

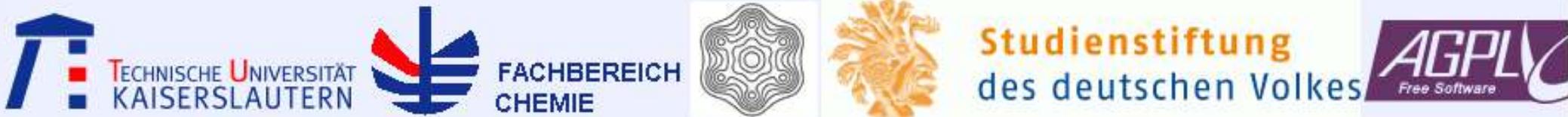
OPEN ENVENTORY MANUALS

Khoi N. Van

Monday, July 7, 2014

CREDITS

About open enventory



open inventory Credits

- open enventory is free software. You may redistribute copies of it under the terms of the GNU Affero General Public License V3 <http://www.gnu.org/licenses/agpl.html>. There is **no warranty**, to the extent permitted by law.
- Development: [Prof. Dr. Lukas Gooßen](#) and [Dr. Felix Rudolphi](#)
- open enventory is a registered trademark of Felix Rudolphi and Lukas Gooßen
- Programming: Felix Rudolphi and Thorsten Bonck
- In memory of Dr. Klaus Angermund.
- The development was generously supported by the Fonds der Chemischen Industrie
- The included applet to enter chemical structures was developed by Otmar Ginkel

OUTLINES

1. Add chemicals
2. Edit chemicals
3. Search for chemicals
4. Borrow/return chemicals

ADD CHEMICALS

Add Storage location if not exists

The screenshot shows the open inventory software interface. On the left, there is a sidebar with the Texas A&M Chemistry logo and a navigation menu. The menu includes options like 'Change password', 'global settings', 'Permission levels', 'About open inventory' (which is circled in green), 'Users', 'Other databases', 'Storage' (which is also circled in green), 'Institutions', 'Disposed chemicals', 'Barcodes for stock-keeping', 'Check supplier search', 'Check substructure search', 'Check reaction mapping', 'Double entries', 'Import tab-separated text file', 'Recreate users', 'Reset block-list', 'Reset locked datasets', 'Manage databases', 'Recalculate structures in databases', and a 'sciformation ELN' section. Below the sidebar, there is a message: 'sciformation ELN is even better or support this project with a donation?'.

The main area of the interface is titled 'open inventory' and shows a chemical database. It includes a top navigation bar with 'Search', 'Change to lab journal', 'Settings', 'Logout', and 'Selected: nothing'. Below this, it says 'You are logged in as root on localhost/romo.' and 'Databases: linchpin'. There are buttons for 'edit mode' (highlighted in red) and 'list mode' (highlighted in blue), and a '10 Results per page' dropdown.

The main content is a table listing storage locations:

storage name	institution	
312-F (flammable)		0 X <input type="checkbox"/>
315-R (Refridgerator)		7 X <input type="checkbox"/>
321-G (General)	Texas A&M University, College Station - TX 77842	0 X <input type="checkbox"/>
FH-2315 (315)	Texas A&M University, College Station - TX 77842	4 X <input type="checkbox"/> 5 X <input type="checkbox"/>



ADD CHEMICALS

Add Storage location if not exists

The screenshot shows the open inventory software interface. At the top left is the Texas A&M Chemistry logo. The top right features the software title "open inventory" in large blue and red letters, with the subtitle "chemical database - © 2012 Felix Rudolphi, Lukas Gooßen" below it. The top navigation bar includes links for "Search", "Change to lab journal", "Settings", "Logout", and "Selected: nothing". A "Databases: linchpin" link is also present. On the left, a sidebar menu lists various administrative functions: Change password, global settings, Permission levels, About open inventory (with sub-options like Users, Other databases, Storages, Institutions, Disposed chemicals), Barcodes for stock-keeping, Check supplier search, Check substructure search, Check reaction mapping, Double entries, Import tab-separated text file, Recreate users, Reset block-list, Reset locked datasets, Manage databases, Recalculate structures in databases, and a "sciformation ELN is even better" section with a "donation?" link. A green circle highlights the "Storages" link in the sidebar. The main content area displays a list of storage locations in "list mode". The columns are "storage name" and "institution". The results are as follows:

storage name	institution	
312-F (flammable)	Texas A&M University, College Station - TX 77842	0 X <input type="checkbox"/>
315-R (Refridgerator)		7 X <input type="checkbox"/>
321-G (General)	Texas A&M University, College Station - TX 77842	0 X <input type="checkbox"/>
FH-2315 (315)	Texas A&M University, College Station - TX 77842	4 X <input type="checkbox"/>
		5 X <input type="checkbox"/>

At the bottom left of the main area is a small "left arrow" icon.

ADD CHEMICALS

Add *Storage location* if not exists

ATM | **CHEMISTRY**
TEXAS A&M UNIVERSITY

open inventory

chemical database - © 2012 Felix Rudolphi, Lukas Gooßen

Search / Change to lab journal / Settings / Logout

You are logged in as root on localhost/romo.

Databases: linchpin

Selected: nothing

Change password
global settings
Permission levels
About open inventory
Users
Other databases
Storages
Institutions
Disposed chemicals
Barcodes for stock-keeping
Check supplier search
Check substructure search
Check reaction mapping
Double entries
Import tab-separated text file
Recreate users
Reset block-list
Reset locked datasets
Manage databases
Recalculate structures in databases

edit mode list mode

Edit storage

storage name	312-F (flammable)
Barcode	
<input type="checkbox"/> Poison cabinet	
at	Texas A&M University
<input type="checkbox"/> Keep storage secret	

1 / 5

10

sciformation ELN
is even better
or support this project with a
donation?



ADD CHEMICALS

Method A: Add via supplier

Step 1: change to supplier search and search chemical

ATM | CHEMISTRY
TEXAS A&M UNIVERSITY

open inventory
chemical database - © 2012 Felix Rudolphi, Lukas Gooßen

Search / Change to lab journal / Settings / Logout
Selected: nothing

Databases: linchpin

20 + page: 1 / 10 10

Search criterion: Name, CAS-No., sum form.
all words

in (select all): own database linchpin

Search: Selected items only, ALL, list mode, edit mode

Result list: New search

sciformation ELN is even better
or support this project with a donation?

	Standard view	Inventory management	Safety data	Physical data	10 Results per page	Show column		
	(1S,2S)-(+)-N-p-Tosyl-1,2-diphenylethylenediamine (98 %)	C ₂₁ H ₂₂ N ₂ O ₂ S	167316-27-0	!	Van, Khoi	H: 315-319-335 P: 261-305+351+338	1 g / 1 g	FH-43:
	1-Acetyl-1-cyclohexene (97 %)	C ₈ H ₁₂ O	932-66-1			H: P:	2 g / 5 g	315-R
	N-BENZOYLIMIDAZOLE (96 %)	C ₁₀ H ₈ N ₂ O	10364-94-0		Van, Khoi	H: P:	5 g / 5 g	315-R



ADD CHEMICALS

Method A: Add via supplier

Step 1: change to supplier search and search chemical

The screenshot shows the 'open inventory' software interface. At the top, there is a navigation bar with links for 'Search', 'Change to lab journal', 'Settings', 'Logout', and 'Selected: nothing'. Below the navigation bar, it says 'You are logged in as root on localhost/romo.' and 'Databases: linchpin'. On the left side, there is a sidebar with links to 'molecules.com', 'Chemie.de', 'SDBS', 'My orders', and 'Confirm orders'. It also contains a 'Search for' section with icons for a flask, a tree, and a benzene ring, and buttons for 'advanced search' and 'Search' (which has a green circle around it). Below this is a 'search criterion' section with dropdown menus for 'Name, CAS-No., sum form.' and 'all words', and a search input field containing '(-)-benzotetramisole'. There is also a dropdown for 'at' and 'all suppliers'. At the bottom of the sidebar, there is a message: 'sciformation ELN is even better or support this project with a donation?'.

The main area displays a table of results from the 'own database'. The columns are labeled: 'sender' (with up/down arrows), 'recipients' (with up/down arrows), 'issued' (with up/down arrows), 'subject' (with up/down arrows), 'do until' (with up/down arrows), and 'completion status' (with a checkbox). The table rows show the following data:

sender	recipients	issued	subject	do until	completion status
	Van, Khoi		Welcome to the list of chemicals of the .	unread	<input checked="" type="checkbox"/> X
	Romo, Daniel, Dr.		Welcome to the list of chemicals of the .	unread	<input checked="" type="checkbox"/> X
	Vellalath, Sreekumar		Welcome to the list of chemicals of the .	unread	<input checked="" type="checkbox"/> X
	Morgan		Welcome to the list of chemicals of the .	unread	<input checked="" type="checkbox"/> X
	Get		Welcome to the list of chemicals of the .	unread	<input checked="" type="checkbox"/> X

ADD CHEMICALS

Method A: Add via supplier

Step 2: choose **Create new molecule based on data**

ATM | CHEMISTRY TEXAS A&M UNIVERSITY

open inventory
chemical database - © 2012 Felix Rudolphi, Lukas Gooßen

Search / Change to lab journal / Settings / Logout
You are logged in as root on localhost/romo. / Order system / Selected: nothing
Databases: linchpin

Search for Advanced
advanced search

search criterion Name, CAS-No., sum form. all words
benzotetramisole

at all suppliers

Search

sciformation^{ELN} is even better or support this project with a donation?

Results from **TCI EUROPE**

name	Catalog number		price		
			amount	price	possible purchase
(+)-Benzotetramisole	B3296	Create new molecule based on data details	200 mg	39.45 EUR	<input type="checkbox"/>
(-)-Benzotetramisole	B3549	Create new molecule based on data details	1 g	122.40 EUR	<input type="checkbox"/>
			5 g	379.50 EUR	<input type="checkbox"/>
amount	price	possible purchase			
1 g	108.45 EUR	<input type="checkbox"/>			

No hits found at **ACROS ORGANICS**



ADD CHEMICALS

Method A: Add via supplier

Step 3: add more info: ammount, person responsible, etc.

The screenshot shows the 'open inventory' chemical database interface. At the top, there is a navigation bar with links to 'Search', 'Change to lab journal', 'Settings', 'Logout', and 'Selected: nothing'. Below the navigation bar, it says 'You are logged in as root on localhost/romo.' and 'Databases: linchpin'. On the left side, there is a sidebar with links to 'emolecules.com', 'Chemie.de', 'SDBS', 'My orders', 'Confirm orders', and search filters for 'Search for' (with icons for molecule, reaction, and structure) and 'Advanced' search. There is also a 'search criterion' section for 'Name, CAS-No., sum form.' and 'all words' dropdowns, and a 'at' dropdown for 'all suppliers'. A 'Search' button with a magnifying glass icon is present. A blue banner at the bottom left reads 'sciformation ELN is even better or support this project with a donation?'. The main content area shows a list of chemical properties for '(+)-Benzotetramisole'. The properties listed are:

CAS number	885051-07-0	Read data from suppliers
stereo-SMILES:	c1ccc(cc1)[C@H]4N=C3Sc2cccc2N3C4	
empirical formula	C15H12N2S	
MW	252.34	
density (20°C)		
hazard codes (GHS)	GHS0	
hazard		



ADD CHEMICALS

Method A: Add via supplier

Step 3: add more info: ammount, person responsible, etc.

The screenshot shows the 'open inventory' software interface. At the top, there's a navigation bar with links to 'Search', 'Change to lab journal', 'Settings', 'Logout', and 'Order system'. Below this, it says 'Databases: linchpin'. The main area displays a search result for '(+)-Benzotetramisole'. The 'edit mode' button is highlighted with a green circle. The form fields include:
- amount: 1 g
- still available: 0.9 g
- tara with lid: kg
- total mass of container: kg
- Update amount automatically: default
- Type of container: glass
- description (e.g. solid support):
- storage location: FH-4315 (315)
- in compartment: Dessicator (marked with a red X)
- Responsible person: Van, Khoi
- Properties checkboxes: light sensitive (unchecked), air sensitive (unchecked), moisture sensitive (checked), refrigerate (unchecked), hygroscopic (unchecked), stabilized (unchecked), denatured (unchecked)
- barcode: (empty field)
- Generated barcode: 20000066



ADD CHEMICALS

Method B: Create new chemical

Step 1: choose **New**



ADD CHEMICALS

Method B: Create new chemical

Step 2: use CAS number to pull info from suppliers

ATM | CHEMISTRY
TEXAS A&M UNIVERSITY

open inventory
chemical database - © 2012 Felix Rudolphi, Lukas Gooßen

Search / Change to lab journal / Settings / Logout
Selected: nothing

Databases: linchpin

You are logged in as root on localhost/romo.

Information about the molecule

molecule names

The first entry will be set as standard name. Mark non-scientific names by appending a hash (#).

CAS number	XXXX-XX-X	Read data from supplier
empirical formula		
MW		
density (20°C)		
hazard codes (GHS)		
hazard statements		

Search
 Selected items only
 ALL
 list mode edit mode

sciformation ELN
is even better
or support this project with a donation?



ADD CHEMICALS

Method B: Create new chemical

Step 3: add more info

The screenshot shows the 'open inventory' chemical database interface. At the top, there is a navigation bar with links to 'Search', 'Change to lab journal', 'Settings', 'Logout', and 'Selected: nothing'. Below the navigation bar, it says 'Databases: linchpin'. On the left side, there is a sidebar with links to 'emolecules.com', 'Chemie.de', 'SDBS', 'My orders', and 'Confirm orders'. It also includes a search section with 'Search for' dropdowns for 'Name, CAS-No., sum form.' and 'all words', and a 'Search criterion' dropdown set to 'own database linchpin'. There are also buttons for 'advanced search' and 'NEW'. Below this, there is a 'Search' section with 'Selected Items only' checked, 'list mode' selected, and buttons for 'ALL' and 'edit mode'. A banner at the bottom left says 'sciformation ELN is even better' and 'or support this project with a donation?'. The main content area is titled 'Select: new molecule'. It has fields for 'purity/concentration' (set to %), 'amount' (set to g), 'storage location' (set to 'not set'), and 'in compartment' (marked with a red X). There is a dropdown for 'Responsible person' set to 'none'. A checkbox for 'Keep package secret' is unchecked. Under 'Properties', there are checkboxes for 'light sensitive', 'air sensitive', 'moisture sensitive', 'refridgerate', 'hygroscopic', 'stabilized', and 'denatured'. A 'barcode' field is also present.



EDIT CHEMICALS

Step 1: Search chemical in the database (more info followed)

Step 2: Click on the structure

ATM | CHEMISTRY TEXAS A&M UNIVERSITY

open inventory
chemical database - © 2012 Felix Rudolphi, Lukas Gooßen

Search / Change to lab journal / Settings / Logout
Selected: nothing

You are logged in as root on localhost/romo.
Databases: linchpin

1 + 10

edit mode Standard view Inventory management Safety data Physical data 10 Results per page Show column

structure	name	empirical formula	CAS number	haz. cod.	Pos.	Responsible person	hazard / precautionary statements	amount	storage	
	Crotonoyl chloride (90 %)	C ₄ H ₅ ClO	625-35-4			Van, Khoi	H: 226-314-335 P: 261-280-305+351+338-310	3 g / 5 g	315-R (Refridgerator)	

Results from own database

Search these services: **NIST** National Institute of Standards and Technology **eMolecules®**

Search criterion: Name, CAS-No., sum form.
all words: crotonoyl chloride
in (select all): own database linchpin

Search: Selected items only (radio button), list mode (radio button), edit mode (radio button)
Result list: New search

sciformation ELN is even better
or support this project with a donation?

EDIT CHEMICALS

Step 3: Click on ‘Go to molecule’ button to edit structure and structural info (MW, Formula, etc.)

The screenshot shows the 'open inventory' chemical database interface. At the top, there is a navigation bar with links to 'Search', 'Change to lab journal', 'Settings', 'Logout', and 'Selected: nothing'. Below this, it says 'Databases: linchpin'. A green circle highlights the 'edit mode' tab in the navigation bar. The main content area displays the details for 'Crotonoyl chloride'. The purity/concentration is listed as 90 %. The data is presented in a table:

amount:	5 g	storage location:	315-R (Refridgerator)
still available:	3	Responsible person:	Van, Khoi
Type of container:	glass	<input type="checkbox"/> Keep package secret	
supplier:	Sigma-Aldrich	Properties:	refridgerate
safety data sheet by:	Search	Generated barcode:	20000172
alt. safety data sheet by:	Search		

Below the table, there is information about the molecule: 'Created by: khoi Date of creation: 03.07.2014 21:24:39', 'Last change by: khoi Date of last change: 03.07.2014 21:24:39', and 'checked by: khoi date of last check: 03.07.2014 21:24:39'. There is also a section for 'information about the molecule' with the 'molecule names: Crotonoyl chloride'.

EDIT CHEMICALS

Step 3: or To change the lab related (person responsible, amount, etc.) info, double click on any where around these info

ATM | CHEMISTRY
TEXAS A&M UNIVERSITY

open inventory
chemical database - © 2012 Felix Rudolphi, Lukas Gooßen

Search / Change to lab journal / Settings / Logout
Selected: nothing

Databases: linchpin

emolecules.com Chemie.de SDBS My orders Confirm orders

Search for Advanced advanced search NEW

search criterion Name, CAS-No., sum form. all words crotonoyl chloride

In (select all) own database linchpin

Search Selected items only ALL list mode edit mode

Result list New search

sciformation ELN is even better or support this project with a donation?

You are logged in as root on localhost/romo.

edit mode Standard view Inventory management Safety data Physical data

Edit package

Crotonoyl chloride

purity/concentration: 90 %

amount:	5 g	storage location:	315-R (Refridgerator)
still available:	3	Responsible person:	Van, Khoi
Type of container:	glass	Keep package secret	
supplier:	Sigma-Aldrich	Properties:	refridgerate
safety data sheet by:	Search	Generated barcode:	20000172
alt. safety data sheet by:	Search		

Created by: khoi Date of creation: 03.07.2014 21:24:39
Last change by: khoi Date of last change: 03.07.2014 21:24:39
checked by: khoi date of last check: 03.07.2014 21:24:39

information about the molecule

molecule names:
Crotonoyl chloride

CAS number: 625-35-4

17 / 20

✉ 10

SEARCH CHEMICALS

Search with names, cas, supplier #,

Step 1: choose database(s)

Step 2: choose options: *contain (~ similar to), exact*

Step 3: click Search

open inventory

chemical database - © 2012 Felix Rudolphi, Lukas Gooßen

You are logged in as root on localhost/romo.

Databases: linchpin

page: 1

Selected: nothing

structure	name	empirical formula	CAS number	haz. cod.	Pos.	Responsible person	hazard / precautionary statements	amount	storage
	Cinnamyl chloride	C ₉ H ₉ Cl	2687-12-9			Vellalath, Sreekumar	H: 302-314-330-334 P: 260-280-284-305+351+338-310	3 ml / 5 ml	315-R compa Compa
	3-Bromo-1-phenyl-1-propene	C ₉ H ₉ Br	4392-24-9			Vellalath, Sreekumar	H: 314 P: 280-305+351+338-310	15 g / 25 g	315-R compa Compa



SEARCH CHEMICALS

A. Search with names, cas, supplier #,

Note: if **Suppliers search mode** is on (see [add chemical via suppliers](#)),
the program includes the local database(s) first

The image shows two side-by-side screenshots of chemical search interfaces.

Left Interface (emolecules.com):

- Logo:** Texas A&M Chemistry logo.
- Navigation:** Links to emolecules.com, Chemie.de, SDBS, My orders, and Confirm orders.
- Search:** "Search for" dropdown with icons for molecule, reaction, and search. Buttons for "advanced" and "advanced search".
- Search Criterion:** "Name, CAS-No., sum form." dropdown set to "all words". Input field contains "1-acetyl-1-cyclohexene".
- Suppliers:** "all suppliers" dropdown.
- Search Buttons:** Standard search and advanced search.
- Sciformation ELN:** A blue banner with the text "sciformation ELN is even better" and "or support this project with a donation?".

Right Interface (open inventory):

- Logo:** open inventory logo.
- Header:** "chemical database - © 2012 Felix Rudolphi, Lukas Gooßen". Navigation links: Search, Change to lab journal, Settings, Logout, Order system, Selected: nothing.
- Message:** "You are logged in as root on localhost/romo." and "Databases: linchpin".
- Chemical Structure:** A benzene ring with an acetyl group attached.
- Results from own database:**

	1-Acetyl-1-cyclohexene	C ₈ H ₁₂ O	932-66-1	H: P:	124.18	
--	------------------------	----------------------------------	----------	----------	--------	--
- molecules at suppliers:** A section stating that information originates from suppliers with no responsibility for correctness. It lists results from Sigma-Aldrich.
- Results from Sigma-Aldrich:**

name	Catalog number	price	possible purchase
1-Acetyl-1-cyclohexene (97% (Aldrich))	A14405	Create new molecule based on data details	<input type="checkbox"/>

SEARCH CHEMICALS

B. Search with Structure

Step 1: choose search with Structures

The screenshot shows the 'open inventory' chemical database interface. At the top, there is a navigation bar with links to 'Search', 'Change to lab journal', 'Settings', 'Logout', and 'Selected: nothing'. Below the navigation bar, it says 'You are logged in as khoi on localhost/ROMO.' and 'Databases: linchpin'. On the left, there is a sidebar with a list of search criteria, including 'Name, CAS-No., sum form.', 'CAS number', 'structure' (which is highlighted with a green circle), 'empirical formula', 'MW', 'Keep molecule secret', 'Number of containers', 'Number of commercial offers', 'SMILES', 'stereo-SMILES', 'monoisotopic mass', 'deg. of unsat.', 'density (20°C)', 'refractive index (20°C)', 'melting point', 'boiling point', 'risk statements', 'hazard statements', 'safety statements', 'precautionary statements', 'hazard codes', 'hazard codes (GHS)', and 'comment'. The main area displays a search result for 'Van, Khoi' with the message 'Welcome to the list of chemicals of the ..'. There are buttons for 'unread' and a red 'X' icon. At the bottom, there are icons for printing and exporting.



SEARCH CHEMICALS

B. Search with Structure

Step 2: draw structure

Step 3: choose options: *contain* (~ similar to), exact

Step 4: click search

The image shows two side-by-side web pages. On the left is the Texas A&M Chemistry website, featuring a navigation bar with links to emolecules.com, Chemie.de, SDBS, Borrowed chemicals, My orders, and Confirm orders. Below this is a search interface with a 'Search for' field containing a benzene ring icon, an 'Advanced' button, and a 'NEW' button. A dropdown menu labeled 'search criterion' is open, showing options: 'structure', 'is similar to', 'contain', 'is exactly', and 'stereo isomers'. The 'contain' option is highlighted with a green circle and a circular arrow. Below the dropdown is a chemical structure of a benzene ring. On the right is the 'open inven' chemical database interface, which includes a logo, a user login message ('are logged in as khol on localhost/ROMO.'), and a tool palette with various chemical drawing and selection tools. The main area displays a search results table with columns for 'recipients', 'issued', 'subject', 'do until', and 'completion status'. One result row is visible, showing 'Van, Khoi' in the recipient column and a link to 'Welcome to the list of chemicals of the ...'.

ORDER CHEMICALS

A. Reordered existing chemicals

Step 1: Pull up the existing chemical data (see [Edit chemicals](#))\

Step 2: Click on Search Suppliers button

The screenshot shows two windows side-by-side. The left window is a search interface for 'Borrowed chemicals' at Texas A&M University, with a search term 'cinnamyl chloride' entered. The right window is the 'open inventory' chemical database, also showing 'cinnamyl chloride' as the search result. A green circle highlights the 'Search Suppliers' button in the top navigation bar of the open inventory window.

open inventory
chemical database - © 2012 Felix Rudolphi, Lukas Gooßen

You are logged in as khoi on localhost/romo.

Databases: linchpin

Search | Change to lab journal | Settings | Logout | Selected: nothing

edit mode Standard view Inventory management Safety data Physical data

Cinnamyl chloride

amount:	5 ml	storage location:	315-R (Refridgerator)
still available:	3	in compartment:	Upper Compartment
Type of container:	glass	Responsible person:	Vellalath, Sreekumar
supplier:	Sigma-Aldrich	<input type="checkbox"/> Keep package secret	
safety data sheet by:	Search	Properties:	moisture sensitive, refridgerate
alt. safety data sheet by:	Search	Generated barcode:	20000011

Created by: khoi Date of creation: 03.07.2014 20:41:12
Last change by: khoi Date of last change: 03.07.2014 20:58:09
checked by: khoi date of last check: 03.07.2014 20:58:09

information about the molecule

molecule names:
Cinnamyl chloride

CAS number:	2687-12-9
stereo-SMILES:	Cl/C=C/c1ccccc1
empirical formula:	C ₉ H ₁₁ Cl

c1ccccc1/C=C\CCCl

ORDER CHEMICALS

A. Reordered existing chemicals

Step 3: Choose the supplier

Step 4: Check the box *Possible purchase*

Step 5: Click on *Prepare order* button

The screenshot shows the 'open inventory' chemical database interface. At the top, there are links to 'emolecules.com', 'Chemie.de', 'SDBS', 'Borrowed chemicals', 'My orders', and 'Confirm orders'. Below these are search buttons for 'Search for' (with icons for molecule, reaction, and structure) and 'Advanced' search, along with 'advanced search' and 'NEW' buttons. A search criterion dropdown is set to 'Name, CAS-No., sum form.' with 'all words' selected and the term 'cinnamyl chloride' entered. A 'In (select all)' dropdown shows 'own database linchpin' selected. Under 'Search', there are checkboxes for 'Selected Items only', 'list mode' (selected), and 'edit mode'. A 'Result list' section includes a 'New search' button.

The main area displays search results from 'SIGMA-ALDRICH' and 'VWR'. A large green circular icon with a hand cursor is overlaid on the page.

Results from SIGMA-ALDRICH

name	Catalog number	price	possible purchase
Cinnamyl chloride (95% (Aldrich))	187186	Create new molecule based on data details	<input checked="" type="checkbox"/>

Results from VWR

name	purity	Catalog number	price	possible purchase
Cinnamyl Chloride, 95%, Stab. With Sodium Carbonate *keep Cold* (50 g)		A14408.18	Create new molecule based on data details	28.30 EUR <input type="checkbox"/>
Cinnamyl Chloride, 95%, Stab. With Sodium Carbonate *keep Cold* (1 kg)		A14408.0B	Create new molecule based on data details	385.00 EUR <input type="checkbox"/>
Cinnamyl Chloride, 95%, Stab. With Sodium Carbonate *keep Cold* (250 g)		A14408.30	Create new molecule based on data details	107.00 EUR <input type="checkbox"/>
Cinnamylchlorid (5 g)	95%	SAFA187186-5G	Create new molecule based on data details	23.00 EUR <input type="checkbox"/>
Cinnamylchlorid (100 g)	95%	SAFA187186-	Create new molecule based on data details	48.10 EUR <input type="checkbox"/>

ORDER CHEMICALS

A. Reordered existing chemicals

Step 6: add necessary additional info

Note: choose *Planned* in Order status, not *Ordered*

□

Add order for me

Order status	planned
Cost centre for order	
Account number	

Alternative choice

Choice	Product name	CAS number	Catalog number	supplier	Package size	price currency	Number of packages/amount	VAT rate	Total price	
<input checked="" type="radio"/>	Cinnamyl chloride	2687-12-9	187186-5G	Sigma-Aldrich	5 g	27.1 USD	1	0	27.10 USD	 

Allow change of the supplier Yes

Group member must order

Buyer comment

B I U S x x HO ━━ ━━ ━━ ━━ ━━ ━━ ━━ ━━





ORDER CHEMICALS

B. Order new chemicals

Step 1: Search chemical using supplier mode (see [here](#))

Step 2: similar as steps 3-6 above



BORROW/RETURN CHEMICALS VIA WEBSITE

Borrow chemical: using the website

Step 1: search chemical (see [section](#) above)

Step 2: click Borrow button

The screenshot shows the 'open inventory' chemical database interface. On the left, there is a sidebar with various search filters and a search bar containing the chemical structure of benzene. The main area displays a table of search results with columns for chemical structure, name, formula, ID, status, owner, and location. A green circle highlights the 'Borrow' button for the entry of Benzamide.

edit mode	Standard view	Inventory management	Safety data	Physical data	10 Results per page	Show column		
	3-Bromo-1-phenyl-1-propene	C ₉ H ₉ Br	4392-24-9		Vellalath, Sreekumar	H: 314 P: 280- 305+351+338- 310	15 g / 25 g	315-R (Refridgerator), compartment Upper compartment
	Benzamide	C ₇ H ₇ NO	55-21-0	 	Vellalath, Sreekumar	H: 302-341 P: 281	1 g / 5 g	FH-2315 (315), compartment Underhood
	(+)-Benzotetramisole	C ₁₅ H ₁₂ N ₂ S	885051-07-0		Van, Khoi	H: P:	0.9 g / 1 g	FH-4315 (315), compartment Dessicator
	(-)-Benzotetramisole	C ₁₅ H ₁₂ N ₂ S	950194-37-3		Van, Khoi	H: P:	0.9 g /	FH-4315 (315),



BORROW/RETURN CHEMICALS VIA WEBSITE

Return chemical: using the website

Step 1: go to My Borrowed chemicals

The screenshot shows two web pages side-by-side. The left page is the 'molecules.com' search interface, and the right page is the 'open inventory' chemical database.

molecules.com Search Results:

- Search term: Benzamide
- Search criterion: Name, CAS-No., sum form.
- Search in: own database linchpin
- Results:
 - Structure: Benzamide (Chemical structure: C=NC(=O)c1ccccc1)
 - Name: Benzamide
 - Empirical formula: C₇H₇NO
 - CAS number: 55-21-0
 - Haz. cod.: ! (Red diamond)
 - Pos.: Vellalath, Sreekumar
 - Responsible person: H: 302-341
P: 281
 - Amount: 1 g / 5 g
 - Storage: FH-2315 (315), compartment Underhood

open inventory Chemical Database:

- Logged in user: khol
- Databases: linchpin
- Search term: Benzamide
- Standard view results:
 - Structure: Benzamide (Chemical structure: C=NC(=O)c1ccccc1)
 - Name: Benzamide
 - Empirical formula: C₇H₇NO
 - CAS number: 55-21-0
 - Haz. cod.: ! (Red diamond)
 - Pos.: Vellalath, Sreekumar
 - Responsible person: H: 302-341
P: 281
 - Amount: 1 g / 5 g
 - Storage: FH-2315 (315), compartment Underhood



BORROW/RETURN CHEMICALS VIA WEBSITE

Return chemical: using the website

Step 2: click *Return* button

The screenshot shows the 'open inventory' chemical database interface. At the top, there is a navigation bar with links for 'Search', 'Change to lab journal', 'Settings', 'Logout', and 'Selected: nothing'. Below the navigation bar, it says 'You are logged in as khol on localhost/romo.' and 'Databases: linchpin'. On the left, there is a sidebar with links to 'emolecules.com', 'Chemie.de', 'SDBS', 'Borrowed chemicals', 'My orders', 'Confirm orders', and search options ('Search for', 'Advanced', 'advanced search', 'NEW'). The main area displays a search result for 'Benzamide'. The results table has columns for 'structure', 'name', 'empirical formula', 'CAS number', 'haz. cod.', 'Pos.', 'Responsible person', 'hazard / precautionary statements', 'amount', and 'storage'. The 'name' column shows 'Benzamide' with an upward arrow icon. The 'structure' column shows the chemical structure of benzamide (a benzene ring with an amide group). The 'amount' column shows '1 g / 5 g'. The 'storage' column shows 'FH-2315 (315), compartment Underhood'. There are also icons for a flask, a clipboard, and a magnifying glass.

structure	name	empirical formula	CAS number	haz. cod.	Pos.	Responsible person	hazard / precautionary statements	amount	storage
	Benzamide	C ₇ H ₇ NO	55-21-0			Vellalath, Sreekumar	H: 302-341 P: 281	1 g / 5 g	FH-2315 (315), compartment Underhood

Search these services: **NIST**
National Institute of Standards and Technology **eMolecules**



BORROW/RETURN CHEMICALS USING BARCODE SCANNER

Borrow chemical: using barcode scanner

!!! Computer that connected to the scanner must be **ON**

!!! Barcode terminal window must be **ON and ACTIVE**, if not log in with terminal username and pass or contact your local admin

Active barcode terminal look like below:

The screenshot shows a computer screen displaying a barcode terminal interface. The interface is divided into two main sections, each with a header and several input fields.

Top Section (Stock-keeping mode):

- Header: Nobody is logged in. (Logout, Login, Close terminal)
- Checkboxes: Stock-keeping mode, Stock-keeping (last check by), Update, delete.
- Input fields:
 - safety data sheet by: [Search]
 - alt. safety data sheet by: [Search]
 - storage location: []
 - Responsible person: []
 - Keep package secret

Bottom Section (information about the molecule):

- Header: information about the molecule
- Input fields:
 - safety data sheet by: [Search]
 - alt. safety data sheet by: [Search]
 - Keep molecule secret



BORROW CHEMICALS USING BARCODE SCANNER

Borrow chemical: using barcode scanner

!!! Computer that connected to the scanner must be **ON**

!!! Barcode terminal window must be **ON and ACTIVE**, if not log in with terminal username and pass or contact your local admin

Step 1: scan your own barcode

The screenshot shows a web-based application for managing chemical borrowing. At the top, a header bar includes a user profile (Van, Khoi is logged in), logout, login, and terminal status (24). Below the header, there's a section for 'Stock-keeping mode' with a checked checkbox and a note about the last check. There are 'Update' and 'delete' buttons. The main area contains two sets of input fields for safety data sheets and storage details. The first set is for the current user ('Hello, Van, Khoi') and the second is for the molecule being borrowed ('information about the molecule'). Both sets include 'safety data sheet by' and 'alt. safety data sheet by' fields with search buttons, and a 'Keep package secret' checkbox. A large green circle highlights the 'Hello, Van, Khoi' user profile area. At the bottom, a footer displays the Texas A&M logo and the text 'Hello, Van, Khoi'.

BORROW/RETURN CHEMICALS USING BARCODE SCANNER

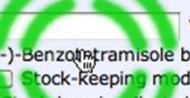
Borrow chemical: using barcode scanner

!!! Computer that connected to the scanner must be **ON**

!!! Barcode terminal window must be **ON** and **ACTIVE**

Step 2: scan chemical barcode

Watch the terminal window to make sure the info is transmitted/recorded.



Van, Khoi is logged in. [Logout](#) 28 [Login](#) [Close terminal](#)

(-)-Benzotetramisole borrowed.
 Stock-keeping mode
Stock-keeping (last check by)
[Update](#) [Delete](#)

(-)-Benzotetramisole

purity/concentration 98 %

amount	1 <input type="button" value="g"/>	storage location	FH-4315 (315)
still available	0.9	in compartment	Dessicator <input checked="" type="checkbox"/>
tara with lid	<input type="button" value="kg"/>	Responsible person	Van, Khoi
total mass of container	<input type="button" value="kg"/>	<input type="checkbox"/> Keep package secret	
Update amount automatically	<input type="button" value="default"/>	Properties:	moisture sensitive
Type of container:	glass	barcode	<input type="text"/>
supplier:	TCI	Protocol entry	<input type="text"/>
safety data sheet by:	<input type="button" value="Search"/>		
alt. safety data sheet by:	<input type="button" value="Search"/>		
Protocol:	...		
07.07.2014 08:54:06 Khoi Van: (-)-Benzotetramisole 1 (0.9) g borrowed.			
07.07.2014 08:54:12 Khoi Van: (-)-Benzotetramisole 1 (0.9) g returned.			
Created by: khoi Date of creation: 03.07.2014 21:04:55			

RETURN CHEMICALS USING BARCODE SCANNER

Return chemical: using barcode scanner

!!! Computer that connected to the scanner must be **ON**

!!! Barcode terminal window must be **ON** and **ACTIVE**

Action: scan borrowed chemical barcode

Note: you don't need to scan the your own barcode beforehand. The scan on a borrowed chemical will return the chemical.

Van, Khoi is logged in. [Logout](#) 41 [Login](#) [Close terminal](#)

(-)Benzotetramisole returned.
 Stock-keeping mode
Stock-keeping (last check by)

[Update](#) [Delete](#)

(-)Benzotetramisole

purity/concentration 98 %	
amount	1 g
still available	0.9
tara with lid	kg
total mass of container	kg
Update amount automatically	default
Type of container:	glass
supplier:	TCI
safety data sheet by:	Search
alt. safety data sheet by:	Search
Protocol:	...
07.07.2014 08:54:12 Khoi Van: (-)-Benzotetramisole 1 (0.9) g returned. 07.07.2014 09:19:43 Khoi Van: (-)-Benzotetramisole 1 (0.9) g borrowed.	
Created by: khoi Date of creation: 03.07.2014 21:04:55	

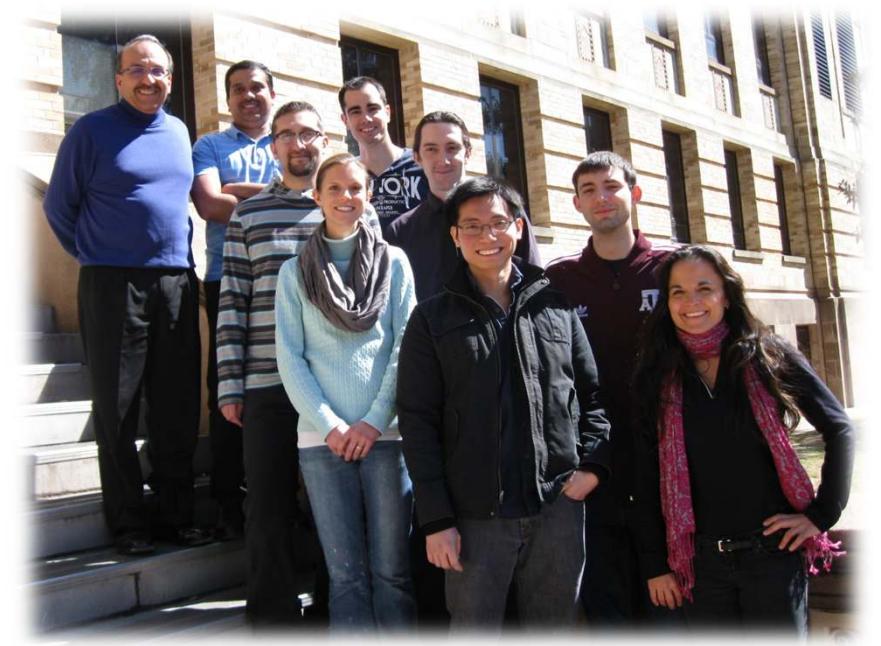
storage location: FH-4315 (315)
in compartment: Dessicator
Responsible person: Van, Khoi
 Keep package secret
Properties: moisture sensitive
barcode:
Protocol entry:

BORROW/RETURN CHEMICALS USING BARCODE SCANNER

Note: if the chemical is free and nobody has logged in, scanning the barcode of that chemical will bring up that chemical's info in the system.

Acknowledgments

- Dr. Felix Rudolphi for tremendous technical support
- Professor Daniel Romo for equipment support
- Sreekumar for heavily testing and procedure planning



March 2014