Temporary_Structures.Salt_Code;1:Salt
Name,TEMPORARY_STRUCTURES.SOLVATE_NAME;0:Solvate
Name,TEMPORARY_STRUCTURES.SALT_MW;2:Salt
MW,TEMPORARY_STRUCTURES.SOLVATE_MW;2:Solvate MW
```

Each field is separated by a comma. So, the notebook page (by default a required field) is noted by  
Temporary\_Structures.Notebook\_Page;0:Page  
The syntax of each entry is the same. That is:  
**<TableName>.<FieldName>;<DataType>;<Displayed Name>**  
so in the notebook page example, the following values hold true:

Syntax Variable	Value
<TableName>	Temporary_Structures
<FieldName>	Notebook_Page
<DataType>	0 (an integer, see DataTypes)
<Displayed Name>	Page

where DataType is one of the Validate Options (also found in the cfserver.ini file)

and Displayed Name is how the name of the field should be displayed to the user.

**MAKING A REQUIRED FIELD NO LONGER REQUIRED**

To no longer require the Notebook page in the REG\_CTRBT\_FORM\_GROUP, simply remove its entry in the REQUIRED\_FIELDS list. In this case, the entry would now look like this:

REQUIRED\_FIELDS=Temporary\_Structures.Structure:Structure,Temporary\_Structures.Salt\_Equivalents;2:Salt Equivalents,Temporary\_Structures.Solvate\_Equivalents;2:Solvate Equivalents,Temporary\_Structures.Compound\_Type;1:Structure Compound,Temporary\_Structures.Sequence\_ID;1:Prefix,Temporary\_Structures.Notebook\_Number;1:Notebook,Temporary\_Structures.Project\_ID;1:Project,Temporary\_Structures.Salt\_Code;1:Salt Name,TEMPORARY\_STRUCTURES.SOLVATE\_NAME;0:Solvate Name,TEMPORARY\_STRUCTURES.SALT\_MW;2:Salt MW,TEMPORARY\_STRUCTURES.SOLVATE\_MW;2:Solvate MW

**ADDING A FIELD TO THE REQUIRED FIELD LIST**

The only information necessary to add a field to the required field list is the table the field is found in, the name of the field, and the field's datatype.

For example, to make the CAS number a required field, we need to know the following values:

Syntax Variable	Value
-----------------	-------

<TableName>	Temporary_Structures
<FieldName>	CAS_Number
<DataType>	0
<Displayed Name>	CAS Number

To make this field required, add the following to the end of the required fields entry:

,Temporary\_Structures.CAS\_Number;0

### Globals

#### ABOUT\_WINDOW

Example: ABOUT\_WINDOW = sample

Description: The text that appears in the about window describing the name of the data view.

Default: Registration Enterprise 9.0.18

Options: Up to one line of text.

---

*NOTE: It is important to note that it is the responsibility of a site's administrator to propagate any changes made to ChemOffice Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

---

#### ADO\_CONNECTION\_NAMES

Example: ADO\_CONNECTION\_NAMES = base\_connection

Description: Names of all ado connection definition sections in the ini file. This list must be comma delimited with no spaces. If the connection name is not here, it will not be loaded by the application. An ADO definition section describes variables for connecting to data source via ADO. In general there is only the

default definition "base\_connection\_group", since most dataviews access the same database. However, this is flexible and allows more definitions than just the default.

ADO\_Connection\_Names are referenced by individual tables.

Default: base\_connection

Options: Comma delimited list of connection definitions found in the ini file.

---

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#### CHEM\_CONNECTION\_NAMES

Example: CHEM\_CONNECTION\_NAMES = base\_cfw\_form

Description: Names of all ChemFinder connection definition sections in the ini file. This list must be comma delimited with no spaces. If the connection name is not here, it will not be loaded by the application. A ChemFinder connection definition section describes variables for connecting to ChemFinder for searching of chemical information. The default definition "reg\_cfw\_form" is normally present (unless there is no chemical information). In dataviews that deal with reaction databases, there may be three (or more) definitions, one for the reaction, one for the solvent and one for the catalyst. (e.g.config/chemprep.ini file in the chemrxn application).

Default:

regreg\_cfw\_form,reg\_struc\_cfw\_form,regtemp\_cfw\_form,reg\_cfw\_form

Options: Comma delimited list of ChemFinder connection definitions found in the ini file.

---

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#### DB\_RECORD\_COUNT

Example: DB\_RECORD\_COUNT = 288

Description: The number of records in the database. This appears in all input and result windows in the upper left corner next to Total Records.

Default: 1

Options: Any integer (equal to the number of records in the database)

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#### DB\_TYPE

Example: DB\_TYPE = STRUC

Description: States the type of database.

Default: STRUC

Options:

---

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*Enterprise application files to future versions of the application. New versions of the ChemOffice Enterprise use default configurations.*

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#### DISPLAY\_NAME

Example: DISPLAY\_NAME = sample

Description: The name used in global search screens to identify the dataview.

Default: Registration Enterprise

Options: Any text

---

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#### FIELD\_MAP\_GROUPS

Example: FIELD\_MAP\_GROUPS =  
gs\_field\_map\_group

Description: Names of field map group definition sections in the ini file. This must be comma delimited, with no spaces. If the field group names are not here, they will not be loaded by the application. Field Map groups specify field mapping used by global search. If global searching is not used, the FIELD\_MAP\_GROUPS (default group created by the wizard) can be set to NULL. FIELD\_MAP\_GROUPS are reference by formgroups.

Default: reg\_map\_group

Options: Comma delimited list of field map group definitions found in the ini file.

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#### FORM\_GROUPS

Example: FORM\_GROUPS =  
base\_form\_group,basemp\_form\_group,gs\_form\_group,add\_record\_form\_group,  
drill\_down\_form\_group

Description: Names of form group definition sections in the ini file. This must be comma delimited, with no spaces. If the form group names are not here, they will not be loaded by the application. Form\_groups specify a sub set of information including the input and result forms to use, the fields that can be searched, the table group to use for searching as well as additional information that will be described in later sections. The default formgroup is "base\_form\_group " this group is used most commonly. There may also be "basemp\_form\_group" which is used for input forms that do not have a plugin, "gs\_form\_group" used for performing global searches over many data views in the application; "add\_record\_form\_group" which is reserved for future use but is not currently implemented and "drill\_down\_form\_group" for displaying results for a drill down link contained in another form groups such as "base\_form\_group". Form\_groups are referenced by hyperlinks from the main.asp page

and carried throughout all functions and sub-routines within ChemOffice Enterprise.

Default:

approve\_form\_group,review\_register\_form\_group,add\_reagent\_ctrbt\_form\_group,  
manage\_users\_form\_group,manage\_roles\_form\_group,manage\_tables\_form\_group,  
manage\_reg\_tables\_form\_group,base\_form\_group,reg\_ctrbt\_form\_group,reg\_ctrbt\_commit\_form\_group,  
reg\_ctrbt\_commit\_user\_form\_group,batch\_ctrbt\_form\_group,identifier\_ctrbt\_form\_group,  
salt\_ctrbt\_form\_group,analytics\_form\_group,add\_analytics\_form\_group,manage\_analytics\_tables\_form\_group,  
sartable\_form\_group,EDIT\_ANALYTICS\_FORM\_GROUP

Options: Comma delimited list of form group definitions found in the ini file.

---

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---

#### INI\_VERSION

Example: INI\_VERSION = "26"

Description: The version number for the ini file.

Default: 26

Options: **Should not be edited**

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the application. New versions of the ChemOffice Enterprise use default configurations.

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#### MAIN\_PAGE

Example: MAIN\_PAGE = 1

Description: Displays main page of the application.

Default: 1

Options: **Should not be edited**

---

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#### MAXHITS

Example: MAXHITS = 100

Description: 100000

Options: Any integer

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---

#### REG\_VERSION

Example: REG\_VERSION = "1.0"

Description: The Registration Enterprise version.

Default: 1.0

Options: **Should not be edited.**

---

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#### SUBFORM\_VIEW\_NAMES

Example: SUBFORM\_VIEW\_NAMES = NULL

Description: Internal Setting.

Default: NULL

Options: **Should not be edited.**

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#### TABLE\_ALIASES

Example: TABLE\_ALIASES = MolTable,Synonyms\_r

Description: Names of all table definition sections in the ini file. This list must be comma delimited with no spaces. If the table name is not here, it will not be loaded by the application. Table definition sections describe all the information needed by ChemOffice Enterprise for searching tables.

Default:

ALT\_IDS\_CHEM\_NAME,ALT\_IDS\_ALL,B  
ATCHES\_FOR\_DELETE,PARAMETERS\_F

OR\_DELETE,  
Cmpd\_Mol\_Utilization\_ID,Cmpd\_Mol\_Utilizations,Utilizations,Batch\_Proj\_Utilization\_ID, Batch\_Proj\_Utilizations,Batch\_Projects,solves,Sites,chem\_reg\_PRIVILEGES, Privilege\_Tables,Security\_Roles,People,Supervisors,Reg\_Quality\_Checked\_Cmpd,Reg\_Quality\_Checked, Reg\_Approved,Structures,Compound\_Salt,Reg\_Numbers,Temporary\_Structures,Compound\_Molecule, Compound\_Project,Projects,Duplicates,Sequence,Test\_Samples,Batches,Notebooks,Salts,Compound\_Type,Alt\_IDs, Identifiers,Spec-tra,dba\_users,dba\_role\_privs,RESULTTYPE,PARAMETERTYPE,EXPERIMENTTYPE, EXPERIMENTS,PARAMETERS,RESULTS

Options: Comma delimited list of tables.

---

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---

#### TABLE\_GROUPS

Example: TABLE\_GROUPS =  
base\_table\_group

Description: Name of table group definition sections in the ini file. This must be comma delimited, with no spaces. If the table group names are not here, they will not be loaded by the application. A table group specifies information about the order of searching tables, what the base table (searched via ADO) is and

what the molecule table (searched via Chem-Finder) is. The majority of applications use the default table group named "base\_table\_group". Table\_groups are referenced by Form\_Groups.

Default:

base\_table\_group,temp\_table\_group,reg\_commit\_table\_group

Options: Comma delimited list of table group definitions found in the ini file.

---

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#### ADO Connection Definitions

##### CONN\_TYPE

Example: CONN\_TYPE = DBQ

Description: Specifies the type of connection string.

Default: "FILE NAME"

Options: DBQ | DSN | OLEDB

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##### CONNECTION\_PASSWORD

Example: CONNECTION\_PASSWORD = ""

Description: Contains the password for the connection. The way the password is entered is

different for different datasources. Otherwise, this entry are probably left empty.

Default: ""

Options: N/A

---

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---

#### CONNECTION\_STRING

Example: CONNECTION\_STRING = C:\Inet-pub\wwwroot\ChemOffice\chem\_reg\config\Reg.udl

Description: The connection string for the CONN\_TYPE specified.

Default: C:\Inet-pub\wwwroot\ChemOffice\chem\_reg\config\Reg.udl

Options: A Connection String

---

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---

#### CONNECTION\_TIMEOUT

Example: CONNECTION\_TIMEOUT = 30

Description: The amount of time in minutes before a connection will automatically close upon no activity. We suggest 15 to 30 minutes.

Default: 15

Options: An integer indicating a number of minutes.

---

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---

#### CONNECTION\_USERNAME

Example: CONNECTION\_USERNAME= ""

Description: Contains the username for the connection.

Default: ""

- Options: N/A

---

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#### COMMAND\_TIMEOUT

Example: COMMAND\_TIMEOUT = 30

Description: The amount of time in minutes before a command object will automatically close upon no activity. We suggest 15 to 30 minutes.

Default: 30



Options: An integer indicating a number of minutes.

---

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#### DBMS

Example: DBMS = ORACLE

Description: The version number for the ini file.

Default: ORACLE

Options: **Should not be edited**

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---

#### PWD\_KEYWORD

Example: PWD\_KEYWORD = pwd

Description: This is a password descriptor used to build the connection string.

Default: password

Options: **Should not be edited**

---

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*the application. New versions of the ChemOffice Enterprise use default configurations.*

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#### USERID\_KEYWORD

Example: USERID\_KEYWORD = uid

Description: This is a user ID descriptor used to build the connection string.

Default: user id

Options: **Should not be edited**

---

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#### Table Group Definitions

[BASE\_TABLE\_GROUP]

Description: As with other items in the globals section the TABLE\_GROUP key specifies individual table groups else where in the ini file. Table Groups specify information about what table is the base table for searching, and what table holds the structures.

The Base Table Group is the base table group. The reg.ini definition is as follows:

```
BASE_TABLE=Reg_Numbers
MOLECULE_TABLE=Reg_Numbers
TABLE_SQL_ORDER=Compound_Molecule,
Reg_Numbers,structures,Compound_Salt,Compound_Project,Projects,Temporary_structures,Batches,Notebooks,Salts,Compound_Type,Alt_IDs,ALT_IDS_CHEM_NAME,ALT_IDS_ALL,Identifiers,People,Supervi-
```

sors,reg\_quality\_checked,reg\_approved,Spec-  
tra,Security\_Levels,Batch\_Proj\_Uti-  
lizations,Batch\_Projects,sol-  
vates,Sites,Utilizations

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---

#### [REG\_COMMIT\_TABLE\_GROUP]

Description: As with other items in the globals section the TABLE\_GROUP key specifies individual table groups else where in the ini file. Table Groups specify information about what table is the base table for searching, and what table holds the structures.

The reg.ini definition is as follows:

```
[REG_COMMIT_TABLE_GROUP]
BASE_TABLE=Temporary_Structures
MOLECULE_TABLE=Compound_Molecule
TABLE_SQL_ORDER=Reg_Numbers,Compound_Molecule,structures,Compound_Salt,Compound_Project,Projects,Temporary_structures,Batches,Note-books,Salts,Compound_Type,Alt_IDs,Identifiers,People,Supervisors,reg_quality_checked,reg_approved,Security_Levels,Batch_Proj_Utilizations,Batch_Projects,sol-vates,Sites,Utilizations
```

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---

#### [TEMP\_TABLE\_GROUP]

Description: As with other items in the globals section the TABLE\_GROUP key specifies individual table groups else where in the ini file. Table Groups specify information about what table is the base table for searching, and what table holds the structures.

The reg.ini definition is as follows:

```
[TEMP_TABLE_GROUP]
BASE_TABLE=Temporary_Structures
MOLECULE_TABLE=Temporary_Structures
TABLE_SQL_ORDER=Compound_Molecule,Compound_Project,Projects,Temporary_structures,Duplicates,Molecules,Sequence,Test_Samples,Batches,Note-books,Salts,Compound_Type,Alt_IDs,Identifiers,People,Supervisors,reg_quality_checked,reg_approved,Spectra
```

---

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---

### ChemFinder Connection Definitions

#### [REG\_STRUC\_CFW\_FORM]

Description: ChemFinder connection names specified in the chem\_connections section of

the globals section reference connection sections elsewhere in the ini file. If a table contains chemical information stored by ChemFinder then the CHEM\_CONNECTION name is referenced by the table definition. The keys specify data necessary to create the ChemFinder connection.

The reg.ini definition is as follows:

```
[REG_STRUC_CFW_FORM]
STRUC_ENGINE=CARTRIDGE
STRUC_FORM_NAME=Reg
STRUC_DB_PATH=C:\Chemoffice_data\C
hem_Reg\RegDB.mst
STRUC_TABLE_NAME=Structures
```

---

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#### [REGREG\_CFW\_FORM]

Description: ChemFinder connection names specified in the chem\_connections section of the globals section reference connection sections elsewhere in the ini file. If a table contains chemical information stored by ChemFinder then the CHEM\_CONNECTION name is referenced by the table definition. The keys specify data necessary to create the ChemFinder connection.

The reg.ini definition is as follows:

```
[REGREG_CFW_FORM]
STRUC_ENGINE=CARTRIDGE
STRUC_FORM_NAME=Reg
STRUC_DB_PATH=C:\Chemoffice_data\C
```

```
hem_Reg\RegDB.mst
STRUC_TABLE_NAME=Reg_Numbers
```

---

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---

#### [REG\_CFW\_FORM]

Description: ChemFinder connection names specified in the chem\_connections section of the globals section reference connection sections elsewhere in the ini file. If a table contains chemical information stored by ChemFinder then the CHEM\_CONNECTION name is referenced by the table definition. The keys specify data necessary to create the ChemFinder connection.

The reg.ini definition is as follows:

```
[REG_CFW_FORM]
STRUC_ENGINE=CARTRIDGE
STRUC_FORM_NAME=Reg
STRUC_DB_PATH=C:\Chemoffice_data\C
hem_Reg\RegDB.mst
STRUC_TABLE_NAME=Compound_Molecule
```

---

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---

#### [REGTEMP\_CFW\_FORM]

Description: ChemFinder connection names specified in the chem\_connections section of the globals section reference connection sections elsewhere in the ini file. If a table contains chemical information stored by ChemFinder then the CHEM\_CONNECTION name is referenced by the table definition. The keys specify data necessary to create the ChemFinder connection.

*Figure 1.1 The reg.ini definition is as follows:*

```
[REGTEMP_CFW_FORM]
STRUC_ENGINE=CARTRIDGE
STRUC_FORM_NAME=RegTemp
STRUC_DB_PATH=C:\Chemoffice_data\C
hem_Reg\RegDB.mst
STRUC_TABLE_NAME=Temporary_Structu
res
```

---

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## Optional Features

### Row Level Security (RLS)

Row-level security is a level of security implemented above the standard Oracle roles. The purpose of using Roles in Chemical Registration is to restrict access to elements of the interface and data to certain users. 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; User A can register

data and edit that data, User B can only register.

On the other hand, Roles do not distinguish which rows a user has access to within a given table. In the pre-row-level-locking (RLS) system, User A sees all compounds in the registry, as does User B. With the implementation of RLS, the rows (records) of data are linked to projects and projects are linked to people. Thus, User A is assigned to a particular project, and will only be able to see compounds that are linked to that project.

#### HOW IT IS IMPLEMENTED

RLS is implemented through the use of Oracle's Fine Grain Access Control. Tables are assigned policies. When a table is accessed, the policy is enforced. A policy is an additional piece of SQL that enforces a rule so a user can only select records that are linked to a project for which he has rights. Since policies are in Oracle, if there is an attempt to access data from any application (e.g. SQL Worksheet), the rule is enforced.

#### DIFFERENCES IN APPLICATIONS THAT CAN REGISTER COMPOUNDS IN REGISTRATION ENTERPRISE

Applications with the ability to register compounds in Registration Enterprise do not necessarily allow the user to specify a project. With RLS, if a post to Registration Enterprise is performed and a project\_id is not linked to the user found - the record is dumped to the Temporary Table and the project is assigned to Unspecified.

#### CHEMLOADER

Since ChemLoader accesses data in Registration Enterprise, it too reflects the changes RLS implements. When a user logs into ChemLoader, the Projects drop-down shows the

projects they are allowed to view - just like the user interface.

#### INI SETTINGS

These settings are located in the Registration Enterprise cfserver.ini file, usually found in:

<webroot>/ChemOffice/chem\_reg/config

ADD\_BATCH\_FROM\_REG\_RESULTS

If the

ADD\_BATCH\_FROM\_REG\_RESULTS

Cfserver.ini setting is as follows:

ADD\_BATCH\_FROM\_REG\_RESULTS=1

a button is enabled in detail view called Add Batch/Lot. This button performs the same function as the button on the homepage with the same name performs, but the user does not have to enter a registration number. After adding a batch the user is returned to the record last viewed.

#### PRIMARY\_STRWHERE

If the PRIMARY\_STRWHERE Cfserver.ini file setting is as follows:

PRIMARY\_STRWHERE=COMPOUND\_PROJECT

Registration Enterprise inspects both the compound and the project when deciding if a duplicate exists. If the compound being added is a duplicate in the entire system, but not a duplicate within a project an end user would see no duplicate window appear and the compound is registered as usual. However since the same compound is a system duplicate the record is placed in the Duplicates Table. If a compound

is a duplicate within a project, the Duplicate Window appears.

#### MAKING PROJECT A REQUIRED FIELD

If the project field (in a record) is not populated and RLS is implemented, the record will not be visible to users. If you implement RLS, it is important to make the project field required for all input forms. For more information about making a field required, see Changing Required Fields.

#### Salt and Solvate Recognition

Both compound level records as well as batch level records contain salt and solvate information. There are a number of options which indicate how salt and solvate information is recorded.

The following settings (found in the Registration Enterprise cfserver.ini file) control how salts and solvates are recognized in the Registration Enterprise:

BATCH\_LEVEL=COMPOUND|SALT

The default is COMPOUND. If set to COMPOUND, salts and solvates are properties of a batches record. If set to SALT, salts are interpreted as parent compounds of a record and make a composite registry number

SHOW\_MF\_WITH\_SALT\_NAME=0|1

The default is 0. If set to 1, salt listboxes display both the salt name and molecular formula rather than the salt name alone.

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# Index

## A

Adding a Batch or Lot 4  
Adding a Compound 3  
Adding a Container 6  
Adding a New Experiment 24  
Adding a New Parameter 26  
Adding a New Project 17  
Adding a New Result Type 26  
Adding a New Salt Record 21  
Adding a New Sequence 18  
Adding a New Solvate Record 22  
Adding a New Structure Comment 19  
Adding a Salt to a Compound 4  
Adding Analytics Data 11  
Adding Identifier Information 11  
Adding New Compounds, Batches, and Containers 2  
Administration 16  
Assigning Users to Projects (for RLS) 32

## B

Batch Attributes 35  
Batch Search 14  
Benefits of using Registration Enterprise 1

## C

Changing Passwords 23  
Compound Attributes 35  
Compound Search 13  
Customizable Fields 33

## D

Defining New Experiments 23  
Deleting a Duplicate 32

Deleting a Parameter 26  
Deleting a Project 18  
Deleting a Result Type 27  
Deleting a Salt Record 22  
Deleting a Sequence 19  
Deleting a Solvate Record 22  
Deleting a Structure Comment 20  
Deleting an Experiment 25  
Deleting Records in Temporary Table 9  
Duplicate Checking 32

## E

Editing a Parameter 26  
Editing a Project 18  
Editing a Result Type 27  
Editing a Salt Record 21  
Editing a Sequence 19  
Editing a Solvate Record 22  
Editing a Structure Comment 20  
Editing an Experiment 24  
Editing Records in Temporary Table 8  
Experiment Type 24  
Exporting Registration Enterprise Records to SDFiles 30

## F

Form Fields 35

## I

Importing SDFiles 28  
Integrating ChemScript with Registration Enterprise 33

## L

Linkage of Projects With People 32

## M

Managing Analytics Tables 23  
Managing Duplicates 12  
Managing Tables 17  
Managing Users and Roles 23  
Managing Workgroups 27  
Marking Records 15  
Matching Fields in the Input and Output  
Databases 30

## O

Optional Features 31

## P

Parameter Type 25  
People 20  
Privileges 37  
Projects 17

## Q

Query and Reporting 12

## R

Registering a Batch Record 10  
Registering a Compound Record 9  
Registering a Temporary Record 9  
Registering All the Temporary Table  
Records 10  
Registering Records 9

Registration Enterprise Workflow 1  
Required Fields 2  
Result Type 26  
Roles 36  
Row Level Security 31

## S

Salt and Solvate Recognition 33  
Salts 21  
Searching and Viewing Records in Tempo-  
rary Table 7  
Searching Registered Compounds 12  
Sending Marked Records 16  
Sequence 18  
Solvates 22  
Specifying Import Options 30  
Specifying Input and Output Databases 29  
Structure Comments 19

## U

Unmarking Marked Records 16  
Unspecified Project 32  
User Interface 31

## V

Viewing Analytics Spreadsheet 16  
Viewing Marked Records 15  
Viewing System Duplicates 32