

Chapter 11:Chemical Inventory

Overview

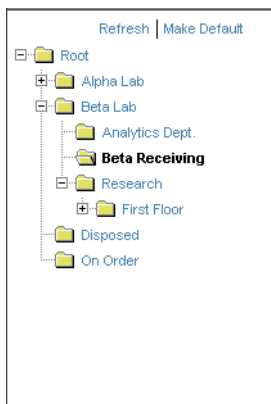
CambridgeSoft's Chemical Inventory Management System (ChemInv) is a ChemOffice WebServer based application designed to manage the reagent tracking needs of chemical and pharmaceutical research centers. The system manages data associated with both commercially procured and internally produced chemical substances from their procurement or initial production through their depletion and disposal.

The three primary entities in the system are *Locations*, *Containers*, and *Substances*, described below:

Terminology

Locations

An inventory *Location* represents a physical location where one or more *Containers* may be stored. Locations can be nested within other locations to produce a hierarchy. The location hierarchy is represented as nested folders on a tree control analogous to that found in the Windows file explorer. Following is an example of a typical location tree:



For a complete list of attributes see, “Record Fields” on page 179.

Containers

An inventory *Container* represents a physical container capable of storing chemical substances. While a Container may physically contain a complex mixture of chemical substances, the Chemical Inventory System only allows for the assignment of a single (primary) chemical structure to each *Container*. Additional text fields are available to track other chemical contents such as the solvent, or other (secondary) chemical substances associated with the Container. Typical containers include: bottle, vial, tube, cylinder, box, etc...

For a complete list of attributes see, “Record Fields” on page 179.

Substances

An inventory *Substance* represents a single pure chemical entity which can be expressed as a two dimensional chemical structure drawing. The system maintains its own internal chemical structure database containing unique substances that can be associated with inventory *Containers*. A new substance will only be added to the inventory system if its chemical structure and chemical name are not already present in the system. A single *Substance* may be associated with each inventory *Container*. Aside from structure and name, substances can be identified via unique registry numbers such as CAS or ACX ID.

For a complete list of attributes see, “Record Fields” on page 179

In This Chapter

You this chapter you will learn to:

- Install Chemical Inventory, see “Installation” on page 166.
- Search for Substances and Containers, see “Searching Chemical Inventory” on page 168.
- Create and Search for Substances, see “Creating a New Substance” on page 170 and “Searching for a Substance” on page 170.
- Manage and Manipulate Locations, see “Location Management” on page 172.
- Create and Search for Containers, see “Creating a New Container” on page 176 and “Searching for a Container” on page 176.
- View and Manipulate the Contents of a Container, see “Viewing the Contents of a Container” on page 176.

Installation

Minimum Server Requirements

Operating Systems

- WinNT Option Pack 4.0 (IIS 4)
- Service Pack 6a
- Microsoft Data Access Components 2.5sp2 or later service pack
- Internet Explorer 4.01 or later

Windows 2000 Server or Windows 2000

Advanced Server

ChemOffice WebServer 2002

Chemical Registration

Installing Chemical Inventory

1. Run the ChemInv installer
2. Create a Blank ChemInv Database

Creating and Testing a Blank ChemInv Database

Note: The sql scripts provided have been designed to be executed with the command line version of SQL*Plus.

This scripts contain substitution variables which will not be processed correctly when run from SQL*Plus Worksheet. To execute the scripts with SQL*Plus just double click the provided command files.

1. Browse to
/cheminv/config/oracle_intall_scripts/create_blank_cheminv_db/

2. Install the Database:

If a previous version of ChemInv is installed

Execute the **Drop_ChemInvDB.cmd**file.

Execute the

Create_Blank_ChemInvDB.cmdfile.

If no previous version of ChemInv is installed

Execute the

Create_Blank_ChemInvDB.cmd file.

Execute the

Import_ChemInvDB_PickLists.cmd file.

3. Browse to
/cheminv/config/oracle_intall_scripts/create_test_cheminv_db/

Execute the

Create_Test_ChemInvDB.cmd file.

Execute the

Import_Test_ChemInvDB.cmd file.

4. Copy the mst and msi files to the ChemOffice_Data folder. If using the test database, be sure to copy the mst and msi from the Test Database folder.
5. Browse to **/cheminv/config/**. Open **ChemInv.udl** and test the connection.

6. Open the **cfserver.ini** file and set the Oracle Server Name.
7. Create a system DSN in ODBC. Use **Chem_Inv** for DSN name, Oracle ODBC driver and **ChemInvDB** as user ID.
8. Reset IIS.

Setting up the Report Writer

The report writer is necessary to print any type of report in Chemical Inventory.

1. Browse to **webserver_source/cfserverasp/RPT**
2. Add a shortcut of the **reports.exe** to the Startup menu (in Documents and Settings) under 'all users'
3. Create a COM+ application for the **ReportQ.dll**. You will need to create the application and the component. Complete instructions regarding creating the COM+ application can be found in **RPTSoftwareInstructions.doc**.
4. Copy the **ChemInv_Reports.mdb** file located in the **RPT** folder to **ChemOffice_Data\ChemInv** folder.

Setting up PDF and Barcode Support

Setting up PDF Support

1. Browse to **ChemInv\Installation\win2pdf**.
2. Install the win2pdf driver.
3. Go to the **Control Panel>Printers** and check that the win2pdf printer is the default Windows Printer.

4. Right click on the win2pdf printer and select properties. Enter the regcode: **9532-9429-9024-9054**.

Setting up Barcode Support

1. Browse to **ChemInv\Installation\Tbarcode**.
2. Run the Tbarcode ocx installer.

Check ini File Settings

ChemInv.ini and **cfserver.ini** are located in **ChemOffice\ChemInv\config**. These files define parameters necessary for Chemical Inventory to perform correctly.

ChemInv.ini

Be sure that:

STRUC_DB_PATH points to location of the **mst** file

the settings to the **RPT** folder and to **Reports_DB_Path** are correct.

Cfserver.ini

Be sure that **ORA_SERVICENAME** points to correct Oracle instance.

Starting Chemical Inventory

When Chemical Inventory is opened, you must log in to start working.

To open and log in to Chemical Inventory:

1. Type **http://hostname** into your web browser.
The main ChemOffice WebServer window appears.

NOTE: *Hostname is the name of the ChemOffice WebServer machine. Contact your server administrator to obtain the correct hostname.*

2. Click **Chemical inventory**.

The Chemical Inventory login page appears.

ChemInventory

Please enter your Username and Password

Username:

Password:

3. Type your **Username** and **Password**, and then click **Log In**.

The Chemical Inventory homepage appears.

ChemInventory

Manage Containers | Manage Substances | Log Off

Print | Preferences | Help | About | Log Off

Search | Clear Form | Refresh List | Retrieve All

Total Containers: 53766

Current login: INVADMIN

Simple Search | Advanced Search | Substructure Search

CAS Registry#:

Substance Name:

Container ID (barcode):

Container Name:

Location Barcode:

Location Name: Browse

Catalog Number:

PO Number:

☐ Search Sublocations

NOTE: Your Administrator may set different privileges for different users, so some options described in this guide may not be available.

Searching Chemical Inventory

Searching is the easiest way to find particular substances or containers in Chemical Inventory. The system allows for combined chemical and text searches of all attributes associated with a *Container*. Several different search forms are available to accommodate the search preferences of different users. For example, the *Substructure Search* form which allows searches based on chemical structure, substance name, CAS number and other attributes is particularly well suited for use by chemists. Similarly, the *Advanced Search* form

which exposes fields such as container and location barcode is particularly well suited for use by stock room or receiving room personnel.

Three different search forms are available on the homepage of Chemical Inventory through the use of tabs. Click on the tab indicating the type of search you would like to perform, and enter your search parameters.

Simple Search

The simple search option allows searching through the use of CAS Number, Container Barcode, Location Barcode, Catalog Number, PO Number, Substance Name, Container Name, and Location Name (select Search Sublocations checkbox if you want to search all sublocations of the chosen location).

CAS Registry#:

Substance Name:

Container ID (barcode):

Container Name:

Location Barcode:

Location Name: Browse

Catalog Number:

PO Number:

☐ Search Sublocations

How to search:

1. Enter the desired information to search for. For more information about entering search criteria, see Searching in the WebServer Users Guide.
2. Click **Search** in the Toolbar.

A list of containers matching your search parameters is returned. Clicking on one of the containers will allow you to view, the location of the container (left frame), container information (upper right frame), and the contents of the container (lower right frame)

Advanced Search

The advanced search option allows searching through the use of CAS number, ACX number, Registry Batch ID, Purity, Concentration, Grade,

Size, Container Cost, Location Name (select Search Sublocations checkbox if you want to search all sublocations of the chosen location), Container ID (barcode), Container ID (internal), Container Name, Container Type, Container Status, Unit of Measure, Qty Remain, Qty Available, Location Barcode, Catalog Number, Supplier, Lot Number, Expiration Date, Date Ordered, Date Received, PO Number, Owner ID, and Current User ID.

For more information regarding these fields, see “Record Fields” on page 179.

This search concentrates more on container properties as opposed to substance properties.

How to search:

1. Enter the desired information to search for. For more information about entering search criteria, see Searching ChemOffice WebServer Applications in the ChemOffice WebServer Users Guide.
2. Click **Search** in the toolbar.

A list of containers matching your search parameters is returned. Clicking on one of the containers will allow you to view, the location of the container (left frame), container information (upper right frame), and the contents of the container (lower right frame).

Substructure Search

The substructure search option allows searching through the use of all of the attributes in the Advanced Search in addition to Substance Name, Molecular Formula, MolWeight Range, and of course, Substructure.

To allow you to draw your substructure, a ChemDraw Plug-in will open along with this search tab. For more information about using the ChemDraw Plug-in, see Drawing Chemical Structures in the ChemDraw User's Guide.

Additionally, the structure drawn can be searched for assuming it to be a Substructure, the exact Structure, or with Tanimoto Similarity, just select the correct type under Search Type. For more information regarding your search type options, see Searching ChemOffice Webserver Applications in the ChemOffice WebServer manual.

How to search:

1. Enter the desired information to search for. For more information about entering search criteria, see Searching ChemOffice WebServer Applications in the ChemOffice WebServer Users Guide.
2. Click **Search** in the toolbar.

A list of substances matching your search parameters is returned. Clicking on the details button of one of the substances will allow you to view, all of the inventory containers that contain that

substance. For information about Searching for substances and their properties, see “Searching Chemical Inventory” on page 168

Deselecting the "Group results by chemical structure search box" will lead directly to a list of containers matching the search criteria (bypassing the substance grouping).

Substance Management

The substance management area of Chemical Inventory is available in the uppermost toolbar of the homepage.

This area allows you to search for substances by substructure, registration numbers, and other physical properties. Although similar to the types of searches found on the homepage, this area concentrates on the searchable aspects of substances and returns a table of substances as opposed to containers.

If you have the appropriate privileges, in addition to allowing you to search for substances previously entered, this area also gives you the opportunity to add a new substance to the database. This option is available after entering the substance management area and clicking on Add Mode.

Creating a New Substance

To see if you have the appropriate privileges to create a new substance, see “Chemical Inventory Role Dependencies” on page 187 and “Chemical Inventory Privileges” on page 188, or ask your system administrator.

The "New Substance" form is available in the Substance Management area of Chemical Inventory.

To reach this form, do the following:

1. From the homepage, click **Manage Substances**.

2. Click **Add Mode**.

How to create a new substance:

3. Enter information about the new substance. For more information about individual fields, see, “Record Fields” on page 179.
4. Click **Add Record** in the toolbar.

Searching for a Substance

A form made to make finding a substance easier is available in the Substance Management area of Chemical Inventory. To reach this form, simply click Manage Substances from the homepage.

This form is a simplified version of the Substructure Search form found on the homepage. The following attributes are available to search under from this

page: Substructure, Substance Name, CAS number, ACX number, Molecular formula, MolWeight Range, and Compound ID.

How to search:

1. Enter the desired information to search for. For more information about entering search criteria, see Searching ChemOffice WebServer Applications in the ChemOffice WebServer Users Guide.

2. Click **Search** in the toolbar.

A list of substances matching your search parameters is returned. Clicking on the details button of one of the substances will allow you to view, all of the entered properties of the given substance.

For more information about other ways to search in Chemical Inventory, see “Searching Chemical Inventory” on page 168.

Managing Synonyms

The synonym management area of Chemical Inventory is available as part of substance management. To access this section, please take the following steps:

1. From the Substance Management area, access the search form.

2. Perform a search for the appropriate substance. For more information about searching for a substance in Chemical Inventory, see “Searching Chemical Inventory” on page 168.

3. While in List View click the **Details** button for the substance.

4. Click on the Manage Synonyms link.

The Synonym Management window opens.

Synonym	New
(u)annulene	Edit Delete
benzol	Edit Delete
benzolene	Edit Delete
Coal naphtha	Edit Delete
Phene	Edit Delete
Phenyl hydride	Edit Delete
benzine	Edit Delete
bicarburet of hydrogen	Edit Delete
carbon oil	Edit Delete
cyclohexatriene	Edit Delete
mineral naphtha	Edit Delete
motor benzol	Edit Delete
nitration benzene	Edit Delete
pyrobenzol	Edit Delete

This area allows you to add new synonyms for a substance edit the synonyms which are already listed, or delete a synonym from the list.

After accessing the Synonym Management window, to add a new synonym:

1. Click **new**.

A text field allowing the addition for a synonym appears.

2. Enter a synonym.

3. Click **OK**.

To edit a synonym

1. Click **Edit** next to the synonym to be edited.
2. Edit the name of the synonym.

3. Click **OK**.

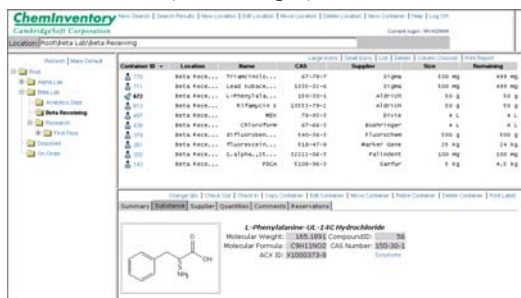
To delete a synonym:

1. Click **Delete** next to the appropriate synonym.
2. If you want to delete the synonym, click **OK**.

Container Management

The container management area of Chemical Inventory is available in the uppermost toolbar of the homepage.

This area is split into 4 frames, shown below:
Current Location Frame (top), Location Tree Frame (left), Container List Frame (top right), Container Contents Frame (bottom right).



Location Management

A location is defined as any "place" that a container can be stored. This includes a shelf, a refrigerator, or even a particular laboratory. Different facilities can decide how best to organize locations. For more information about locations, see "Location Tree Frame" on page 173.

Current Location Frame

The location text box indicates the currently selected inventory location. Actions performed via the links on this frame apply to the currently selected location. In addition, you may enter a location id value into the location box to rapidly

access a location on the tree. A barcode reader may be used to enter a location id value into this box further expediting navigation to a given location.



The following controls and functions are available within the current location frame:

Available to all users:

Function	Description
New Search	Returns to <i>Search Mode</i> screen. The last search form selected by the user will be automatically preselected.
Search Results	Returns to last hit list viewed while on <i>Search Mode</i> . If no search has been performed the link brings up the search default search form.

Available to only some users:

Function	Description
New Location	Creates a new inventory <i>Location</i> at the currently selected location
Edit Location	Allows setting of the following <i>Location</i> attributes: location name, location type, location barcode and location description.

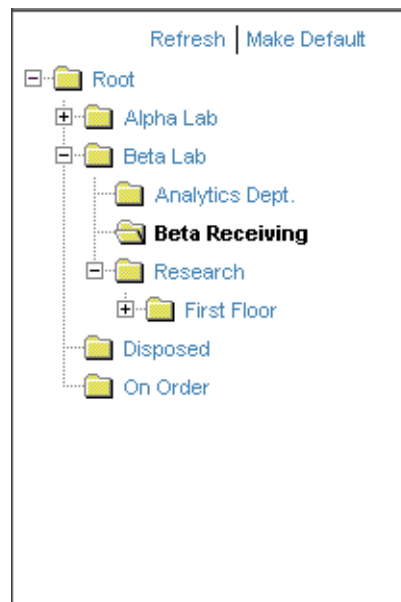
Function	Description
Move Location	Allows moving a location to a different node on the location tree. Enter a location id value or use the browse link to select the destination locations. All containers and sub locations will follow with the moved location.
Delete Location	Deletes the currently selected location. A location must be empty before it can be deleted.
New Container	Creates a new container in the currently selected location. For more information about creating a new container, see “Creating a New Container” on page 176.

For more information about which functions are available to you, see “Chemical Inventory Role Dependencies” on page 187 and “Chemical Inventory Privileges” on page 188.

Location Tree Frame

The location tree control allows navigation of the *Location* hierarchy. Click on the +/- symbols to expand/contract location folders. Click on the location name to display its contents on the container list frame. The refresh link at the top right

of the page repopulates the tree from the latest available location data and returns it to its fully contracted position.



Manipulating Locations

A number of functions are available in the current location frame of the container management area of Chemical Inventory:

- New Location
- Edit Location
- Move Location
- Delete Location
- Default Location

Creating a New Location

To see if you have the appropriate privileges to create a new location, see “Chemical Inventory Role Dependencies” on page 187 and “Chemical Inventory Privileges” on page 188.

Containers are located in different places throughout a facility. The types of locations necessary in your inventory system is highly dependent upon your setup.

In order to create a new location:

1. From the homepage, click **Manage Containers**.
2. Use the location tree to select where the new location should be created.
3. Click **New Location** in the Current Location Frame.
4. Click **OK**.

Enter the desired information in the window that opens. For more information about a particular field, see, “Record Fields” on page 179.

Editing a Location

To see if you have the appropriate privileges to edit a location, see “Chemical Inventory Role Dependencies” on page 187 and “Chemical Inventory Privileges” on page 188.

After a location is created, its properties may be changed. For example, when a particular laboratory was initially arranged, a number of containers were placed on a shelf. As the laboratory grew, it was necessary to move the containers to a cabinet. In

order to change the location type in your inventory system, you don't have to create a new location, you can edit the existing location.

In order to change the properties of a particular location:

1. From the homepage, click **Manage Containers**.
2. Browse to the location to be edited in the Location Tree Frame.
3. Click **Edit Location** in the Current Location Frame.

Make sure the information listed in the window that opens is for the correct location.

Enter the desired new information in the window. For more information about a particular field, see, “Record Fields” on page 179.

4. Click **OK**.

Moving a Location

To see if you have the appropriate privileges to move a location, see “Chemical Inventory Role Dependencies” on page 187 and “Chemical Inventory Privileges” on page 188.

After a location is created, it may be necessary to move the location to somewhere else in the tree. For example, a refrigerator may have been located in a lab on the first floor, but is being moved to a lab on the third floor. Of course all of the containers inside

the fridge are moved along with it. It is easy to move a location along with all of it's contents in the Chemical Inventory system.

In order to move a location:

1. From the homepage, click **Manage Containers**.
2. Browse to the location to be moved in the Location Tree Frame.
3. Click **Move Location** in the Current Location Frame.

Make sure the information listed in the window that opens is for the correct location.

4. Enter the new destination for the location to be moved. For more information about the destination field, click on the field in the image below.

5. Click **OK**

Deleting a Location

To see if you have the appropriate privileges to delete a location, see “Chemical Inventory Role Dependencies” on page 187 and “Chemical Inventory Privileges” on page 188.

If a location needs to be removed from the inventory system, you should use the delete location tool. If the location is merely being moved, see “Moving a Location” on page 174.

In order to change the properties of a particular location:

1. From the homepage, click **Manage Containers**.
2. Browse to the location to be deleted in the Location Tree Frame.

A location can only be deleted if it is empty, so make sure there are no containers in the location to be deleted.

3. Click **Delete Location** in the Current Location Frame.

NOTE: *You can not undo the deleting of a location.*

Saving a Default Location

The location tree frame allows the user to save a default location. If a default location is chosen, each time the user accesses the Container Management section, the default location will be opened in the location tree frame.

To save a default location, please do the following:

1. From the **Container Management** section, browse to the location to be saved as the default in the **Location Tree Frame**.
2. Open that location by double clicking on the folder icon next to the location name.

The default location window appears.

3. Click **OK**.

Creating a New Container

To see if you have the appropriate privileges to create a new container, see “Chemical Inventory Role Dependencies” on page 187 and “Chemical Inventory Privileges” on page 188.

The “New Container” form is available in the Container Management area of Chemical Inventory. To reach this form, do the following:

1. From the homepage, click **Manage Containers**.
2. Click **New Container** in the Current Location Frame.

A window with multiple tabs labeled Required, Substance, Supplier, Contents, Optional, Owner, and Comments opens.

Location ID: 1036
Container name: Phosphoric Acid, 99.999% LAR, 100 mg
Container type: bottle
Unit of measure: milligram
Container size:
Initial amount:
Number of Copies: 1
Container Status: Available
Supplier Name: Unknown
Catalog Number:
Lot Number:
Expiration Date:
Date Received: 2/22/2002
Container Cost(\$):
PO Number:
Compound ID:
Grade:
Purity: percent
Concentration: mill molar
☐ Autogenerate Barcode ID
☐ Print barcodes immediately
Cancel OK

3. Enter information about the new container.
4. Click **OK** in the toolbar.

Searching for a Container

There are two ways to search for a particular container. If you have some information about the container, but don't know its actual location, using the search forms is often the easiest way to locate one or more inventory *Containers*. The system allows for combined chemical and text searches of all attributes associated with a *Container*. A search form configured to return matching *Containers* will result in a hit list comprised of containers matching the search criteria. Containers matching the search criteria appear on screen as a tabular report which

can also be reproduced as a printable report. For more information about these search forms, see “Simple Search” on page 168 and “Advanced Search” on page 168.

If you know the location of the container you are looking for, you can use the location tree to navigate through all inventory locations to find the container. The Location Tree is displayed in the Container Management area. For more information about the Location Tree and how to navigate it, see “Location Management” on page 172.

Viewing the Contents of a Container

After performing a search, or navigating through the location tree, a list of containers is displayed. For more information about searching for containers, see “Searching for a Container” on page 176.

Container List Frame

Container ID	Location	Name	CAS	Supplier	Size	Remaining
94	Shelf A	triamine	59-43-8	Tocris	100 mg	100 mg
95	Shelf A	retinol	49-24-9	ChemService	10 g	10 g
97	Shelf A	retinol	316-75-4	Cayman	5 g	5 g
77	Shelf A	cyclobutane	25-25-1	Acros - Int.	100 ml	100 ml
70	Shelf A	Fluorescein std	2321-67-5	Marker Gene	100 g	100 g

Both the container list frame found in the upper right hand frame of the Container Management area, and the report displayed after container based search results show a list of containers with some summary information.

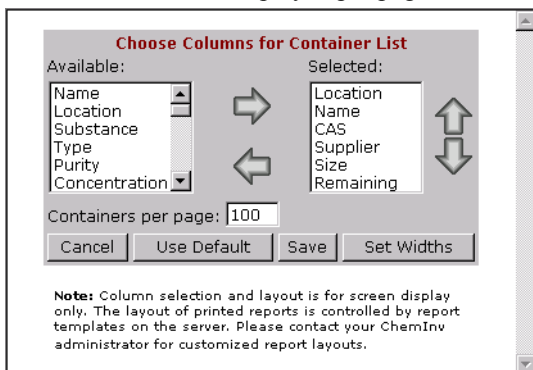
Containers are sorted in descending order by container id, but can be resorted by clicking any of the column headers. The small triangle next to the column name indicates the sorting order. Sorting affects containers regardless of whether they are displayed on the current page.

Each container ID is preceded by a small flask. If the container information is open, the flask tips to the side. Click on one of the containers in the list to see the container details on the frame below.

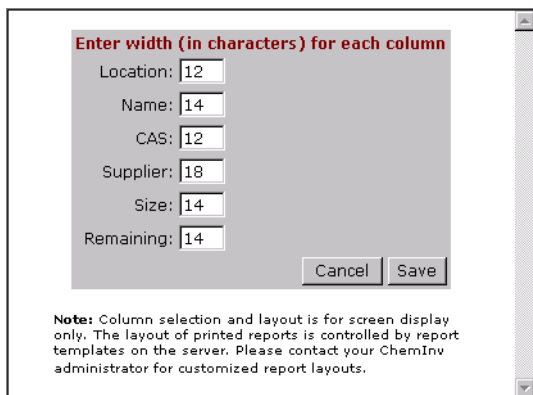
Column Chooser

The Column Chooser link, allows the user to customize what columns appear and the width of columns in the Container List Frame, as well as other result lists within Chemical Inventory.

The Column Chooser window allows the user to customize the appearance of result lists. It allows control over the selection, order, and width of columns to be displayed on screen as well as the number of containers displayed per page.



By clicking the Set Widths button, another window opens that allows the user to enter specific widths for each column.



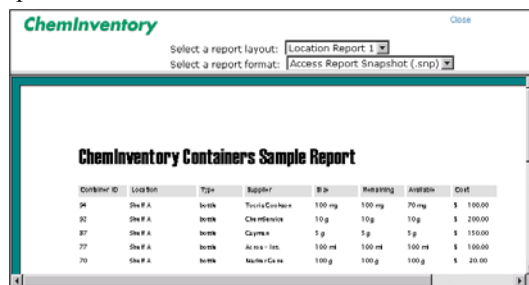
Custom column settings are saved by the user's browser and remembered even after the browser has been closed. The settings available via the Column Chooser affect only the screen report. The

appearance of printed reports is controlled by report templates managed by the application administrator. Multiple report templates can be associated with the screen report. Please contact the administrator if you need additional report templates produced.

Print Report

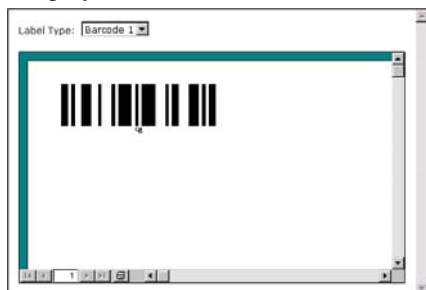
The Print Report link, found in the far right of the frame, creates, displays, and gives the option to print a report containing information about the containers listed in the frame.

Reports can be printed from three places in Chemical Inventory: the container list frame, the container view frame, and the search results window. All three of these reports are generated in the same way, but can display different information. Reports are driven by report templates on the server. Typically the system administrator creates report templates with the appropriate layout and content to be printed. Please contact the administrator if you need additional reports created to satisfy your need. Different templates and formats can be accessed from the list boxes at the top of the report. Once a report is created on the server it can be printed from the browser by using the print icon button in the report viewer window.



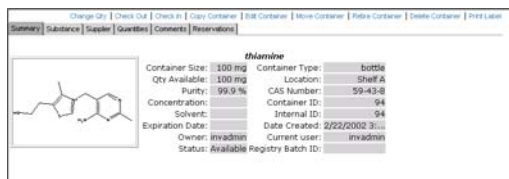
Because reports are printed according to previously created report templates, information in a report is not necessarily the same information displayed in the window or frame that you choose to print. For example, the Print Report link in the container list frame will generate a report about the containers

listed in that frame, but the report template may not include the container's cost, while the container list frame displays the container cost.



Container labels are printed via the report writer as well. A label is considered a special kind of report which can include any of the attributes associated with a single container. The report writer is also able to encode any of the container attributes into a scannable barcode.

Container Details Frame



All container attributes are displayed within the *Container Details Frame*. Given the large number of attributes associated with a container, they are subdivided into tabs which group the attributes into more manageable subsets.

The first tab includes a summary of the most essential container attributes including container name, container id, barcode, location etc.... Other notable tabs include the substance tab, which summarizes the substance attributes and the supplier tab which brings together data related to the purchase of a chemical substance such as supplier name, catalog number, lot number, container cost, and purchase order number.

For more info about available functions see, “Special Functions in Container Details Frame” on page 185.

Choosing Preferences

For more information, see the ChemOffice WebServer User’s Guide.

Printing

You can print records from Chemical Inventory.

To print records:

1. Click **Print**.

The Print dialog box appears.

2. Check the settings and then click **OK**.

A Chemical Registration record is printed.

Logging Off

You can end your Chemical Inventory at anytime by logging off.

To log off:

- Click **Log Off**.

The Chemical Inventory Log In dialog page appears. You can log back in and continue using Chemical Registration, or browse to a different site.

Record Fields

When creating a new record, or searching for a record in the database, the web form displayed includes numerous fields. These fields are listed below with a brief description of what is contained in each field.

Substance/Batch Attributes

Field Name	Description
ACX number	The ACX Number is a unique identifier and registry number for substances in ChemACX, ChemFinder.Com, and submitted via Open Chemistry. ACX Numbers can also be extended to point to physical material, and may contain information relating to the vendor, quality, and package size.
CAS Registry Number	The CAS Registry Number is a unique accession number assigned by the Chemical Abstracts Service, a division of the American Chemical Society. Other than being guaranteed unique to a given compound, this number has no particular meaning. CAS Registry Numbers are assigned to every uniquely-identifiable substance.
Compound ID	The Compound ID number identifies the compound in the Chemical inventory database. It is automatically generated when a compound is entered into the Chemical Inventory system. This number is linked to a compound name and other information in the database.
Concentration	The concentration is a calculation which gives information about the amount of a substance in a mixture. The concentration can be entered in any of the following units: percent, moles, millimoles, normal, and parts per million. To indicate units, select the appropriate abbreviation (% , M, mmol, N, ppm respectively) in the list box directly to the right of the concentration text box.
Grade	The grade is a way to categorize the certain attributes of the contents of a container.
Molecular Formula	The molecular formula is a method of describing a substance's makeup on an atomic level. This field is filled automatically after a substance is inserted into a form. If the user is searching, this field contains the molecular formula of a substance.

Field Name	Description
MolWeight Range	The molecular weight is a calculation reflecting the average mass of a molecule of a substance. This field is filled automatically after a substance is inserted into a form. If the user is searching, this field contains the molecular weight range of a substance.
Purity	The purity is a calculation reflecting how much of a mixture is purely the substance recorded. The purity can be entered in any of the following units: percent, moles, millimoles, normal, and parts per million. To indicate units, select the appropriate abbreviation (% , M, mmol, N, ppm respectively) in the listbox directly to the right of the concentration text box
Solvent	A solvent is a substance capable of dissolving another substance. This field is intended to contain the name of the solvent for the substance.
Substance Name	This field is meant to list the name of the substance.
Structure	This field contains the structure for, or a substructure of a substance. Drawing this structure is facilitated through the use of the ChemDraw plug-in which appears when drawing a structure is an option. For more information about drawing structures, see "Drawing Chemical Structures" in the ChemDraw manual.

Container Attributes

Field Name	Description
Catalog Number	The Catalog Number is a number created by the supplier of a substance for ordering purposes.
Container Cost	This field holds information about the cost of the container. The number entered into this field is assumed to have dollars as its units.
Container ID (barcode)	This field provides a unique ID for a container that can be converted into a barcode with the Print Label function.
Container ID (internal)	This ID number is automatically generated when the container is entered into the inventory system. This number is used to identify the container in the Chemical Inventory database.

Field Name	Description
Container Name	This field is meant to list the name of the container. This name can be anything that will allow a user to identify the container and makes sense to the rest of the facility.
Container Status	This field requires the user to choose a status describing the container's current state. The following is the list to choose from: Available, Disposed, Empty, In transit, Missing, Order Pending, Ordered, Unknown.
Container Size	This field records the size of a container in the units recorded in the Units of Measure field.
Container Type	This field requires the user to choose a type describing the container's appearance. The following is the list to choose from: bag, bottle, box, can, case, cylinder, drum, fiber drum, palette, plate.
Date Ordered	This field is meant to contain the date a particular container was ordered. An icon that looks like a small calendar will display a calendar. When a date is clicked on from the calendar, that date is inserted into the field.
Date Produced	This field is meant to contain the date the contents of a container was produced. An icon that looks like a small calendar will display a calendar. When a date is clicked on from the calendar, that date is inserted into the field.
Date Received	This field is meant to contain the date a particular container was received. An icon that looks like a small calendar will display a calendar. When a date is clicked on from the calendar, that date is inserted into the field.
Destination	This field contains a location ID and is used when a location is being moved. The location ID in this field should be that of the new desired location.
Expiration Date	This field is meant to contain the expiration date for the contents of the container. An icon that looks like a small calendar will display a calendar. When a date is clicked on from the calendar, that date is inserted into the field.
Location ID	The Location ID number identifies the location in the Chemical inventory database. It is automatically generated when a location is entered into the Chemical Inventory system. This number is linked to a location name and other information in the database.

Field Name	Description
Location Name	This field is meant to list the name of the location. This name can be anything that will allow a user to identify the location and makes sense to the rest of the facility.
Location Type	This field requires the user to choose a type describing the location attributes. The following is the list to choose from: Bench, Bin, Box, Building, Cabinet, Company, Cylinder Storage, Disposal/Neutralization Room, Dry box, Freezer, GMP, Hood, Instrument Room, Laboratory, Pan, Receiving, Refrigerator, Safe, Shelf, Site, Solvent Cabinet, Solvent Room, Stock Room, Ultra-Freezer, Utility Room, unknown.
Location Description	This field contains a description of where a location is, or attributes related to a location.
Lot Number	This field is meant to list the supplier's lot number.
Minimum Stock Threshold	This field indicates the minimum amount of a given substance that should be held in stock.
Maximum Stock Threshold	This field indicates the maximum amount of a given substance that should be held in stock.
Number of Copies	This field indicates how many copies of a container should be made during the creation process.
PO Number	This field contains the purchase order number for the container.
Quantity Remaining	This field contains the amount of a mixture remaining in a container. The units of the amount are the same as the units recorded in the units of measure field.
Quantity Available	This field contains the amount of a mixture available in a container. This field is also used to enter the initial amount under the Contents Tab when creating a new container. The units of the amount are the same as the units recorded in the units of measure field.
Registry Batch ID	This field contains the registry batch ID. The registry batch ID is the registration + batch number identifier assigned by the Chemical Registration application. This number will allow you to relate compounds in the registry to inventory.
Requisition Number	This field contains the supplier's requisition number.

Field Name	Description
Reservation Date	This field is meant to contain the date a reservation is made for. A reservation can be made for a particular amount of the contents of a container. An icon that looks like a small calendar will display a calendar. When a date is clicked on from the calendar, that date is inserted into the field.
Reservation ID	This field is meant to contain the ID that is automatically generated when a reservation is made. A reservation can be made for a particular amount of the contents of a container. This ID number is linked to information about the reservation in the Chemical Inventory database.
Reservation Quantity	This field is meant to contain the amount a reservation is made for. A reservation can be made for a particular amount of the contents of a container.
Reservation Status	This field is meant to contain the status of a reservation. A reservation can be made for a particular amount of the contents of a container.
Reservation Type	This field is meant to contain the type of reservation entered. A reservation can be made for a particular amount of the contents of a container. The following is a list of options in the reservation type listbox: External Hole, Internal Hole, Sale Pending, Sold, Undeclared.
Supplier	This field is meant to contain the name of the supplier.
Unit of Measure	This field is a list box that allows the user to choose a unit of measure for the container. This unit of measure is used as the units for all quantity measurements entered. The following is a list of options in the units of measure listbox: ampulle, cubic centimeter, cubic feet, cylinder, each, gallon, gram, kilogram, liter, microgram, microliter, milligram, milliliter, ounce, pack, pint, pound, quart.

Other Attributes

Field Name	Description
Comments	This field is available for the user to enter information that hasn't already been entered in another field, or needs to be expanded on.

Field Name	Description
User ID	The listbox available lists all registered users of the Chemical Inventory system.
Owner ID	The listbox available lists all registered users of the Chemical Inventory system. Select the appropriate user to be listed as the owner of the container.

Special Functions in Container Details Frame

The following functions can be available from the Container Details Frame. For more information about what functions should be available to you, see “Chemical Inventory Role Dependencies” on page 187 and “Chemical Inventory Privileges” on page 188.

Function Name	Description
Change Qty	The Change Qty function allows the modification of the quantity of material remaining in the container. Quantities are measured in the predefined unit of measure associated with the container.
Check Out	The Check Out function is typically used when a user removes a container from a central storage location for subsequent use at a different location. The act of checking involves a change in container location plus a change in the current user responsible for the container.
Check In	The Check In function performs the reverse of the check out process. It is typically performed when a user returns a chemical container to its central storage location. The system remembers the location and user under which the container was created and uses them as the default values during the check in process.
Copy Container	The Copy Container function allows you to create one or more containers using a preexisting container as a starting template. Typically attributes such as lot number, container cost of expiration dates may need to be modified before the new container/s are created.

Function Name	Description
Edit Container	The Edit Container function allows editing of all container attributes. You may switch between the various tabs to access all container attributes. Changes to the container are only committed to the database once the <i>Update Container</i> button is clicked.
Move Container	The Move Container function moves the currently selected container to a new location. The destination location id can be directly entered or scanned into the text box in the dialog, or the browse link can be used to select a location from the tree.
Delete Container	The Delete Container function deletes the currently selected container. The container is permanently removed from the system.
Retire Container	The Retire Container function retires the currently selected container. When a container is retired, it is not deleted, but is no longer in use.
Print Label	See “Print Report” on page 177

Chemical Inventory Role Dependencies

Different users will use Chemical Inventory for different reasons. For this reason, when setting up new user accounts, your system administrator assigns certain roles to each individual. Some roles cannot access specific areas of Chemical Inventory, or cannot perform particular functions. This may be why some screenshots differ slightly from what you see, or why you are unable to access certain areas. Please see your system administrator if you have questions about your roles.

An individual role can contain a number of privileges. For example, although the BROWSER only has the privilege to read the contents of a container, INV_CHEMIST is allowed to Move and Edit the contents of a container as well. For a list of privileges associated with these roles, see “Chemical Inventory Privileges” on page 188.

The roles available are listed below:

Role Name	Oracle Role Name	Privileges
BROWSER	INV_BROWSER	Read Only
CHEMIST	INV_CHEMIST	Edit/Move Containers
RECEIVING	INV_RECEIVING	Create/Edit/Move Containers
FINANCE	INV_FINANCE	Create/Edit/Move Containers + Create/Move/Delete Locations
REGISTRAR	INV_REGISTRAR	Create/Edit/Delete inventory substances
ADMIN	INV_ADMIN	Full Access

Chemical Inventory Privileges

The privileges associated with the available Chemical Inventory roles are listed below:

Privilege	Oracle Privilege Name	Roles Including Privilege
Create a new location	INV_CREATE_LOCATION	FINANCE, ADMIN
Edit a location	INV_EDIT_LOCATION	FINANCE, ADMIN
Move a location	INV_MOVE_LOCATION	FINANCE, ADMIN
Delete a location	INV_DELETE_LOCATION	FINANCE, ADMIN
Create a new container	INV_CREATE_LOCATION	FINANCE, ADMIN
Edit a container	INV_EDIT_CONTAINER	CHEMIST, FINANCE, ADMIN
Move a container	INV_MOVE_CONTAINER	CHEMIST, FINANCE, ADMIN
Delete a container	INV_DELETE_CONTAINER	CHEMIST, FINANCE, ADMIN
check out/in a container	INV_CHECKOUT_CONTAINER	CHEMIST, FINANCE, ADMIN
Create a new substance	INV_CREATE_SUBSTANCE	REGISTRAR, ADMIN
Edit a substance	INV_EDIT_SUBSTANCE	REGISTRAR, ADMIN
Delete a substance	INV_DELETE_SUBSTANCE	REGISTRAR, ADMIN
Reserve a container	INV_RESERVE_CONATINER	ADMIN