

CSD Portfolio Release Notes

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1.1 Conditions of Use

The Cambridge Structural Database Portfolio (CSD Portfolio) including, but not limited to, the following: ConQuest, CSD-Editor, Decifer, Mercury, Mogul, IsoStar, CSD Conformer Generator, Hermes, GOLD, SuperStar, the CSD Python API, web accessible CSD tools and services, WebCSD, CSD sketchers, CSD data files, CSD data updates, the CSD database, sub-files derived from the foregoing data files, documentation and command procedures, test versions of any existing or new program, code, tool, data files, sub-files, documentation or command procedures which may be available from time to time (each individually a Component) encompasses database and copyright works belonging to the Cambridge Crystallographic Data Centre (CCDC) and its licensors and all rights are protected.

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Web: <https://www.ccdc.cam.ac.uk/>

Telephone: +44-1223-336408

Email: admin@ccdc.cam.ac.uk

2 CSD Release Package

The installer is supplied via download, for Windows, Linux and macOS. The installer contains:

- The Cambridge Structural Database, Version 5.46
- ConQuest 2024.3
- Mercury 2024.3
- enCIFer 2024.3
- CSD Editor 2024.3
- IsoStar 2024.3
- Mogul 2024.3
- CSD Conformer Generator 2024.3
- Hermes 2024.3
- GOLD 2024.3
- CSD-CrossMiner 2024.3
- CSD Ligand Overlay 2024.3
- SuperStar 2024.3
- CSD Python API 3.3.1

Supported platforms are listed elsewhere (see [Supported Platforms](#)). Note that CSD Editor is currently only available on Windows and Linux platforms. Additionally, you may have access to other components that are supplied separately:

- WebCSD (accessed via <https://webcsd.ccdc.cam.ac.uk>)

Access to these will depend on what your licence gives you access to.

2.1 CSD-Core

- ConQuest, Mercury, Hermes, Mogul, IsoStar, WebCSD, enCIFer, CSD Editor and the CSD Python API.

2.2 CSD-Materials

Everything in CSD-Core as well as:

- Additional functionality within Mercury and the CSD Python API.
- CSD Conformer Generator.

2.3 CSD-Discovery

Everything in CSD-Core as well as:

- Additional functionality within Mercury and the CSD Python API.
- GOLD, SuperStar, CSD Ligand Overlay, CSD-CrossMiner and CSD Conformer Generator.

2.4 CSD-Enterprise

All of the above

3 Database Content and Information

CSD version 5.46 (November 2024) contains 1,308,537 unique structures and 1,341,400 entries.

The 5.46 release of the Cambridge Structural Database (CSD) contains over 35,000 new structures compared v5 45, an increase of almost 3%. The database also contains updates to over 50,000

existing database entries and also provides new versions of CSD subsets and an updated Mogul data library including the latest data.

4 What's New

See the following web page for an overview of what's new across the CSD Software Portfolio over the last 12 months: <https://www.ccdc.cam.ac.uk/solutions/whats-new/>

5 Known Problems

5.1 Running CCDC programs on linux under Wayland fails with a Qt mismatch error

If you encounter this problem then CCDC can be started correctly using this workaround:

```
cd /path/to/CCDC/ [the installation directory of the CCDC software]
find . -name "libqwayland-egl.so" -delete
find . -name "libqwayland-generic.so" -delete
```

5.2 Hydrate Analyser Water H-Bonding tab gives inconsistent results in disordered structures when packing is turned on

When analysing the hydrogen bonds around a water molecule in a disordered structure, changing the packing setting can change the motif hits. Until this is resolved, it is recommended you use the Hydrate Analyser with packing turned off.

5.3 Synthons tool in VisualHabit

Morphology displays the 'All' disorder state in the visualiser the second time the tool is used

The VisualHabit Morphology tool when working on a disordered CIF generates synthon results for the correct disorder state the first time it is used. However, if you move away from the structure, come back and recalculate, or if you switch disorder states and recalculate the morphology, while the synthon table updates correctly, the visualiser will now only show the 'All' disorder state.

It is recommended you close and open Mercury if you need to run it twice until this issue is resolved.

5.4 CSD Python API not working on RHEL 9

There is a known issue where the version of python which is bundled with the CSD Portfolio will not run on RHEL 9 and clones. This is caused by incompatible libraries and the workaround is to set LD_LIBRARY_PATH before starting the Python session.

```
LD_LIBRARY_PATH=~/.CCDC/ccdc-software/csd-python-api/  
miniconda/lib
```

Change the path to the CCDC folder if necessary.

5.5 ConQuest fails with "ValueError: No JSON object could be decoded" on RHEL 8

On some versions of Linux including RHEL 8 and clones, ConQuest will fail to start with an error message

```
ValueError: No JSON object could be decoded
```

The workaround is to rename or delete the file CCDC/ccdc-software/conquest/lib/libcrypto.so.1.1 so that ConQuest uses the system libraries instead.

5.6 Unable to run the CCDC maintenance tool on macOS 15

For installations carried out with the 2024.2 and earlier versions of the CSD installer, you will get the error message 'The application "ccdc-maintenance-tool.app" can't be opened' when attempting to run the CCDC Maintenance Tool on macOS 15. This is due to macOS 15 introducing new requirements to allow applications to run.

We have resolved these issues, but as upgrades are not possible with existing installs you will need to re-install again using the CSD Portfolio installer to obtain the latest version that will allow you to apply future updates normally.

5.7 ConQuest will not start when used with the latest version of VMWare

We are aware of issues with the latest versions of VMWare tools that cause ConQuest to fail to start, due to changes in the graphics drivers on this platform.

Solutions for this issue include:

1. Start ConQuest from a command prompt (in ccdc-software\conquest\exe type csds.exe -no3d). This will start ConQuest without a 3D visualizer but you can choose the export to Mercury option to view the results there.
2. Downgrade VMWare to an older version to use the older graphics drivers.

5.8 The Aromatics Analyser may fail on linux

When using the Aromatics Analyser functionality in Mercury, the calculation may fail with an error relating to the neural network calculation failing to finish. The underlying cause of this is due to a

problem loading and using TensorFlow in the underlying Python code that is running. Similarly, Aromatics Analyser functionality in the CSD Python API may fail with a glibc error for the same reason.

A workaround is to set LD_LIBRARY_PATH to include the ccdc-software/csd-python-api/miniconda/lib of your installation, e.g.

```
export LD_LIBRARY_PATH=/path/to/ccdc/ccdc-software/csd-python-api/miniconda/lib:$LD_LIBRARY_PATH
```

5.9 Use of ConQuest's 3D Visualiser on Retina Displays

On macOS systems with retina displays only, there is a known issue with being unable to select atoms in ConQuest's 3D visualiser. We would recommend exporting your hits to Mercury for further analysis instead.

5.10 Use of ConQuest, Mogul's sketcher and scripts in Mercury on Windows accounts where the username contains non-ascii characters

On some Windows systems where the user's username contains non-ascii characters or spaces this can cause problems with components of the CSD Portfolio that use Python (specifically ConQuest and Mogul). For ConQuest we would recommend adding the following line to the .csds_defaults3 file in your user home area to work around this issue:

```
csds_data_directory = 'C:\\conquest_workspace'
```

5.11 ConQuest is not compatible with dark mode in macOS

ConQuest will not change its display in macOS dark mode but will instead use the same display as found in standard display mode.

5.12 On macOS, ConQuest may occasionally not display interface elements correctly

On macOS, ConQuest may sometimes open an interface panel and not properly render all of its elements correctly. If this happens, closing and re-opening the element should resolve the issue.

5.13 Aromatics Analyser and POV-Ray image creation are not compatible with Apple ARM-chipsets (M1)

The Aromatics Analyser and POV-Ray functionality in Mercury are currently not compatible with Apple ARM chipsets running macOS and are not supported. All other functionality should work correctly with Apple ARM chipsets. We plan to improve support for these chipsets with subsequent releases.

5.14 Starting programs on Apple ARM chipsets (M1) for the first time has a delay

When running on Apple Silicon via Rosetta 2 emulation, it is normal that the first time a program runs, it takes extra time to start, usually in the region of 15-60 seconds. This delay no longer occurs the second time you use the program.

5.15 On Windows, the Conformer Generator does not run as it cannot find a Python distribution

Execution of the Conformer Generator scripts requires Python to be set up to execute python scripts on your system. This FAQ provides some details on how to resolve this problem: <https://www.ccdc.cam.ac.uk/support-and-resources/support/case/?caseid=5ee48c7d-a5de-ed11-96a2-00505695c114>

5.16 The Conformer Generator functionality of the CSD Python API may not work correctly on macOS virtual machines

In our testing we've found some issues with the Conformer Generator functionality in the CSD Python API failing to work inside macOS 12 virtual machines and instead raising a RuntimeError exception with the message 'Unknown library requested in library store'. We were unable to reproduce this on "bare metal" installations of macOS 12 for this release, so only virtual machines should be affected.

5.17 On Ubuntu 22.04 only, running Python API scripts from Hermes and Mercury does not work

On Ubuntu 22.04 only, the Python API script window in Hermes and Mercury does not display its web view of the output HTML.

6 Installation Overview

Sections 6 to 8 describe how to perform a typical installation, which is the recommended method of installing the CSD software and data. This will involve the following steps:

1. Download the online CSD Release installer from <https://www.ccdc.cam.ac.uk/support-and-resources/csdsdownloads/>. This will require your Customer Number and Activation Key.
2. Install the CSD Software and Database files for Windows (see [Windows Installation](#)), Linux (see [Linux Installation](#)), and/or for macOS (see [macOS Installation](#)) and register the software.
3. Install the IsoStar 2023 server (Linux) (see [IsoStar Server Installation](#)).

More advanced methods of installation are also possible and are described in section 9.

6.1 System Requirements

6.1.1 Supported Platforms

Executables in this release are supported on the following platforms and operating systems. Those platforms that are actively tested on prior to release are denoted with an asterisk:

- Windows - Intel compatible, 64-bit:
 - Windows 10* and 11*

Use of CCDC applications on Windows will require the Microsoft Visual Studio C++ redistributable libraries for Intel x64 architecture to be installed. These can be obtained via the x64 installer available at <https://learn.microsoft.com/en-US/cpp/windows/latest-supported-vc-redist> or directly via this link https://aka.ms/vs/17/release/vc_redist.x64.exe.

- Linux - Intel compatible, 64-bit:

- RedHat Enterprise 8 and 9
- Rocky Linux 8 and 9*
- Ubuntu LTS 22* and 24*

We do not support Wayland as a display server protocol (see known issues).

Note: As we add support for newer versions of Linux, support for older versions may have to be withdrawn. If you are using a Linux version near the minimum that we support, we would recommend updating in the near future to ensure you are able to use future CSD software updates without interruption.

- macOS - Intel compatible, 64-bit:

- macOS 13*, 14* and 15*

- macOS - Apple ARM (via Rosetta 2 emulation), 64-bit:

- macOS 13, 14* and 15*

Note: Apple ARM-based (M1,M2) systems are supported with this release via emulation with Rosetta 2, but with the caveat that there are some issues with certain functionality as detailed in the known issues section. We plan to improve support with subsequent releases.

If you choose to use a version other than those listed above we cannot guarantee that the software will work correctly, although we will attempt to assist you with any problems you may encounter.

Linux platforms will require the Network Security Services (NSS), OpenGL, Fortran and libXScrnSaver packages to be installed. Ubuntu 22 requires the libxcb-xinerama0 to be installed to run the installer (see Linux Installation below for more details).

6.1.2 Changes to Supported Platforms

CentOS and RedHat 7 are now unsupported platforms. The CSD Portfolio will no longer function on these platforms starting with 2024.2 due to improvements to the underlying technologies that the CSD Portfolio uses. If you are using CentOS or RedHat 7, then do not upgrade past 2024.1. If this will cause you difficulties, please contact support@ccdc.cam.ac.uk to discuss further.

Please note that there may be new system library requirements on Linux with this version. Please see the Linux installation chapter for new details.

Windows 10 is due to reach end of life for Microsoft support at the end of October 2025 and it is anticipated that CCDC will also drop support at this time. Please contact support@ccdc.cam.ac.uk to discuss further.

The 2025.1 release will see us change the version of the CSD Python API installed with the desktop software to use Python 3.11 rather than 3.9.

6.1.3 Changes to Supported Products

DASH is no longer a core CCDC product and will not be distributed as part of the CCDC Software Portfolio. In order to support development for its enthusiastic user base, we are opening DASH up for others to contribute to. DASH certainly won't be going away, it will simply be moving to a different home - in particular, an open source project on GitHub. To find out more about the future direction of DASH, please visit this page: <https://www.ccdc.cam.ac.uk/solutions/open-source/dash-open-source/>.

The `cqbatch` and `mogulbatch` command line utilities are now deprecated - while these remain a part of the CSD Release software during 2023, their use is no longer recommended, and we would instead encourage switching to use of the CSD Python API. We anticipate that `cqbatch` will be removed entirely in a future release.

If any of the above will cause insurmountable difficulties, please contact us at support@ccdc.cam.ac.uk to discuss possible solutions.

6.1.4 Graphics System Requirements

Products with 3D graphical display functionality are supported only on graphics cards and chipsets that have up to date installers and are still in support from the graphics system manufacturers. The graphics drivers in use should support OpenGL 2.1.

6.1.5 Access of CSD software by X-forwarding

Remote access of CSD software by X-forwarding, such as via ssh on Linux, or a mixed system such as use of an X-emulator on Windows to access a Linux installation, is not supported.

While such methods may work, success can depend on many variables, including both the remote and local system as well as any emulation software that may be used and we cannot fully test or provide support for all of these combinations. If you do encounter any difficulties, we would recommend using the native software for the platform you are accessing from, and if all possible do so locally rather than remotely. If disk space is a concern, a compromise can be installing the software locally and accessing a remote data install.

6.1.6 Stereoscopic Viewing Graphical System Requirements

Please check the following support solution on our website to see the most recent recommendations for 3D stereoscopic viewing in Mercury:

<https://www.ccdc.cam.ac.uk/SupportandResources/Support/pages/SupportSolution.aspx?supportsolutionid=284>

We would appreciate receiving feedback to support@ccdc.cam.ac.uk on your experiences of using stereo display on different hardware configurations to those suggested in the support solution above, if successful, so that we may inform other users of valid hardware configurations. On machines without appropriate hardware, the **Stereo** checkbox will be disabled.

6.1.7 Disk Space and Memory Requirements

A complete installation of the 2024.3 CSD Release requires approximately 37 GB of disk space. This includes all software (7 GB) and all data files (30 GB). Approximately 50 GB of free disk space will be required during installation.

The minimum recommended RAM is 8GB. The software update mechanism can require more RAM to be available during the update activity. We advise that additional swap space or RAM is available at that moment to accommodate a further 4GB.

7 General Installation Instructions

7.1 Online Installation (recommended)

On all platforms the recommended online installer will give you the option to install CSD Software, CSD Data or a combination of the two. The installer will download the selected components first to a local cache and then will install to the selected install location. The online installer connects to CCDC's software and data repository to download the latest versions that are available. If you desire access to an older version of the software then please see the offline installer section below.

7.2 Online Installer Settings

The Settings can be accessed from the first dialog page of the online installer. Here you can manually set proxy settings (the installer should set these automatically, but it is possible to change that here), configure the use of a different repository from which to download the software and data (see the [Creating a Local Repository](#) section below), and lastly to set the location of the cache

for the downloaded files (this can be used to select a location with enough free storage to host the temporary files if the default location does not have enough space).

7.3 Selecting the components to install

The installer allows you complete control over which parts of the CSD Portfolio software and data you would like to install. The user is first presented with the option to select from a complete install, or one of several pre-configured packages we believe will be of use for certain types of user. It is possible to completely customise your selection after this choice, and software or data can be added or removed post installation via the installed maintenance tool. Where one component is dependent on another to operate correctly then the other component will be automatically selected.

7.4 Data installation strategies

The default option is to install both the CSD Software and the CSD Data to the same location. However, it is possible to install the CSD Software and CSD Data separately. The most common reason to do so is to install the data to a remote location where it can be accessed by one or more software installations.

See [Configuring the use of a remote database location](#) for details on how to configure a software only installation to use a remote installation of data.

7.5 Offline installation

If you cannot access the internet from the install system, or you do not wish to need to access the internet during installation for any reason then an offline installer is also available. The installer is a snapshot of the software and data available at the time of its creation, so it is possible to use the offline installer to obtain older versions of the software. As there is no connection to the internet there is no settings option from the first dialog, but otherwise the installer operates the same as the online version.

7.6 Creating a custom offline installer

You can create an offline installer with select components from the CSD portfolio from the online installer. First, download the online installer, then from the command line within the folder where the installer is downloaded, run the following command:

```
CSDInstallerOnline-windows.exe search
```

This command will list the packages available, you can identify which components you want to generate an offline installer for. This example will show you how to create an offline installer for the free version of Mercury, enCIFer and utilities that depend on it:

```
CSDInstallerOnline-windows.exe create-offline pkg  
uk.ac.cam.ccdc.csd.mercury uk.ac.cam.ccdc.csd.encifer -  
root C:\Users\myusername\Desktop -c --accept-licenses
```

- uk.ac.cam.ccdc.csd.mercury will select Mercury and dependent components
- uk.ac.cam.ccdc.csd.encifer will also include enCIFer in the offline installer
- - root sets the folder where the installer will be placed, in this case C:\Users\myusername\Desktop
- -c confirms the process will continue with no user input
- --accept-licenses accepts the user licence for the installer

Once the installer has been created, you can run it by either double-clicking or running the installer from the command line.

7.7 Creating a local software and data repository

It is also possible to create a local version of the software and data repository that the online installer connects to. you may then configure the online installer to use this local repository instead of the default CCDC online repository. This allows you to keep all install files behind your firewall. Software installed this way will also use

this local repository to check for updates so can be used to control when you make updates available to users. To set up a local repository, follow these instructions:

1. Download the offline installer and run it at the command line with the argument `--cl`. The installer can be run either in GUI mode or at the command line as long as this extra argument is given.
2. Install all software and data. Once done, a repository directory will be created in the entered install location. This repository can be moved to a different location after creation if required.
3. When running the online installer, use the settings repository tab and deselect the default CCDC repositories and add the local repository as a user defined repository. This can be done either using `file:///` and the system path to the repository folder, or the repository folder can be made available on a web server and accessed via `http://`.

To update the local repository to a more recent version, repeat steps 1 to 2 above with a newer version of the offline installer. This newer version of the repository can then replace the older one and existing installs can use it to perform an update operation.

7.8 Running via the command line

Nearly all dialog options can be entered via arguments at the command line in order to install without use of the installer GUI. The only options that cannot be run from the installer command line are the custom CCDC licensing and telemetry options. These will require licensing and telemetry options to be selected as post-installation steps.

To see what command line options are available, run the installer with the `--help` argument.

For example, to install with no user input all software and data components you would use a command like

```
./CSDInstallerOnline-linux --root /local/myinstall -c --accept-licenses install uk.ac.cam.ccdc
```

-root sets the root installation folder, in this case /local/myinstall -c confirms the start of the installation with no user input --accept-licenses accepts the user licence for the installer install uk.ac.cam.ccdc will install all software and data

For details on the package names that can be used to install individual components, run

```
./CSDInstallerOnline-linux search
```

7.9 Further Help

Visit our installation support page at https://www.ccdc.cam.ac.uk/csds_install_help. This page contains all of the above details and will also be updated with further assistance as we determine other use cases that would be useful to highlight.

8 Windows Installation

8.1 Requirements

The CSD software will require both of the following Microsoft Visual Runtime Libraries to be installed:

1. Visual C++ 2008 Redistributable x64 package: <https://www.microsoft.com/en-us/download/details.aspx?id=26368>.
2. Visual C++ 2015, 2017, 2019, 2022 x64 Redistributable package: https://aka.ms/vs/17/release/vc_redist.x64.exe.

8.2 Installation Procedure

Administrator privileges are required for installation to a restricted location such as C:\Program Files. Installing to a user accessible location does not require administrator privileges.

Installation of the CSD Python API requires long path support to be enabled on Windows. If installing with administrator rights then this will be done automatically. Otherwise prior to installation you will need to ensure that the registry key LongPathsEnabled in Computer\HKEY_LOCAL_MACHINE\SYSTEM\CurrentControlSet\Control\FileSystem is set to 1.

For more information on installation of the CSD Python API please see this FAQ: <https://www.ccdc.cam.ac.uk/support-and-resources/support/case/?caseid=95672bfa-adcc-ed11-96a2-00505695c114>.

Do not install directly on top of a previous installation; use a new folder.

To install on Windows:

1. Download the online (recommended) or offline windows installer.
2. Double-click on the installer exe file. The installer menu will take you through the steps necessary to complete the installation.
3. Installation will install the selected software components in a ccdc-software folder, the selected data components in a ccdc-data folder, and a selection of utilities in the ccdc-utilities folder. A maintenance tool will also be installed in the root installation directory which can be used to add or remove programs post install, check for updates and also uninstall.
4. If you used the offline installer, copy the ccdc-data folder from the unzipped installer directory to the root installation directory so that it is alongside the ccdc-software folder.

9 Linux Installation

9.1 Package Requirements

The CSD software requires the Network Security Services (NSS), OpenGL, Fortran, libXss.so.1, libxcb-iccmm.so.4 and libatomic libraries to be present on your system. These can be installed on RHEL / Rocky Linux 8 or 9 with the command:

```
sudo dnf install nss libXScrnSaver libglvnd-opengl libgfortran5  
libxkbcommon-x11 xcb-util-wm xcb-util-cursor xcb-util-  
keysyms libatomic
```

Or on Ubuntu:

```
sudo apt-get install libnss3 libxss1 libopengl0 libgfortran5  
libxkbcommon-x11-0 libxcb-xinerama0 libxcb-cursor0 libxcb-  
keysyms1 libatomic1
```

These prerequisites assume a desktop deployment of the Linux OS. For headless installs additional packages which are included in a desktop installation may need to be installed manually.

9.2 Installation Procedure

Do not install directly on top of a previous installation; use a new folder.

To install on Linux:

1. Download the online (recommended) or offline linux installer.
2. Ensure that the installer executable has execute permissions via a command like (substitute in the name of the downloaded file):

```
chmod a+x ./CSDSInstaller-linux
```

3. In a terminal window on the machine where you intend to run the CSD Portfolio, type (substitute in the name of the downloaded file):

```
./CSDInstaller-linux
```


4. Follow the on-screen instructions to install the software and databases.
5. Installation will install the selected software components in a `ccdc-software` folder, the selected data components in a `ccdc-data` folder, and a selection of utilities in the `ccdc-utilities` folder. A maintenance tool will also be installed in the root installation directory which can be used to add or remove programs post install, check for updates and also uninstall.

9.3 IsoStar Server Installation

This step may be skipped entirely if you wish to use our publicly hosted IsoStar server at <http://isostar.ccdc.cam.ac.uk>.

The Linux IsoStar Server installer contains the IsoStar Software for all supported Linux platforms, as well as the IsoStar data files.

To install IsoStar on Linux:

1. Download the `IsoStar-linux-x64-installer.run` installer file.
2. Ensure that the installer executable has execute permissions via the command:

```
chmod a+x ./IsoStar-linux-x64-installer.run
```

3. In a terminal window as a **non-root** user on the machine where you intend to run the CSD Portfolio, type:

```
./IsoStar-linux-x64-installer.run
```

4. Follow the on-screen instructions to install the software and databases.

10 macOS Installation

10.1 Installation Procedure

Administrator privileges are required for installation to a restricted location such as /Applications. Installing to a user accessible location does not require administrator privileges.

Do not install directly on top of a previous installation; use a new folder.

To install on macOS:

1. Download the online (recommended) or offline macOS installer.
2. Double-click on the installer dmg file to mount it, then double click on the installer exe. The installer menu will take you through the steps necessary to complete the installation.
3. Installation will install the selected software components in a `ccdc-software` folder, the selected data components in a `ccdc-data` folder, and a selection of utilities in the `ccdc-utilities` folder. A maintenance tool will also be installed in the root installation directory which can be used to add or remove programs post install, check for updates and also uninstall.

11 WebCSD Access

The CCDC hosts a WebCSD server which can be accessed at <https://www.ccdc.cam.ac.uk/structures>

You can register a username and password in order to obtain access. Alternatively, those with unlimited site licences can contact admin@ccdc.cam.ac.uk with details of their institution's IP address range(s) in order to arrange access by IP address.

12 Starting and Configuring CSD Portfolio Software

12.1 Windows

To start any CSD Portfolio software component on Windows select the appropriate link from the Windows Start menu:

Programs -> CCDC.

Or use one of the desktop shortcuts created for ConQuest, Mogul, Mercury, IsoStar, enCIFer, Hermes, CSD-CrossMiner and GOLD by the installation process.

12.2 Linux

Using a command line console, change directory to <INSTALLDIR>/ccdc-software (where <INSTALLDIR> is the path to your installation directory), or ensure that this is in your system PATH.

Then for ConQuest, type:

```
./conquest/bin/cq
```

For Mogul, type:

```
./mogul/bin/mogul
```

For Mercury, type:

```
./mercury/bin/mercury
```

For IsoStar client, type:

```
./isostar/bin/run_isostar
```

For Hermes, type:

```
./hermes/bin/hermes
```

For the GOLD interface in Hermes, type:

```
./hermes/bin/gold
```

For CSD-CrossMiner, type:

```
csd-crossminer/bin/crossminer
```

12.3 macOS

To start any CSD Portfolio software component on macOS click on the appropriate icon in the Dock, or in the installation folder for ConQuest, Mercury, Mogul, IsoStar, enCIFer, Hermes, CSD-CrossMiner and GOLD.

12.4 Using Hermes to access CSD-Discovery functionality

Hermes acts as both a visualiser and as an interface and client for GOLD, SuperStar and the CSD Ligand Overlay. Access to these requires a CSD-Discovery enabled licence.

SuperStar and the CSD Ligand Overlay can be accessed via the Calculate menu and GOLD can be accessed via the GOLD menu.

To start Hermes or GOLD, please refer to the instructions given earlier in this section.

12.5 Testing your Installation

A number of tutorials are available to complement the software.

To test your installation and to learn something about the features of the software, it may be useful to try one or more of these tutorials which are located at the end of the User Guide for each product.

The HTML version of each User Guide can be found in the docs subdirectory of each product or via the product's **Help** menu.

12.6 Activation of CSD Portfolio Components

The CSD Portfolio Installer will offer you the opportunity to activate the CSD Portfolio as part of the installation process, either by accessing our online activation servers, or by entering details of a local licence server. Activation online will require your activation key.

If a valid licence is not present, then when using any component of the CSD Portfolio software (e.g., ConQuest, Mogul or IsoStar client) for the first time you will be prompted to activate.

For more information about activation and licensing see [Licensing Overview](#) .

Mercury and enCIFer may be installed and used with a free CSD-Community licence. Activating with a CSD-Core or greater licence will, however, allow access to additional features that are only available to CSD Portfolio users.

12.7 Configuring the use of a remote database location

If using locally installed data then all CSD Portfolio software components should automatically locate and use that local data. If, however, you have no locally installed data and wish to access a remote set of data, then the CSD Portfolio software will need to be told where that data is.

If required data is not present, then the CSD Software that requires that data will present you with the option to install or locate the data it needs. Select the 'install' option to install locally using the maintenance tool. Select the 'configure' option to navigate to the location of the root ccdc-data folder of a remote data location. Once this choice is made it is stored for future use in a CSD.ini file (see below).

It is not possible to use a mixture of local and remote data - you should choose to access data via one of these routes.

12.7.1 ConQuest

ConQuest uses its own mechanism for accessing data in a remote location. The location of these files is identified by selecting a CSD database information file. For ConQuest this file will be called `as545be.inf` and will be found in the `csd` subdirectory in the location where you installed the database files. If installed locally this should be found automatically.

12.7.2 The CSD.ini configuration file for data location

The `CSD.ini` file stores the location of the data once that is configured by the steps above. This is placed in one of the following user locations:

Windows: `"C:\Users\%USERNAME%\AppData\Roaming\CCDC"`

Linux: `"~/ .config/CCDC"`

macOS: `"~/Library/Preferences/CCDC"`

It is also possible to set this on a system-wide level for all users. To do so copy an existing user-based `CSD.ini` to one of these locations:

Windows: `"C:\ProgramData\CCDC"`

Linux: `"/etc/xdg/CCDC"`

macOS: `"/Library/Preferences/Qt/CCDC"`

or create one with the following content

```
[General]
```

```
root=/path/to/ccdc-data
```

where `/path/to/ccdc-data` is the full path to the location of the `ccdc-data` folder of your remote data install

12.8 Configuration of CSD Portfolio Components

12.8.1 ConQuest

12.8.1.1 Search Data Directory

Before using ConQuest you may be required to identify a Search Data directory. This will be used to store temporary files for running searches. It will also be the default directory for saving some ConQuest files.

12.8.1.2 Viewing PDF files Produced by ConQuest

ConQuest is able to generate PDF files for viewing or printing entries from the CSD (including 2D diagrams).

In order to view or print these files you will need to use a PDF reader, such as Adobe Acrobat Reader. Adobe Acrobat Reader is available from the Adobe website: <https://www.adobe.com>. Other free PDF readers are available, see <https://pdfreaders.org>

12.9 Desktop launchers for Linux

The CSD software installs .desktop files suitable for use with most modern Linux desktop's launcher mechanism including both Ubuntu and RHEL/Centos.

The files are installed into the desktop directories of each software component in your Linux installation.

To associate a CCDC application with the desktop launcher, use the command `sudo desktop-file-install application.desktop`, which will require your account to be able to run commands as root via `sudo`. For example, to add IsoStar use:

```
sudo desktop-file-install isostar.desktop
```

Once done, you should find that application now appears in your desktop's **Applications** menu.

In order to allow the **Open With** dialog in browsers on Ubuntu to offer IsoStar or Hermes as options when viewing IsoStar scatterplots or mol2 files, this step will be required with the `isostar.desktop` and `hermes.desktop` files respectively.

See <https://specifications.freedesktop.org/desktop-entry-spec/latest/index.html> for more details.

13 CSD Python API

The installer includes a version of the CSD Python API and a distribution of miniconda Python in order to allow for easy use. This will be automatically installed together with the CSD software.

13.1 Use of the CSD Python API in Mercury

The **CSD Python API** menu in Mercury allows the running of Python scripts in an interactive manner, typically acting on the currently viewed structure. This menu should default to using the included miniconda python installed in the `csd-python-api` directory alongside the CSD software. The **Options...** menu may be used to specify a different Python installation or clicking the **Default** button will return to using the bundled version of the API.

For more details on the use of the API in Mercury, please refer to the Mercury User Guide.

13.2 Use of the CSD Python API via the command line

The CSD Python API can also be used via the command line. The CSD Release installer will setup some convenient shortcuts and/or scripts to allow you to start the API with the correct environment already set. More details on using the Python API can be found in the CSD Python API documentation.

13.2.1 Using the CSD Python API on Windows

A Python command prompt may be started via the **CSD Python API** shortcut that will have been created on your desktop, or in the Windows Start Menu.

To set up the environment correctly in the terminal without starting Python, navigate to the `miniconda/Scripts` directory and type:

```
activate
```

A (base) prompt should appear at the start of the command line prompt, indicating that the correct environment has been created. The miniconda Python is now the default to be started by just typing `python`.

To go back to a normal terminal, type the following in the `miniconda/Scripts` directory:

```
deactivate
```

13.2.2 Using the CSD Python API on Linux

Start a terminal and navigate to the `csd-python-api` directory. To get a Python prompt where the API can be used, run the `run_csd_python_api` script. A Python terminal should start, reporting Python version 3.9.16.

To set up the environment correctly in the terminal without starting Python, navigate to the `miniconda/bin` directory and type:

```
source activate
```

A (base) prompt should appear at the start of the command line prompt, indicating that the correct environment has been created. The miniconda Python is now the default to be started by just typing `python`.

To go back to a normal terminal, type the following in the `miniconda/bin` directory:

```
source deactivate
```

13.2.3 Using the CSD Python API on macOS

Open Finder and navigate to the `csd-python-api` folder. To get a Python prompt where the API can be used, double-click on the `run_csd_python_api` script. A Python terminal should start, reporting Python version 3.9.16.

The `run_csd_python_api` script can also be run from a terminal.

To set up the environment correctly in the terminal without starting Python, navigate to the `miniconda/bin` directory and type:

```
source activate
```

A (base) prompt should be created, and the correct environment for macOS will now be set to allow use of Python scripts that utilise the API. To deactivate, type:

```
source deactivate
```

13.3 Use of the CSD Python API with your own Python installation

The CSD Python API may be installed into your own Python installation via use of pip or conda package managers. This method of use is recommended only for expert Python users who are experienced with installing Python packages.

14 Licensing Overview

CSD Release software is licensed on a node-locked basis. Your site has a Licence of Access Agreement that entitles you to install the CSD Release on a specified number of machines.

The first time you attempt to run any of the CSD Release components (e.g., ConQuest, Mercury, Mogul) on a particular machine that has not been activated you will be prompted to activate the installation using the process described below.

Note: For those institutions with a site licence, a local licence server alternative is available. This mechanism provides site-wide access to the CSD without the need to activate individual machines, by accessing your local licence server instead of activating online.

CCDC licensing is primarily node-locked which means that each licence is tied to a specific computer system. In order to use CCDC software there are primarily three methods to access the software:

1. Activate access to free CSD-Community features (e.g., Mercury, enCIFer)
2. Activate additional features with a CCDC licence activation key
3. Access a local licence server that has been set up and started on your network

To facilitate this process, your CCDC software installation will contain the CCDC Software Activation tool. This may be accessed in an interactive way by a graphical user interface, or at the command line by passing appropriate arguments. Additionally, you may select the option to perform activation or set up access to a local licence server when performing an installation of the CSD Release.

14.1 Activating via CCDC software application

If activation has not yet been carried out, then starting one of the CCDC software applications such as Mercury or Hermes will automatically start the activation interface.

14.2 Starting the CCDC Software Activation tool graphical user interface

14.2.1 Windows

The CCDC Software Activation tools will be located in the

`<INSTALLDIR>\ccdc-utilities\software-activation`

folder of a CSD installation, or

To start the graphical user interface, double-click on

`ccdc_activator_gui.exe`

14.2.2 Linux

The CCDC Software Activation tools will be located in the

`<INSTALLDIR>\ccdc-utilities\software-activation/bin`

folder of a CSD installation, or

To start the graphical user interface, run `ccdc_activator_gui`.

14.2.3 macOS

The CCDC Software Activation tools will be located in the

`<INSTALLDIR>\ccdc-utilities\software-activation`

folder of a CSD installation. To start the graphical user interface, double-click the CCDC-Software-Activation application.

14.3 Running the command line CCDC Software Activation tool

The command line variant of the CCDC Software Activation tool may be found in the same location as the graphical user interface version detailed above. You will need to start a command line prompt/terminal and then:

On Windows run:

`ccdc_activator.exe`

On Linux run:

`./ccdc_activator`

On macOS run:

```
./CCDC-Software-Activation.app/Contents/macOS/ccdc_activator.x
```

This should display the available command line arguments that may be passed to the activation tool. To perform activation or setup of a local licence server, the correct arguments will need to be provided. These are detailed in each licence activation/setup type below.

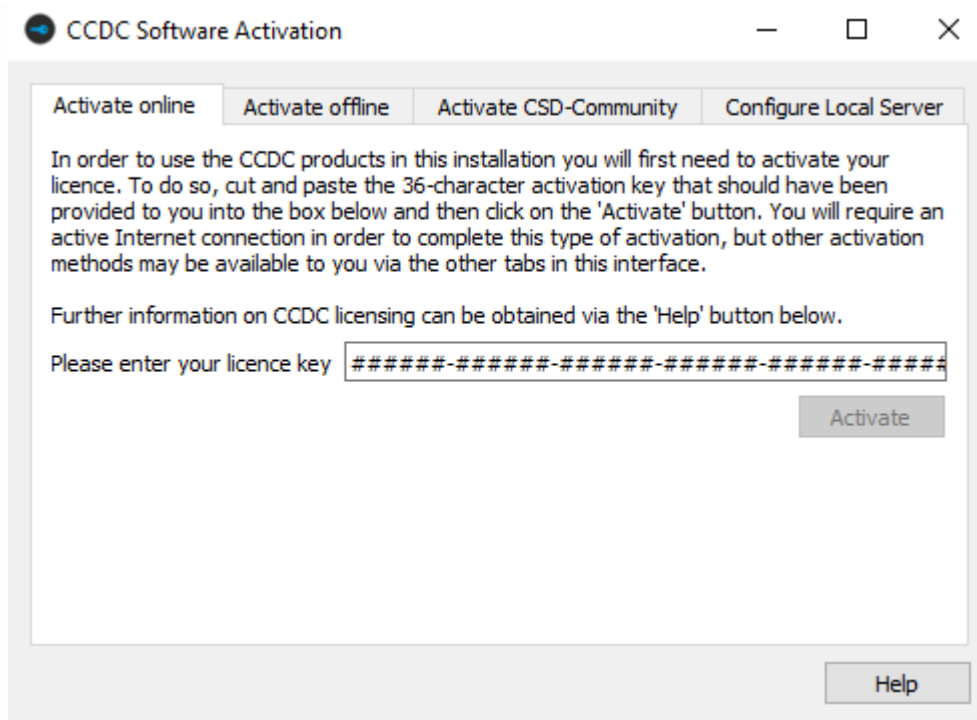
14.4 Activating online with a CCDC licence activation key

If you have purchased a CCDC product such as the CSD Portfolio, then you will have been provided with an activation key. This key can be used to perform an activation on the computer system you are using the CCDC software, and the easiest method to do so is by directly communicating with our licence server. This will require internet access on the computer you wish to activate. If you have previously activated with another licence key, you can enter a new one to change to use that licence.

This will utilize one of your available licenses and allow use on that computer for any user. Note that each user will need to activate the CCDC software individually, although this will use the same single licence seat if performed on the same computer system. It is also possible to configure your system to auto-activate for all users.

14.4.1 Via the graphical user interface

1. Start the **CCDC Activation Tool** as described above.
2. Click on the **Activate online** tab if it is not already selected.



3. Copy and paste the activation licence key into the box and then click on the **Activate** button. You should be informed that activation was successful. Access to the CCDC products and features your licence allows should now be possible.

14.4.2 Via the command line interface

Run the `ccdc_activator` command line tool with the `-a` and `-k` arguments, followed by your activation key. For example, on Windows:

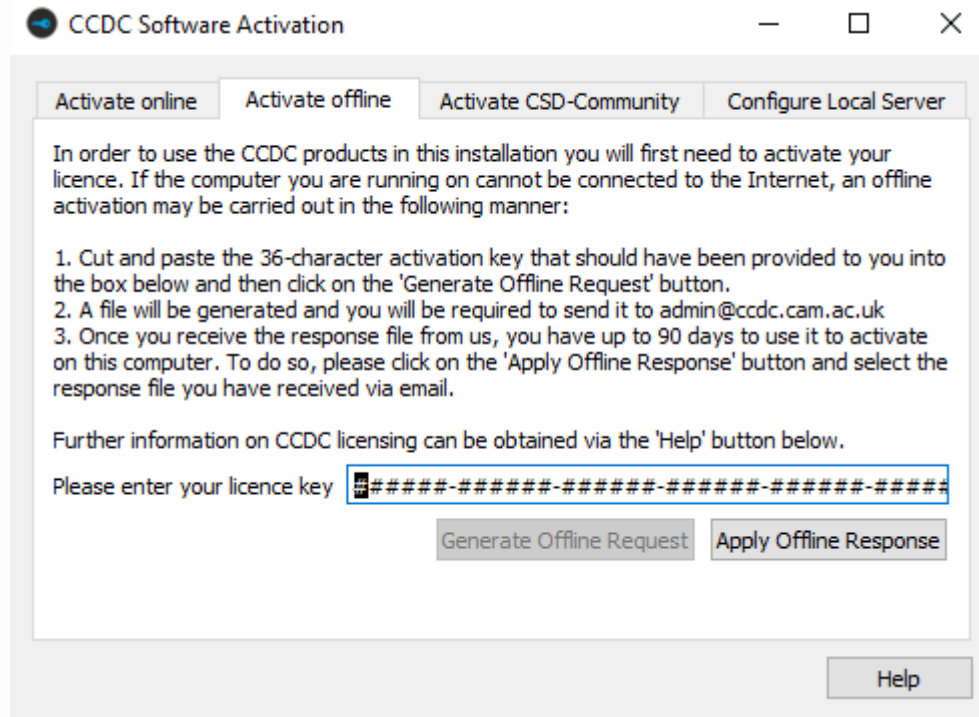
```
ccdc_activator.exe -a -k 123456-123456-123456-123456-123456-123456
```

14.5 Activating offline with a CCDC licence activation key

If you have an activation key but the system you are installing on has no direct internet access, then you can instead utilize the **Activate offline** option. This will save licensing information from the target computer and allow you to use another internet enabled computer elsewhere to complete activation. If you have previously activated with another licence key, you can enter a new one to change to use that licence.

14.5.1 Via the graphical user interface

1. Start the **CCDC Activation Tool** as described above.
2. Click on the **Activate offline** tab if it is not already selected.



3. Copy and paste the activation licence key into the box and then click on the **Generate Offline Request** button. You will be prompted to save a LicenceRequest.licreq file to your computer.
4. Transfer this file to an internet enabled computer and visit <https://www.ccdc.cam.ac.uk/licensing>. Use the licensing portal to upload your licence request file and then download the corresponding licence response file.
5. Repeat steps 1-3 but this time use the **Apply Offline Response** button to select the response file sent to you by CCDC.
6. You should be informed that activation was successful. Access to the CCDC products and features your licence allows should now be possible.

14.5.2 Via the command line interface

Run the `ccdc_activator` command line tool first with the `-k` argument, followed by your activation key, then the `-g` and `-f` arguments followed by a file location to save the request file. For example, on Windows (this command is all on one line):

```
ccdc_activator.exe -k 123456-123456-123456-123456-123456-123456 -g  
-f C:\Users\myusername\LicenceRequest.licreq
```

Send the request file to admin@ccdc.cam.ac.uk. A response file should be returned to you – complete activation with the `-o` argument instead of `-g` (all on one line again):

```
ccdc_activator.exe -k 123456-123456-123456-123456-123456-123456 -o  
-f C:\Users\myusername\LicenceResponse.dat
```

14.6 Setting up access to a local CCDC licence server

If you have an unlimited site-wide licence for CCDC products, then it is possible to request access to a local licence server that can be installed within your network. You can then allow individual installations to access that local licence server to get permission to run, instead of performing node-locked activations. If you have previously activated with another licence key or set up use of a different local licence server, you can enter new details to change to use that licence instead.

14.6.1 Obtaining the local CCDC licence server

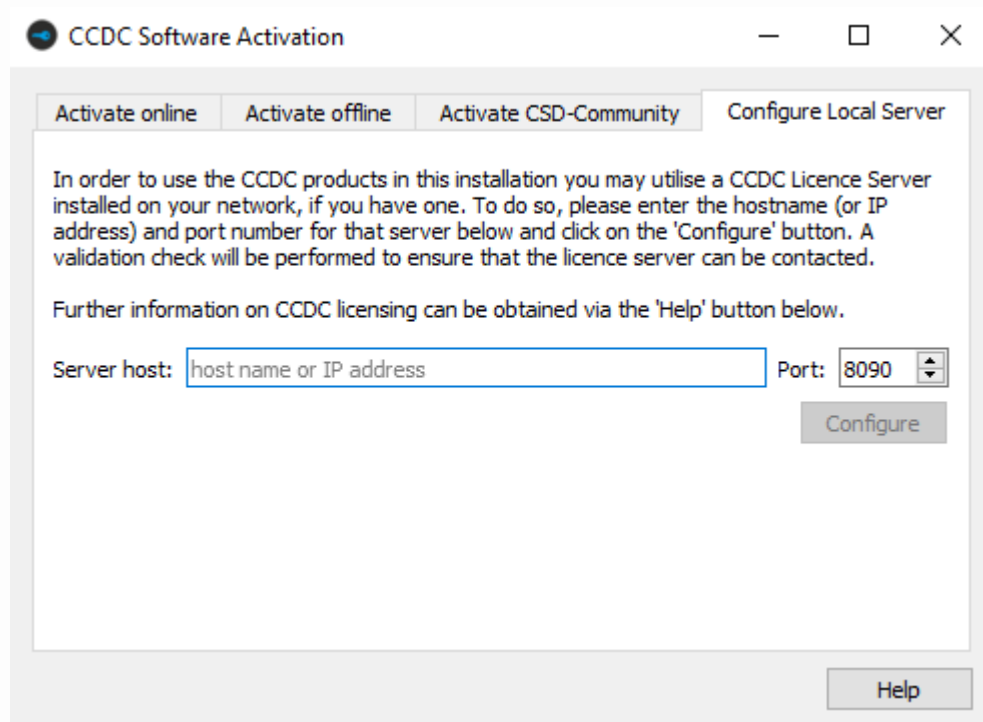
To obtain the local CCDC licence server, please send a request to admin@ccdc.cam.ac.uk, quoting your customer details and existing node-locked activation key.

The local licence server is provided as an installer for macOS, Linux or Windows and should be installed on a physical machine (it is NOT possible to use the local licence server on a virtual machine). More detailed instructions for installation and configuration of the local CCDC licence server are provided with the installers.

Once installed, you will need to know the hostname (or IP address) of the system it is installed on, as well as the port number it has been configured to use. This information is used by each client that connects to the licence server.

14.6.2 Configuring access to the local CCDC licence server via the graphical user interface version of the activation tool

1. Start the **CCDC Activation Tool** as described above.
2. Click on the **Configure Local Server** tab if it is not already selected.



3. Copy and paste the server hostname or IP address into **Server host** and select the port number the local licence server is using in **Port**.
4. You should be informed that activation was successful. Access to the CCDC products and features your licence allows should now be possible.

14.6.3 Via the command line interface

Run the `ccdc_activator` command line tool with the `-s` argument, followed by the URL and port that the server is running on in the format `http://myserver:port`. For example, on Windows:

```
ccdc_activator.exe -s http://myserver:1234
```

14.7 Using the activation tool in administrative mode to allow access for all users on a system

It is possible to use the activation tool to configure the licensing system to either auto-activate for all users of a system, or else configure all users to connect to a local licence server. To do so, the command line `ccdc_activator` tool must be used as Administrator or root (depending on the system in use). This is primarily intended as a means for system administrators to deploy the CSD Software and not require any licensing action by individual users.

To use the `ccdc_activator` tool in administrative mode, use the `-A` argument as an addition to one of the commands detailed above. For example, to set up a CSD installation to attempt to auto-activate with a particular key for users of that system use:

```
ccdc_activator.exe -A -a -k  
123456-123456-123456-123456-123456-123456
```

To set up all users to connect to a local licence server at `http://myserver:1234` use

```
ccdc_activator.exe -A -s http://myserver:1234
```

14.8 Licensing via an environment variable

It is possible to use the `CCDC_LICENSING_CONFIGURATION` environment variable instead of using the activation tool to provide licensing information. This mechanism overrides all other licensing

information and will be used in preference to any of the other licensing actions detailed above that may have previously been carried out.

A system administrator can use this mechanism to set the environment variable on a system-wide level, thereby granting access for all users.

The `CCDC_LICENSING_CONFIGURATION` variable can be set in two ways:

- A licence key can be used to automatically activate CCDC programs by setting `CCDC_LICENSING_CONFIGURATION` to:

```
lf-code;123456-123456-123456-123456-123456-123456
```

where `123456-123456-123456-123456-123456-123456` is the licence key provided by CCDC.

- A local floating licence server can be used by setting `CCDC_LICENSING_CONFIGURATION` to:

```
lf-server;http://myserver:1234
```

where `myserver` is the server hostname or IP address or your local licence server, and `1234` is the port it is using.

Care must be taken to follow the provided syntax or CCDC programs will not run, providing an error message stating 'Invalid Licensing configuration. Please contact your System Administrator to correct the issue'.

14.9 Optional values in the environment variable

It is possible to pass optional values via the `CCDC_LICENSING_CONFIGURATION` environment variable. These must be present in addition to the base parameters detailed above. The optional values are formed as key=value pairs, separated by semi-colons. There is currently one such optional value:

- Number of Retries. This setting allows the specified number of retries to occur to try to attempt licensing and can be useful in cases where access to either the CCDC's main licence server, or your own local licence server, may be temporarily disrupted. The value takes the form:

```
num-retries=X
```

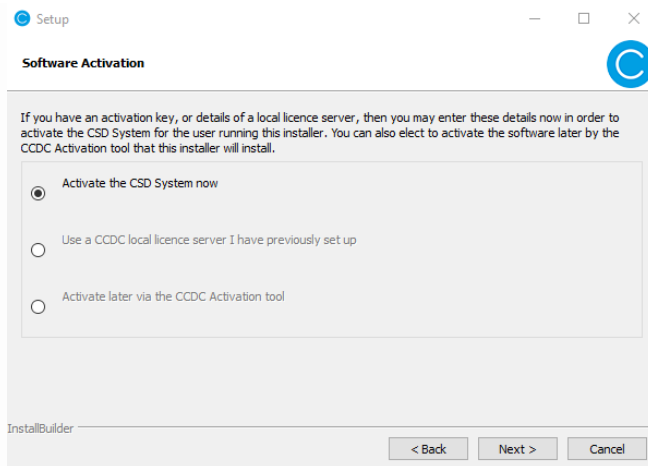
where X is the number of retries, e.g. `num-retries=5`. An example value of `CCDC_LICENSING_CONFIGURATION` using your own licence server with up to 5 retries would be:

```
lf-server;http://myserver:1234;num-retries=5
```

14.10 Performing licensing tasks with the CSD Portfolio installer

It is possible to both activate the CSD Portfolio and setup access to a local licence server when using the CSD Portfolio installer.

When installing the CSD Portfolio, you will be presented with the following dialog:



You may select to either activate the CSD Portfolio now, use a CCDC local licence server, or you can choose to perform activation later with the CCDC activation tool as described in the earlier sections.

Licensing may only be carried out when using the installer in the interactive GUI mode. If using via the command line, licensing tasks will need to be carried out with the installed software activation tool as post installation tasks.

15 Public IsoStar Server

A public IsoStar server is hosted at CCDC: <http://isostar.ccdc.cam.ac.uk>. Access to scatterplots from this public server requires a licensed copy of the IsoStar client package.

16 CCDC Maintenance Tool

The installer will always create a maintenance tool to help manage your installation. This can be found in the root folder of the installation.

The maintenance tool can be used to

1. Add or remove software or data data components
2. Check for updates
3. Uninstall

16.1 Adding or removing components

This operates similarly to a new installation. You may view the currently installed components and choose to remove or add new ones. Added components will be downloaded and installed as with a standard online install.

16.2 CSD Software & Data Updates

A check is automatically made for the existence of software and data updates when running Mercury or Hermes and if an update is found you will be prompted to run the maintenance tool to apply it.

Alternatively a check can be made directly with the CCDC maintenance tool.

If an update to any of the software or data components you currently have installed is detected then you may choose to perform the update via the maintenance tool interface.

16.3 Updating an install made by an offline installer

The online installer configures the CCDC maintenance tool to check the CCDC repositories for updates but the offline installer does not. It is however possible to add them as temporary repositories in order to carry out a one-off online update (this will require internet access). The process for this is:

1. Start the CCDC Maintenance Tool
2. Click on the Settings button and select the Repositories tab
3. In the Temporary Repositories section, add the following URL for a data update:

`https://install.ccdc.cam.ac.uk/online_repo/data`

Also add the appropriate URL for your OS for a software update:

https://install.ccdc.cam.ac.uk/online_repo/windows-dynamic-64

https://install.ccdc.cam.ac.uk/online_repo/linux-64

https://install.ccdc.cam.ac.uk/online_repo/mac

4. On Linux or Mac, click OK, select the Update Components option, and keep clicking Next to go through the update process.
5. On Windows the above step will fail to locate data updates because when using the offline installer the data is copied rather than installed as a component. After setting up the temporary repositories select Add Or Remove Components instead, then add the top-level CSD Data Portfolio component. This is a large download but it will enable future data updates to be installed via Update Components.

17 Activating In-House Databases

Since the 2019 CSD Release, ConQuest and the other CSD Portfolio programs no longer recognize our old ASER format database (.ind, .msk and .tcd). In order to use an existing ASER database you will first need to convert it to our new database format. Details on how to do so can be found in this support FAQ: <https://www.ccdc.cam.ac.uk/support-and-resources/support/case/?caseid=d5e44a8b-41ee-e811-9044-005056975d8a>

ConQuest can search in-house databases in addition to the main CSD. These databases are created using the CSD Editor or similar utilities. If you have created an in-house database that you wish to search using ConQuest you must first activate it using the procedure described below.

In order to activate your in-house database, you must copy (or soft-link: Linux only) the in-house database file (.sqlite) to the same directory as the CSD V5.45 database files. This is typically:

<INSTALLDIR>/ccdc-data/csd

You must then run the Activate program.

For Linux, ensure that <INSTALLDIR> is in your PATH and type:

```
<INSTALLDIR>/ccdc-software/conquest/bin/activate
```

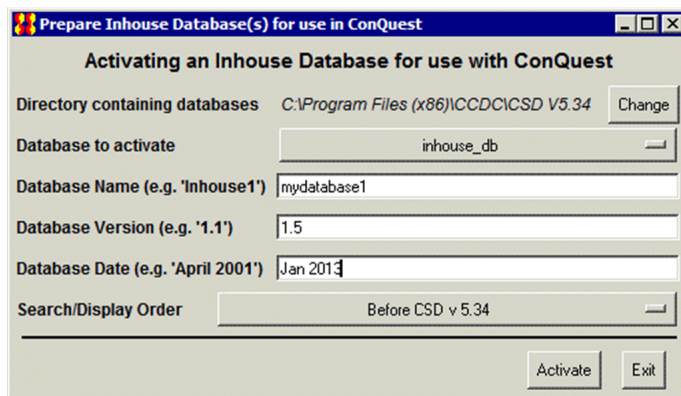
To run the activate database program on Windows use:

```
<INSTALLDIR>/ccdc-software/conquest/exe/activate
```

On macOS, start a terminal window and run the command:

```
<INSTALLDIR>/ccdc-software/conquest.app/Contents/Resources/bin/  
activate
```

In all cases a pop-up window like the one shown below will be displayed:



The activation program attempts to find the directory where the database is located by examining your ConQuest defaults file. However, if the correct directory cannot be found then use the **Change** button to locate the required directory.

All databases in the selected directory which have not been activated will be displayed in the **Database to activate** pull-down menu. Simply select the databases you wish to activate.

The contents of the **Database Name** dialogue box will be used by ConQuest to identify which database you wish to search or view. Choose a name relevant to the database contents.

Enter a version number for the database in the **Database Version** dialogue box. If you have an earlier version of a database, with the same Database Name in the same directory, it is important to make sure that the most recent version has the largest version number so that it is used in preference to the others.

Enter the date for the database in the **Database Date** dialogue box.

Use **Search/Display Order** pull-down menu to select the order in which activated databases will be displayed and searched by ConQuest. Taking the above example, if you select **After CSD v5.45**, when both databases are selected for searching in ConQuest the main CSD database will be searched before the in-house database.

When you are happy with your selections, press the **Activate** button. This will create a .inf file for the database, which will then be viewable and searchable the next time you start ConQuest. You can activate additional databases by repeating the procedure described above.

To close the activate database program press the **Exit** button.

