Compound Registration FAQ

The FAQ (Frequently asked questions) page contains listed questions and answers, commonly asked about the system when using the Compound Registration web application.

1. ## How can I register a compound with parent multiplicity 2 and salt multiplicity 3?

   On the Registration, Submission or Browse-Edit page you can add the salt or solvate then set the appropriate multiplicity. After setting the salt/solvate multiplicity the parent multiplicity can be also set. Please note, that only positive integer numbers can be set for salt multiplicities and positive numbers with one decimal can be set for solvate multiplicities (the decimal places in case of salts/solvates can be configured).

2. ## Can I set fractional salt or solvate multiplicities?

   Yes. The precision of the salt and solvate multiplicities is configurable, it can be set on the Administration/Chemistry/Salts & Solvates/Settings. By default, the precision of the salt multiplicities is 0 (only positive integer numbers are accepted), the precision of the solvate multiplicities is 1 (fractional value with one digit is allowed).

3. ## Can I register multicomponent structures?

   Yes, different types of multi-component compounds exist, based on the level of accuracy of the composition information: alternate, formulation, and mixture. A multi-component compound is distinct from a structure having multiple fragments within a structure field that has been registered as a single compound (without registering each fragment individually). An alternate is a multi-component compound without quantitative composition information. A formulation is a multi-component compound with exact quantitative composition information. A mixture is a multi-component compound with semi-quantitative composition information.

   It is possible to register polymers as multi-component compounds. Polymers can be stored with its monomer units, that are created by stripping the "leaving groups" (configurable) from the monomers. More details can be found here.

4. Can I register multi fragment structures?

Multifragment structures can be registered, and are handled as a single molecule. Fragments representing salts/solvates can be automatically extracted and converted to the proper salt/solvate and multiplicity information during the registration process.

5. Can I register dimer structures by drawing the monomer and setting 2 for the parent multiplicity?

No. Greater than 1 parent multiplicities must be used with salt/solvate info. For registering dimer structures you must draw or import the dimer.

6. Can I register peptides?

Yes. Peptides can be registered as single-type structures. Peptides are stored with all their atoms as chemical entities. Using Marvin JS structure editor, peptide sequences can be imported as 1-letter or 3-letter aminoacid sequences. It is possible to register in a contracted, expanded or ungrouped form. In case if autoregistration is not possible, you can register it from the Staging area (manual registration).

7. Can I register polymers?

Yes. Polymers can be registered as single-type structures, but as multi-component compounds as well. In order to register as single structures, you can just simply draw structures then click on the Repeating Group tool on the toolbar, select the atoms you want to be included and set the repeat pattern. For more info click here.

Registering as multi-component compounds p olymers can be stored with its monomer units, that are created by stripping the "leaving groups" (configurable) from the monomers. More details can be found here.
The molecular weight and molecular formula of polymers cannot be calculated. Polymers can be stored with its monomer units, that are created by stripping the "leaving groups" (configurable) from the monomers. More details can be found here.

8. Can I register Markush structures?

Yes, it is possible to register Markush structures within the system. The registered Markush structures are stored separately, but treated the same way as all the other ones: parents, versions and preparations are created; Markush matches are offered during the registration, etc. There are two major limitations: (1) Markush structures cannot be registered automatically, all of them are forced to be reviewed, (2) Markush structures cannot be used as components in multi-component structures.

Searching for Markush structures is possible on the Search page, even against the non-Markush structures (in that case all members of the Markush query will be returned as hits, even if they are only part of a multi-component structure).

9. Can I bulk register structures?

Yes, there is a specific Upload option for this purpose. You can load an SDFile and map its fields to the appropriate Compound Registration fields (or use a previously saved mapping template), and you can even reset the system switches and the Structure Checker and Autofixer options on the fly. The original and fixed structures can be previewed before initiating the registration.

Please note that currently only Single type compounds can be uploaded.

10. Can I configure the system to store my compounds only on 2 levels (parent-lot)?

It is possible to configure the system to hide the version level on all the GUI pages and in all confirmation messages, so from the user perspective, the system behaves like the data would be stored only on 2 hierarchy levels. You can also configure the system to generate registration IDs on the lot (preparation/batch) level (e.g.CXN1234-01), which takes care of the lot counter even if you move a lot from one parent to another (it is regenerated according to the new parent). In addition, you can configure the downstream service to neglect the version level, so your downstream systems do not need to even know about it. And, which is the most important: if later you decide to upgrade your system to a 3-level hierarchy, it can be simply done by a configuration!

11. Can I autoregister a preparation (lot) under a given Id?

Yes, use the Register with CN option, which is available on the Registration, Submission pages and Browse pages. Note that on the Browse page the option is available only for the selected parent or version level.

12. How can I register a compound without structure, or with only partially known structure?

Compounds without structures can be registered on the Registration page after selecting the ‘No structure’ structure type. In order to provide additional information a Chemically Significant text (CST) can be added to the compound. It is also possible to register a ‘No structure’ without CST.

‘No structure’ structure type is available from version 18.03.12-2503.
In older versions compounds without structures can be registered only together with CST.

There is a switcher option available on the Configuration that controls whether the CST only records should be autoregistered or not. If the records fall to the Staging area with "UnknownCST" status message, they can be registered easily from there (Submission page). If the CST is present in the Chem. Sig. Text dictionary (Administration page), the record will be always autoregistered.
CSTs can be used also for the user wants to register the same structure but as different compounds (receiving two different parent IDs in the database). If the structures of two compounds are the same (or empty), but the CSTs are different, then these compounds are considered as 2D matches (not as duplicates).

13. Is JChem Oracle Cartridge supported on the back-end?

The DB storing of the Registry contains normal JChem tables, and the direct support of the Cartridge is not needed, because the Registry tabled can be directly joined to other JChem Cartridge tables, if required.

14. Can I use other editors than Marvin JS on the GUI pages?

Yes, Marvin applet and ChemDraw are supported, but for the latter one you need a valid installation of ChemDraw on your computer. More details can be found here.

15. I changed the Structure editor to Marvin applet, but I cannot use it in Chrome or Firefox.

Java applets are not supported by Chrome and Firefox (since Firefox 52 version). But Marvin applet can be still used with InternetExplorer11. Note that you have to allow Java in the browser and the applet is loading very slowly.

16. I changed the Structure editor to ChemDraw, but I cannot use it in my 64-bit InternetExplorer.

ChemDraw has not plugin support for 64-bit web browsers. ChemDraw, if Active X plugin installed, can work fine in 32-bit Internet Explorer (11) or FireFox (older versions than FireFox 52) browsers. Note that ChemDraw has to be installed locally on your computer.

17. What to do if my compound fell to staging due to a quality check, but I believe that this is the correct structure?

You should switch off the Perform Quality Checks option on the Submission page. You need to have the corresponding privileges to do so.

18. What to do if my compound fell to the Staging Area because of a Structure Checker error that not belongs to the quality checks (e.g. Racemate Checker error)?

If you have an automatic fix available for this checker, you can select it from the popup list of that checker, and, then it will be applied on the fly when you register your structure (in the case of the Racemate Checker the Convert to Unknown fixer can be a possible option). Prior to registration, you can test the effect of the fix using the Check option.

If you do not find any appropriate fix for the checker, you have to modify the structure to pass the failing structure checker, or you can contact a Registrar to fix the submission for you.

19. Can I modify a submission in the Staging area without registering it?

Yes. Submissions can be modified (e.g. LnbRef, Molweight, Restriction, CST, structure) and then saved. These will be marked as "Saved submissions" in the Staging and their original structure can be restored later or they can be registered.

20. Can I have a detailed status message in the Staging area about the submissions?

For the submissions in the Staging area, a status message is displayed in the last column. When hovering over the status message a detailed message is also displayed for the given submission. If a submission is opened from the Staging in the Submission page, the short and detailed message is also displayed.

21. What are the meanings of the different molecular weights indicated in the result table on the Search page?

Molweight (structure) refers to the calculated molecular weight of the version structure (including charges, isotopes), whereas the Molweight (structure + salt) refers to the calculated molecular weight of the preparation structure together with the salt or solvate which belongs to the version/lot. Molweight (parent) Molweight (version) and Molweight (lot) are molweights supplied by the user.

22. Can I add a salt or isotope to an already registered compound?

Yes, on the Browse-Edit page, from version or lot level, salts/solvates and/or isotopes can be added to the structure. Then click on the Save button. User that have a privileged role can do this.

23. **Will the IDs be kept, if I modify the structure?**

In the case when the structure change was performed on the parent level, yes. In other cases, when the change was made on version or lot level, new IDs (PCN, CN, LN) will be given.

24. **If I add a salt or isotope on the Browse page to an already registered structure, will my compound receive a new parent Id?**

No. In case of salt/solvate and/or isotope additions, which can be performed only from lot or version level, the parent Id (PCN) will be always kept.

25. **Can I amend an already registered single type compound to be a multi-component compound?**

Yes. From version or lot level single compounds can be amended to multi-component ones. The multi-component compound will receive a new PCN, and the new components, if they were not registered yet as single compounds, will receive new parent Ids, to which the components are linked in the multi-component compound.

26. **Can I amend a multi-component compound?**

Yes. Multi-component compounds can be amended from lot or version level. They cannot be amended from parent level.

27. **What will happen when I amend compounds that are used as components in multi-component compounds?**

Single compounds used as components in multi-component compounds can be amended only on parent level. When amending compounds that are used as components in multi-component compounds, the modified structure will be moved to a new tree (and will receive new PCN, CN, LN), in case there is no match in the DB, while the reference of the multi-component compound will be kept with the original compound.

28. **What are the match actions in the case when amending a compound and having an exact match?**

In case of exact match, the only option is to Accept the match. If other matches (e.g. 2D) besides the exact are also present, no match options will be available for those.

29. What are the match actions in the case when amending a compound and having a 2D match?

In the case when there is no exact match and there is one or more 2D / Tautomer / 2D&Tautomer match(es), the match actions are Accept and Unique.

30. Can I amend a compound from version level when there is no lot under it?

No. Version level amendment is not allowed for versions without lots. "Editing the structure is not permitted. Amendment of an empty parent/version is not allowed." message can be seen above the structure editor and the Save button (in the Edit mode) is disabled.

31. What are the mandatory fields for a registration on the Registration page?

It is configurable. When registering a lot, a structure and/or CST and a valid source are needed for a registration. Usually valid, unique external Ids (like LnbRef) are also set to be required for the registration, but any other fields can be set.

32. Can Project based access be used to the registered compounds?

Yes, the Project based access can be enabled (configurable). In this case, registration and access (to be viewed or to be modified) of compounds will be available only if the logged in user has the specified permission within the given project. For a logged in user, the available projects will be displayed in the field drop-down list. No registration will be possible using newly given Project name(s) as additional data. Otherwise, when Project based access is disabled, Project fields can be freely used as additional data, no filtering is made.

33. Can I change the content of the additional data dropdown fields?

Additional data fields, in general, can be configured only by the privileged user. When defining the additional data (Administration/Forms and Fields tab), a list of values and even default values can be set.

34. How can I migrate the compounds from my old registration system?

There are 2 options:

a.) You can use our REST API. For details click here.

b.) Using the Upload page SDFiles can be uploaded. It is possible to keep the original PCN and CN provided with the record if there is no match to a previously registered compound. Different mappings can be set between the SDF fields and the system (e.g. salts and multiplicities, additional data fields, users, etc.). Note that using the Upload page only single structures can be registered.

35. Is it possible to load all of my salts/solvates in a single action into the dictionary?

Yes, similarly to the compound upload, salt/solvates can be bulk loaded from the Upload page of the application. Salts and/or solvates can be imported from an SDFile after mapping its fields to the appropriate fields (Name and salt solvate flag).

36. What should I do if I receive an error like “An error occurred while bootstrapping the application” after upgrading to a newer Compound Registration version?

*The “An error occurred while bootstrapping the application” error means that the application cannot be loaded. You always need to clear the browser cache. If you are using Internet Explorer, Edge, Google Chrome, or Mozilla Firefox you can quickly clear cache with a keyboard shortcut. While in your browser, press **Ctrl** + **Shift** + **Delete** simultaneously on the keyboard to open the appropriate window. Make sure that "Cookies" and "Cached images and files" and items "From the beginning of time" is selected when clearing the browsing data, then restart your browser and try to reload again the Compound Registration web application.*

37. Why do I receive a Marvin JS related error?

The Marvin JS license file is most probably provided in a separate license file than the Compound Registration license file.

- ***Using the latest Compound Registration version****: using the installer wizard both files can be uploaded and the system will automatically merge the two licenses. No "Valid license cannot be found" message should be received in this case.*
- ***Using C ompound Registration versions older than 17.06.12:*** *the content of the MarvinJS license should be copied into the same license.cxl file that is used for Compound Registration.*

38. Is it possible to configure Compound Registration to send an email when existing structures are edited?

Not possible at the moment. Emails can be sent by the system during successful /unsuccessful registrations and for the ending submissions (Staging area).

39. What is the reasonable number of compounds in an sd file that I can upload through bulk upload? Is there any size limitation?

On the count of compounds there is no limitation directly, however the bulk upload is limited in size of the uploaded file to ~ 100 Mbytes/file. It can be modified as follows:

Edit the ***{tomcat_home}/webapps/RegistryCxn/WEB-INF/classes /applicationContext.xml*** *file and edit the* ***<bean id="multipartResolver">*** *tag by increasing the value of* ***maxUploadSize*** *property (after saving the file, you have to restart the server):*

```
<bean id="multipartResolver" class="org.springframework.
web.multipart.commons.CommonsMultipartResolver">
<!-- the maximum file size in bytes (100MB) -->
  <property name="maxUploadSize" value="104857600" />
</bean>
```

40. Is there a way to query in Compound Registration for the library identifier?

If you turn on the Administration / General Settings / 'Keep unmapped fields as "Uncategorized Data" during bulk uploads' option, the Library identifier of a given upload will be added to each uploaded compound as an additional data field. If you create a new field in the Form Editor with the Field Identifier "LIBRARY" and enable it for all levels, you will be able to search for this field on the Search page on all levels.

41. *Is there a way to upload SDFs that contain more salt components per structure with different multiplicities?*

Yes, it is possible. You need to have defined separately each salt Id and multiplicity in the SDF, then you need to map consecutively each salt Id field with "Version saltsolvate ID" and each salt multiplicity field with "Version saltsolvate muliplicity".