

CSD Release and Installation Notes

2022.2 CSD Release

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1 CSD Release Package

The 2022.2 CSD Release installer is supplied via download, for Windows, Linux and macOS. The installer contains:

- The Cambridge Structural Database, Version 5.43
- ConQuest 2022.2
- Mercury 2022.2
- enCIFer 2022.2
- IsoStar 2022.2
- Mogul 2022.2
- CSD Conformer Generator 2022.2
- Hermes 2022.2
- GOLD 2022.2
- CSD-CrossMiner 2022.2
- CSD Ligand Overlay 2022.2
- SuperStar 2022.2
- CSD Python API 3.0.13

Supported platforms are listed elsewhere (see Supported 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.

CSD-Core

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

CSD-Materials

Everything in CSD-Core as well as:

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

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.

CSD-Enterprise

All of the above

2 Database Content and Information

- The 2022.2 CSD Release contains 1,138,368 unique structures and 1,161,919 entries (CSD version 5.43). More structures will be made available in the CSD data updates throughout 2022.

3 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/>

4 Known Problems

- **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.
- **Use of ConQuest, Mogul's sketcher and API scripts in Mercury/Hermes 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's). 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'
```

- **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.
- **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.
- **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.
- **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.
- **CSD Portfolio software fails to run on linux systems using Wayland as a display protocol**
If using our software on a system using Wayland you will receive an error similar to:

WARNING: Warning: Ignoring XDG_SESSION_TYPE=wayland on Gnome. Use QT_QPA_PLATFORM=wayland to run on Wayland anyway.

Use of the CSD Portfolio on systems using Wayland is unsupported at this time, but if required our software can run by setting the following environment variable:

```
export XDG_SESSION_TYPE=xcb
```

It is likely that graphical interfaces will not be displayed to our usual standard with this workaround, although command line use should work as normal.

- **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=57580dd5-151a-ec11-9693-00505695c114>

- **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.

- **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. We plan to fix this in a later release and to add Ubuntu 22.04 to our supported platforms.

- **On linux platforms Help and other documentation links may not work**

When using the documentation links in the Help section of various CCDC products (e.g. Mercury, IsoStar, CrossMiner) then the documentation may fail to load correctly in your browser. The documentation can be viewed manually via the files in the documentation folder of your installation, or from our website at <https://www.ccdc.cam.ac.uk/support-and-resources/ccdcresources/>

5 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 required CSD Release installers from http://www.ccdc.cam.ac.uk/csds_download. 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 registering the software.
3. Install the IsoStar 2022.2 server (Linux) (see IsoStar Server Installation).

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

5.2 System Requirements

5.2.1 Supported Platforms

Executables in this release are supported on the following platforms and operating systems, unless noted that some platforms are unavailable in section 1:

- Windows - Intel compatible, 64-bit:
 - Windows 10 and 11
- Linux - Intel compatible, 64-bit:
 - RedHat Enterprise 7.6 or higher, and 8
 - CentOS 7.6 or higher
 - CentOS Stream 8
 - Ubuntu LTS 18 and 20

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 or Apple ARM (via Rosetta 2 emulation)*, 64-bit:
 - macOS 10.15, 11 and 12

Note: Apple ARM-based (M1) 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 2022.2 CSD Release 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 (see Linux Installation below for more details)

5.2.2 Changes to Supported Platforms

From the 2022.3 release onwards we will add support for Ubuntu 22 and remove support for Ubuntu 18.

5.2.3 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 2022, 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.

5.2.4 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.

5.2.5 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.

5.2.6 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:

<http://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.

5.2.7 Disk Space Requirements

A complete installation of the 2022.2 CSD Release requires approximately 24 GB of disk space. This includes all software (7 GB) and all data files except for Crossminer (17 GB). The optional CrossMiner data install will occupy another 11 GB.

6 Windows Installation

6.1 General Installation Options

On all platforms the installer will give you the option to install:

- CSD Software
- CSD Data

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. In this case we recommend installing the CSD Data to your desired location first, then re-run the installer and install only the CSD Software - you will be prompted to locate the CSD Data so that individual users will not need to do so themselves when first starting CSD software that requires it.

6.2 Installation Procedure

Administrator privileges are required for installation.

Do not install directly on top of a previous installation; use a new folder. We recommend that you uninstall previous versions of all CSD Portfolio software, any previous version of the CSD Python API, as well as Mogul and CSD database files, and remove all CSD update files, before you install the current version.

To install on Windows:

1. Download the `csds-2022.2.0-windows-installer.zip` file and unpack its contents to a location on your computer. Note that the installer cannot be run from within the zip file and both the installer and dist file must be located in the same directory.
2. Double-click on the `csds-windows.exe` file. The installer menu will take you through the steps necessary to complete the installation.
3. Installation will place ConQuest, Mercury, Mogul, Conformer Generator, IsoStar Client, enCIFer in a 'CSD_2022' sub-directory, and Hermes, GOLD and SuperStar in a 'Discovery_2022' sub-directory, and the CSD Python API in a 'Python_API_2022' sub-directory. Shortcuts to these programs will also be placed on your desktop and Start Menu (where available).

6.3 Uninstalling CSD Software and Database files

The CSD Release software can be removed from your computer by selecting:

Start Menu -> CCDC -> CSD Portfolio Software 2022 -> Uninstall CSD Portfolio 2022

7 Linux Installation

7.1 Package Requirements

The CSD software requires the Network Security Services (NSS), OpenGL, Fortran and libXss.so.1 libraries to be present on your system. These can be installed on CentOS/RedHat 7 with the command:

```
sudo yum install nss libXScrnSaver libglvnd-opengl libgfortran5
```

Or on CentOS/RedHat 8:

```
sudo yum install nss libXScrnSaver libglvnd-opengl libgfortran
```

Or on Ubuntu 18.04/20.04:

```
sudo apt-get install libnss3 libxss1 libopengl0 libgfortran5
```

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.

7.2 Installation Procedure

Do not install directly on top of a previous installation. We recommend that you uninstall previous versions of the CSD software, database files including all CSD update files before you install the current version.

To install the CSD Release, and/or data on Linux.

1. Download `csds-2022.2.0-linux-installer.tar` and unpack its contents to a location on your computer. Note that both the installer and dist file must be located in the same directory.
2. Ensure that the installer executable has execute permissions via the command:

```
chmod a+x ./csds-linux-x64.run
```

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

```
./csds-linux-x64.run
```

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

7.3 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 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.

8 macOS Installation

8.1 General Installation Process

Administrator privileges are recommended but not usually required for installation.

Do not install directly on top of a previous installation. We recommend that you uninstall previous versions of the CSD Portfolio, database files including all CSD update files before you install the current version.

We suggest that all software and database components are installed in the `/Applications` directory, which will usually require Administrator privileges. However, you are free to use any other location.

8.2 Installation Procedure

To install on macOS:

1. Download the `csds-2022.2.0-macos-installer.dmg` file and unpack its contents to a location on your computer.
2. Double click on `csds-osx` and follow the on-screen instructions to install the software and databases.

8.3 Troubleshooting

IsoStar is a client-server application and only the client software can be installed on Windows or macOS. 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 (see Public IsoStar Server). Alternatively, you can use an HTTP server to make the IsoStar data available. The HTTP server can be run on any of the supported IsoStar Linux platforms (see Supported Platforms). Please note that it is currently not possible to run the IsoStar server on Windows or macOS. Further information on setting up your HTTP server is provided (see IsoStar Server Installation).

On macOS, Safari does not employ Helper Applications so if this browser is being used to access IsoStar data you will need to download the scatterplot file then open the file within the IsoStar client manually. Alternatively, Firefox can be configured to launch an application associated with a particular file extension.

If you are experiencing any problems with installation or use of the CSD Portfolio, please review our support database at <http://www.ccdc.cam.ac.uk/support> where you should be able to find help with common issues.

9 Advanced installation strategies

There are several options to adjust the installation of the CSD Portfolio to your needs.

9.1 Installing the CSD data and CSD Portfolio software separately

It is possible to install the CSD data and the CSD Portfolio software to different locations. This can be useful to, for example, have a single data installation on a network accessible location that multiple software-only installations can use. This will allow you to save space on the systems where the software is installed.

Using the standard graphical installation interface, you will have the option to install both data and software (the default), only the data, or only the software. To install the data to a different location, it is highly suggested to perform the data-only install first. If this is done, you can supply the path to the location of the data during installation of the software and have this location automatically used when running the software.

9.2 Running the installer at the command line

More advanced use of the CSD Portfolio installers usually involves running via the command line, which allows various arguments to be added that changes the installer's behaviour or provides information normally entered via installer dialogs.

Windows:

Ensure you are in the same directory as the .exe installer file and then just type its name, e.g.

```
csds-windows.exe
```

Linux:

You will normally need to specify the location of the installer executable to run it - this is most easily done by being in the same working directory as the .run installer executable and prepending `./` (which means "in this directory"), e.g.

```
./csds-linux-x64.run
```

macOS:

To run the installer application at the command line, ensure you are in the same working directory and use the open command, e.g.:

```
open csds-osx.app
```

9.3 Installing without GUI access

If you do not have graphical access to the machine where you are installing, the installation program can be run using a text-only interface. This can be useful for cases when running over slow connections or as a simplified interface. This interface should automatically be invoked if it senses there is not a graphical interface, but can also be manually specified if desired by adding the **--mode text** argument when running the CSDS installer at the command line, for example:

```
./csds-linux-x64.run --mode text
```

You will be walked through the same installation procedure as in the graphical interface and have the same options.

9.4 Silent and other install methods using the command line

The technology used by the CSD installers allows all data normally entered in the graphical installer interface to instead be specified directly via command line arguments when running the installer in a terminal window.

In particular, the **--mode** and **--unattendedmodeui** options can be used to control the amount of output and interactivity of the installation, such as silent and unattended installation, which can be useful for mass deployments of the software in an automated fashion.

Running the installation program in a terminal/shell with the **--help** option will provide a complete list of the command-line options available. For example:

```
csds-windows.exe --help
```

Below are some of the more common options or scenarios.

- **--mode unattended** will force the installer to operate in batch/unattended mode. There are several associated options that are required for automated installations:
- **--prefix** give the root directory of the installation. On Linux, it will default to \$HOME/CCDC, on Windows to C:\Program Files\CCDC and /Applications/CCDC on macOS.
- **--unattendedmodeui** can take the values:
 - **none** for an unattended silent install
 - **minimal** for limited feedback during installation
 - **minimalWithDialogs** for dialog driven feedback if possible
- **--licensing** can take the values of:
 - **NotNow** to skip registration. Activation will need to be completed manually later `ActivateAfterInstall LocalLicenceServer NotNow`
 - **ActivateAfterInstall** to attempt to activate the software automatically immediately after the installation process. Will additionally require the activation key. This mode requires the machine to have access to the internet as it will contact the CCDC licensing server.
 - **LocalLicenceServer** will use a specified existing local licence server. You will require the hostname or IP of the licence server, and the port it is using.

- **--activation_key <activation_key>** is used in conjunction with **--Licensing ActivateAfterInstall** to activate the software during the installation process.
- **--activate_admin true** is used in conjunction with **--Licensing ActivateAfterInstall** to activate the software during the installation process for all users of a system. This requires running as administrator or root user. This causes the software to auto-activate online when each user first starts one of the components of the CSD Portfolio.
- **--server_host <server_host>** and **--server_port <server_port>** are used in conjunction with **--Licensing LocalLicenceServer** to configure access to a local licence server.
- **--server_admin true** is used in conjunction with **--Licensing ActivateAfterInstall** to setup access to a local licence server for all users of a system. This requires running as administrator or root user.
- **--enable-components** and **--disable-components** will enable and disable the installation of the data (datagroup) and the software (softwaregroup) components of the CSD Portfolio. Allows the values:
 - **datagroup** installs the data component
 - **vcredist** (Windows only) installs the Microsoft Visual Studio runtime libraries required by the CSD software.
 - **softwaregroup** installs the software component. This option additionally allows the specification of the location of your data install:
- **--csdsoftwareonly**
 - **true** enables definition of the data directory via **--csdsoftwareonlydatadir**
 - **false** no link to a data directory will be carried out (default)
- **--csdsoftwareonlydatadir <data directory>** should be set to the location of the main CSD database files, for example on Windows: "C:\Program Files\CCDC\CSD_2022\CSD_543"

Note that if an argument contains a space you will need to enclose it in double quotes. This is most common with Windows paths that contain elements like "Program Files".

The two most common scenarios are for batch mode installations with activation during installation:

- Windows
 - `csds-windows.exe --prefix "C:\Program Files\CCDC" --mode unattended --unattendedmodeui none --Licensing ActivateAfterInstall --activation_key 123456-123456-123456-123456-123456`
- Linux
 - `./csds-linux-x64.run --prefix /soft/ccdc --mode unattended --unattendedmodeui none --Licensing ActivateAfterInstall --activation_key 123456-123456-123456-123456`
- macOS
 - `open csds-osx.app --prefix /Applications/CCDC --mode unattended --unattendedmodeui none --Licensing ActivateAfterInstall --activation_key 123456-123456-123456-123456`

or with a local licence server for all users (must be run as administrator or root user):

- Windows

- o `csds-windows.exe --prefix "C:\Program Files\CCDC" --mode unattended --unattendedmodeui none --Licensing LocalLicenceServer --server_host myserver --server_port 1234 --server_admin true`
- Linux
 - o `./csds-linux-x64.run --prefix /soft/ccdc --mode unattended --unattendedmodeui none --Licensing LocalLicenceServer --server_host myserver --server_port 1234 --server_admin true`
- macOS
 - o `open csds-osx.app --prefix /Applications/CCDC --mode unattended --unattendedmodeui none --Licensing LocalLicenceServer --server_host myserver --server_port 1234 --server_admin true`

9.5 MSI-based installers

MSI (MicroSoft Installer) based installers are available as an alternative to the Bitrock installers we provide by default. MSI-based installers are mainly of use for those organisations that have mechanisms in place to deploy using Microsoft technologies that require MSI-based installers. If this would be of use to your organisation please contact support@ccdc.cam.ac.uk.

The MSI installers are provided as separate software and data installers. During install time, if the data is not being installed on the same computer then the software installer allows the user to select where the data is installed. If installing silently, the following msi parameters will achieve the same result:

```
USE_NETWORK_CSD_DATA=1 DATABASE_PATH="C:\path\to\CSD_543"
```

9.6 Uninstallation using the command line

In much the same way as the installer executable, the uninstaller that is created in the CSD_2022 installation folder can also be run either interactively via a GUI, or at the command line. Like the installer executable, you can view the options available with the uninstaller by using the **--help** argument, e.g.

```
uninstall.exe --help
```

To perform a silent uninstall with no further user prompts, use:

```
csds-windows.exe --mode unattended
```

Note that it can take some time for the uninstall to complete.

9.7 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.

10 CSD-CrossMiner

CSD-CrossMiner is now installed as part of the CSD Portfolio package. In order to be used you will need to download the optional data that it requires. This can be done via the update options in the program itself, or the data can be manually downloaded and installed from our website downloads page (<https://www.ccdc.cam.ac.uk/support-and-resources/downloads/>).

11 WebCSD Access

The CCDC hosts a WebCSD server which can be accessed at:

`https://www.ccdc.cam.ac.uk/structures`

Access to this server can be set up by IP address if you send us your IP ranges or you can register a username and password in order to obtain access. If your institution has purchased a campus licence you will receive unlimited, site-wide access to WebCSD.

Those with unlimited site licenses can contact admin@ccdc.cam.ac.uk with details of their institution's IP address range(s) in order to arrange access.

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>/CSD_2022/bin (where <INSTALLDIR> is the path to your CSD_2022 installation directory), or ensure that this is in your system PATH.

Then for ConQuest, type:

```
cq
```

For Mogul, type:

```
mogul
```

For Mercury, type:

```
mercury
```

For IsoStar client, type:

```
run_isostar
```

For Discovery software, change directory to <INSTALLDIR>/Discovery_2022/bin (where <INSTALLDIR> is the path to your Discovery_2022 installation directory), or ensure that this is in your system PATH.

Then for Hermes, type:

```
hermes
```

For the GOLD interface in Hermes, type:

```
gold
```

For CSD-CrossMiner, type:

```
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 in 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 (i.e. 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 Portfolio or greater licence will, however, allow access to additional features that are only available to CSD Portfolio users.

12.7 Configuration of CSD Portfolio Components

12.7.1 ConQuest

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.

Database Location

Before using ConQuest you may be required to locate the main database files. The location of these files is identified by selecting a CSD database information file. For ConQuest this file will be called `as541be.inf` and will be found in the `csd` subdirectory in the location where you installed the database files.

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 web-site:

<http://www.adobe.com>. Other free PDF readers are available, see <https://pdfreaders.org>

12.7.2 Mogul

Database Location

Before using Mogul, you may be required to locate the main database files (as detailed for ConQuest above) as well as the mogul database files. The location of these files is identified by selecting a mogul path information file. For Mogul this file will be called `mogul543.path` and will be found in the data subdirectory in the location where you installed the database files.

12.7.3 Mercury

When Mercury is launched, it tries to detect whether or not the CSD is installed. If the CSD can be found, it is opened, and the structure navigator on the right-hand side of the main Mercury window will then contain the refcodes of all the entries in the database.

If you have a CSD-format database that is not detected automatically by Mercury, you can open it by clicking Databases, followed by Database Location... Once opened, the database will be added to the Databases menu.

You can use Mercury to view either your own crystal structures, or those retrieved from a ConQuest search. To view the hits from a ConQuest search in Mercury select Analyse Hitlist, from within ConQuest, and then View in Mercury from the pull-down menu. Alternatively, within ConQuest, select File from the top-level menu and View in Mercury from the resulting pull-down menu.

Different Mercury features are unlocked depending on your licence.

12.8 Setting up the CSD Portfolio Environment on Linux and macOS

Setting the `CSDHOME` environment variable on Linux and macOS can aid in the location of the CSD software and data installation if you have a non-standard setup. Additionally, adding `<INSTALLDIR>/CSD_2022/bin` and `<INSTALLDIR>/Discovery_2022/bin` to your `PATH` on linux can allow you to start the CSD software without use of the full path to its location.

For example:

1. To set `CSDHOME` for Bourne shell (sh) or Korn shell (ksh), type:
`CSDHOME=<INSTALLDIR>/CSD_2022; export CSDHOME`
where `<INSTALLDIR>` is the top level CCDC directory of your CSD Portfolio installation.

For example:

```
CSDHOME=/usr/local/CCDC/CSD_2022; export CSDHOME
```

Or

```
CSDHOME=/Applications/CCDC/CSD_2022
```

2. Similarly, to set CSDHOME for C-shell (csh), type:

```
setenv CSDHOME <INSTALLDIR>/CSD_2022
```

For example:

```
setenv CSDHOME /usr/local/CCDC/CSD_2022
```

3. To add <INSTALLDIR>/CSD_2022/bin and <INSTALLDIR>/Discovery_2022/bin to your PATH for Bourne shell (sh) or Korn shell (ksh), type

```
PATH=<INSTALLDIR>/CSD_2022/bin:<INSTALLDIR>/Discovery_2022/bin:
$PATH; export PATH
```

4. Or for C-shell (csh) type:

```
setenv PATH
<INSTALLDIR>/CSD_2022/bin:<INSTALLDIR>/Discovery_2022/bin:$PATH;
rehash
```

To make these changes permanent, add the commands executed in steps 1 and 2 to all your CSD Portfolio users' .login (csh) or .profile (sh, ksh) files. Alternatively, place the commands in a system-wide login or profile script such as /etc/profile.

12.9 Desktop launchers for Linux

The CSD software now 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 CSD_2022/desktop and Discovery_2022/desktop directories of your Linux installation for the respective programs that can be launched from the CSD software in those locations.

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 2022.2 CSD Release 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 `Python_API_2022` 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 run in an existing command prompt window, navigate to the `Python_API_2022\miniconda` directory and type 'python'.

13.2.2 Using the CSD Python API on Linux

Start a terminal and navigate to the `Python_API_2022` 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 3.7.12.

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

```
source activate
```

A (root) prompt should appear at the start of the command line prompt, indicating that the correct environment should have 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 `Python_API_2022` 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 3.7.12.

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 (root) 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 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 setting up access to a local licence server when performing an installation of the CSD Release. Additionally, you may select the option to perform activation or setting 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>\CSD_2022\Software Activation`

folder of a CSD installation, or

`<INSTALLDIR>\Software Activation`

in other CCDC product installers. 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>/CSD_2022/bin`

folder of a CSD installation, or

`<INSTALLDIR>\software_activation`

in other CCDC product installers. 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>/CSD_2022`

folder of a CSD installation, or

`<INSTALLDIR>\Software_Activation`

in other CCDC product installers. 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

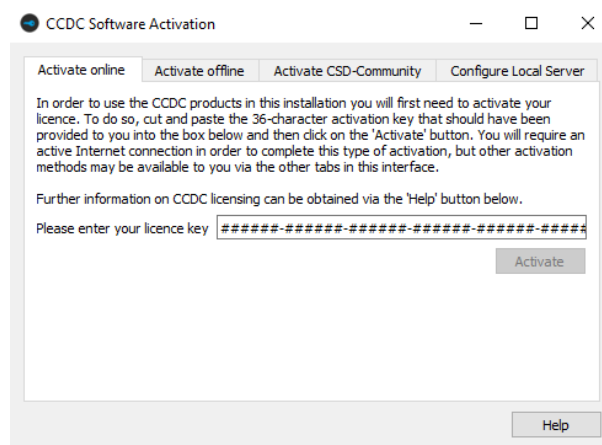
If you have purchased a CCDC product such as the CSD Portfolio, then you will have been provided with an activation key. This key can be used to perform an activation on the computer system you are using the CCDC software, and the easiest method to do so is by directly communicating with our licence 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:

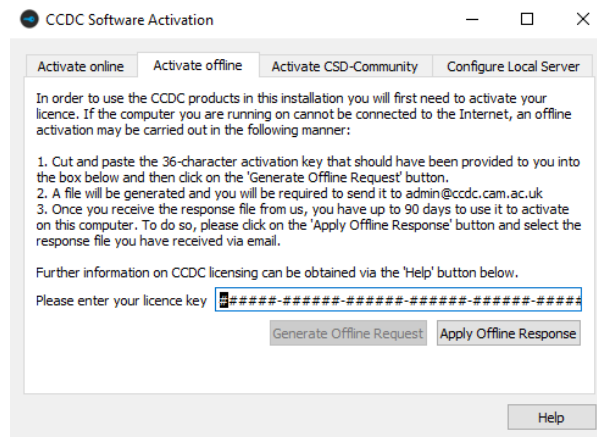
```
ccdc_activator.exe -a -k 123456-123456-123456-123456-123456-123456
```

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:

```
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*:

```
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

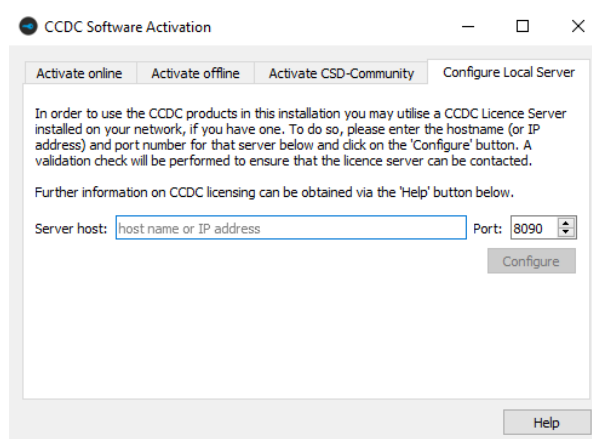
To obtain the local CCDC licence server, please send a request to admin@ccdc.cam.ac.uk, quoting your customer details and existing node-locked activation key.

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 instruction 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 of 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
```

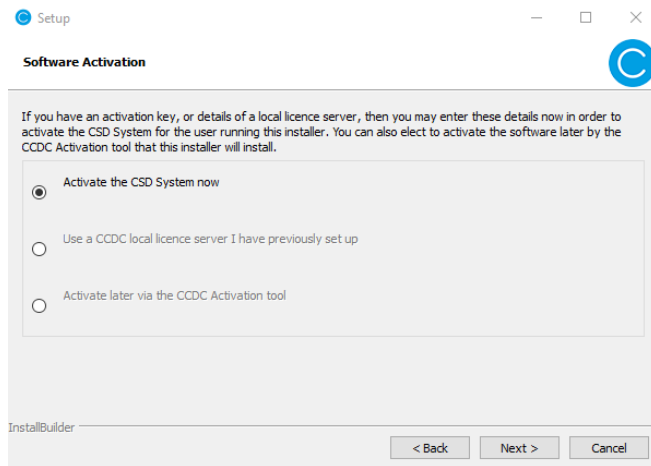
where `X` is the number of retries, e.g. `num-retries=5`. An example value of `CCDC_LICENSING_CONFIGURATION` using your own licence server with up to 5 retries would be:

```
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. If installing as an administrator or root user, then this allows you to both install to a system and set up licensing so that the end user can immediately start using the software.

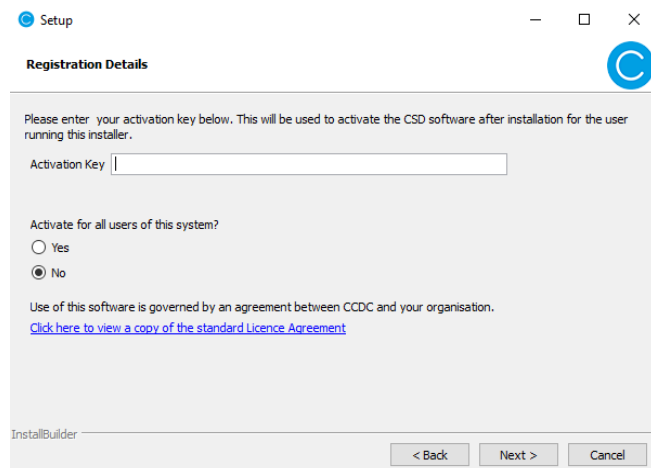
When installing the CSD Portfolio, you will be presented with the following dialog:



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.

14.10.1 Activate the CSD Portfolio now

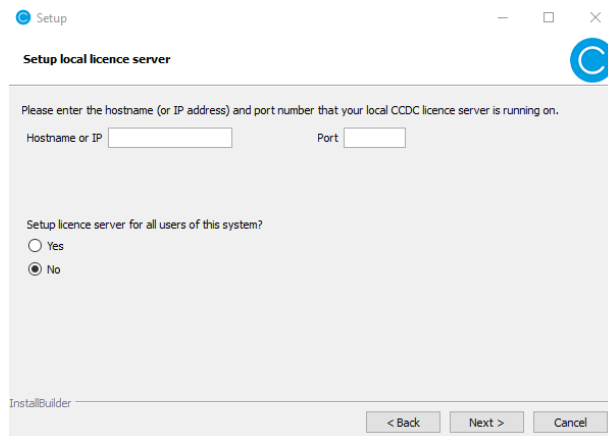
You will be presented with the following dialog which allows you to enter your activation key.



If you have administrator or root user access, then you will also be able to select whether to perform this activation for all users. Selecting 'no' (which is also the default option) will activate only for the user that is carrying out the installation, selecting 'yes' will set up the install to perform an auto-activation with the entered activation key when a user first starts a CSD Portfolio software application.

14.10.2 Use a CCDC local licence server

You will need to have first set up a local licence server on your network and know the hostname (or IP address) and port number that it uses. You will then see this dialog:



You will need to enter the hostname or IP address of your local licence server, as well as the port that it has been configured to use. If installing as an administrator or root user, you can also select to install for all users of the system, or just for the user performing the installation (the default).

14.11 Command line use of the CSD Portfolio installer

The CSD Portfolio installer can also be used at the command line by providing suitable arguments. Please see the following support FAQ that details the current command line options available in the installer: https://www.ccdc.cam.ac.uk/csds_install_help

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 CSD Software & Data Updates

It is possible to check for the existence of software and data updates which are made available at regular intervals (approximately every 3 months). This will keep your software and copy of the CSD database more current between each major CSD Release.

Updates can be obtained automatically via the **Help... Check For Updates** option in either Mercury or Hermes.

Alternatively, the following URL will take you to the CCDC download page where the updates can be obtained manually as they become available:

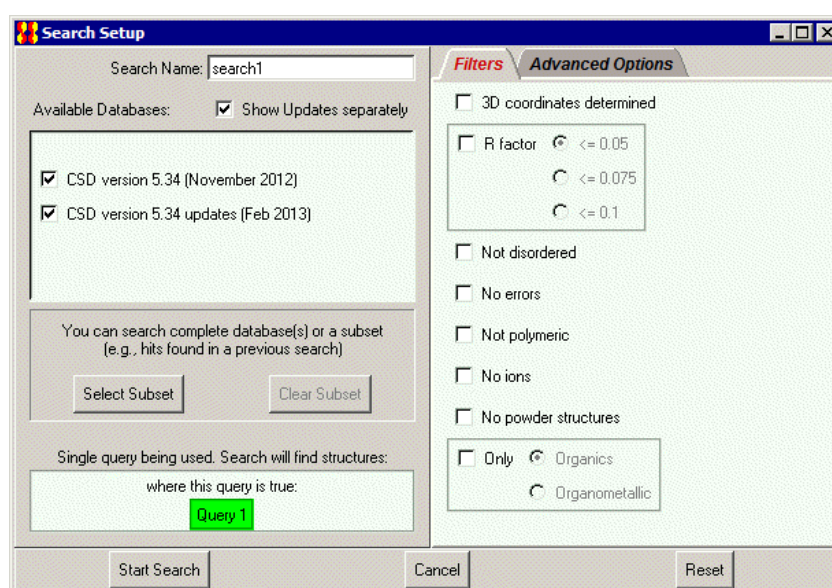
<https://www.ccdc.cam.ac.uk/support-and-resources/downloads/>

You will be required to enter your Customer Number and Activation Key in order to download an update. For data updates only:

- Updates will need to be downloaded in numeric order and added to the same directory as your CSD database files.
- Follow the instructions for installation and the update(s) will be visible when restarting ConQuest.

Note: You will need write permission to the main CSD folder to install each update.

- Each update will be shown separately in the *View Databases* menu.
- The update packages can be searched either with the main database or separately as desired; this is controlled via options in the *Search Setup* dialogue box:



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 PreQuest 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 V5.41 database files. On Linux this is typically:

```
<INSTALLDIR>/CSD_2022/csd
```

While on Windows, this is normally:

```
C:\Program Files\CCDC\CSD_2022\CSD_543
```

And on macOS:

```
/Applications/CCDC/CSD_2022/DATA/CSD_543
```

You must then run the Activate program.

1. For Linux, ensure that `<INSTALLDIR>/CSD_2022/bin` is in your `PATH` and type:
`activate`

To run the *activate database* program on Windows select:

```
Programs -> CCDC -> CSD Portfolio Software 2022 -> Activate in-house database
```

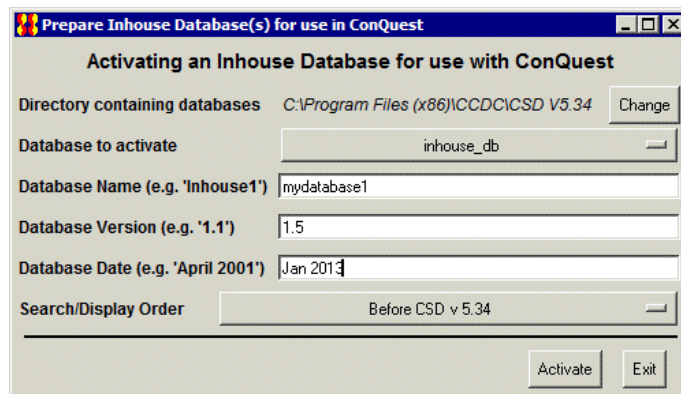
from the Windows Start menu.

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

```
/Applications/CCDC/CSD_2022/conquest.app/Contents/Resources/bin  
/activate
```

Note: Windows users will require escalated administrator privileges to activate databases. To do so, right-click on the **Activate Inhouse Databases** menu item and select **Run as Administrator**.

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 v5.43**, 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.

Search Setup

Search Name:

Available Databases:

- CSD version 5.31 (November 2009)
 - Restricted to 11181 refcodes*

You can search complete database(s) or a subset (e.g., hits found in a previous search)

Single query being used. Search will find structures:
where this query is true:

Filters **Advanced Options**

- 3D coordinates determined
- R factor
 - ≤ 0.05
 - ≤ 0.075
 - ≤ 0.1
- Not disordered
- No errors
- Not polymeric
- No ions
- No powder structures
- Only
 - Organics
 - Organometallic