Autoregistration

Registration is the process of calling the registration service to register a compound automatically, based on a predefined configurable set of business rules (validation, standardization, structure checking and fixing).

The form page of the application from where the registration can be initiated is the Registration page.

Before registering a structure and/or CST, the compound is first validated, standardized, checked and fixed. Finally, the structure to be registered is checked for any exact parent matches (considering also CSTs).

Specific IDs (like PCN, CN, LN) can be set for the compounds to be registered.

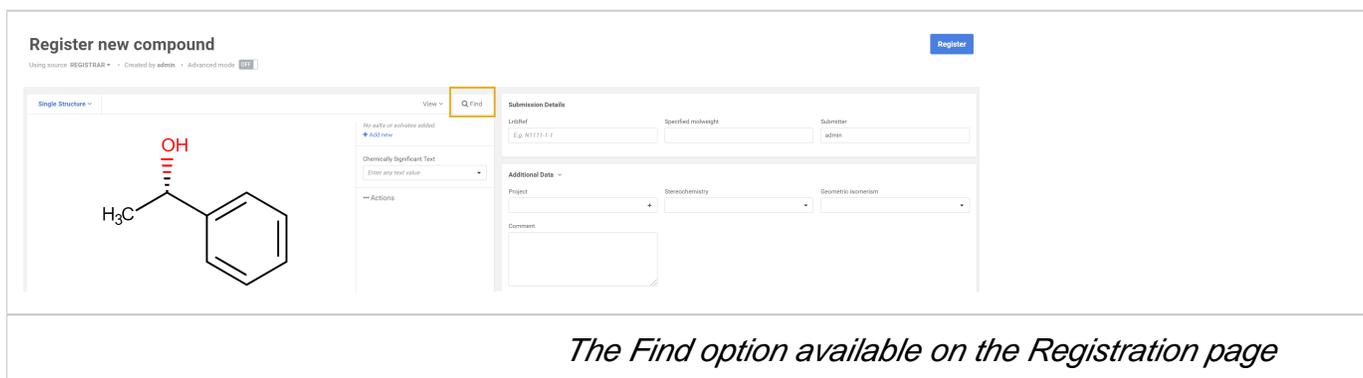[Registration] [Check for matches] [Copy structure] [Assign]

Registration

Compound Registration's structure matching logic is based on ChemAxon's JChem Stereochemistry. During structure registrations the JChem Global Stereo model is used.

Examples for how to register new and matching structures:
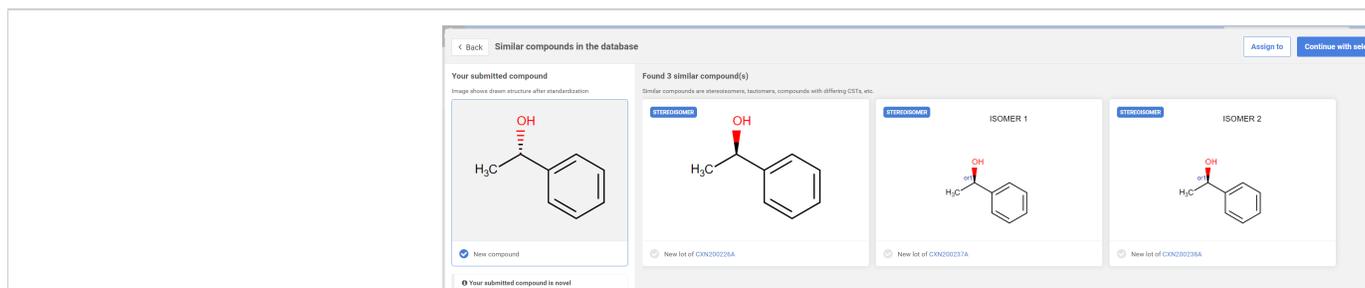
- New structure
- Matching structure

Check for matches

A Suggestion list that contains the already registered matching compounds can be accessed from the Find option located on the top right corner of the structure editor.

The Find option available on the Registration page

Consequently, after checking the "suggestions" from the database, the user can decide which structure should be chosen for registration, the drawn one can be kept, but other suggestions can be selected. This list is the same as the one displayed in the case of an advanced mode registration, the only difference is the Register as selected button instead of the **Continue with selected** button.
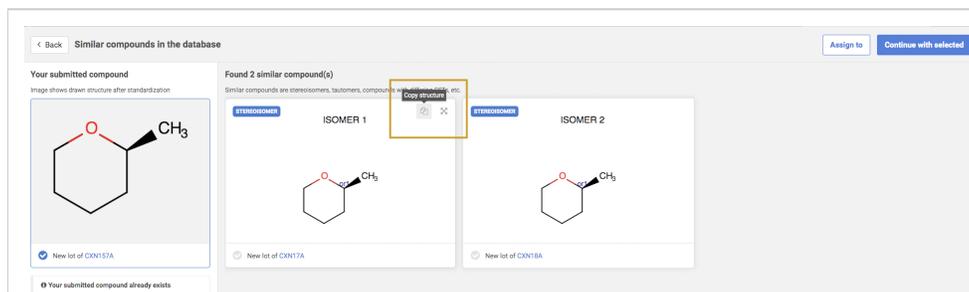

The Suggestion list containing the drawn structure and the matching compounds f...

In the case of a submission cannot be registered automatically, it will fall to the Staging area and a user with corresponding privileges will need to review and manually register it.
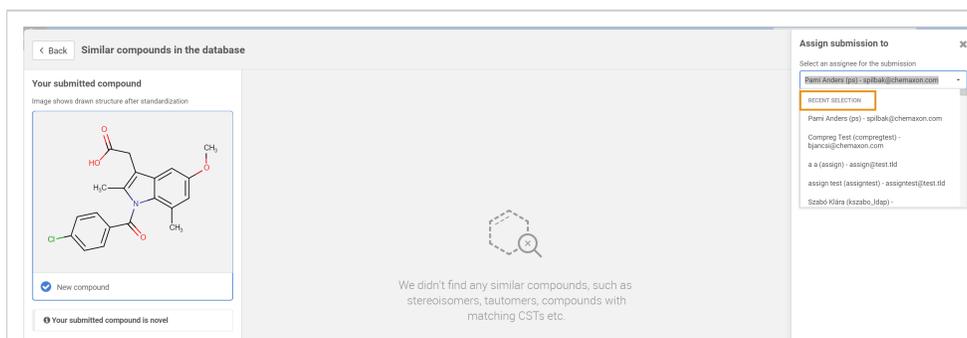
Copy structure

It is possible to copy to clipboard the 'Your submitted compound' or the found 'similar compounds' also. For this purpose please find the Copy structure icon in the top right corner. After clicking on this icon the structure is copied to the clipboard in molfile V3000 format and it can be pasted somewhere else.
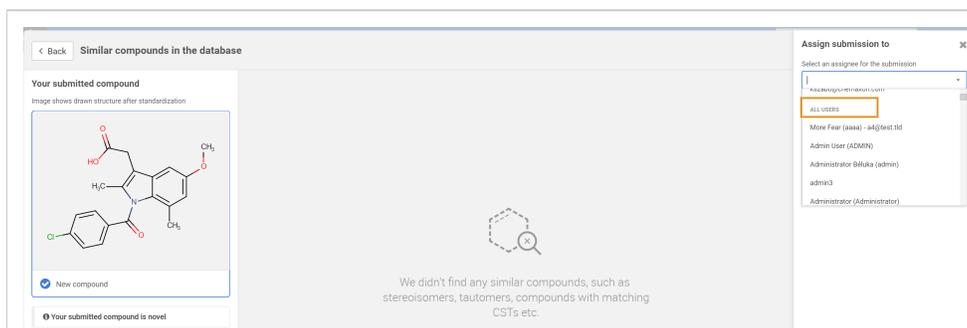

The Copy structure icon

Assign

Submissions can be assigned to other users even before the registration process is started. After drawing the compound, the current user can click the Autoregistration#Find button in order to check the existing matches in the database or to assign the compound to other users. (In advanced mode or on the submission page this suggestion list is also available after clicking to the Register button and the assignment can be done here with the help of 'Assign to' button.) All users (from the DB and from external sources) are displayed here. The logged-in user can select the assignee of the submission from a list of users. The list contains all users (from the DB and from external sources). In the top of this list the *recent selection*, the last 5 choices are shown and below this, the list of *all users* is shown. The username, e-mail address and full name properties of a user are displayed in the user selector dropdown and are all searchable through a typeahead filter.

The list of assignees on the Registration page - Recent selection

The list of assignees on the Registration page - All users

ⓘ The last user choice will always determine the new default assignee for the given user in the given web browser.

ⓘ If the E-mail notification is ON, the users will get notifications *via* E-mail upon assignment of submissions.