

Chemical and Biological Information System

User's Quick Guide

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Introduction

Welcome to Chemical and Biological Information System (CBIS). CBIS provides Web-based applications for managing chemical and biological materials and data.

Chapter 1. Compound Module

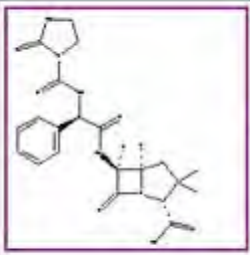
Compound module manages corporate compounds' structures and their properties. It allows you to search and view information in the compound database. This module also provides links to the Inventory, Assay, and other modules.

The **Compound** tab allows you to

- View compound structures and properties
- Sort the database by one or more fields
- Search the database by matching substructures or property data
- Register compounds into the database

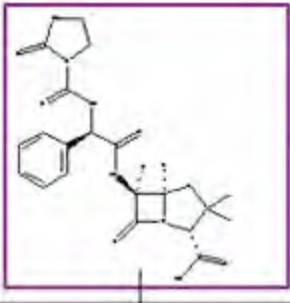
You can also perform the following tasks in the **Compound** tab,

- To view, withdraw, or deposit inventory batches
- To view or create assays

Compound ID	Structure	Name	Project Name	Formula	Mol Wt	Salt Forms	Inventory	Assays
CMP-000003		azlocillin	G-Protein	C ₂₀ H ₂₃ N ₅ O ₆ S	461.501696	sodium potassium	View Withdraw Deposit	View Create
							to view, withdraw or deposit batches	to view or create assays

1. Viewing Compound Structures and Properties

- To view a compound structure, click on the structure picture to open **Chemistry 4-D Draw** program
- To view a salt structure, click on the salt name in the **Salt Forms** column

Compound ID	Structure	Name	Project Name	Formula	Mol.Wt	Salt Forms
CMP-000003		azlocillin	G-Protein	C ₂₀ H ₂₃ N ₅ O ₆ S	461.501696	sodium potassium

click to view the details

click to view the structure

click to view salt structure

c. To view a compound's detail information

- Click the compound ID in the **Compound ID** column.
- Or click the **Compound Details** link. Use the Page Navigator buttons to see other compounds.



show / hide search and sort panel

page navigator buttons

2. Sorting the Database

You can sort the data table using one of the following methods:

- To sort the table by multiple fields, click the **Sort by** button. Select the fields to sort in the **Sort by** dialog box, specify the sort order (Ascending 123..., or Descending 987...) and click the '<' button. Click OK to sort the table
- To sort the table by a single field, click on the column header

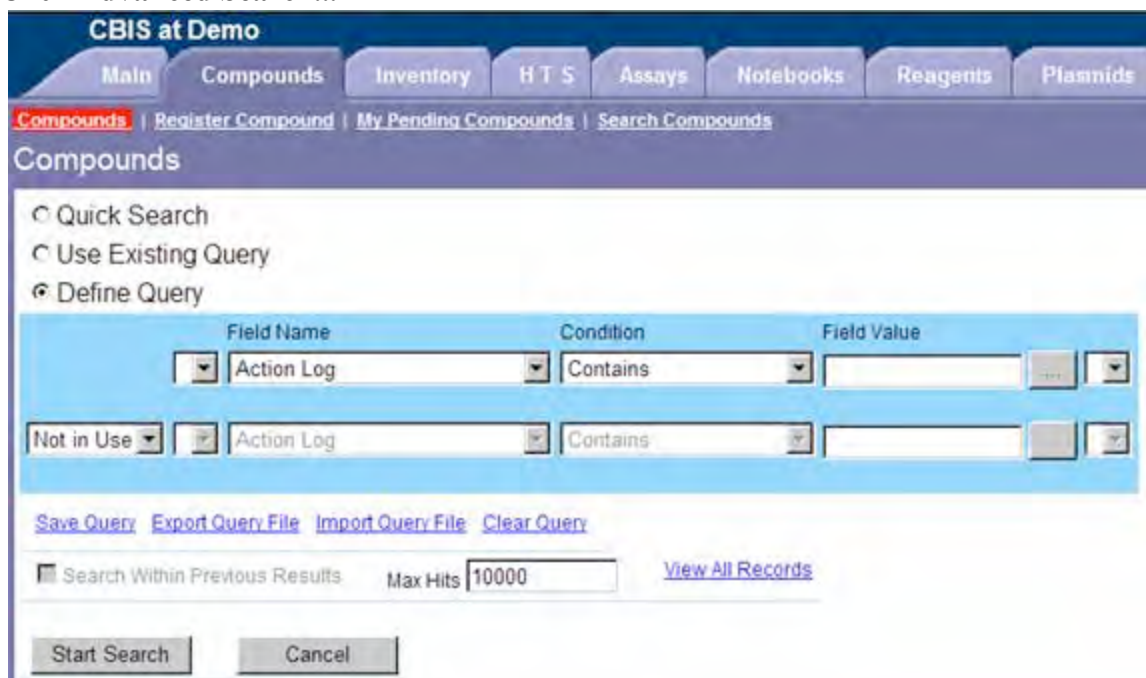
3. Searching the Database

You may search the database with a structure query, or a data query.

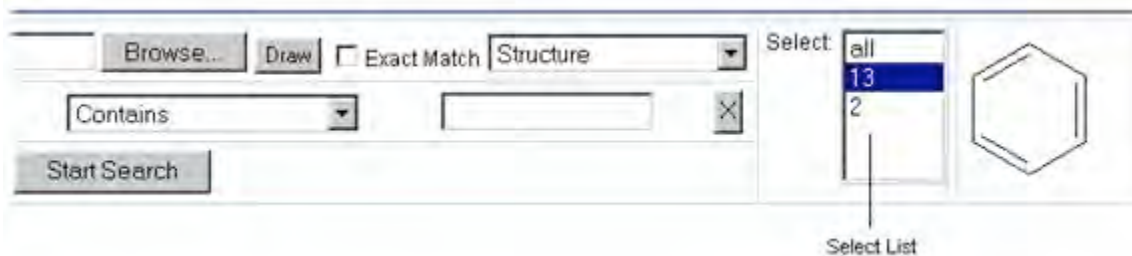


Enter data query and Click the **Quick Search** button to do a quick search.

Click **Advanced Search...** link



You can perform a filtering search on the results of prior searches by specifying the new query and clicking the **Start Search** button. Click an item on the **Select list** to view the result of the selected search step.

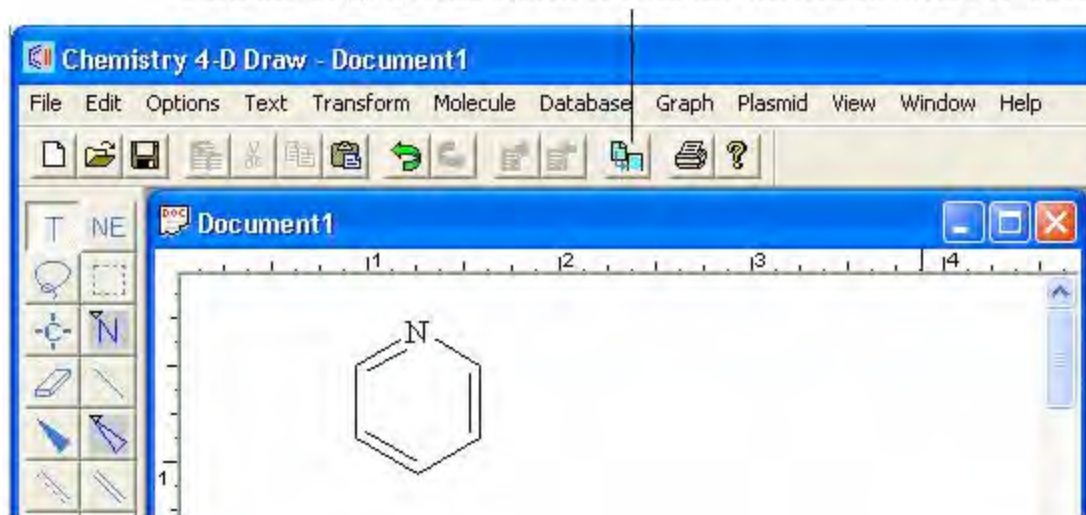


Specifying a Structure Query

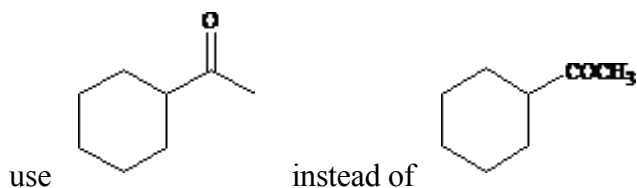
You can specify a structure query with one of the following methods:

- Specify a MOL file or CNS file (Chemistry 4-D Draw file) by clicking the **Browse** button and choose a file on your computer
- Send a structure to CBIS server directly from Chemistry 4-D Draw program by selecting the structure and clicking the **Copy Special** button. If Chemistry 4-D Draw is not running on your computer, click the **Draw** button to start the program.

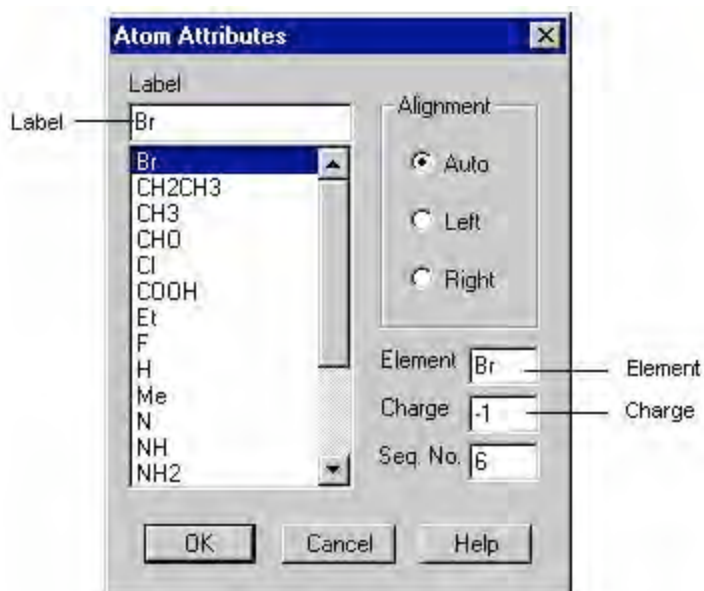
Click the **Copy Special** button to send the selected structure to CBIS



Important Note: Please expand all labels in structures before searching. For example:



In Chemistry 4-D Draw, please use the **Atom Label tool**  to set the charges, labels, and elements.



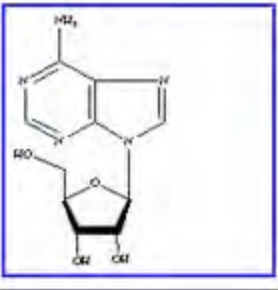
4. Registering a Compound

Before you register a compound, prepare the following:

- Structure of the compound (expand all labels) whose elements, charges, valences have been verified (using commands in the Molecule menu)
- Salt forms associated with the compound (structures, formulas and masses)
- Compound name and other properties

To register a compound:

- Click the **Registration** link
- Click the **Register Compound** button at the bottom of the page

Status	Action	Compound ID	Structure	Salt Forms	Name	Formula	Mol Wt	Project Name	Be Inf
Pending	Change Status	CMP-000013			adenosine	C10H13N5O4	267.245766		

Register Compound Register SD File

- In the **Structure** dialog box, specify the structure by

- Specifying a file with the **Browse** button (a MOL file or CNS file)
- Or sending a structure from Chemistry 4-D Draw. Click the **Draw** button to start the program if it is not yet started. Draw the structure, select it, and click the **Copy Special** button within Chemistry 4-D Draw. Go to the CBIS and click the **Paste Chem4D Structure** button

- d. Click the **Next** button to specify the properties; Please verify the formula and molecule weight carefully. Enter other properties and click the **Register Compound Only** button. The compound is now in the Pending area where only you (the owner) see the item

- e. Now salt forms can be registered. Click on the **Edit Salt Forms** link to add a new salt form, which is defined by structures of the compound and counter ions. Please verify that the salt form's formula and molecule weight carefully
- f. Continue to add other salt forms for the compound

- g. To promote the compound to the public database, click the **Change Status** link and set the status to “Approved”. The compound is now in the public area.

Chapter 2. Inventory Module

Inventory module tracks the amounts, locations and properties of compound batches.

The **Inventory** tab allows you to:

- View, search and sort batches
- Deposit a batch of vials. Print barcode labels for vials
- Submit a withdrawal request
- Approve requests and process withdrawals

Chemical and Biological Information System at [redacted]

Main | Compounds | **Inventory** | Plates | Assays | Reagents | Documents | Reports

Batches | Batch Details | Deposit | Withdrawal Request | Pending Withdrawals | Logs | Logout | Henry Li | 8/11/2002 9:02:43

Batches

Batch ID: [] Contains: [] Select: all

Sort By: [] Max Hits: 100 Start Search

page size: 10 |< |> Page 1 of 1 (6 records)

Compound ID	Batch ID	Amount	Original Amount	Unit	Available Amount	Location	Action	Analytical Data	Purity	Physical Form
CMP-000003	CMP-000003_0001	80	100	uL	80	Ryoka Urayasu Building:1st Floor	Remove Print COA Withdraw Print Label Logs	GC-MS test Tigloidine.cns	98%	Crystal

1. Viewing, Searching and Sorting Batches

You can view the detailed properties of a batch by:

- Clicking the batch ID in the **Batch ID** column
- Or clicking the **Batch Details** link. Use the Page Navigator buttons to see other batches' data

You can sort the data table by:

- To sort the table by multiple fields, click the **Sort by** button. Select the fields to sort in the **Sort by** dialog box, specify the sort order (Ascending 123..., or Descending 987...) and click the '<' button. Click OK to sort the table.
- To sort the table by a single field, click on the column header.

To search batches with a data query:

Select the field name, search operator (e.g. contains, starts with). Enter the value to search and click the **Start Search** button.

You can perform a filtering search on the results of prior searches by specifying the new query and clicking the **Start Search** button. Click an item on the **Select list** to view the result of the selected search step.

To search batches with a structure query:

Go to Compound module, search the compound database by matching substructure (see the Compound Module chapter). Then click the View link in the Inventory column. All batches containing the selected compound will be displayed in a table.

2. Depositing a Batch (Vials)

- Click the **Deposit** link, and then click the **Deposit Batch** button;
- Specify data of the batch;
- Click on **Edit Table** button to enter amounts;
- After all data are entered, click the **Register** button. The batch is now in the Pending area where only you (owner) can see the data;
- Click the **Print Label** link to print vial labels;
- Click the **Change Status** link to promote the batch to the public area (“Approved”).

Register Batch

Location : Specify...

Compound ID : Specify...

Salt Form : Specify...

Source Type : Specify...

Source : Specify...

Notebook Page :

Physical Form : Specify...

Color : Specify...

Analytical Data :

Purity :

Purity Method : Specify...

Unit :

Quantity :

Comments :

Please choose a location:

- [Kyoka](#)
- [Urayasu Building](#)
 - [1st Floor](#)
 - [RoomA](#)
 - [2nd Floor](#)
 - [3rd Floor](#)
 - [4th Floor](#)
 - [5th Floor](#)
 - [ChemCenter II](#)

Click + to expand
Click a link to select

Edit Table

Column Name	Vial ID	Amount
Row 1	1	200
Row 2	2	300

You may deposit a batch from Compound module by clicking (1) **Compounds tab** (2) **Compound link** (3) **Deposit/Inventory** link of the selected compound.

You may deposit a batch when you are registering a compound.

3. Submitting a Withdrawal Request

To submit a withdrawal request

- a. Click the **Withdrawal Request** link;
- b. Specify Compound and Batch ID, or use the barcode scanner to scan a vial label (Form the browser click the Barcode on Vial text box, scan the barcode. The program will fill in the form);
- c. Specify request amount, date;
- d. Click the **Submit Request** button. The owner of the batch will be notified of the request;
- e. To check the status of the request, click the Pending Withdrawals link.

Withdrawal Request	
Barcode on Vial	<input type="text"/> <input type="button" value="Scan"/>
Compound ID :	<input type="text" value="KOSN-000010"/> <input type="button" value="Specify..."/>
Batch ID :	<input type="text" value="KOSN-000010.0001"/> <input type="button" value="Specify..."/>
Date Required :	<input type="text" value="4/28/2002"/> <input type="button" value="Specify..."/>
Current Amount :	<input type="text" value="381"/>
Available Amount :	<input type="text" value="381"/>
Amount Requested :	<input type="text" value="23"/>
Unit :	<input type="text" value="mg"/>
Comment :	<input type="text" value="urgent please"/>
<input checked="" type="checkbox"/> Email Request to Owner : Mary Wang	
<input type="button" value="Submit Request"/> <input type="button" value="Cancel"/>	

You may submit a withdrawal request from the Compound module by clicking (1) **Compounds tab** (2) **Compound link** (3) **Withdraw/Inventory** link of the selected compound.

4. Approving a Withdrawal Request

If you are the owner of a batch, you can approve a request.

- Click the **Pending Withdrawals** link to check the requests that need to be approved;
- Click the **Change Status** link to approve or reject the request;
- The person who submitted the request will be notified of the status change.

While in the Pending Withdrawals page, you can also search a batch using the barcode on a vial. From the browser click the Barcode on Vial text box, scan the barcode. The program will display all requests of the batch.

5. Withdrawing Vials

Once a request has been approved, you can withdraw vials of the batch.

- Click the **Pending Withdrawals** link to view a list of requests that have been approved;
- Click the **Withdraw** link to record the withdrawal. Specify the amount for each vial;
- Click the **Withdraw** button to process the withdrawal.

Vial ID	Available Amount	Withdraw Amount
1	250	
2	500	

Click to specify vial amounts

Chapter 3. Assay Module

In addition to storing assay information and results, the Assay module provides data analysis tools for assays. You can optionally register raw experimental data of assays and view fitted response curves within CBIS.

The **Assays** tab allows you to:

- Register assays;
- Enter assay data or load data from files;
- Fit response curves and obtain EC50/IC50;
- View fitted response curve;
- View and search assay data;
- Build SAR (Structure-Activity Relationship) table;

Compound ID	Structure	Result Graph	Assay Type	Assay Name	Assay Target	Scientist	Notes/Other Page ID
CMP-000001	<chem>O=C(O)CC(c1ccccc1)(c2ccccc2)c3ccccc3</chem>		Cell proliferation/Cytotoxicity	MTT	NCIH460	Henry Li	

1. Registering an Assay

You can register an assay with or without experimental data (concentrations vs. measurements). However, if experimental data are available, you will be able to fit response curves and obtain IC50/EC50. Also, the fitted graph will be displayed and available for download in the assay table.

To register an assay:

- Click the **Registration** link;
- Click the **Register Assay** button;
- Specify assay information and results;
- If you want to enter multiple assays, select the **Multiple Assays** checkbox. Please note that with this option, you cannot load experimental data and store response curves in CBIS database;
- You can now load result data and fit a response curve, obtaining EC50 or IC50 data (see next section).

Edit Assay Data

Compound ID :	<input type="text" value="CMP-000003"/>	<input type="button" value="Specify..."/>
Batch ID :	<input type="text" value="CMP-000003.0002"/>	<input type="button" value="Specify..."/>
Scientist :	<input type="text" value="Henry Li"/>	
Notebook Page ID :	<input type="text"/>	
Project Name :	<input type="text" value="G-Protein"/>	
Assay Date :	<input type="text" value="8/11/2002"/>	<input type="button" value="Specify..."/>
Assay Type :	<input type="text" value="Cell proliferation/Cytotoxicity"/>	
Assay Name :	<input type="text"/>	<input type="button" value="Specify..."/>
Assay Target :	<input type="text"/>	<input type="button" value="Specify..."/>
Result Table :	<input type="text" value="(empty)"/>	
	<input type="button" value="Edit Table..."/>	
Result Value :	<input type="text"/>	<input type="button" value="Calculate..."/>
Result Type :	<input type="text" value="IC50"/>	
Value Prefix :	<input type="text"/>	
Result +/- :	<input type="text"/>	
Control 1 :	<input type="text"/>	
Control Value 1 :	<input type="text"/>	
Control 2 :	<input type="text"/>	
Control Value 2 :	<input type="text"/>	
Comments :	<input type="text"/>	

Click to load/input
result data

Multiple Assays

Click to input data for multiple assays

Edit Assay Data

Compound ID : Specify...

Batch ID : Specify...

Scientist : Henry Li

Notebook Page ID :

Project Name :

Assay Date : Specify...

Assay Type : Cell proliferation/Cytotoxicity

Assay Name : Specify...

Multiple Assay Result :

Assay	Target	Result	Value	Result	Type	Result	Error

 Edit Table...

Comments :

Process Cancel Multiple Assays

enter multiple assays

2. Loading or Entering Experimental Data

You can store experimental data (concentrations vs. measurements) in the database.

- Click the **Edit Table** button;
- Enter the data;
- Or click the **Browse** button to specify the data file. Click the **Read Table File** button. The input file is in tab-delimited format and can be created using Microsoft Excel.

Edit Assay Data

Edit Table

Column Name	Log C	Response1	Run 2
Row 1	-9	1000	1050
Row 2	-8	950	1000
Row 3	-7	750	800
Row 4	-6	500	600
Row 5	-5	400	350
Row 6	-4	100	150
Row 7	-3	50	60
Row 8			
Row 9			
Row 10			

Read Table File:

3. Fitting Result Data to a Response Curve

To fit a response curve

- a. Click the **Calculate** button;
- b. Specify curve fitting options (use the defaults if you are not sure):
 - Variable Slope – By default, CBIS automatically fit the response curve to either 1.0 or -1.0. Select this option if you want to allow the slope to be fitted to other values;
 - Fix Minimum at 0 – Whether to fit the curve so that the curve's minimum is 0 or to allow variable minimum;
- c. The fitted curve will be displayed, and EC50 or IC50 will be calculated.

Edit Assay Data

Response Curve Fitting Options:

Variable Slope

Fix Minimum at 0

Calculate Cancel

Edit Assay Data

Compound ID: CMP-000006 Specify...

Batch ID: CMP-000006.0001 Specify...

Scientist: Henry Li

Notebook Page ID: 12345-123

Project Name: G-Protein

Assay Date: 8/11/2002 Specify...

Assay Type: Cell proliferation/Cytotoxicity

Assay Name: ³H-thymidine Specify...

Assay Target: Primary Cells Specify...

Result Table:

Log C	Response 1	Run 2	Run 3
-9	0	250	
-8	250	150	
-7	50	350	
-6	750	500	
-5	1200	1150	
-4	1250	1150	
-3	1350	1250	

Edit Table...

Result Value: 1.319046E-06 Calculate... Click

You may register an assay for a compound from the Compound module by clicking (1) **Compounds tab** (2) **Compound link** (3) **Create/Assays link** of the selected compound.

4. Building and Downloading SAR Table

You can create an SAR (Structure-Activity Relationship) table for assays for a list of compounds by clicking on the **Show SAR Table** on the Assays page. The table summarizes results for selected compounds and assays. Data can be downloaded by clicking on the Download Table link.

Chapter 4 Notebooks Module

CBIS E-Notebook allows your company to store experimental procedures and data in the database while meeting FDA requirements for maintaining hardcopy documents. You can search the structures, sequences, experimental conditions and other fields in the notebook databases. You can also quickly create a new experiment by using an existing notebook page as a template.

CBIS Notebooks module manages different formats of E-Notebook. The current installed format is designed for organic reactions. (Please ask your CBIS administrator about other installed Notebook formats). This format of E-Notebook allows users to record reactions and print hardcopies for maintaining physical notebooks.

The **Notebooks** tab allows you to:

- Create and edit notebooks
- Create and edit notebook pages
 - a. Create a new reaction
 - b. Copy an existing reaction
- Record reactions
 - a. Store reaction schemes
 - b. Specify reactants, solvents, products
 - i. Equivalents
 - ii. Molarity
 - iii. Percent purity
 - iv. Density
- Calculate reactions
 - a. Required amounts or volumes for reactants and solvents
 - b. Expected product amounts
 - c. Percent yield
- Search and sort notebook pages
 - a. Search structures in reaction schemes, reactants, products
 - b. Search data associated with the reactions
- Download and view reactions

A notebook in CBIS has a corresponding physical notebook. Notebook pages are printed on papers and glued to a bound notebook for keeping physical record.

1. Registering a Notebook

To register a notebook:

- a. Click the **Register Notebook** link;

- b. Click the **Register Notebook** button;
- c. Specify notebook information; You may change the Notebook ID. CBIS will check that the ID is unique in your company;
- d. Click the Register button.

You then change the status of the notebook to “Approved” by clicking the **Change Status** link.

2. Registering a Notebook Page

To add a page to a notebook, you must first create a notebook. You may add pages only to your own notebooks.

To register a notebook page:

- e. Click the **Register Page** link;
- f. Click the **Register Page** button;
- g. Specify notebook page information;
- h. Click the Register button.

You are now in the Edit Notebook page. Use the following steps to enter reaction information:

a. Reaction Scheme

Click the **Specify** link to paste a reaction scheme from Chemistry 4-D Draw (or use Browse button to import a CNS file). CBIS will interpret the reaction scheme by finding an Arrow. Structures on the left side and above the arrow are reactants (CBIS can also be configured to recognize reactants or solvents below the arrow). Products molecules are on the right side.

Notes: By default, whenever you import a new reaction scheme, all existing reactants and products of the editing page will be deleted. It is possible to configure CBIS to keep existing information.

b. Reactants

After the reaction scheme is imported, reactants and products are added to the tables automatically. You can add or delete reactants. You must specify the limiting reagent, MW, equivalents of reactants.

For liquid reagents, you need to specify molarity or density.

c. Solvents and Other Reagents

Notes: Depending the configuration of CBIS at your company, there may not be a table for Solvents and Other Reagents.

To calculate the required solvents and reagents, you need to specify the concentration for the

limiting reagent and Wt. / Vol. Multiplier. Enter the volume ration for each solvent. Enter either the Wt or Vol for other chemicals. CBIS will calculate the required amounts and volumes automatically.

d. Products

Enter the MW and actual amount for the product. CBIS will calculate the expected amount and percent yield.

After you have finish editing a notebook page, you can promote it to Approved by using the **Change Status** link.

3. Searching and Sorting Notebook Pages

Please see the Compound Module chapter for general procedures for searching and sorting databases.

You may search structures in reaction schemes, reactants and products.

4. Viewing and Printing Notebook Pages

In the Notebook Pages tab, the Notebook Tree on the left side lists notebook pages in your company by:

- a. Types of notebook (e.g. reactions or assays)
- b. Scientists
- c. Notebook

You can click on Page Details link to view one page at a time.

To print a page, click on the Print link. Then use the File | Print command on your browser to print the current page.

Chapter 5 HTS Module

CBIS HTS module allows your company to automate High-Throughput Screening experiments. CBIS provides all the features and tools for HTS:

- Manage plate inventory
- Reformat plates
- Primary screens
 - i. Prepare plates
 - ii. Data loading and analysis
 - iii. Well invalidation
 - iv. Hits identification
- Secondary screens
 - i. Plate preparation
 - ii. Data loading and analysis
 - iii. Point invalidation
 - iv. Response curve fitting
 - v. Create assays

Definitions:

Plate – Plates are containers of wells for measuring many compounds' bioactivity in a single run. Plates come with the sizes of 96, 384 and 1536 wells.

Well – Wells are small containers in a plate that contain solutions. Each well has a coordination of (Row-Col). E.g. B08 stands for second row, eighth column.

Primary Screen – Measurement of one or more plates of compounds to determine “hits” or active compounds. The definition of “hits” is based on comparing activity measurements to that of a reference compound. User can control the threshold (percent activity).

Secondary Screen – HTS runs to create the response curves for a group of compounds. The compounds' IC50 or EC50 are determined from the curves.

CBIS-HTS helps you to manage HTS plates and data. The program tracks compounds, batches, wells, plates, parent plates, plate reading, plate data, hit list, assay lists all through the simple web interface. CBIS automatically consolidates data from multiple plates and perform primary screen analysis by calculating averages, std err. The hit lists are identified by the user controllable percent efficacy of the reference compound.

Secondary screens are performed with either one plate or more plates simultaneously. The response curves are fitted and displayed on the screen. Users can invalidate points (ignore some out-of-place points during curve fitting) on the curves. The resulting data can be transferred to Assays module automatically where SAR tables can be built with a single click.

1. Registering HTS Plates

You can register plates in two ways:

A. Compounds/Plates purchased from a supplier

You will receive the compounds and plates in SDF format. To register the compounds and plates, you must login as Admin or a user with “admin” privilege. Because the number of compounds imported may be in tens of thousands, you must backup the SQL database before importing an SDF file.

1. Go to Compounds module, click Registration link. Click the Register Plate File button. Browse in the SDF file and click the Next button.

If the SDF file is too large, you will receive an error. You need to copy the SDF file to the C:\Program Files\ChemInnovation\Cbis\temp directory. Enter the file name without path.

2. In the form, specify:

Location : where the HTS plates will be stored
Plate Size : 96 Wells
Source : Name of the supplier
Amount : Volume of wells (e.g. “400”)
Unit : uL
Concentration in M (e.g. “5e-3”)
Non-Stop : Yes
Pre-Approved Yes

Click the Register button. You will see the progress page which refresh every 15 seconds. Wait until the job is completed. Click the Done button.

All the compounds in the SDF file are not registered. The plates are also registered.

3. Go to the HTS module, click the Registration link. Click the View Details button. Click the Show Compound Name checkbox. Verify that the plates have the correct compounds and concentrations.

Click the Registration link. Click the Approve All My Plates button to update all plates that have been imported by you to the public area.

B. Build new plates using compounds from the company inventory

You can define a new plate for different usages:

- (1) Storage – Storage plates can be used to build new plates by dilution and/or

reformatting.

- (2) Primary Screen – Each well on a plate contain a compound. The concentrations of all compounds in a plate are the same. There are a few wells for holding the reference compound.
- (3) Secondary Screen - Each plate contains a set of compounds with various concentrations so that the measurement can be used to fit a response curve.

A new plate can be defined and the compounds on the wells can be specified one by one after selecting the “Edit” checkbox.

A pre-defined plate can also be imported via Excel files.

C. Reformatting Plates

Depending on the plate reader a company has installed, it may be necessary to reformat plates. CBIS allows you to reformat plate easily by selecting the original plates and target plates. E.g. four 96-well plates can be used to build a 384-well plate.

To define a new format, select the size from the New Plate dropdown. Then select the source plates.

Chapter 6 Documents Module

Documents module manages all types of corporate documents (Word, PowerPoint, PDF, GIF, etc) and their information such as title, author, date, abstract, keyword.

The **Documents** tab allows you to:

- Register documents
- Search and sort documents
 - a. Search data associated with the documents
 - b. Search text within the documents
 - c. Search Structures within the documents
- Download and view documents

The screenshot shows the 'Chemical and Biological Information System at Ryoka' interface. The 'Documents' tab is active. The search area includes a 'Query File' field, a 'Browse...' button, a 'Draw' button, and an 'Exact Match' checkbox. There are also dropdown menus for 'Document ID' and 'Contains', and a 'Start Search' button. The results table is as follows:

Title	Author	Project	Date	Key Words	Abstract	Action
CBIS Features	Admin Cbis	G-Protein	8/2/2002	Cheminformatics, Bioinformatics, Word document	CBIS provides a full suite of Web-based applications for managing chemical and biological materials and data throughout their lifespan	View
CBIS Presentation	Admin Cbis	DNA Cloning	8/2/2002	PowerPoint File	This is a sample PowerPoint file stored in CBIS. The file can be opened from the Web. The content can be searched.	View

1. Registering a Document

To register a document:

- i. Click the **Registration** link;
- j. Click the **Register Document** button;
- k. Specify document information;
- l. Click the Register button.

2. Searching and Sorting Documents

Please see the Compound Module chapter for general procedures for searching and sorting databases.

In addition to search data associated with the documents, you may search text (keywords) within the documents. Further more, if there documents contain structural information (such as .CNS files or MOL files), you can perform substructure search.

Chapter 7 Reports Module

Reports module manages project reports or monthly reports. It stores report information such as title, results, conclusions, and short term plans. You can attach files to a report. You can also add references to compounds and assays within CBIS.

The **Reports** tab allows you to:

- Register reports
- View, sort reports
- Search reports
 - a. Search data in a report
 - b. Search attached documents
 - c. Search referenced compounds
 - d. Search referenced assays

Title	Reported By	Date	Project Name	Objectives	Results	Conclusions	Short Term Plans	Reference Compounds	Reference
Solvent Effect the Asymmetric Epoxidation	Henry Li	8/12/2002	G-Protein	The study of the solvent effec...	EtOEt 6.3% ee, CH ₂ Cl ₂ 41%ee	Higher optical yield in non hydrogen acceptor solvent.	Test different solvents: CHCl ₃ , EtOH	CMP-000003	Name: SRB Re: 1:0E

1. Registering a Report

To register a document:

- a. Click the **Registration** link;
- b. Click the **Register Report** button;
- c. Specify information;

2. View, Searching, and Sorting Reports

You can view the detailed reports by:

- Clicking the **ReportDetails** link. Use the Page Navigator buttons to see other reports

You can sort and search the report:

- Please see the Compound Module chapter - Searching the Database and Sorting the Database

Chapter 8 Tutorials

Tutorial Lesson 1 Registering a Compound and Its Salt Forms

Select the **Compounds** tab to open the Compounds page.
Select the **Registration** link to open the Pending Compounds page.
Click on the **Register Compound** button to register a compound.

Structure: Click on the **Browse** button, select the file *c:\Program Files\cheminnovation\chem4dd\samples\tutor1.cns*, and click the **Next** button.

*Or, click the **Draw** (PC only) button.*

*In the **File Download** dialog box, select the “Open this file from its current location”, and then click **OK** button.*

*Chemistry 4-D Draw drawing program is started. The **NE** tool is selected.*

Move the curser to the center of the screen and click the mouse button.

Type: benzoic acid

Press the <Enter> key. The chemical structure of benzoic acid appears on the screen and is selected.

*Click the **Copy Special**  button.*

*Go to CBIS Browser; click the **Paste Chem4D Structure** (PC only) button.*

Compound ID: CMP-000010
Formula: C7H6O2
Mol Wt: 122.12424200

Please check the formula and molecular weight.

Name: Click the **Assign** button.
Other Names: Click the **Edit Table** button, type “benzenecarboxylic acid”, click the **Add Data** button, and then the **Done** button.
Project Name/PI: Click the **Specify** button, select G-Protein from the list, and click the **OK** button.
Background Info: Description: NMR
Data File: *c:\Program Files\cheminnovation\chem4dd\samples\tutor1.cns*

Now click the **Add Data** button and then the **Done** button.

Key Words: Click the **Specify** button. Select the aromatic from the list and click the **OK** button.

Comments: Type none

Click the **Register Compound Only** button.

The above compound is now in the Pending status.

*If you wish to make any changes, click the **Edit** link in the **Action** column.*

Next, add a salt form using the following procedures.

Click the **Edit Salt Forms** link of CMP-000010 in the **Action** column.

Click **Add Salt Form** button.

Structure: Click the **Browse** button, select the file *c:\Program Files\chem4dd\samples\tutor1s.cns*, and then click the **Next** button.

Description: Type *Sodium*
Formula: $C_7H_5O_2Na$
Mol Wt: 144.1060360

Please check Formula and molecular weight and make any change.

Click the **Add** button.

You may repeat the same procedures to add other salt forms of CMP-000010.

Now Click the **Change Status** of CMP-000010 in the **Action** to open the **Update Compound** page.

Compound ID: CMP-000010
Name: benzoic acid
Registered by: Henry Li
Registration Status: Select **Approved**
Comment:

Click the **Update** button.

You have successfully registered a compound and its salt into the database.

(End of Tutorial Lesson 1)

Tutorial Lesson 2 Depositing a Batch of Vials

Click the **Inventory** tab to open the **Inventory** page.

Click the **Deposit** link to open **Pending Batches** page.

Click the **Deposit Batch** button to open the **Register Batch** dialog page.

Location: Click **Specify** button and select Ryoka/Urayasu Building/1st Floor/Room A.

Compound ID: Click **Specify** button, select CMP-000010 the list, and click the **OK** button.

Salt From: Click on the **Specify** button, select sodium from the list, and click **OK** button.

Source Type: Select In-house from the list.

Source: Type Chemical Group

Made By: Type Henry

Notebook Page: Click the **Edit Table** button
Notebook Page: Type 12345-123
(the format is #####-####).

Click the **Add Data** button and then the **Done** button.

Physical Form: Click the **Specify** button, select Crystal from the list, and click the **OK** button.

Color: Click the **Specify** button, select White from the List, and click the **OK** button.

Analytical Data: Click the **Specify** button
Method: Select HPLC trace from the list
Comment:

Data File:
Click the **Add Data** button and then the **Done** button.
Purity: Type: 100%
Purity Method: Click the **Specify** button, select HPLC trace from the list, and the **OK** button.
Unit: Select mg from the list.
Quantity: Click the **Edit Table** button.

Row 1
Vial ID: 1
Amount: Type 100

Click **Add Row** button to add Row 2

Row 2 :
Vial ID: 2
Amount: Type 50

If you want to delete a row, select the checkbox at the end of the row and click Delete Row/Column button.

Click the **Update** button

Comment: None

Click the **Register** button

The batch is now in the Pending status.

*If you want to make any changes, click the **Edit** link in the **Action** column*

Click **Change Status** link in the **Action** column to open the **Update Container** page.

Registration Status: Select Approved
Click the **Update** button.

You have deposited a batch of two vials.

(End of Tutorial Lesson 2)

Tutorial Lesson 3 **Withdrawing a Batch the Inventory**

Click the **Withdrawal Request** link to open the **Withdrawal Request** page.

Barcode on Vial:
Compound ID: Click the **Specify** button, select CMP-000003 from the list, and click the **OK** button.
Batch ID: Click the **Specify** button, select the CMP-000003.0001 from the list.
Date Requested: Click the **Specify** button, select a date, and click the **Select** button.
Amount Requested: Type 20
Comment: none
Checked Email Request to Owner: Admin Cbis.

If the Owner is yourself, you may uncheck the Email Request

Click the **Submit Request** button.

Now your withdraw request is waiting for the approval of Admin Cbis.

Admin Cbis receives an e-mail of the request.

*He logins his account. Click the **Inventory** tab and then the **Pending Withdrawal** link. Click the **Change Status** in the **Action** column of Batch ID CMP-000003.0001 to open the **Update Request Status** page.*

Change the status to Approved

*Check Email Request to Requester:
Click the **Update** button.*

You will receive an email from Admin Cbis notifying the approval. Click the **Inventory** tab and then **Pending Withdrawals** link.

Click the **Withdraw** link in the **Action** column of **Batch ID** CMP-000003.0001.

Click the **Edit Table**

Row 1
Withdraw amount: Type 20

Click the **Update** button and then **Withdraw** button.

You have successfully withdrawn a vial from the inventory.

(End of Tutorial Lesson 3)

Tutorial Lesson 4 Registering an Assay

Click the **Assays** tab to open the **Assays** page.

Click the **Registration** link to open the **Pending Assays** page.

Click on **Register Assay** button to open **Edit Assay Data** dialog page.

Compound ID: Click the **Specify** button, select the CMP-000010 from the list, and click on **OK** button.

Batch ID: Click the **Specify** button, select the CMP-000010.0001 from the list and click **OK** button.

Notebook Page ID: Type 12345-123 (the format is #####-###)

Project Name: Select G-Protein from the list.

Assay Date: Click the **Specify** button and then the **Select** button.

Assay Type: Select MIC from the list.

Assay Name: Click the **Specify** button, select the MTT from the list, and then click the **OK** button.

Assay Target: Click the **Specify** button, select the SF-268 from the list, and click **OK** button.

Result Table: Click the **Edit Table** button to open the **Edit Table** page.

You may enter the data to the table or click **Browse** button to browse your existing data file: *c:\Program Files\cheminnovation\chem4dd\samples\assay1.txt*, click the **Read Table File** button, and then **Update** button.

Result Value: Enter the data, or click the **Calculate** button, then select Variable Slope or Fix minimum at 0, and click the **Calculate** button.

Value Prefix: >

Result Type: Select IC50 from the list.

Result +/-: Enter the data

Control 1:

Control Value 1: Enter the data

Control 2:
Control Value 2:
Comments:

*If you want to enter multiple assays, click the **Multiple Assays** checkbox, and then click **Edit Table** button to enter data.*

Click the **Process** button.

The assay is now in the Pending status.

*If you want to make any changes, click the **Edit** link in the **Action** column*

Click **Change Status** link in the **Action** column to open the **Update Assay** page.

Registration Status: Select Approved

Click the **Update** button.

You have registered an assay.

(End of Tutorial Lesson 4)

Tutorial Lesson 5 Registering a Notebook and a Notebook Page

Select the **Notebooks** tab to open the Notebooks page

1 Registering a Notebook

Select the **Register Book** link to open View Pending Notebooks page.

Click the **Register Notebook** button to open the Register Notebook page.

Notebook ID: NB-00004

Scientist: Click the **Specify** button, select the scientist from the list, and click the **OK** button.

Title: Type: Enkephalin Analogs
 Description: Type: Design and synthesis
 Click the **Register** Button.

Now the notebook NB-00004 is in the Pending status.

Click **Change Status** link in the **Action** column to open the **Update Notebook** page.

Registration Status: Select Approved

Click the **Update** button.

You have registered a notebook.

2. Registering a Page

Select the **Register Page** link to open the **Pending Notebook Pages** page.

Click the **Register Notebook Page** button to open the Register Notebook Page dialog box.

Notebook ID: Click the **Specify** button, select NB-00004 from the list, and click the **OK** button.

Template Reaction: None

Scientist: Click the **Specify** button, select a scientist from the list, and click the **OK** button.

Project Name: Select G-Protein from the list.

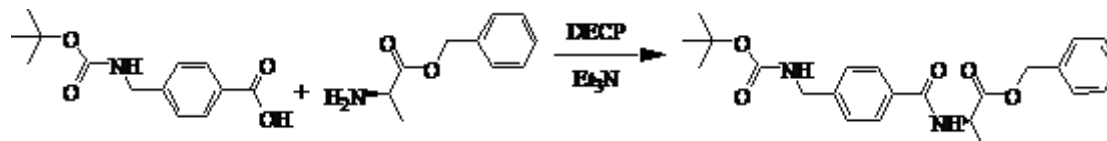
Title: Type: Synthesis of Boc-PAMB-Ala-Obz

Comment:

Click the **Register** button to go to Edit Notebook Page.

Reaction: Click the **Edit** button, then click the **Draw** button to open the **Chemistry 4-D Draw** Program.

 In Chemistry 4-D Draw program, draw the following reaction scheme:



click the **Specify Copy**  button.

Return to CBIS, click the **Past Chem4D Structure** button.

Reactants:

Click the first **Edit** button

Name: type Boc-PAMB-OH
Formula: C13H17NO4
Limiting: Check the box.
Formula Mass: 251.28
Mol Wt: 251.28
Amount: Type: 0.20

Click the **Update** button.

Click the second Edit button.

Name: Type: H-Ala-OBz
Formula: C10H13NO2
Formula Mass: 179.22
Mol Wt: 179.22
Eq: Type: 1

Click the **Update** button

Click the **Edit** button of DECP

Eq: type: 1.2

Click the **Update** button.

Click the **Add** button of Reactants

Name: Type: triethylamine
Formula: Type C6H15N
Eg: Type: 1.5

Click the **Update** button

Products:

Click the **Edit** button.

Name: type Boc-PAMB-Ala-OBz
Actual(g): type: 0.28

Click the **Update** button.

Solvent

Click the **Edit** button

Type: DMF 5 ml

Click the **Update** button

Procedures

Click the **Edit** button and type:

Boc-PAMB-OH and H-Ala-Obz were dissolved in DMF. DECP and then triethylamine were added dropwise. The mixture was stirred at 0°C for 30 mins and then at 25°C for five hours. Water (5 ml) and ethyl acetate (15 ml) were added. The organic phase was

Click the **Update** button.

Analytical Data

Click the **Edit Table** button.

Method: Select Melting Point from the list

Comment: Type 106-109 °C

Click the **Add Data** button.

Method: Select 1H NMR from the list.

Date File: Click the **Browse** button to select the file.

Click the **Add Data** button.

Click the **Done** button.

Click the **Done** button

Now the notebook page NB-00004.001 is in the Pending status.

*If you want to make any changes, click the **Edit** link in the **Action** column*

Click **Change Status** link in the **Action** column to open the **Update Notebook Page** page.

Registration Status: Select Approved

Click the **Update** button.

You have registered a notebook page.

Tutorial Lesson 6 Registering a Document

Select the **Documents** tab to open the Documents page.

Select the **Registration** link to open the Pending Documents page.

Click on the **Register Documents** button to open Register Document dialog page.

Document ID: 100008
Title: Type: Peptide I Analogs
Author: Click the **Specify** button, select Henry Li from the list, and click the **OK** button
Project Name: Select G-protein from the list
Date of Creation: 8/11/02
Key Words: Type: Enkephalin, Peptide T
Abstract: Click the **Edit** button. Type:
This document details the design and synthesis of an analog of peptide T, an inhibitor of human immunodeficiency virus infection.....
Click the **OK** button.

Comments:
File Data: Click the **Browse** button to find C:\Cheminnovation\sample\test.txt. Click the **OK** button

The document is now in the Pending status.

*If you want to make any changes, click the **Edit** link in the **Action** column*

Click **Change Status** link in the **Action** column to open the **Update Document** page.

Registration Status: Select Approved

Click the **Update** button.

You have registered a document.

(End of Tutorial Lesson 6)

Tutorial Lesson 7 Registering a Report

Select the **Reports** tab to open the Reports page.

Select the **Registration** link to open the Show Pending Reports page.

Click on the **Register Report** button to open Create Report dialog page.

Author: Henry Li

Date: 8/12/02

Project Name: Select G-Protein from the list

Title: Type: Solvent Effect....

Objectives: Click the **Edit** button, Type:

The study of the solvent effect on the asymmetric epoxidation of allylbenzene with....

Click the **OK** button

Results: Click the **Edit** button. Type:

EtOEt 6.3%ee, CH₂Cl₂ 41%ee

Click the **OK** button.

Conclusions: Click the Edit button. Type:

Higher optical yield in non hydrogen acceptor solvent.

Click **OK** button.

Short Term Plan: Click the **Edit** button. Type:

Test different solvents: CHCl₃, EtOH

Click the **OK** button.

Reference Compounds: Click the **Edit Table** button, then **Specify** button, select CMP-000003 from the list, click the **Add Data** button, and then **Done** button.

Reference Assays: Click the **Edit Table** button, then **Specify** button, select CMP-000003.0001 from the list, click the **Add Data** button, and then **Done** button.

Attachment: Click the **Edit Table** button.

Description: Type: Solvent Effect Table 1

File Data: Click the **Browse** button.
Select file: C:\cheminnovation\sample\test.txt
Click the **Add Data** button and then **Done** button

Click the **Create** button.

The report is now in the Pending status.

*If you want to make any changes, click the **Edit** link in the **Action** column*

Click **Change Status** link in the **Action** column to open the **Update Report** page.

Registration Status: Select Approved

Click the **Update** button.

You have create a report.

(End of Tutorial Lesson 7)

Tutorial Lesson 8 HTS Primary Screen

A. Registering Compounds and Plates

Select the **Compounds** tab
Select the **Registration** link
Click on the **Register Plate File** button

In the Register SD Compounds and Plates form, specify

SD File:	P0305.sdf
Plate Location:	Pick a location
Plate Size:	96
Source:	ChemInnovation (the name of the supplier of plates)
Amount:	400
Unit:	uL
Concentration:	5e-3
Amount:	400
Non-Stop:	Yes
Pre-Approved:	Yes

Click the Register button. Wait until job finishes. Click the Done button.

The compounds are now in the Approved status. The plates are in Pending status.

Select the **HTS** tab
Select the **Registration** link
Click on the **View Details** button to verify compounds and concentrations are correct.

Select the **Registration** link
Click **Approve All My Plates** button to change plates' status to Approved.

B. Defining a Plate for Primary Screen

Select the **HTS** tab
Select the **Registration** link
Click on the **Register Plate** button

In the Register Plate form, specify

New Plate:	96->96
------------	--------

Parent Plate ID: Pick the ID of the plate created in the previous step
Dilution Factor: 100 (new wells' concentration is $5e-3M \times 0.01 = 5e-5M$)
Location: Pick a location for the plate will be stored
Plate Type: Primary Screen
Amount: 10
Unit: uL

Click the **Next** button. Verify that the compounds and concentrations are correct for all wells.

Select the "Edit" checkbox. Click the Draw button of the following wells to specify blank and reference compound's wells. Ignore BatchID and Concentration.

A1, B1, C1, D1 Click Draw, then enter "Blank"
A12, B12, C12, D12 Click Draw, then enter "RefCmp"

Click the **Register** button.

Change status to Approved.

C. Defining a Primary Screen Job

Select the **HTS** tab
Select the **Register Primary** link
Click on the **Register Job** button

In the Register Primary Screen form, specify

Job Name: AC-1-020922-01 (User initials, 1 for primary, date, number)
Project Name: Choose a project
Assay Type: MIC
Assay Name: Tube-dilution Method
Assay Target: H. influenzae ATCC9006
Plate: Pick the plate defined in the previous step
Plate Data File: PrimaryReading1.xls

Click the **Next** button. Verify that the compounds and readings are correct for all wells.

Click the **Next** button. Specify:

Blank: Blank

Reference: RefCmp

Click the **Process** button. You have registered a primary screen job.

D. Determining Hits in Primary Screen

Select the **HTS** tab

Select the **Register Primary** link

Click the **Primary Screen** link in the Action column for the Job defined in the previous step.

In the Primary Screen form, specify

Hit Criteria: 95

Click the **Find Hits** button

Click the **Update** button. Click the **Done** button.

Click the **Hit List** link to download the hit list. Keep the list opened (in Notepad) and you will need to use the list for secondary screen in the following step.

You have finished a primary screen study.

(End of Lesson 8)

Tutorial Lesson 9 HTS Secondary Screen

A. Defining a Plate for Secondary Screen

Select the **HTS** tab

Select the **Registration** link

Click on the **Register Plate** button

In the Register Plate form, specify

New Plate:	New from Vials
Location:	Pick a location for the plate will be stored
Plate Type:	Secondary Screen
Amount:	10
Unit:	uL

Click the **Next** button.

In the Compounds tab, specify

Number of Points:	7
Start Concentration:	1e-9
Compounds:	(Copy 5 compounds from the Hit List in the previous step and Paste them into the text area, one per line). E.g CMP-000026 CMP-000046 CMP-000054 CMP-000056 CMP-000060

Click the **Next** button. Verify (using the Compound, Concentration checkbox) that there are 5 compounds, two curves for each compound, 7 points for each curve.

Click the **Register** button.

Change the status to Approved.

B. Defining a Secondary Screen Job

Select the **HTS** tab

Select the **Register Secondary** link

Click on the **Register Job** button

In the Register Primary Screen form, specify

Job Name: AC-2-020922-01 (User initials, 2 for Secondary, date, number)
Project Name: Choose a project
Assay Type: MIC
Assay Name: Tube-dilution Method
Assay Target: H. influenzae ATCC9006
Plate: Pick the plate defined in the previous step
Plate Data File: SecondaryReading1.xls

Click the **Next** button. Verify that the compounds and readings are correct for all wells.

Click the **Next** button. Choose the last compound as Reference (leave Blank field empty).

Click the **Process** button.

C. Performing a Secondary Screen Study

Select the **HTS** tab

Select the **Register Secondary** link

Find the job defined in the previous step and click the **Secondary Screen** link.

You can now see the five fitted curves and the resulting IC50 or RC50. (For actual experiment, a scientist can invalidate bad points by selecting the “Invalidate” checkbox).

Click on the Process Assays button.

Select the **Secondary Screen** link. Find the job you have just completed, and click on the list of assays (under the Result Assays column).

You will see five curves that have been added to the Assays module.

(End of Tutorial Lesson 9)

Glossary:

Salt Form

Compound structure and counter ions

Amount

Sum of vial amounts

Available Amount

Available Amount = Batch amount – Request amount

Special Considerations While Using Web-based Applications

1. Avoid using the “Back” button of your browser. Otherwise, the form you see may not represent the actual status of your data; Use the links and buttons on the pages instead.
2. Avoid leaving an input form with your data “unattended”. A session may time-out and you may lose your data. Click the Submit button before going to a meeting.
3. Do not click the Submit button again while waiting for a response.