Inventory Loader 9.0

Overview

Inventory Loader is an application to load information from ChemFinder databases into the Inventory Manager and Registration System databases.

ChemFinder databases may be created from many sources, most commonly SDFiles. SDFiles are the common currency of chemical information exchange today.

Inventory Loader may be run from any machine with access to the ChemOffice Enterprise application server.

Installation

Requirements

- MSXML 4
- ChemFinder 9.x

Instructions

1. Start the **InvLoaderSetup.exe** application.
2. Click **Next**.
3. Choose the directory where you would like the application files installed. The default is:

   C:\Program Files\CambridgeSoft\InvLoader
4. Click **Next**.
5. Choose the Start menu folder name for the shortcut to InvLoader. The default is

   InvLoader.
6. Click **Next**.
7. Choose whether or not to create a desktop icon for InvLoader.
8. Click **Next**.
9. Review the installation settings.
10. Click **Install**.

Usage

1. Start the Inventory Loader application.

   An introduction screen appears.
2. Click **Next**.
3. Enter the name of the ChemOffice Enterprise application server, your username, and your password.

   NOTE: *The username you use here must have sufficient privileges to add compounds to and create plates in the Inventory Manager system. If you want to register those compounds, you must have sufficient privileges on the Registration System.*
4. Click **Next**.

   NOTE: *If an error message appears saying no plate locations or plate formats are defined, you will have to configure at least one location in Inventory Manager to hold plates, and/or create at least one valid plate format. Consult the documentation for Inventory Manager.*
5. Browse to the ChemFinder database you want to load.
6. Select whether you wish to load compounds into plates, or just load compounds.

Loading Compounds into Plates

1. Click **Next**.

   NOTE: *If an error message appears saying "Cannot open database", you may need to upgrade the database to the current ChemFinder version. To do this, simply open the database within ChemFinder and follow the prompts.*

2. If more than one table is defined in the ChemFinder database, then you will see a drop down list of table names. Select the table that holds the data to be mapped. Typically, the table name is "MolTable".

   A table appears.

   The table's left column shows you the fields in Inventory Manager.

   The table's second column lets you choose to either enter a default value, or to pick a field from your Chemfinder database to insert into that field. If you choose Use Default, you can enter that default value in the 3rd column. The default is to leave the field blank.

3. Enter information for one or more fields. The following is an explanation of the fields:

Field Name	Field Description
Well Coordinate	the address of the well on the plate, e.g. "A02" or "H12"
Row	Row – the row of the well on the plate, either in letter or number format.
Column	the column of the well on the plate, in number format.
Reg Number	the CambridgeSoft registration number of the compound. You will generally leave this blank unless you are importing data from the Registration System into Inventory Manager.
Batch Number	the CambridgeSoft registration batch number of the compound. You will generally leave this blank unless you are importing data from the Registration System into Inventory Manager.
Barcode	the barcode of the plate. This is the barcode that will be used in Inventory Manager. If you leave this blank, Inventory Manager will assign new barcodes to the plates according to a scheme which you set up in a later screen.
Compound Name	an identifier for the compound.
CAS Number	the CAS number for the compound. Many screening libraries do not include CAS numbers.

Field Name	Field Description
ChemACX ID	the CambridgeSoft ChemACX id for the compound. Many screening libraries do not include ChemACX numbers.
Supplier	the supplier of the plate.
Supplier Barcode	the barcode assigned by the supplier to the plate. If you will be re-barcoding the plates upon import, you may assign the original supplier barcode to this field for tracking purposes.
Supplier Compound ID	supplier's identifier for the compound

The remainder of the fields should be self-explanatory.

NOTE: *You do not have to fill in all fields.*

Some notes on filling in this grid:

a. Either Well Coordinate or Row AND Column may be mapped to ChemFinder fields. It is not necessary to map both, and you don't have to do either, but if you map Row, you must map Column. If you map Well Coordinate, you shouldn't map Row or Column.

b. If your plates have identifiers, you should map that identifier to either Barcode, Supplier Barcode, or (if the plate identifier is numeric) to Supplier Plate Number. If you don't, you will receive a warning, and the compounds will probably not be plated according to your expectations.

c. If you map only Supplier Barcode, Supplier Plate Number, or Barcode, and you do NOT map Well Coordinate or Row AND Column, the compounds will probably not be plated correctly.

d. If you do not map ANY of: Supplier Barcode, Supplier Plate Number, or Barcode, Well Coordinate or Row AND Column, then the compounds will be put into plates in the order that they are encountered in the file. This is probably a rare scenario.

4. Click **Next**.
5. Choose the location where you want to create the plates.
6. Choose the plate format you wish to use. The plate format describes the size of the plate (96, 384 well), as well as the layout of the plates – where compounds are located, which wells are empty.
7. Choose the plate type you wish to create. The Plate Types list is an arbitrary list of types.

NOTE: *The number of compounds being imported and the number of plates to be created appears at the bottom of this screen. This is a good place to check if the results are what you expected.*

8. Click **Next**.
9. Choose the library to assign the plates to.

   This is an arbitrary list of classifications.
10. Enter how you want Inventory Manager to barcode your plates.

NOTE: *If you have mapped a ChemFinder field to Barcode in a previous screen, the Barcode section of this screen will be greyed out, indicating that the barcodes from your file will be used.*

11. Assign a starting group number for your plates if desired. This is rarely used.
12. Click **Next**.
13. If you want to register these compounds into the Registration System, check the box.

    Inventory Loader will validate your login against the registration system.

    If it succeeds, a grid containing the options for registering the compounds appears. You can choose what project, prefix and sequence to register the compounds with, as well as other options. For more documentation on what these choices mean, consult the Registration System documentation.

    a. If you want to assign fields to be filled in for the compound when it is registered, click Registration Options…
    b. A dialog appears, with a table similar to the one you used to assign inventory fields. Here you can choose default values or SDFile fields to assign to registration system fields.

NOTE: *Please note that the fields here are named as they are in the database, not as they are in the Registration System interface. The mapping between display name and database name may be found in C:\inetpub\wwwroot\chemoffice\chem_reg\config\cfserver.ini*

14. Click **Next**.
15. If you would like to save a log of the plates that were created in XML format, check the box and specify a path.

    This is usually not necessary unless you are experiencing problems.
16. Click **Next**.
17. Click **Finish** and the plates are imported. Each plate may take a while, as compounds are duplicate-checked and indexed for searching.

Import Compounds Only

1. A screen of inventory fields that can be mapped to ChemFinder fields appears. See step 3. on page 3 for more information.
2. Click **Next**.
3. Click **Finish**.