

Instant JChem FAQ

Instant JChem - Frequently Asked Questions

Administrators

Which RDBMS should I use with IJC

- ✔ There are three options and the one that best suits you is largely dependent upon scale and functionality and since scripting is possible at the IJC level the former becomes less important. Often, a project might be developed to a start point using single session Derby RDBMS (free,bundled). At some point the scale or data or number of concurrent users may dictate a switch to MySQL or Oracle. The Oracle option is mandatory if your organisation will also take advantage of the scalability of the Oracle cartridge.

Should I use 32 or 64 bit Java

- ✔ There is a limit on the size of the cache in 32 bit Java of ~1600MB. There are several options to increase the cache size. If you switch to 64 bit Java this limit is theoretically infinite and should cache tens of millions of structures. You can also switch to using the ChemAxon cartridge which puts the overhead on to the Oracle server and away from the client machine.

How does IJC allow control of sharing

- ✔ This is a complex subject that is best discussed with the Sale/Consultancy services team. In essence IJC supports a security model and choice of policies that are somehow independent of the RDBMS security. At the simplest level one could distribute a derby zip file to the organisations you work with. With more sophisticated RDBMS (Oracle) and with correct network configuration (often VPN), one could allow direct access to external CRO's. At the IJC level the admin user can deploy objects within a schema and other roles exist to control edit/read capability. Each user within the policy owns and independently shares access to their forms. In the case of Oracle, licensing is based upon CPU's. In the case of IJC, the licence varies depending upon number of users and additional items like calculator plugins, reactor...etc...

How do I uninstall Java Web Start client

✔ Uninstallation of IJC JWS needs to be performed manually. It is a two step process.

1. Run the command "jawas -viewer" from the Run dialog or command line and remove the application from the Java Cache Viewer window
2. Other temporary files must be removed by hand. They are stored in \$HOME/.chemaxon folder. There should be a folder named like ws_installation_Ver#. This folder contains the whole IJC and can be removed. There should be also a folder named ws_Ver# which contains shared project configurations and customizable settings for IJC. For complete uninstallation, please remove this folder too.

How to unlock unused space on Apache Derby Database

✔ Apache Derby database offers a possibility to clean the database from unused space, which can occur after, for example, deletion of rows in some tables. For a how-to, please see this [post](#) on our forum.

How to completely uninstall IJC updated by Auto Update Center

- ✔ When updating IJC by the Auto Update Center, the libraries used for the upgrade will be stored in the USERDIR. The uninstaller however does not clean them up and therefore the uninstallation has to be completed manually, by removing those left temporary files. The files are usually located in *C:\Users\username\AppData\Roaming\instantjchem\IJCVERSION* (typically for windows). This folder should be deleted after performing uninstallation. You can find the exact location of the USERDIR in Help -> About InstantJChem.

This special case might be needed when for example downgrading IJC after an update by Auto Update Center, which breaks functionality because of expired license for that particular new version.

- ⚠ Please note that by deleting all the content of *instantjchem* directory (not only the IJCVERSION subdirectory), you might also delete settings for other possible versions of IJC running in parallel.

Users

After reinstalling IJC I can see a different incomplete blank distorted interface

- ✔ Please remove/rename the old/existing userdir. This can be found using Help Instant JChem. Re-start IJC and the problem should be resolved.

Calculated fields are not updating when I change other fields used in their derivation

- ✔ Please try data reload data to refresh calculated field values.

Which data visualisation capabilities exist in IJC

- ✔ Data can be visualised by binding entity data to widgets which is a task completed during form building. There are a number of these "Viz" widgets such as scatter plot, histogram, radarchart and box plot.

IJC does not display some Markush structures

- ✔ IJC structures are usually stored in BLOB or CLOB columns. IJC has some limitation how much data from a BLOB/CLOB column can get for one item. By default it is set to 1024*1024 bytes and hence Markush structures might be pretty big, IJC just shows blank cell. You can workaroud it by setting your own limit by startup option: *ijc.lobSize=<number of bytes>*. Please see more about how to set this option in [admin's guide](#).

IJC does not start on Ubuntu and its derivates

- ✔ This problem is caused by Ubuntu and certain bugs in how Java is treated in the latest versions. The workaround for that is to run the following command from terminal, or put the following command to a startup script so that it runs any time the user logs in.

```
unset GNOME_DESKTOP_SESSION_ID
```

Developers

How can I access API within IJC

- ✔ There are several entry points in the IJC application that facilitate Groovy coding. You can add scripted calculated fields at the entity level or compile full scripts at the data tree or schema levels depending upon the nature of the task. You can use these scripts to complete among other things, data import/export and derivations.

I am finding calculated fields not to perform well in my environment - is there any alternative

- ✔ An alternative to calculated fields are columns populated using triggers. Cartridge functions can be adopted in such a mechanism to utilise ChemAxon functionality. Additionally these are normal fields and can be queried and ordered.