

COMPOUND REGISTRATION

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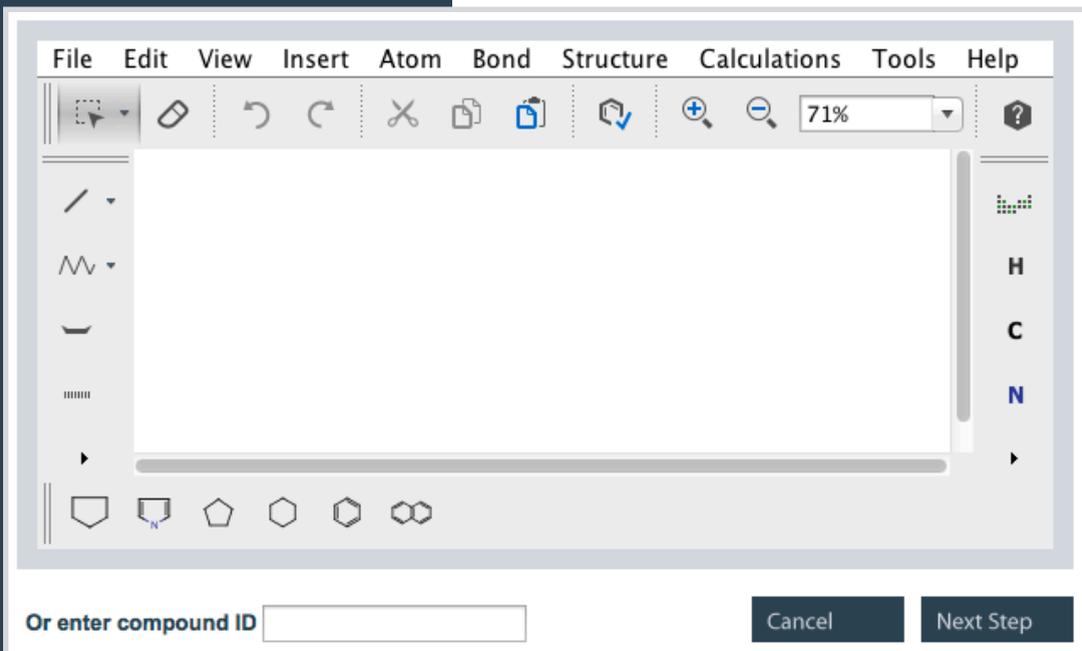
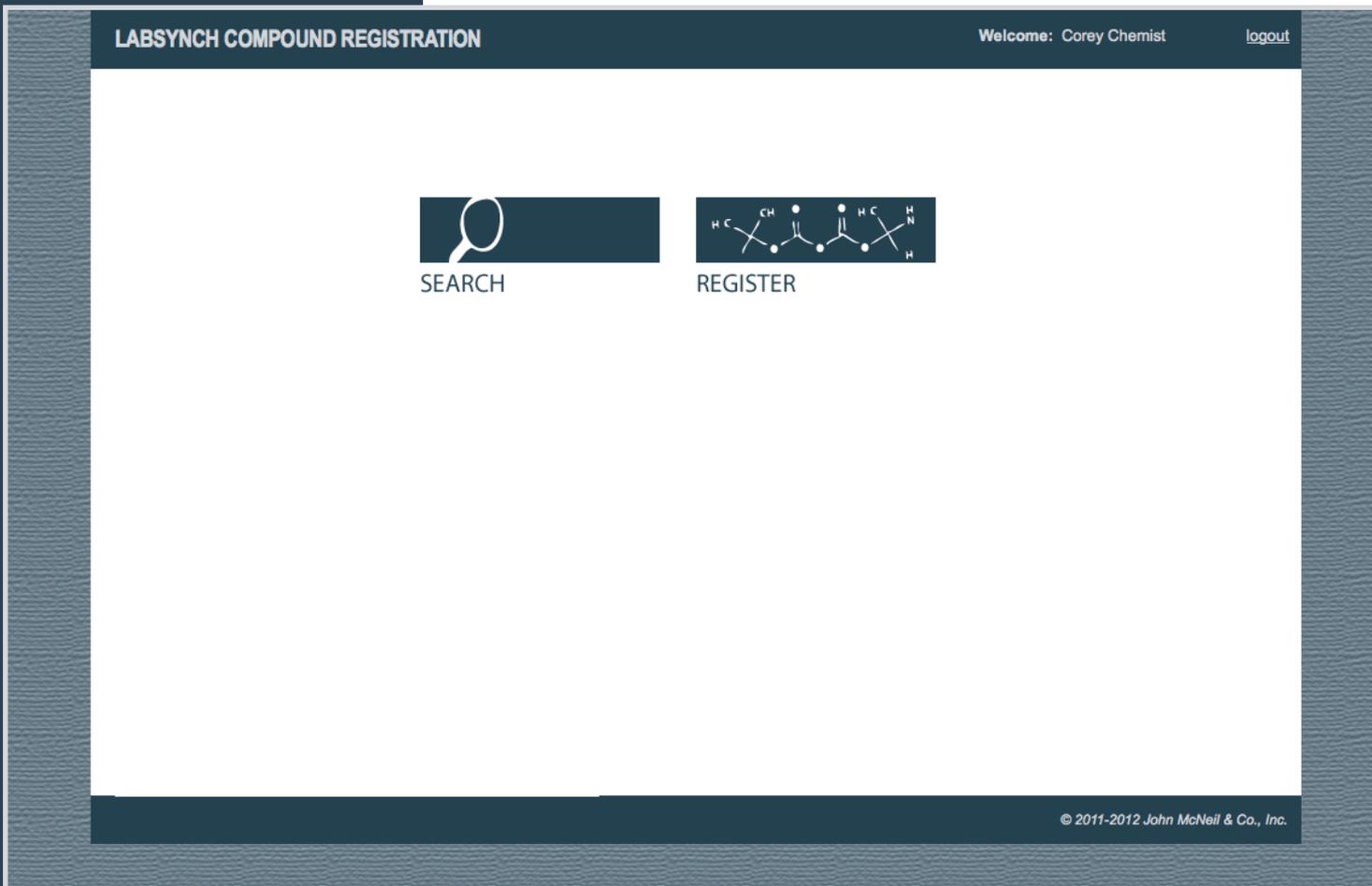
SCHRÖDINGER

JOHN MCNEIL
& Company, Inc.

COMPOUND REGISTRATION

REGISTER A NEW COMPOUND STEP 1

This is what the landing page for Compound Registration looks like. To register a new compound, click **REGISTER**.

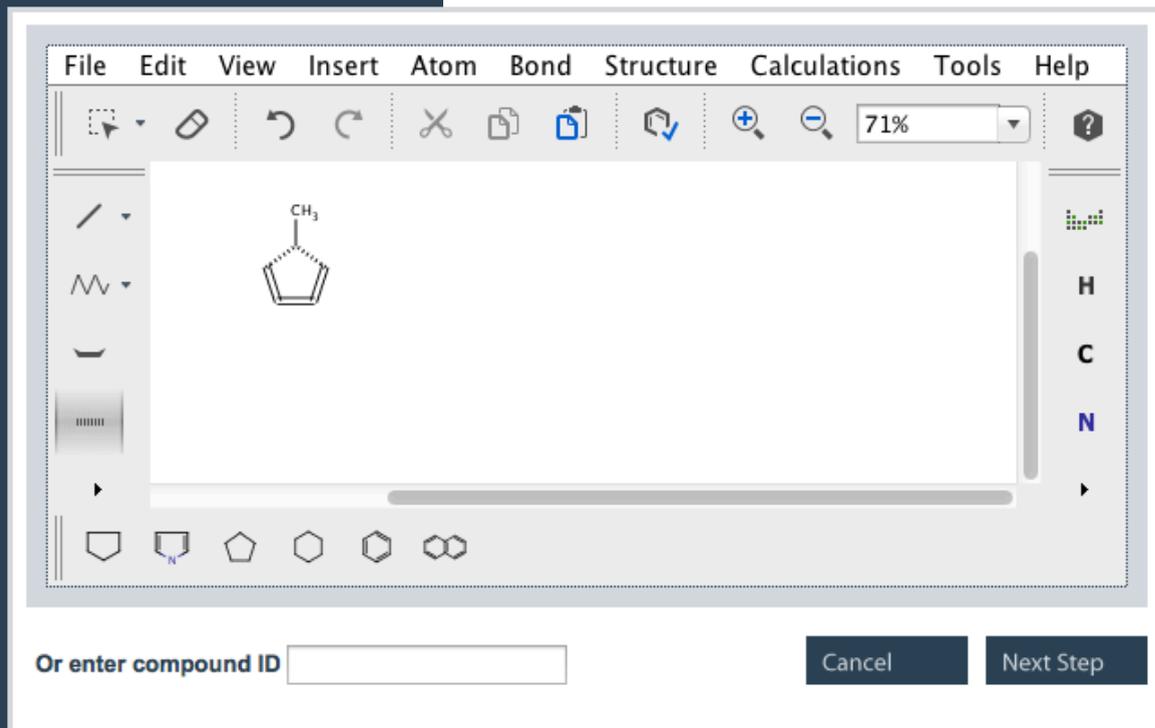


Marvin loads. From here you can draw the structure of the new compound, or enter a compound ID.

COMPOUND REGISTRATION

REGISTER A NEW COMPOUND STEP 2

Draw the desired structure and click **NEXT STEP**.

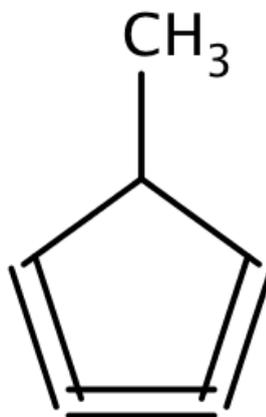


The screenshot shows a chemical drawing software interface. At the top is a menu bar with options: File, Edit, View, Insert, Atom, Bond, Structure, Calculations, Tools, Help. Below the menu is a toolbar with various drawing tools like a selection tool, eraser, undo, redo, delete, copy, paste, and zoom controls. The main canvas displays a 2D skeletal structure of methylcyclopentadiene, consisting of a five-membered ring with two double bonds and a methyl group (CH₃) attached to one of the ring carbons. On the right side, there is a vertical toolbar with buttons for H, C, and N. At the bottom left, there is a text input field labeled "Or enter compound ID" and two buttons: "Cancel" and "Next Step".

If the structure is unique, only the option to register a new structure is shown. Click **NEXT STEP**.

REGISTRATION STEP 2: REVIEW STRUCTURE MATCHES

REQUESTED STRUCTURE:



Register new structure

Virtual

Mol. Wt. 78.11

Mol. Formula C₆H₆

Back

Cancel

Next Step

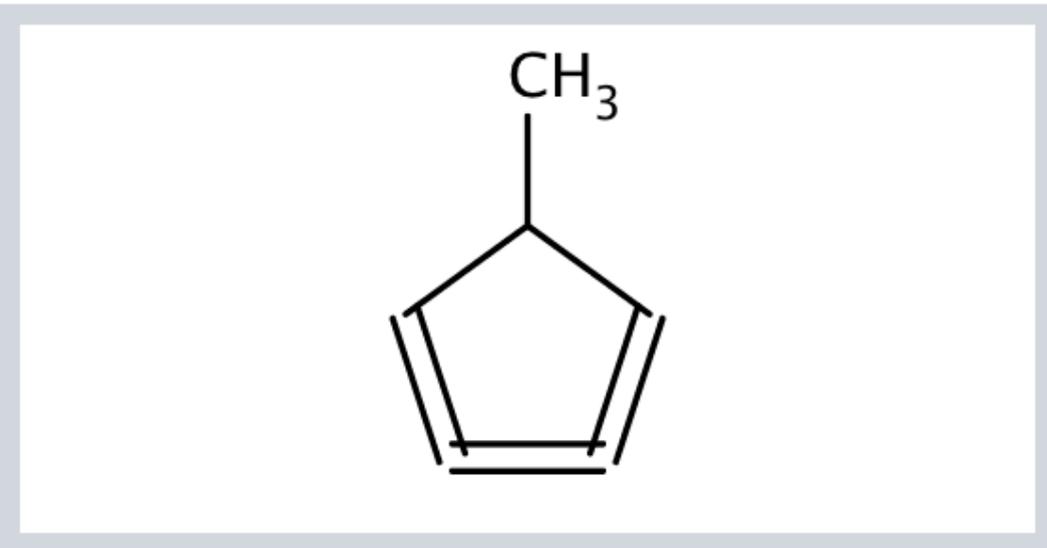
COMPOUND REGISTRATION

REGISTER A NEW COMPOUND STEP 3

A new compound and batch form loads. Here you can fill in the compound parameters. Click **SAVE**.

NEW COMPOUND AND BATCH

PARENT STRUCTURE:



Stereo Category: Stereo Comment: Original ID:

Mol. Formula: Mol. Wt.:

ENTER ISOTOPE/SALT STRUCTURE:

Salt: Equiv: CAS number:

Salt: Equiv:

Salt: Equiv:

Isotope: Equiv:

Isotope: Equiv:

New Salt

New Isotope

BATCH PROPERTIES:

Chemist:

BUID:

*Notebook-Page:

Project:

Batch Mol. Wt.:

*Synthesis Date:

Physical state:

%e.e.:

Batch comments:

Color:

Supplier:

Amount:

Supplier compound ID:

Supplier lot:

MP:

BP:

Purity measured by:

Purity (%):

Analytical Files: Add analytical files by editing batch after it is saved

Back

Cancel

Save

The only required fields are Notebook-Page and Synthesis Date.

The correct format for Notebook-Page is: #####-###

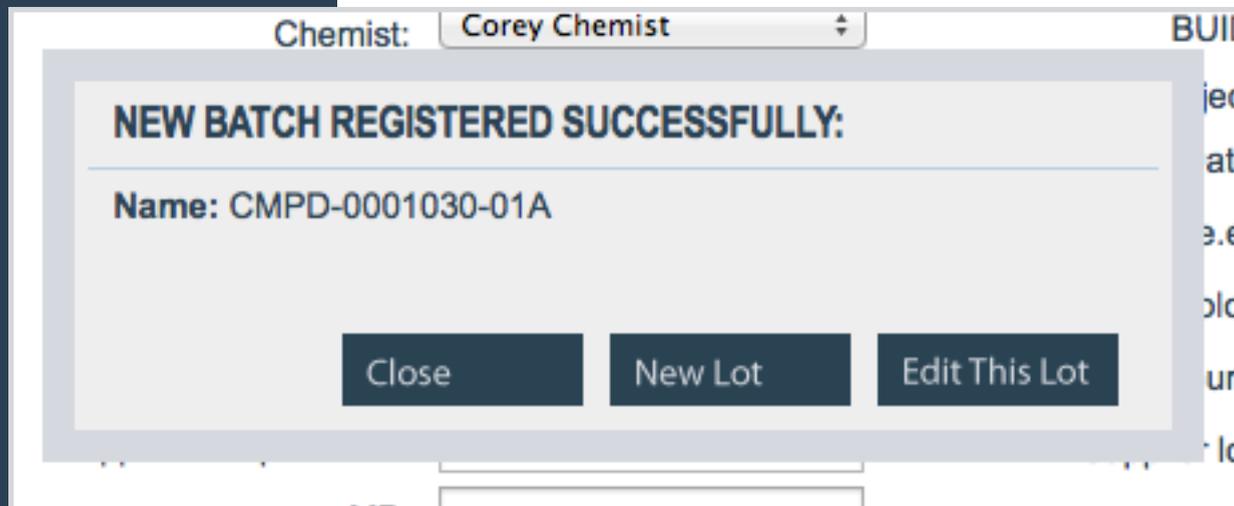
If either of these are not filled out, or are filled out incorrectly, you will be unable to save the compound.

The available fields, required fields, and notebook page format may be different for your installation.

COMPOUND REGISTRATION

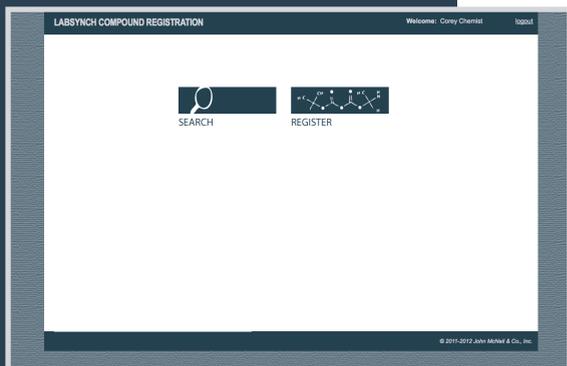
REGISTER A NEW COMPOUND

Once the compound has been successfully saved, an alert will pop up showing the compound name, in this case "CMPD-0001030-01A," along with options to **CLOSE**, make a **NEW LOT**, or **EDIT THIS LOT**.



COMPOUND REGISTRATION

REGISTER A NEW BATCH STEP 1

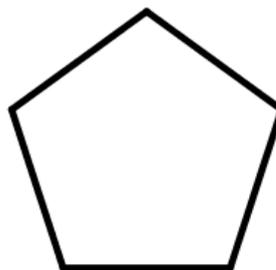


If you draw a structure that has already been registered as a compound, there are two options: register a new structure, or register a new batch from the parent structure.

Select **NEW BATCH**, and click **NEXT STEP**.

REGISTRATION STEP 2: REVIEW STRUCTURE MATCHES

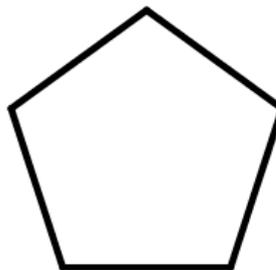
REQUESTED STRUCTURE:



Register new structure Virtual Mol. Wt. Mol. Formula

New batch **CMPD-0001010**

PARENT STRUCTURE:



Stereo Category: Stereo Comment: Original ID:

Mol. Formula: Mol. Wt.:

Back

Cancel

Next Step

COMPOUND REGISTRATION

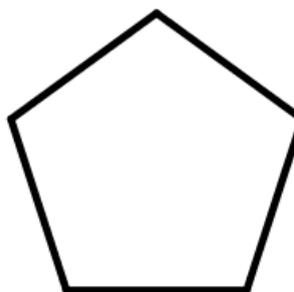
REGISTER A NEW BATCH STEP 2

The parent properties will not be editable.

Fill out the rest of the form with the required information. Then click **SAVE**.

NEW COMPOUND AND BATCH

PARENT STRUCTURE:



Stereo Category: Stereo Comment: Original ID:

Mol. Formula: Mol. Wt.:

ENTER ISOTOPE/SALT STRUCTURE:

Salt: Equiv: CAS number:

Salt: Equiv:

Salt: Equiv:

Isotope: Equiv:

Isotope: Equiv:

New Salt

New Isotope

BATCH PROPERTIES:

Chemist:

*Notebook-Page:

Batch Mol. Wt.:

Physical state:

Batch comments:

Supplier:

Supplier compound ID:

MP:

Purity measured by:

BUID:

Project:

*Synthesis Date:

%e.e.:

Color:

Amount: mg

Supplier lot:

BP:

Purity (%):

Analytical Files: Add analytical files by editing batch after it is saved

Chemist:

BUI

Back

Cancel

Save

NEW BATCH REGISTERED SUCCESSFULLY:

Name: CMPD-0001030-01A

Close

New Lot

Edit This Lot

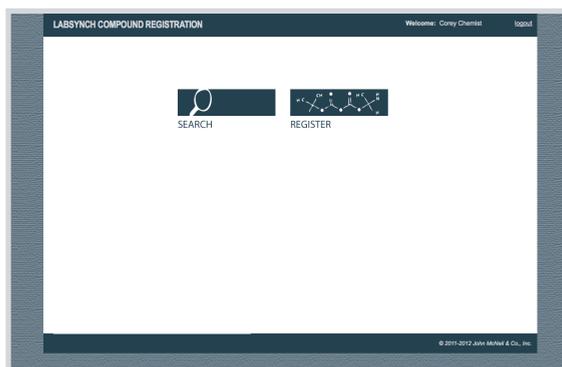
A message will pop up if the new batch was registered successfully.

COMPOUND REGISTRATION

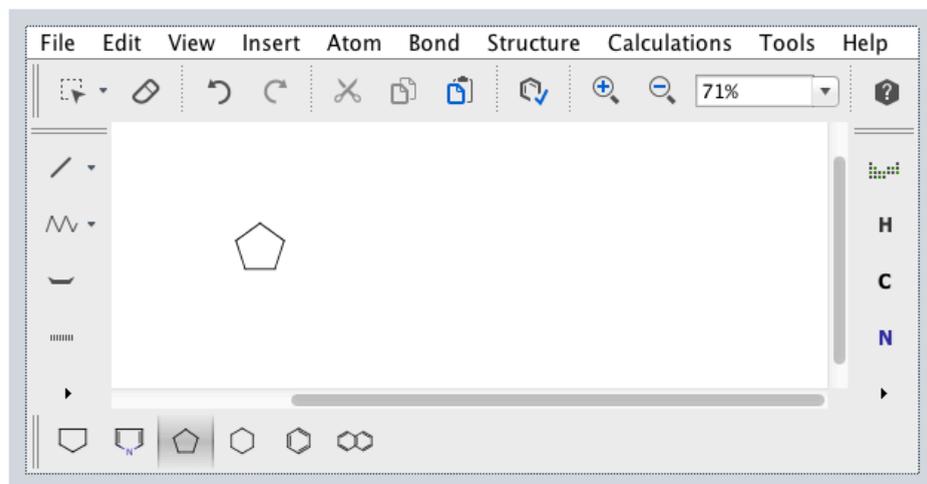
SEARCH FOR A COMPOUND

To search for a compound, click **SEARCH**.

You can search by structure and/or any combinations of the filter fields in the **QUERY STRUCTURE** form.



QUERY STRUCTURE:



CMPD Number to

Alias contains

Synthesis date range to

Chemist anyone

Substructure
 Exact

Draw the structure you wish to search for. The results displayed will include any compound that has the given structure included.

The structure will be displayed as the highlighted portion of the compound.

SEARCH RESULTS

Back Close

CMPD-0000193 Achiral Batch 1 - 09/14/2012

New Lot Details

CMPD-0000244 Achiral Batch 1 - 09/14/2012

New Lot Details

H₃C

O

O-CH₃

The 'SEARCH RESULTS' section shows a list of compounds. The first entry is 'CMPD-0000193 Achiral Batch 1 - 09/14/2012'. Below this entry, a chemical structure is displayed. A black arrow points from the text 'The structure will be displayed as the highlighted portion of the compound.' to a blue-highlighted pentagon ring in the structure. The structure is a complex molecule consisting of a central pentagon ring connected to a chain of atoms, including a hydroxyl group (HO), a triple bond, another hydroxyl group (OH), and another pentagon ring. Below the first entry, the second entry 'CMPD-0000244 Achiral Batch 1 - 09/14/2012' is partially visible, showing a chemical structure with a highlighted bicyclic ring system and a methyl group (H₃C). At the bottom of the results area, there are labels for 'H₃C', 'O', and 'O-CH₃'.

COMPOUND REGISTRATION

EDIT A BATCH/CREATE A NEW LOT

SEARCH RESULTS

Back Close

CMPD-0000193 Achiral Batch 1 - 09/14/2012

New Lot Details



You can edit a batch or create a new lot from a successful compound registration or search result.

Chemist: Corey Chemist

NEW BATCH REGISTERED SUCCESSFULLY:

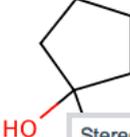
Name: CMPD-0000931-01A

Close New Lot Edit This Lot

Editing the batch or creating a new lot will bring up a familiar page with some fields disabled and not editable.

EDIT BATCH CMPD-0000193-01

PARENT STRUCTURE:



Stereo Category: Achiral Stereo Comment: Original ID:

Mol. Formula: Mol. Wt.: 194.27

ISOTOPE/SALT STRUCTURE:

BATCH PROPERTIES:

Chemist: Corey Chemist

*Notebook-Page: 1234-123

Batch Mol. Wt.: 194.27

Physical state: solid

Batch comments:

Supplier:

Supplier compound ID:

MP:

Purity measured by: HPLC

Analytical Files:

CAS number:

BUID: 3120

Project: Project 1

*Synthesis Date: 09/14/2012

%e.e.:

Color:

Amount: mg

Supplier lot:

BP:

Purity (%): =

View/Edit Files

New Lot Close Update

Chemist: Corey Chemist

*Notebook-Page: 1234-123

Batch Mol. Wt.: 194.27

Physical state: solid

Batch comments:

Supplier:

Supplier compound ID:

MP:

Purity measured by: HPLC

Analytical Files:

BP:

Purity (%):

Analytical Files:

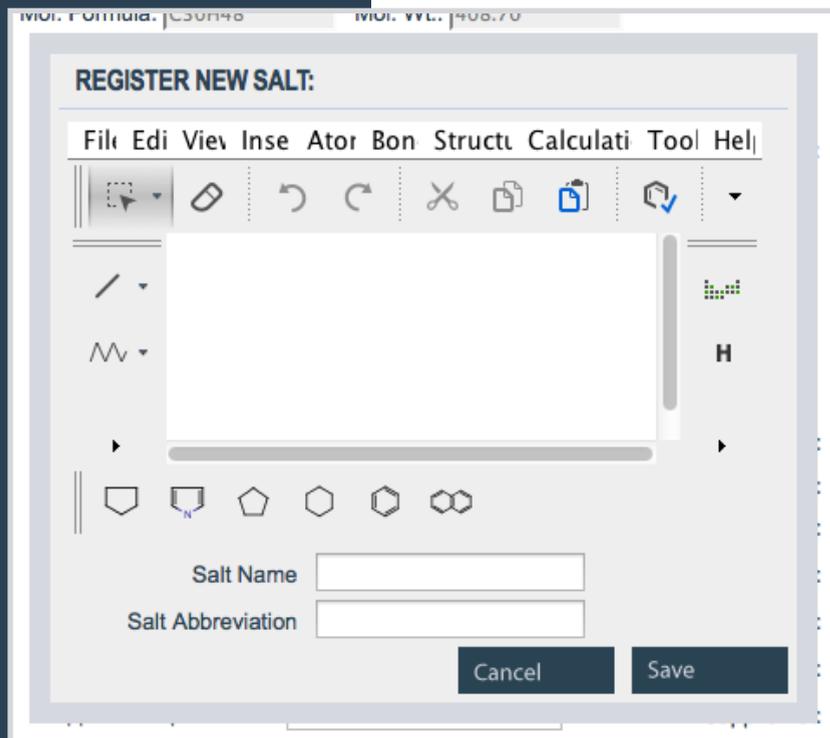
Edit the necessary details and click **UPDATE/SAVE**. A message will pop up with the results (success if successful, or errors if failed).

Lot save succesful

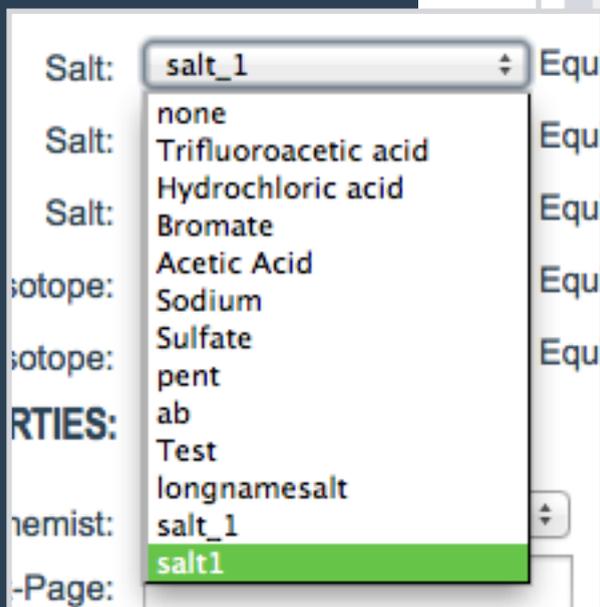
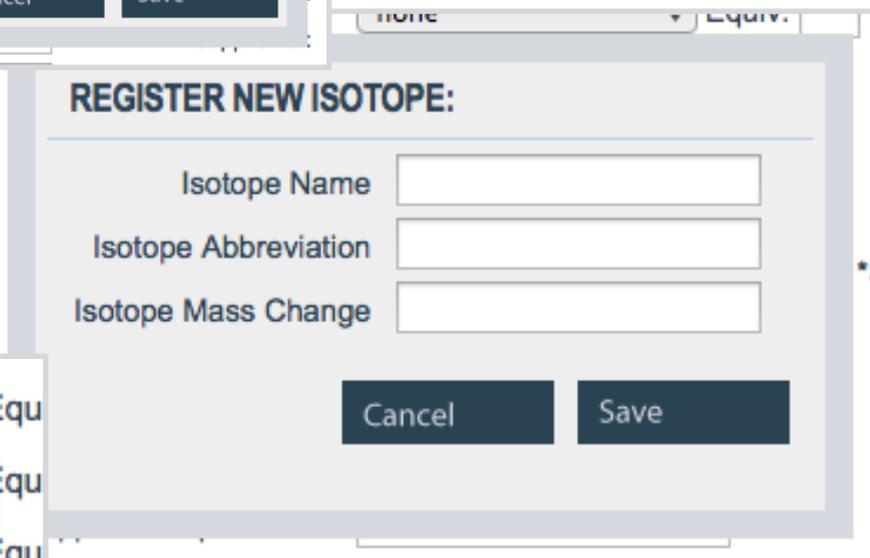
Hide 1 message

COMPOUND REGISTRATION

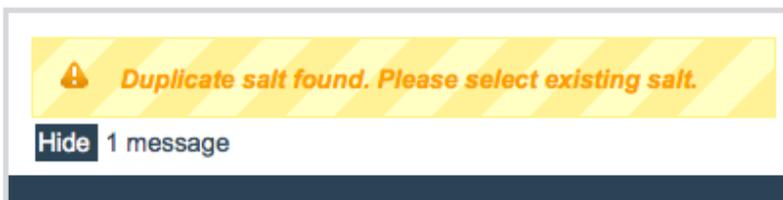
REGISTER A NEW SALT AND ISOTOPE



You can also register a new salt or isotope that can then be associated with the batch being created/edited. After you have created the salt or isotope, it will appear in the dropdown menus for each. You can also associate more than one salt and isotope for a batch.



If a new salt or isotope has already been entered, an error message will pop up, and you can select the existing salt or isotope from the dropdown menus.



COMPOUND REGISTRATION

UPLOAD AN ANALYTICAL FILE

Click **VIEW/EDIT FILES** to upload analytical files.

ity measured by: Purity (%):

Analytical Files:

Browse to the desired file's location and select the file. It will then appear in the menu, where you can change the file type, remove the file, or add another file. Once the files have been uploaded, they will appear at the end of the batch page. Click **UPDATE**.

FILE NAME	FILE SIZE	FILE TYPE	STATUS	REMOVE
<input type="button" value="Browse..."/> No file selected.		<input type="text" value="HPLC"/>		cancel

FILE NAME	FILE SIZE	FILE TYPE	STATUS	REMOVE
<input type="button" value="Browse..."/> HPLC_fiona_test.rtf		<input type="text" value="HPLC"/>		cancel
<input type="button" value="Browse..."/> No file selected.		<input type="text" value="HPLC"/>		cancel

FILE TYPE

- HPLC
- LCMS
- NMR

Analytical Files: Name: HPLC_fiona_test.rtf Description: "HPLC"

COMPOUND REGISTRATION

BATCH PROPERTY ERRORS

BATCH PROPERTIES:

Chemist:	Corey Chemist	BUID:	
*Notebook-Page:	1231124124	Project:	Project 1
Batch Mol. Wt.:		*Synthesis Date:	
Physical state:	solid	%e.e.:	
Batch comments:		Color:	
Supplier:		Amount:	mg
		Supplier lot:	
		BP:	
		Purity (%):	=

⊖ Notebook Page must be provided and formatted like 1234-043

⊖ Synthesis Date must be provided and formatted like mm/dd/yyyy

Hide 2 messages

Cancel

Save

If there are any errors, the compound will not be saved, and errors will be displayed.

Chemist:	Corey Chemist	BUID:	
*Notebook-Page:	7777-001	Project:	Project 1
Batch Mol. Wt.:		*Synthesis Date:	03/21/2014
Physical state:	solid	%e.e.:	

Fix the errors and the error messages will disappear. You can then save the compound.

Chemist:	Corey Chemist	BUID:	
*Notebook-Page:	7777-001	Project:	Project 1
Batch Mol. Wt.:		*Synthesis Date:	03/21/2014
Physical state:	solid	%e.e.:	

In this example, Notebook-Page and Synthesis Date are both required fields. If either of these are not filled out, or are filled out incorrectly, an error message will appear.

The correct format for Notebook-Page is: #####-####