

Register Virtual Compound

Redirection Notice

This page will redirect to [Register a Virtual Compound](#) in about 3 seconds.

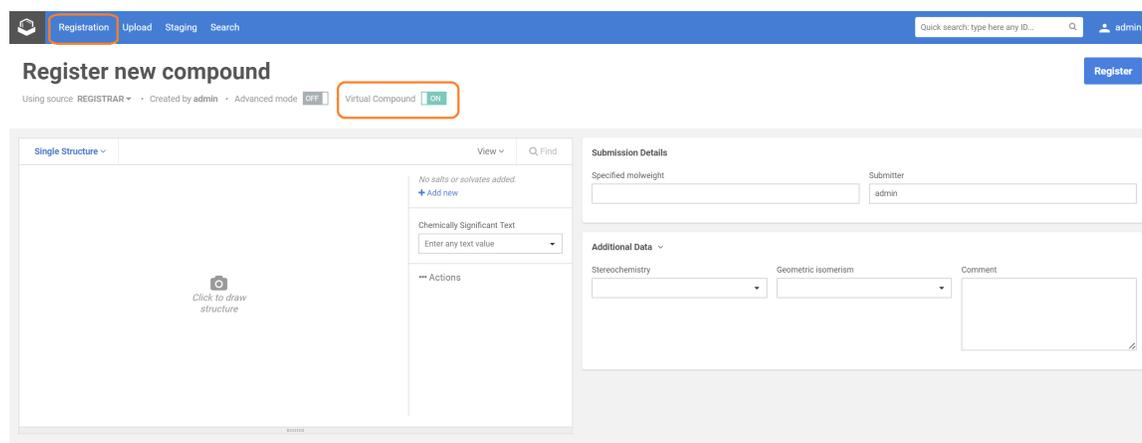
Registration system allows registration of compounds without lots. The registration is made without providing any lot related information. The functionality can be available on the:

- [Registration page](#)
- [Upload page](#)

Registering virtual compounds from the Registration page

The system can be configured to allow the registration of virtual compounds. Make sure your administrator has set the system accordingly ([Administration/General Settings](#)).

Turning on the "Virtual" option will open a new registration form. Here [version](#) and [parent](#) level related information can be set, no [lot](#) specific information should be given.



The screenshot shows the 'Register new compound' interface. At the top, there is a navigation bar with 'Registration', 'Upload', 'Staging', and 'Search' tabs. A search bar and a user profile 'admin' are on the right. Below the navigation, the title 'Register new compound' is displayed, followed by 'Using source: REGISTRAR', 'Created by admin', and 'Advanced mode'. A 'Virtual Compound' toggle switch is highlighted with a red box and is currently set to 'ON'. The main form area is divided into two columns. The left column is titled 'Single Structure' and contains a 'Click to draw structure' button. The right column is titled 'Submission Details' and includes a 'Specified molweight' input field, a 'Submitter' dropdown menu (set to 'admin'), and an 'Additional Data' section with 'Stereochemistry' and 'Geometric isomerism' dropdown menus, and a 'Comment' text area.

In order to register a virtual compound:

1. Turn on the "Virtual" setting on the Registration page. The functionality can be set by your system administrator from the [Administration/Configuration page](#).
2. Draw a structure and/or add any data that is needed for registration, e.g. CST, parent, version level additional data.
3. Click on Register button.

The successful registration will be summarized in a Registration Summary window, which contains Ids for the parent (PCN) and version (CN) level. The created [tree](#) will contain only the [parent](#) and the [version](#) of the registered compound.

<div style="border: 1px solid #ccc; padding: 10px;"> <div style="background-color: #f0f0f0; padding: 5px;">Registration Summary</div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">  <p>Registration successful</p> </div> <div style="border: 1px solid #ccc; padding: 5px;"> <p style="text-align: center; margin: 0;">DETAILS</p> <table style="width: 100%; border-collapse: collapse;"> <tr> <td style="width: 50%;">PCN</td> <td style="width: 50%; text-align: right;">CXN6</td> </tr> <tr> <td>-----</td> <td>-----</td> </tr> <tr> <td>CN</td> <td style="text-align: right;">CXN6A</td> </tr> <tr> <td>-----</td> <td>-----</td> </tr> <tr> <td>LN</td> <td></td> </tr> <tr> <td>-----</td> <td>-----</td> </tr> <tr> <td>LnbRef</td> <td></td> </tr> </table> </div> </div> <div style="display: flex; justify-content: flex-end; margin-top: 10px;"> View Details Ok </div> </div>	PCN	CXN6	-----	-----	CN	CXN6A	-----	-----	LN		-----	-----	LnbRef		<div style="border: 1px solid #ccc; padding: 10px;"> <div style="background-color: #f0f0f0; padding: 5px;">Tree Browser</div> <div style="margin-top: 10px;"> <div style="background-color: #f0f0f0; padding: 2px 5px; margin-bottom: 5px;"> v CXN6 </div> <div style="background-color: #0056b3; color: white; padding: 2px 5px; margin-bottom: 5px;"> CXN6A </div> </div> </div>
PCN	CXN6														
-----	-----														
CN	CXN6A														
-----	-----														
LN															
-----	-----														
LnbRef															
<i>Registration Summary</i>	<i>Tree Browser</i>														

Note that if the virtual compound being registered is already present in the DB (with or without lot) no warning is received and the Registration Summary window will display the Ids.

Note that also [multi-component compounds](#) can be registered as virtual compounds.

Bulk upload virtual compounds

Uploading an SDF file that contains a property field that can be mapped with "Virtual Compound"

1. On the Upload page browse for the SDF
2. Map the appropriate fields, e.g. "virtual" --> "Virtual Compound". The value for the "Virtual Compound" field should be either true or false.
3. Upload. As a result, if the "Virtual Compound" value was true, the compound was registered without lot (as a virtual compound), if the value was false, the compound was registered with lot.

Uploading an SDF file that does not contain a property field that can be mapped with "Virtual Compound"

1. On the Upload page browse for the SDF
2. Map the appropriate fields.
3. If there are no property fields within the SDF that can be mapped with the "Virtual Compound", click on the "Append field" button located at the bottom of the field list. If you want to register all structures from the SDF as virtual compounds, set default value "true" for the appended field "Virtual Compound".
4. Upload. As a result, all compounds will be registered without lot (as a virtual compounds).

Upload File Use text editor

Indoles-200.sdf  

5 field(s) were found: Record nr. 1  

- Structure → Structure
Mrv0541 05081404202D 25 27 0 0...
- CdId 5
- Mol Weight 349.814
- Formula C20H16C1N3O
- External_ID N10005-1-1

+ Append field   

Add new fields using the "Append field"

Upload File Use text editor

Indoles-200.sdf  

6 field(s) were found: Record nr. 1  

- Structure → Structure
Mrv0541 05081404202D 25 27 0 0...
- CdId 5
- Mol Weight 349.814
- Formula C20H16C1N3O
- External_ID N10005-1-1
- Appended field → Virtual Compound 

Virtual Compound

+ Append field   

Add default value "true" to the "Virtual Compound" field