COMPOUND REGISTRATION

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SCHRÖDINGER

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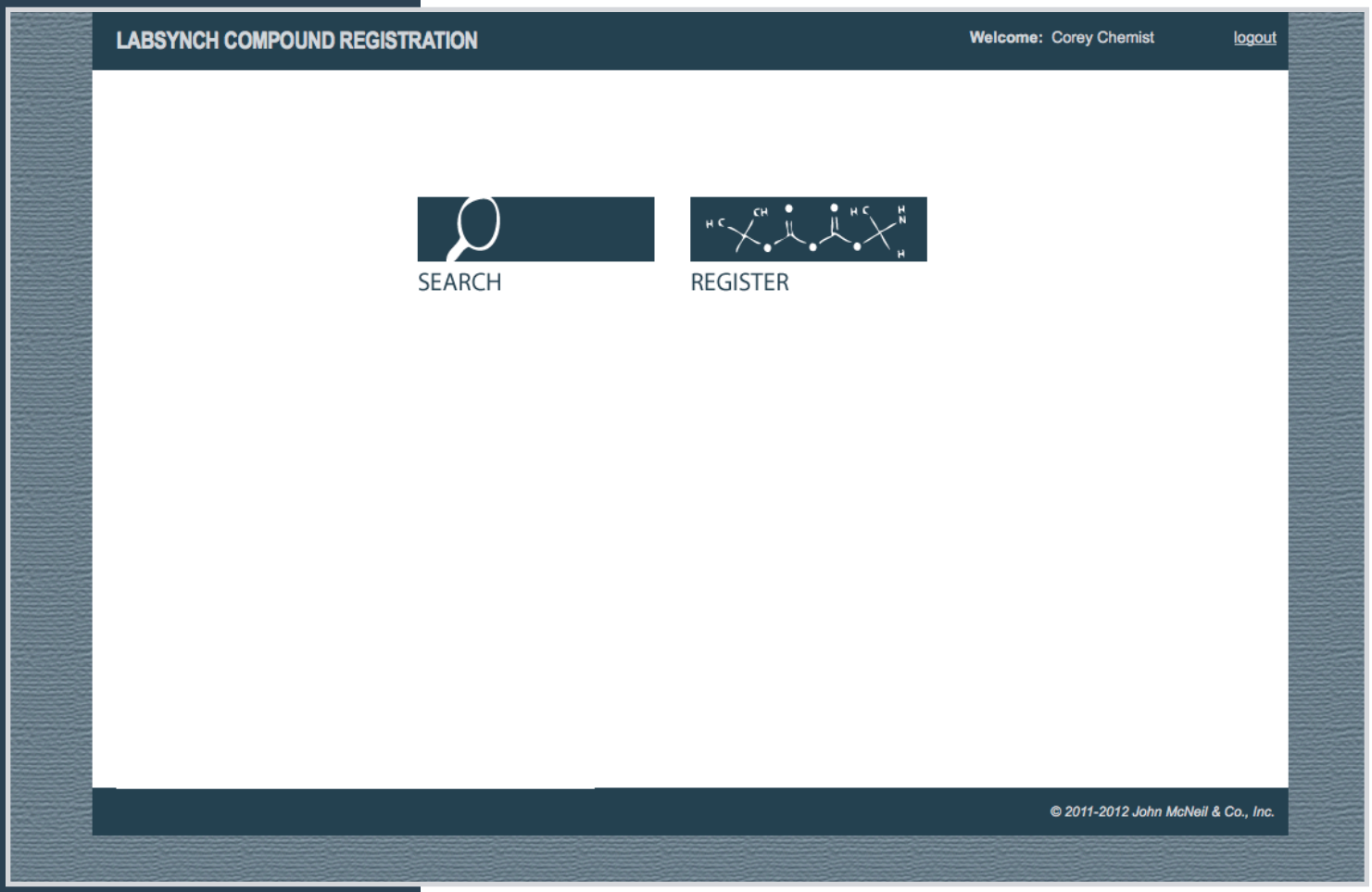
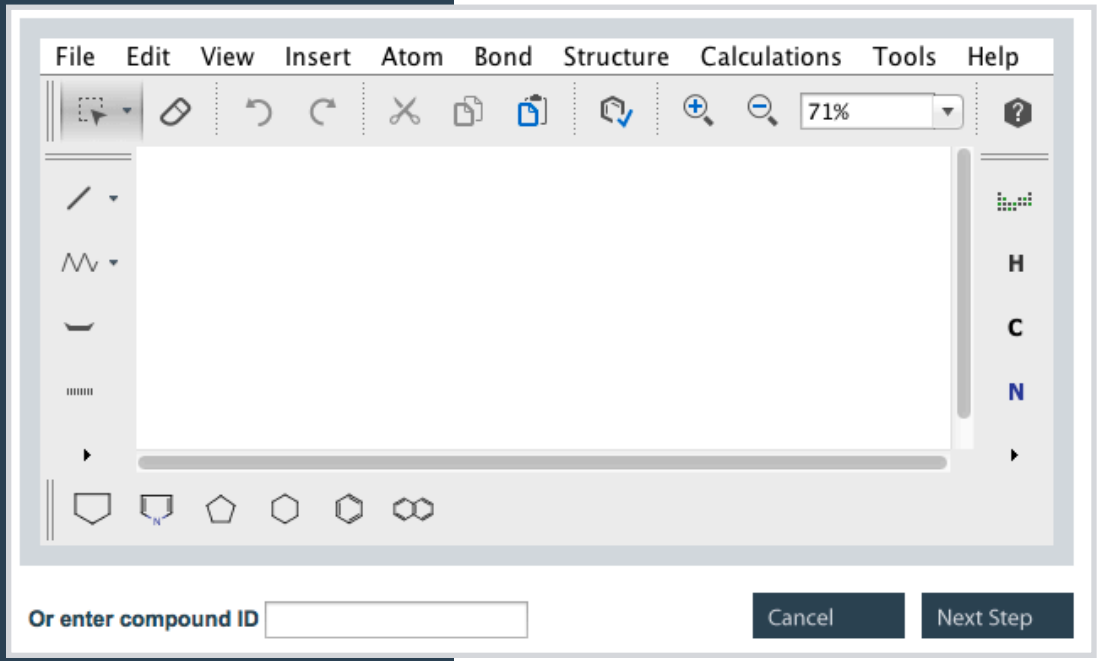
& Company, Inc.

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**.



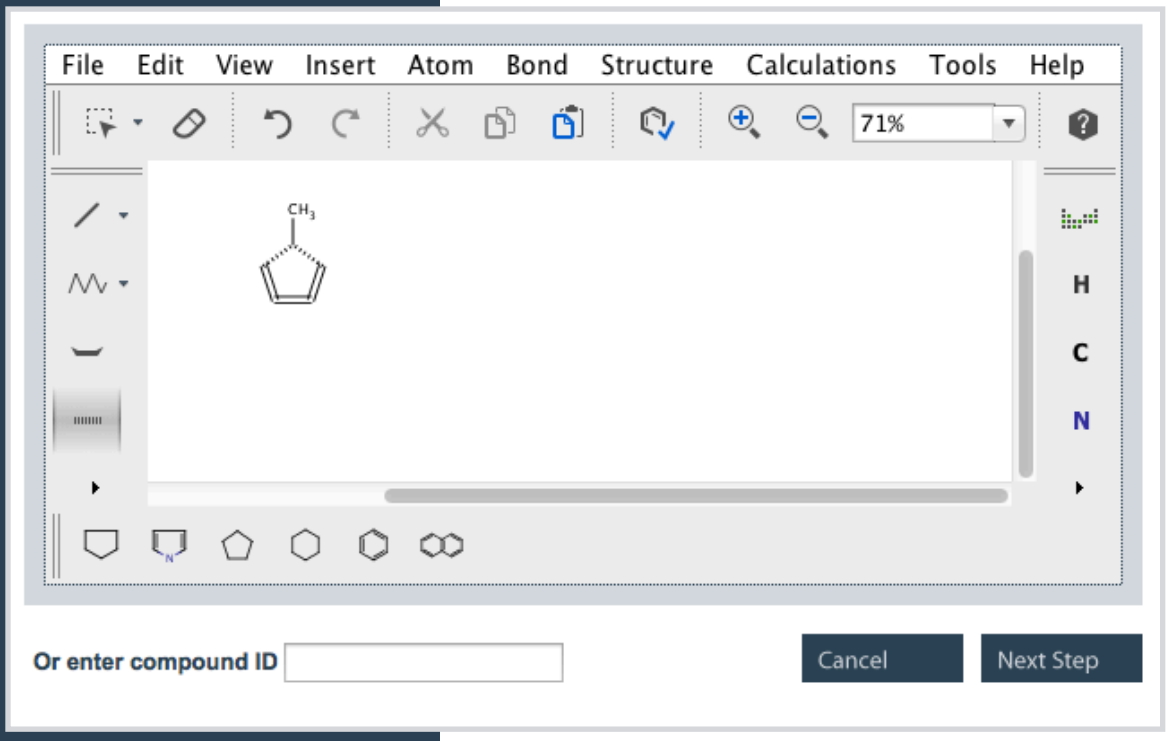


Marvin loads. From here you can draw the structure of the new compound, or enter a compound ID.

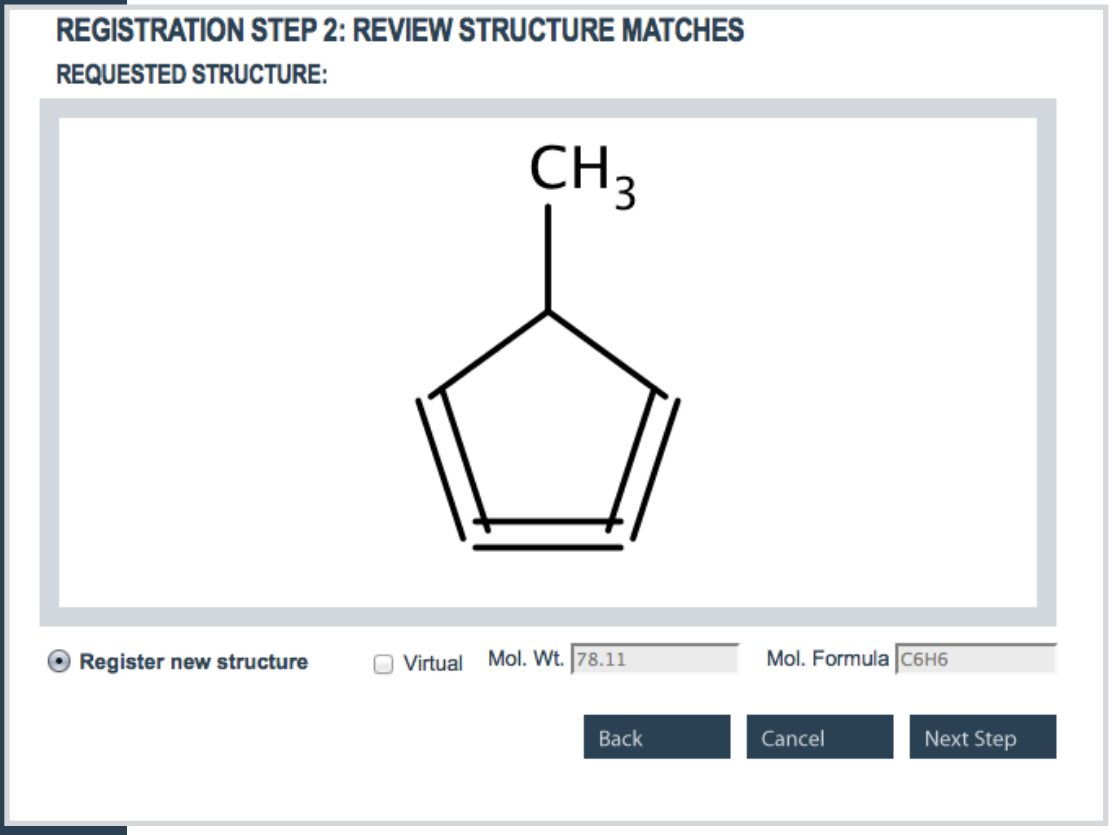
COMPOUND REGISTRATION

REGISTER A NEW COMPOUND STEP 2

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



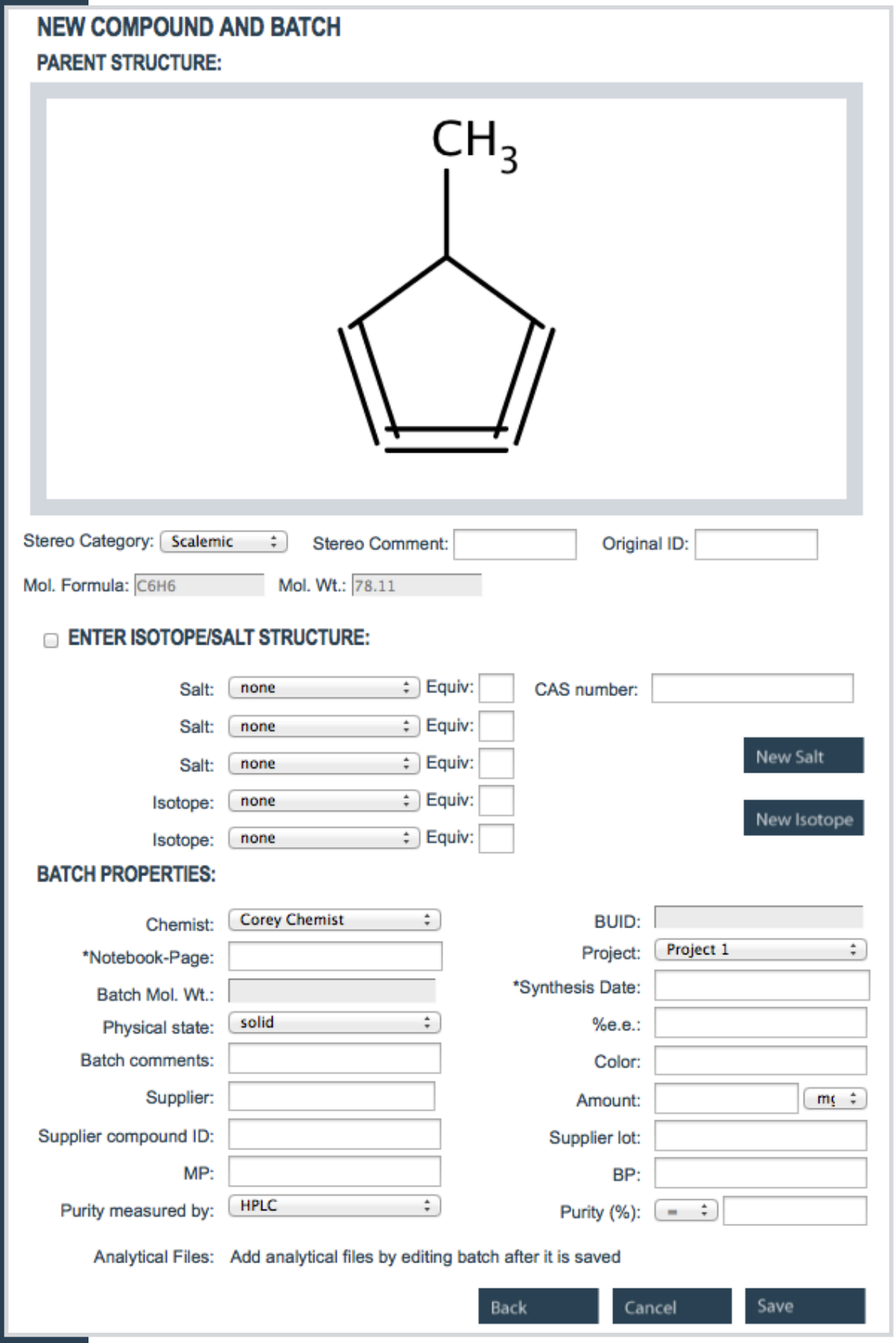
If the structure is unique, only the option to register a new structure is shown. Click **NEXT STEP**.



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**.



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

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

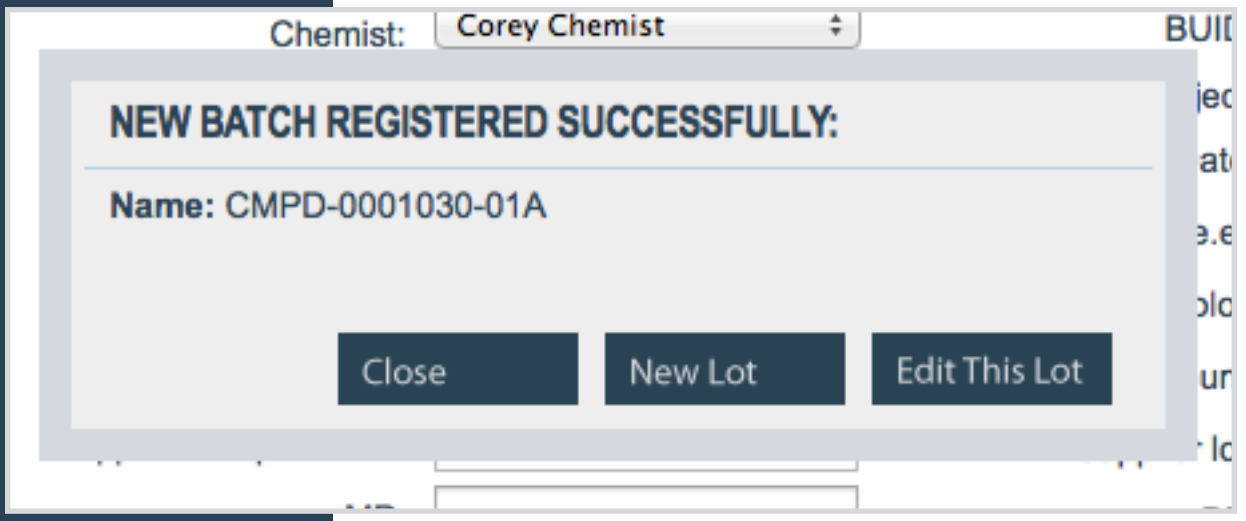
If either of these are not filled out, or are filled out incorrectly, you will be unable to save the compound.

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

COMPOUND REGISTRATION

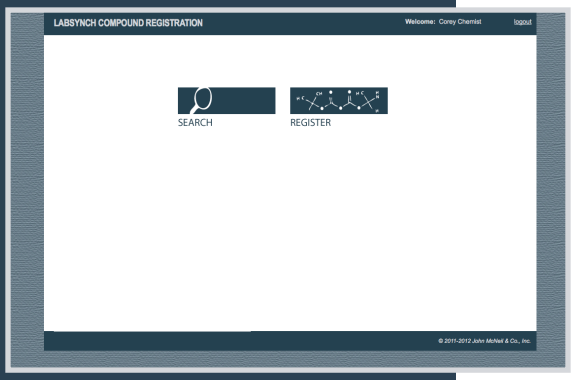
REGISTER A NEW COMPOUND

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**.



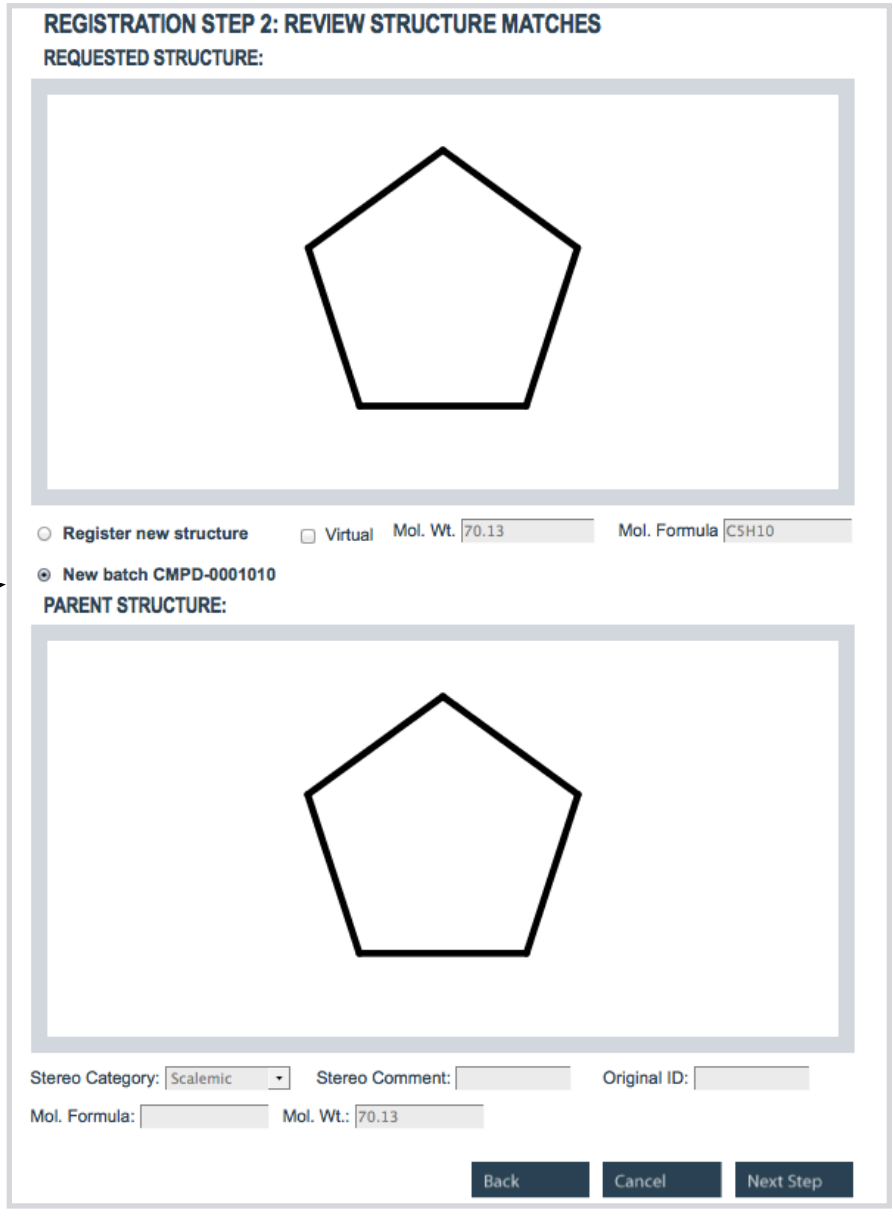
COMPOUND REGISTRATION

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**.

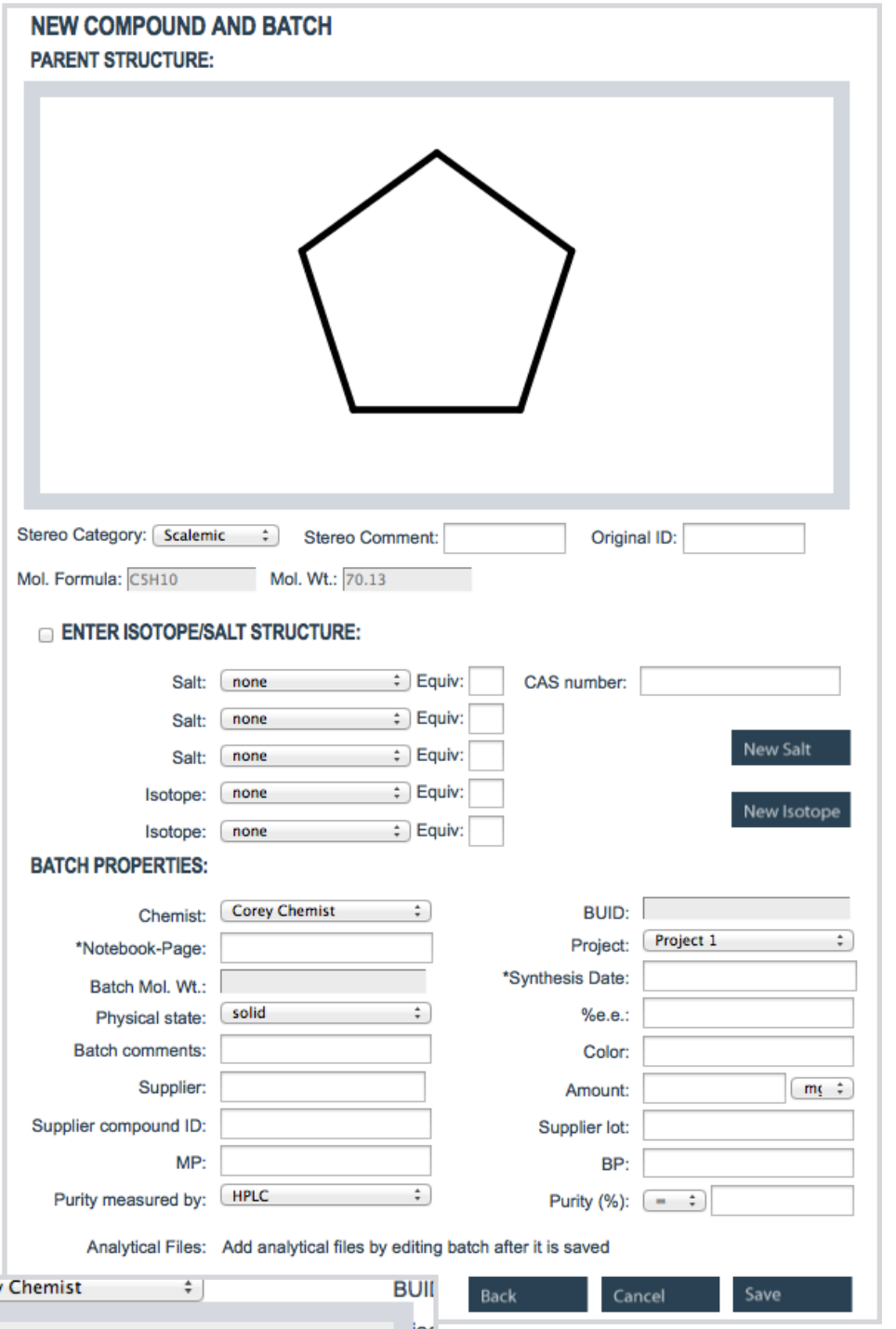


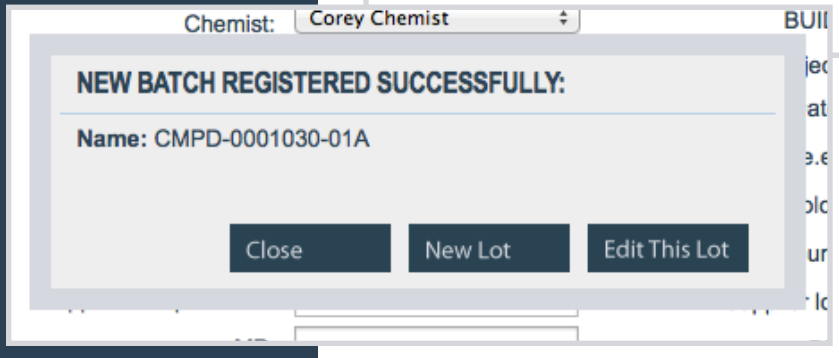
COMPOUND REGISTRATION

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**.





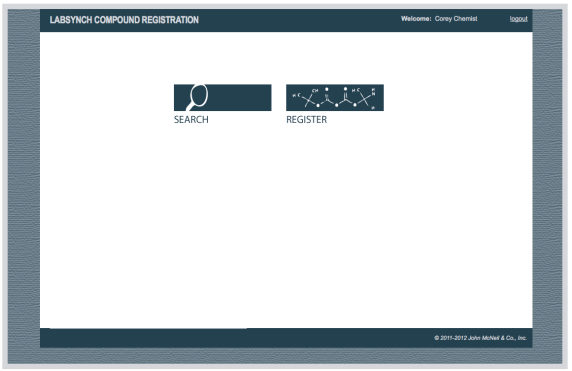
A message will pop up if the new batch was registered successfully.

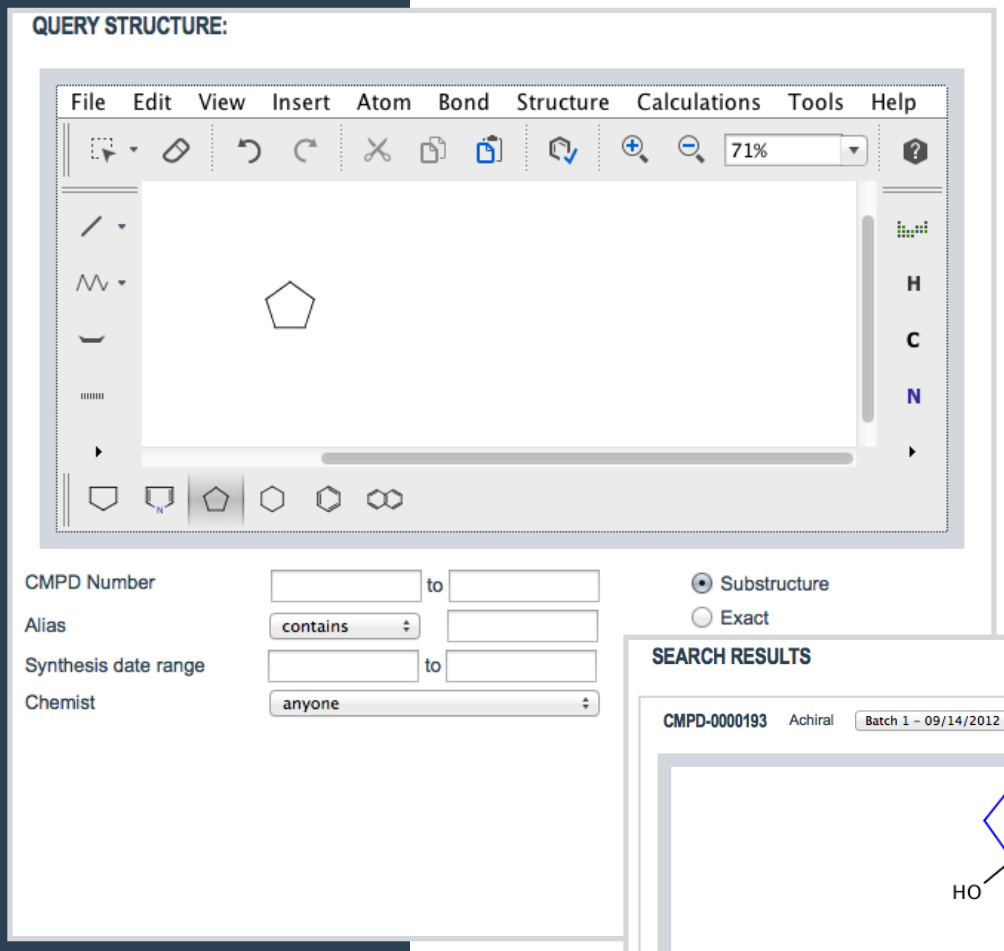
COMPOUND REGISTRATION

SEARCH FOR A COMPOUND

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

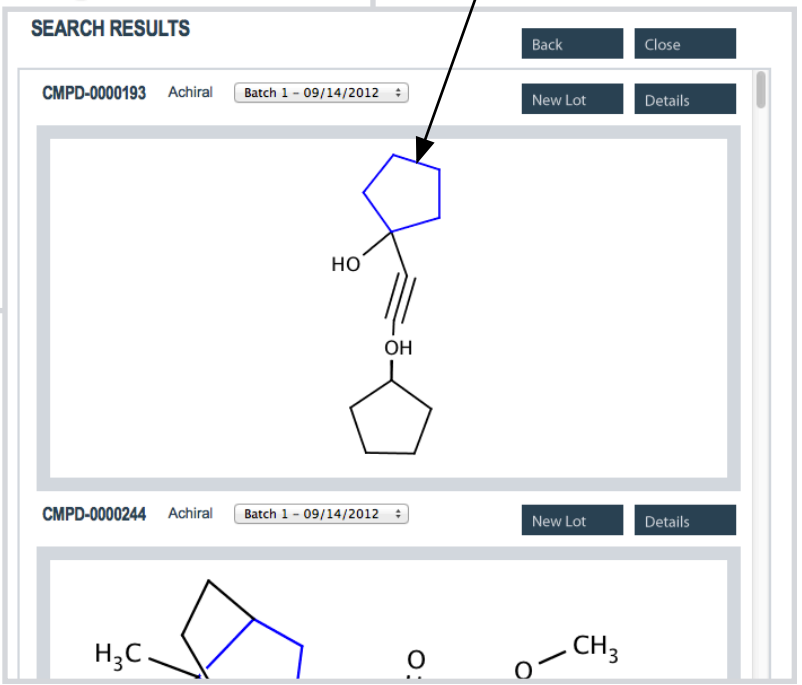
You can search by structure and/or any combinations of the filter fields in the **QUERY STRUCTURE** form.





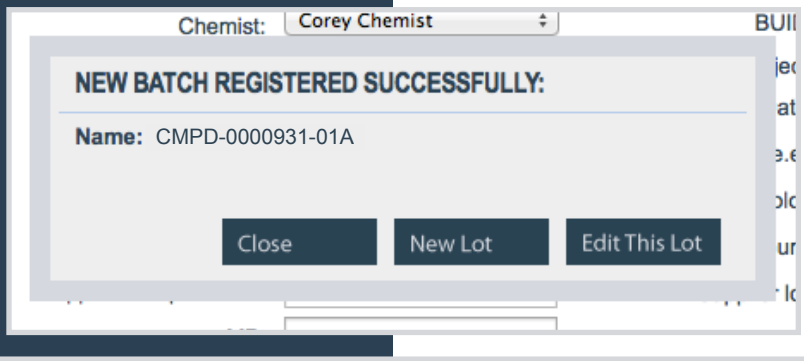
Draw the structure you wish to search for. The results displayed will include any compound that has the given structure included.

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



COMPOUND REGISTRATION

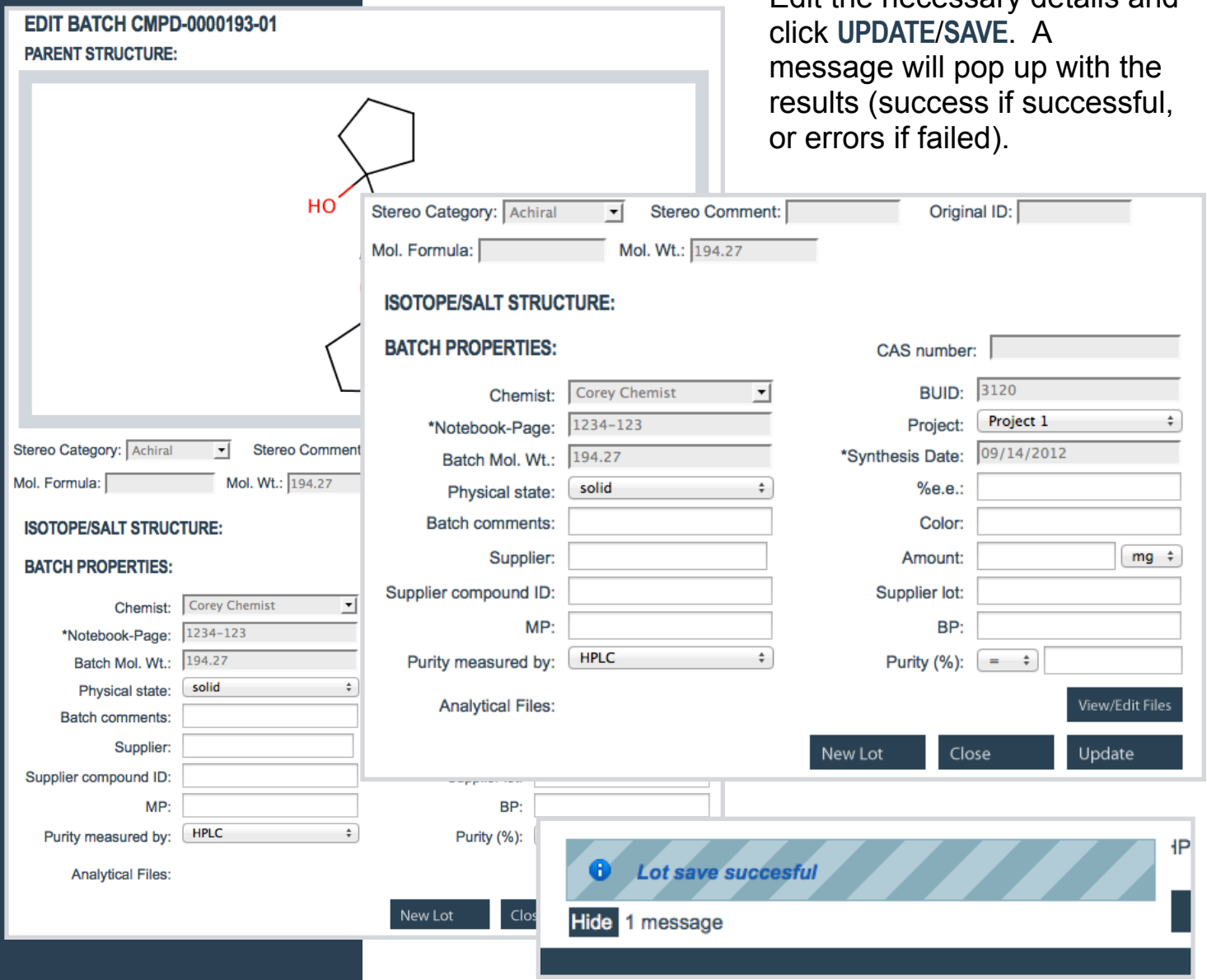
EDIT A BATCH/CREATE A NEW LOT



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

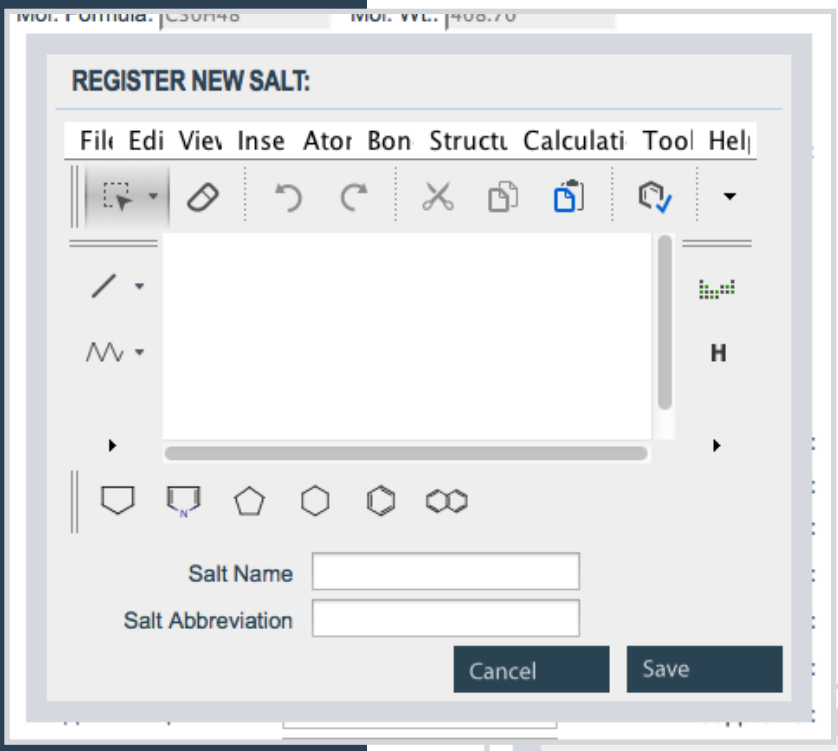
Editing the batch or creating a new lot will bring up a familiar page with some fields disabled and not editable.

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

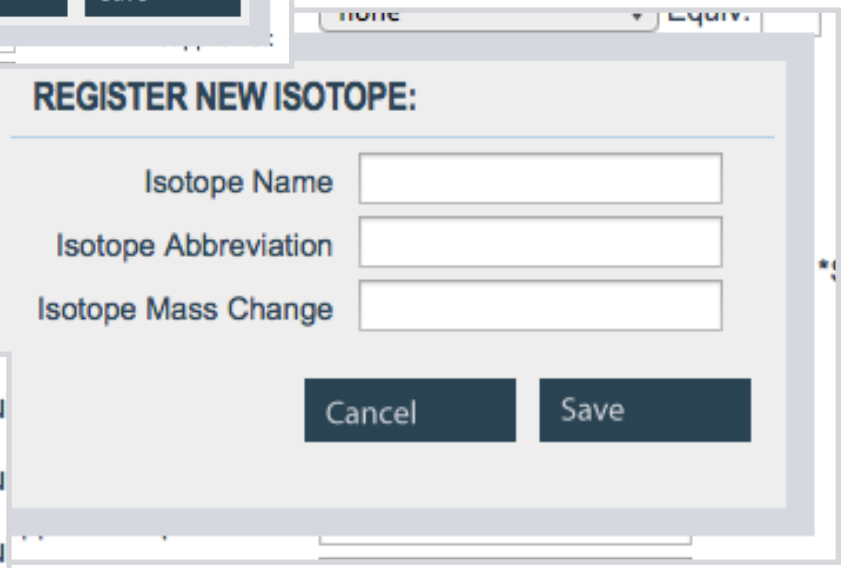


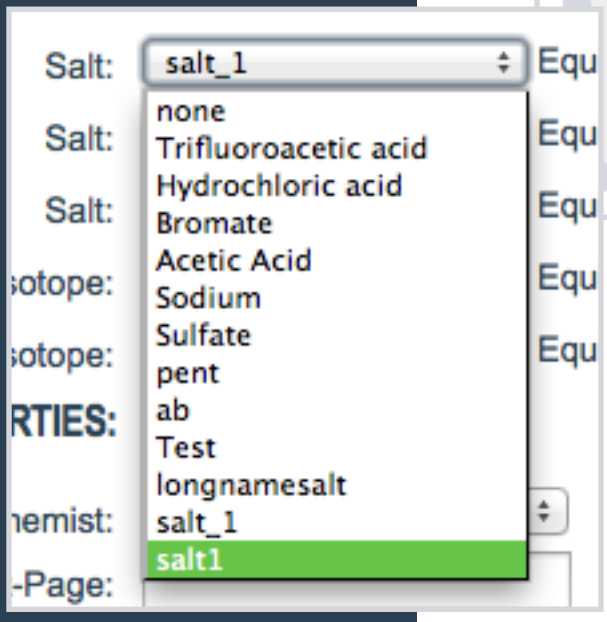
COMPOUND REGISTRATION

REGISTER A NEW SALT AND ISOTOPE

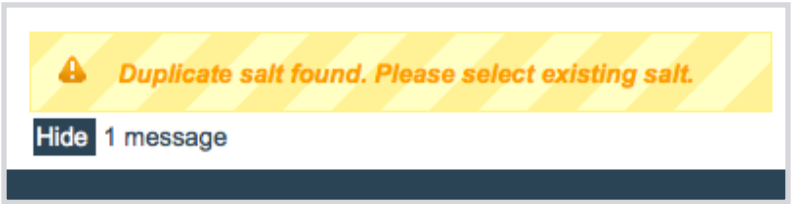


You can also register a new salt or isotope that can then be associated with the batch being created/edited. After you have created the salt or isotope, it will appear in the dropdown menus for each. You can also associate more than one salt and isotope for a batch.





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.

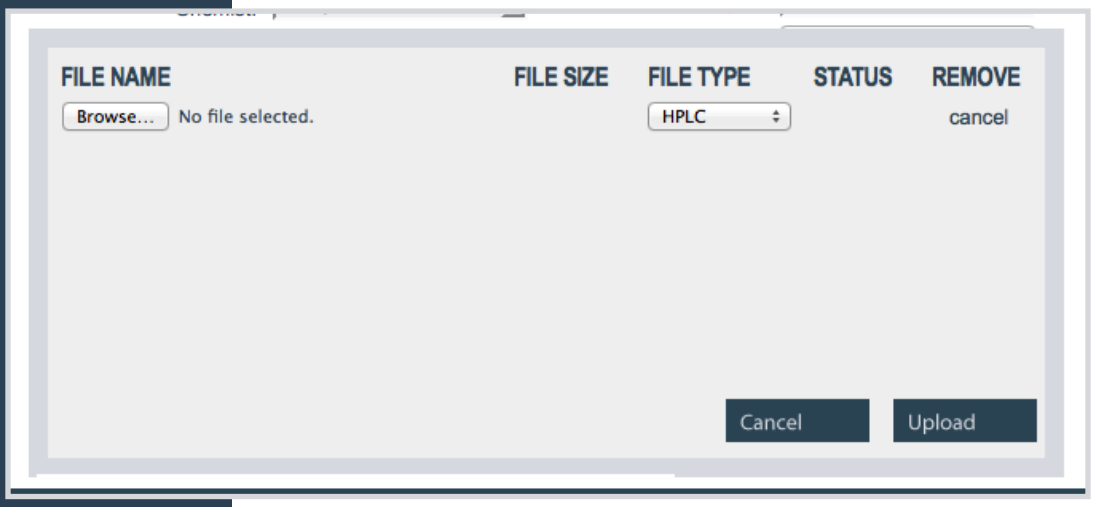


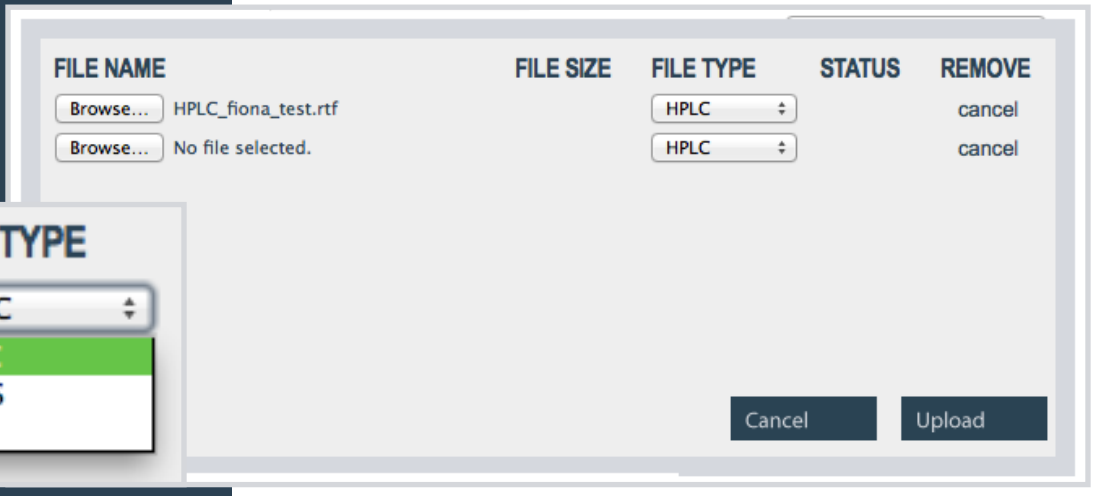
COMPOUND REGISTRATION

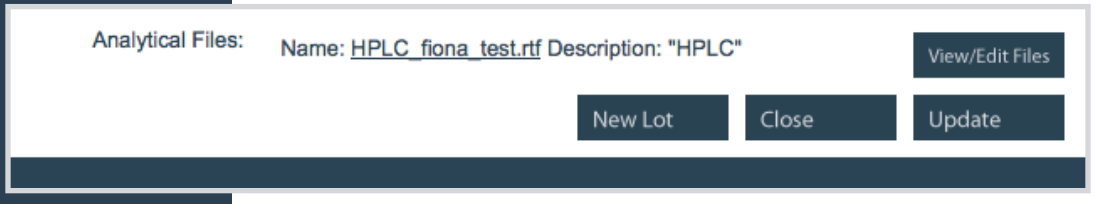
UPLOAD AN ANALYTICAL FILE

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

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**.

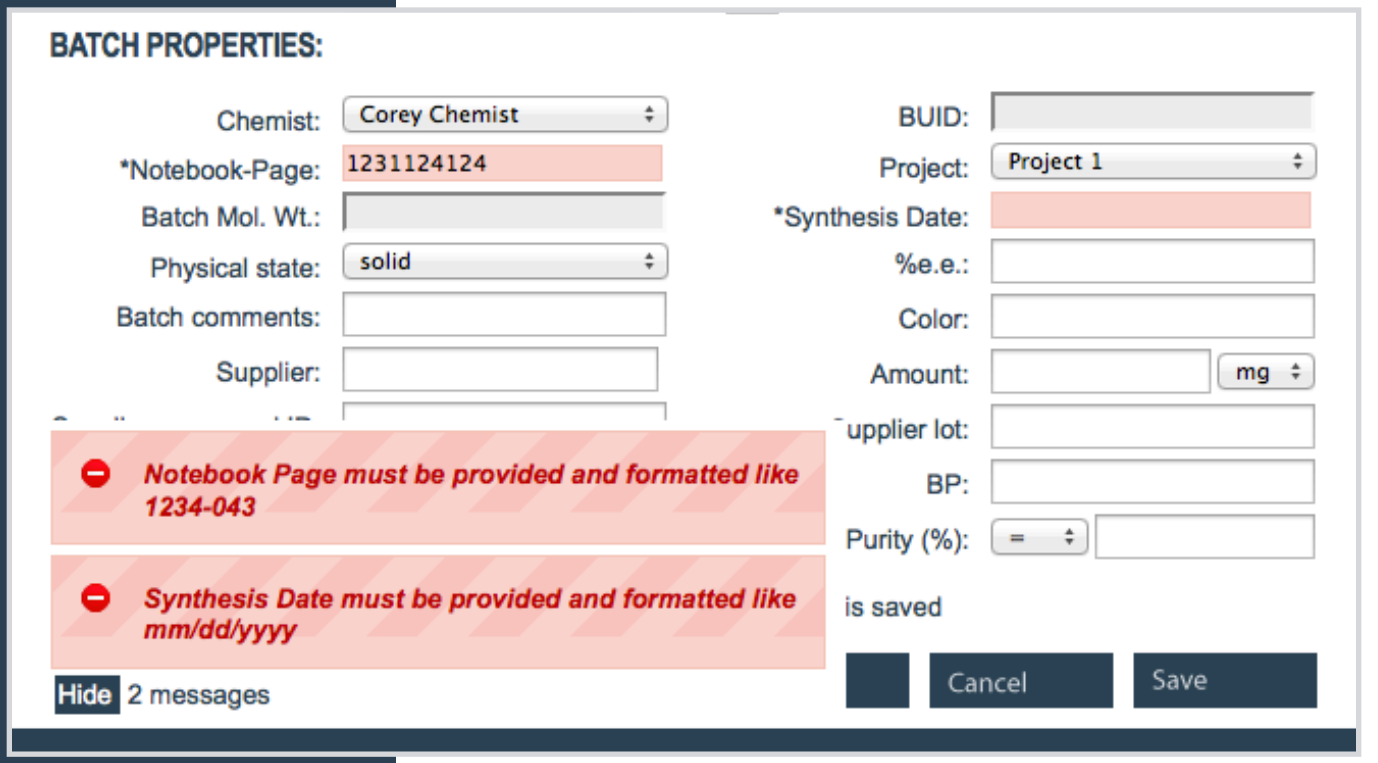




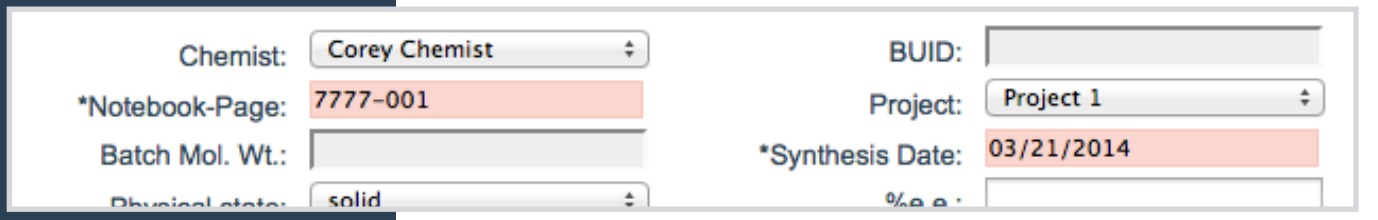


COMPOUND REGISTRATION

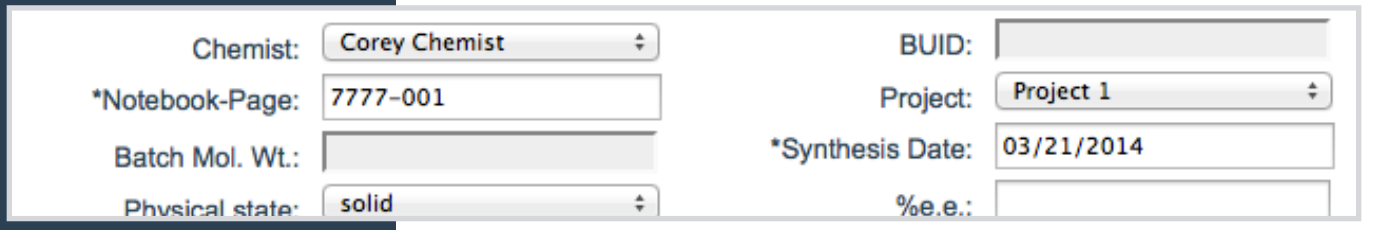
BATCH PROPERTY ERRORS



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



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



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: ####-###