

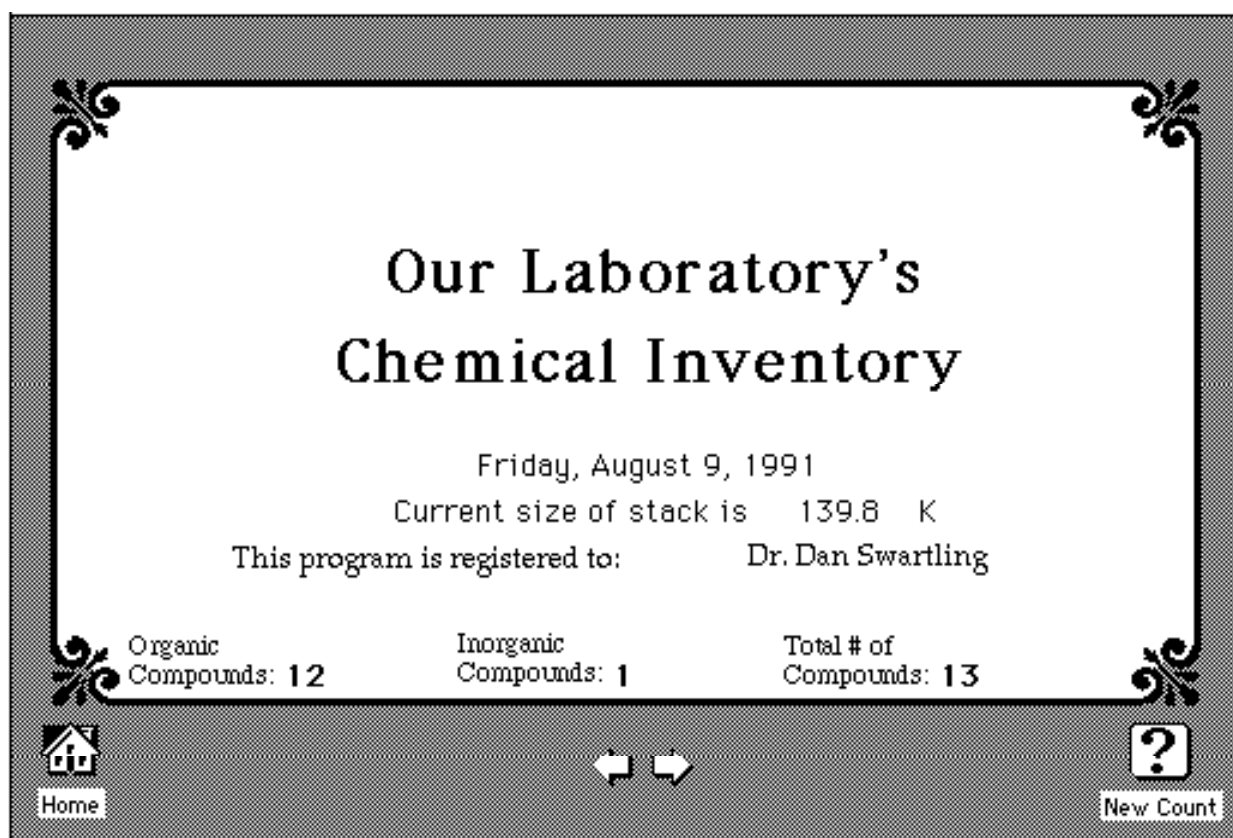
Chemical Inventory 2.2

the Hypercard™ chemical database program

This stack was written to keep track of a large chemical inventory, and it operates as if it were a large collection of 3 by 5 inch index cards. It was designed to be as simple to use as possible, assuming very little computer knowledge on the part of the user. It requires the use of System 6.0.5 or greater and Hypercard 2.0 or greater.

A Brief Overview of Features

Before using the stack you should copy it to your hard disk or to another floppy disk and keep the original in a safe place. To start the program, place the mouse arrow over the stack icon and double-click the mouse. This will open HyperCard and take you to the top card of the stack. Before you can proceed for the first time you must enter your name as you wish it to appear on the screen. The screen will appear as shown below:



When the stack is first opened, you will see the current date and the current size of the database. You will also see the number of organic compounds, inorganic compounds, and total number of chemicals indexed. The functions that appear on the top card are as follows:

Home - If you click here with the mouse, it quits the current application and takes you to the home stack.

Left Arrow - Click here to go to the last card in the stack.

Right Arrow - Click here to go to the first card in the stack.
New Count - Click here after entering new compound data and it will determine how many organic and inorganic compounds have been entered, and calculates the total number of compounds indexed. This may take some time if there is a large amount of data to consider, so be patient.

Clicking on the right or left arrow takes you into the chemical database. An example of what will appear on the screen is shown below:

The screenshot shows a graphical user interface for a chemical database. The main window displays a card for 'S-(4-Chlorobenzyl)thiuronium chloride, 99%'. The card is divided into several sections: 'Compound Name', 'Formula', 'Mol. Wt.', 'Company Name' (Aldrich), 'Catalog No.' (11,565-7), 'Where is it?' (Lab 22 shelf #29), 'How much on hand?' (25g), 'Date Acquired', 'Date Reordered', 'Comments/Safety notes', 'I/O?' (0), 'MSD sheet?', 'Usage Record', 'CAS#', and 'Hazard'. Navigation buttons (left arrow, right arrow, up arrow, down arrow) are placed around the card. A bottom panel contains buttons for 'New Entry', 'Return', 'Find', and 'Delete Card'.

The functions of the chemical index card that appear as buttons at the bottom left corner of the screen are as follows:

New Entry-Click here and a blank card will appear, ready for a new compound and other information to be entered.

Left Arrow- Click here to go to the previous card.

Right Arrow- Click here to go to the next card.

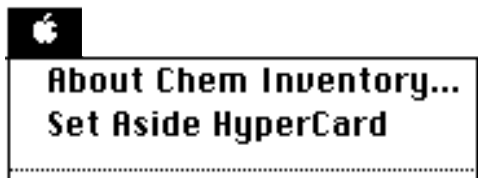
Return- Click here to return to the top card, which is described on page 1.

Find- Click here and a pop-up box will appear with instructions for searching for a particular compound. Click on the OK button to make it go away.

Delete Card- Click here to remove an obsolete entry. To avoid accidental erasure, a dialog box will appear and ask you to make sure that you want to do this. Click on yes and the card is gone for

good.

The Menus:



About Chem Inventory -If you click here with the mouse, a pop-up box appears telling you who wrote this thing. Click on Dr. Dan's head to hear what he has to say. Click on the OK button to make the pop-up box go away.



Open Stack - Allows you to open a different stack, such as an older version of this stack, in a separate window.

Save a Copy - Allows you to make a backup copy of this stack.

Compact Stack - Removes dead space within the stack, thus saving space on the disk. The stack contains empty space after adding new entries or after sorting the cards.

Page Setup - Allows you to choose the printing layout (landscape or portrait) and to set other options for your printer.

Print Card - Prints the current card.

Print Report - Prints out the contents of this stack as either one of two types of reports (explained later).

Quit -When you are done entering data or searching for a compound, click here to quit the stack.

Edit	
Cut	⌘H
Copy	⌘C
Paste Picture	⌘U
<hr/>	
New Card	⌘N

Cut - Use this to remove text from a field in order to paste it somewhere else.

Copy - Use this to copy text in a field in order to paste it somewhere else.

Paste - Use this to paste text into a field.

New card - This will bring up a new, blank card ready for data entry. You must hit the tab key before you start to type.

Go	
First	⌘1
Prev	⌘2
Next	⌘3
Last	⌘4
<hr/>	
Find...	⌘F
Message	⌘M

First - This will take you to the first card in the stack.

Prev - This card will take you to the previous card (same as left arrow).

Next - This will take you to the next card (same as right arrow).

Last - This will take you to the last card in the stack.

Find - This will bring up the message box. Type in the name or part of the name of the chemical you wish to locate.

Utilities	
Import	
Export	
Merge	
<hr/>	
Scan	

Import/Export - Click here to either read data from a text file into the stack or to export all the data from the stack to a text file, which can be opened by another database or a word processor. You will be prompted for the file to save to or to read from. This file should ideally be at the same heirarchical file level as Hypercard.

Merge - This function will copy cards from an earlier version of this stack and paste them into the current version. This function is available only to registered users of this stack.

Scan - Click here to have all the cards flashed up on the screen. You will be returned to the same card you were at before hitting the scan button. To stop the scan on a particular card, quickly type command-period.

Sort by
Name
Formula
Where it is
Date acquired
CAS #
Hazard

Click here to sort alphabetically by compound name or by where the compound is located, by formula, by date acquired, by CAS#, or by hazard class. If you choose to sort by chemical name, this feature does full chemical name and will ignore number and case prefixes and upper and lower case. It can take some time, so grab a cup of coffee and relax for a minute. A 490 card stack takes 14 minutes to sort on a Mac IIcx. Your time will vary accordingly.

Data Entry - Easy as Pi

To enter data into the stack, first click on the "New Entry" button. A fresh, blank card will appear on the screen. Before you can start typing, you must hit the tab key. You will see a blinking cursor in the Compound Name box. Type in the compound name. Hit the tab key to cycle through all of the fields, typing in the relevant data. The fields on each card are pretty much self-explanatory, and are as follows:

"Compound Name", "Formula", "Mol Wt", "Company", "Catalog No.", and "Where it is" are pretty much self-explanatory.

"How Much on hand?" should reflect not just the total quantity on hand but also how it is packaged. Don't type 25 grams if it is actually 5 5-gram bottles. If a chemical has been used up, type "None" in this field and type the date reordered in the "Date Reordered" field. This is to insure that a) a person looking for a particular reagent knows that it is gone, and b) that the person knows that it has been reordered so that a duplicate order is not prepared.

“Who took it?” (The “Comments” box) If you have a large, central stockroom or several laboratories where chemicals are stored, it is nice to know who took an item and where it is now. That way, when you are in the middle of a reaction and go to where a reagent normally is kept and it is not there, you can track it down and kick that person’s butt. The comments box can also be used for noting if something is a carcinogen, flammable, air sensitive, safety notes and waste disposal procedures, or whatever else you wish to note.

“I/O” is the field used by the top card to determine if this card contains an organic (**O**) or inorganic (**I**) entry. The New Count button on the top card uses this field in determining the number of organics, inorganics, and the total number of compounds and displays this information in the appropriate field. O and I can be either upper-case or lower-case. If you have the Material Safety Data Sheet on file for this compound, type an **“x”** into the **“MSD sheet?”** box.

Additional fields are provided for **CAS#**, **Hazard class type**, and the **Date Acquired** for chemicals that decompose or form peroxides over time.

Subscripts, superscripts, and Greek letters are supported for chemical names and formulas. For example:

to type MgSO_4 , type: shift-m, g, shift-s, shift-o, option-4.
to type α -Ketobutyric acid, type option-a for the alpha
to type ^{19}F NMR, type: option-shift-1, option-shift-9 for the 19 part.

The keyboard layout for the font used in this stack is shown in a separate PICT file.

To erase an entry in any field, hit the tab key until you reach that field, then hit the backspace key.

The Cut (**command-X**), copy (**command-C**), and paste (**command-V**) functions are fully supported. To copy text from one card to another, tab to the field that you want to copy (you will see the entire text field highlighted), then type **command-C**. Move to the card that you want to copy the text to, and type **command-V**. To delete highlighted text, type either **command-x** or just hit the backspace key. Using the mouse, you can highlight a portion of text in any card field and cut, copy or paste.

Looking for Something?

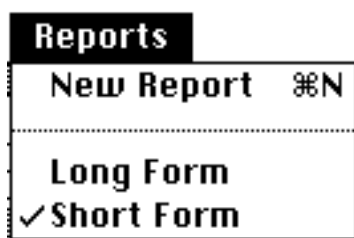
To search for a particular compound or compounds, first, type: **command-F**. A message box will appear with a cursor blinking between two quotation marks. Type in the name or fragment of the name that you wish to search for, then hit the return key. If the program finds a match for this string, the card will appear on the screen and the matching string will appear with a box around it. To find another match, just hit the return key. Hitting the return key will cycle you through all of the cards that have the matching string. If no

match is found, you will be left with the current entry on the screen. To search for another compound, type **command-F** again, and type the name or name fragment, then hit the return key. Click the mouse button and the box will disappear from around the matching string, and also will end the search.

Printing Reports

If you wish to print the current card, choose "Print Card" from the "File" menu.

Once the stack is sorted, you can print a hard copy of the chemical inventory using two templates. First, choose "Page Setup" from the "File" menu. If you wish to use the short-form template (name, location, amount) choose portrait mode. If you wish to use the long-form template (name, company, catalog number, location, amount) choose landscape mode. Next, choose "Print Report" from the "File" menu. You will then see a page layout for the current template. To switch between "Short Form" and "Long Form", choose from the "Reports" menu. Then click on "Print".



In order to print correctly in the background under Multifinder or in System 7, you should install the bitmap font TimesMol3 into your system file, and place the laser font TimesMolPla into your system folder, or the extensions folder under System 7.

Sorting

In order for the chemical sort routine to function correctly, you **must** begin the proper name of the compound with a capital letter. For example:

Diethyl ether
 o-Xylene
 2-Chloropropane
 4-(p-t-Butylphenyl)aniline

If the name has the following characters in the prefix: **D, L, R, S, E, Z** or **N**, you must use option-shift letter for it to be ignored by the sort routine. For example:

D-Ascorbic acid, use option-shift -d for the D.
 L-Glycine, use option-shift -l for the L.
 R-tetramethylethylenediamine, use option-shift -r for the R.
 S-(A)-2-Methylbutyric acid, use option-shift -s for the S.
 E-(U)-2-Butene, use option-shift -e for the E.
 Z-(U)-2-Butene, use option-shift -z for the Z.

Final Comments

All information is automatically saved, which is why there is no "save" button.

Upon opening the stack, the program checks for empty space left from deleted cards or from expansion to allow multiple new entries from the last time the program was used. If it finds empty space, it does an automatic compression. When this happens, it will take a few seconds for the program to open and you will see the current size displayed on the top card decrease. This is normal behavior; don't worry, be happy.

If upon opening the stack, you see an error message stating that the program could not find the menu item "Compact Stack", then this means that the userlevel in the user preferences of the Home stack is set too low. To remedy this, type **command-m**. A message box will appear. Type in the following: set userlevel to 5 (hit return). Then close the message box. This should clear up the problem. The stack will function normally anyway if the userlevel is set too low except that the stack will not remove any dead space left from deleting cards.

Hitting the tab key will move you through the fields. Hitting shift-tab will move you backwards through the fields.

The keyboard arrow keys perform the following functions:

- left - go to the previous card
- right - go to the next card
- up - go forward through the most recent cards
- down - go backwards through the most recent cards.

The cards provided in the stack are for demonstration purposes—you can use them to test sorting and printing. They can be deleted if so desired, with the exception of the 1-pyrenebutyric acid card. This card is the base card for all other entries. To change the contents of this card, simply tab through the fields and replace the contents of each field with your own information.

This stack is shareware. The registration fee is \$15. Registered users are entitled to free updates and unlimited user support. For the address of the author, see the "About" box.

Reports of any bugs, suggestions for new features, improvements, or general comments are more than welcome. See the "About" box for the author's address.