

CSD Release and Installation Notes

2018 CSD Release Update 3

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1 CSD Release Package

The 2018 CSD Release Update 2 installer is supplied via download, or via USB stick, for Windows, Linux (32-bit and 64-bit) and macOS. The installer contains:

- The Cambridge Structural Database, Version 5.39
- ConQuest 1.23
- Mercury 3.10.3
- enCIFer 1.6.4
- IsoStar 2.2.8 (Server is version 2.2.5 and is Linux 32-bit only)
- Mogul 1.7.6
- Conformer Generator 1.2.3
- Hermes 1.9.3
- GOLD 5.6.3
- SuperStar 2.1.9
- DASH 3.3.10 (Windows only)
- CSD Python API 1.5.3

Supported platforms are listed elsewhere (see Supported Platforms). Additionally, you may have access to other components that are supplied separately:

- CSD-CrossMiner (64-bit only)
- WebCSD (accessed via <https://webcsd.ccdc.cam.ac.uk>)
- Relibase (accessed via <http://relibase.ccdc.cam.ac.uk>)
- PreQuest (Windows and Linux 32-bit only; accessible by separate download. For details please contact support@ccdc.cam.ac.uk.)

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

CSD-System

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

CSD-Materials

Everything in CSD-System as well as:

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

CSD-Discovery

Everything in CSD-System as well as:

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

CSD-Enterprise

All of the above

2 Database Content and Information

- The number of CSD entries in the 2018 release of the CSD System is 904,100 in the main database, 11,921 in the Nov17 update, 20,084 in the Feb18 update and 14,411 in the May18 update, making a total of 950,516 entries.

3 What's New

The CSD Database

- The 2018 release contains over 900,000 entries (CSD version 5.39) – an increase of more than 60,000 entries from the previous year
- Targeted enhancements have also been made to over 62,000 existing CSD entries, including:
 - Addition of validated metal oxidation states to over 21,000 entries
 - Enhancement of over 6,000 historical entries from the 1970s and 1980s
 - Review of text fields including refinement, disorder, CSD class and bioactivity
 - Inclusion of article DOIs for older entries
- Work on replacing the underlying technologies in the CSD system has also allowed us for the first time to provide direct display within Mercury of the anisotropic displacement parameters (ADPs) for over 220,000 entries.

CSD-System

- A new suite of features has been introduced in Mercury to help you visualise, understand and modify the symmetry of crystal structures including the ability to:
 - View along unit cell or Miller directions
 - Link directly to International Tables Volume A (Space-group symmetry) online
 - Reduce symmetry from the current space group to any valid subgroup
- During 2017, we have also introduced a new version of WebCSD (v2) which is:
 - Fully cross-platform – for desktop, tablet and mobile
 - Current – with up-to-the-minute data updates
 - Searchable – by 2D structure, unit cell and text/numeric fields
- Further enhancements to the CSD-System software include:
 - Improved searching in ConQuest, incl. more effective unit cell search – the new cell search method, also used in WebCSD and CellCheckCSD, considers unit cell angles
 - Improved handling of bridged & fused rings in Mogul – these are both now supported in the rings library
 - A new contact group in IsoStar – organic iodine

CSD-Materials

- New, more effective simulated annealing parameters have been introduced to DASH resulting from a focused research study in collaboration with the University of Reading.
- Additional enhancements made to the CSD-Materials components include:
 - Streamlining of the Hydrogen-Bond Propensity (HBP) wizard for improved usability
 - New bromine & iodine probes added to Full Interaction Maps to analyse halogen-bonding interactions

CSD-Discovery

- A new application has been introduced called CSD-CrossMiner – an interactive and highly versatile pharmacophore query tool. CSD-CrossMiner is provided with ready-to-use databases for navigating both the CSD and protein-ligand binding sites from the PDB. This delivers an overall interactive search experience with application areas including interaction searching, scaffold hopping and the identification of novel fragments for specific protein environments.
- Other improvements made to CSD-Discovery include:

- Improvements to CSD Conformer Generator to better account for sparse distributions and rarer ring conformations
- A new CSD Python API menu in Hermes allowing you to create and run your own Python scripts within the Hermes application
- Cavity viewing and highlighting of proteins
- Improvements to GOLD for configuration of constraints
- Exposure of pharmacophoric-driven constraints for docking

4 Known Problems

- **Use of the ‘Locate Licence File’ option to specify a licence file:**
This functionality will only allow you to use a licence file in a non-standard location for the session you are using the CSD software for. In order to have a licence permanently used, please use one of the methods detailed in [CSD System Software Licensing](#).
- **Use of Matplotlib and Pillow in the included CSD Python API miniconda:**
The versions of matplotlib (1.4.3) and Pillow (2.8.2) that we bundle with our miniconda distribution can cause crashes to occur if used in interactive mode. A workaround for the problem is to replace "matplotlib.show()" with "matplotlib.show(block=False)".
- **The ‘Copy to Clipboard’ functionality in Mercury and Hermes may fail on some Linux systems:**
We have observed some issues with copying the 3D visualiser contents to the clipboard via the ‘Copy to Clipboard’ option in Mercury and Hermes. The workaround is to export an image via ‘File->Save As’ instead.
- **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.
- **In the CSD Python API, diagram.DiagramGenerator can cause a failure if used twice:**
A workaround for this issue is to use a new DiagramGenerator object for each diagram to be saved, rather than re-using an existing object. The issue has been fixed in 2018 CSD Release Update 2, so this can also be resolved by updating the software.

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 System installers from http://www.ccdc.cam.ac.uk/csds_download. This will require your Site Number and Confirmation Code.
2. Install the CSD System Software and Database files for Windows (see Windows Installation), Linux (see Linux Installation), and/or for macOS (see Mac OS X Installation) and registering the software.
3. Install the IsoStar 2.2.5 server (Linux) (see IsoStar 2.2.5 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, 32-bit executables (compatible with 32-bit and 64-bit versions of Windows) for:
 - Windows 7, 8 and 10
- Linux - Intel compatible. Both 32-bit and 64-bit versions are available for:
 - RedHat Enterprise 6 and 7
 - CentOS 6 and 7
 - Ubuntu 12, 14 and 16

Note: As we add support for newer versions of Linux, support for older versions may have to be withdrawn.
- Mac Intel compatible 64-bit executables for:
 - macOS 10.10, 10.11, 10.12 and 10.13

If you choose to use a version other than those listed above we cannot guarantee that the 2018 CSD Release software will work correctly, although we will attempt to assist you with any problems you may encounter.

5.2.2 Changes to Supported Platforms and Products

This release is the last to include 32-bit linux executables – future releases for linux will be 64-bit and therefore will only function on 64-bit linux distributions. The next release will also drop official support for Windows 8, Ubuntu 12 & 14 and macOS 10.10 and 10.11.

It is anticipated that the next release will support these platforms:

- Windows - Intel compatible, 32-bit executables (compatible with 32-bit and 64-bit versions of Windows) for:
 - Windows 7 and 10
- Linux - Intel compatible. 64-bit executables for:
 - RedHat Enterprise 6 and 7
 - CentOS 6 and 7
 - Ubuntu 16
- Mac Intel compatible 64-bit executables for:
 - macOS 10.12, 10.13 and 10.14

Note that unless explicitly detailed above, withdrawal of support does not necessarily mean that our future software releases will not work on that platform, but that we cannot guarantee they will be able to do so as software will not be fully tested on those systems. If this will cause insurmountable difficulties, please contact us at support@ccdc.cam.ac.uk to discuss possible solutions.

Development work has now started on new database creation and editing tools that will be made available as that work is completed. We therefore anticipate that PreQuest will be retired and will no longer form a part of the 2019 CSD System software package.

5.2.3 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** check-box will be disabled.

5.2.4 Disk Space Requirements

A complete installation of the 2018 CSD Release requires approximately 17 Gb of disk space. This includes all software (3 Gb) and all data files (14 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 recommended 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 System 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-2018-windows.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 and DASH in a 'CSD_2018' sub-directory, and Hermes, GOLD and SuperStar in a 'GoldSuite_2018' sub-directory, and the CSD Python API in a 'Python_API_2018' sub-directory. Shortcuts to these programs will also be placed on your desktop and Start Menu (where available).

6.3 Uninstalling CSD System Software and Database files

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

Start Menu -> CCDC -> CSD System Software 2018 -> Uninstall CSD System 2018

7 Linux Installation

7.1 Installation Procedure

Linux versions of the CSD software are provided for both 32- and 64-bit versions of linux. Please ensure that you download the correct version for your version of linux.

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

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

1. Download `csds-2018-linux.tar` (32-bit) or `csds-2018-linux-x64.tar` (64-bit) 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.run
```

if installing the 32-bit version, or

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

if installing the 64-bit version.

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

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

or

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

Dependent on the version you unpacked in the previous steps.

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

7.2 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 32-bit platforms, as well as the IsoStar data files.

To install IsoStar on Linux:

1. Download the `IsoStar-2.2.5-linux-installer.run` installer file.
2. Ensure that the installer executable has execute permissions via the command:

```
chmod a+x ./IsoStar-2.2.5-linux-installer.run
```

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

```
./IsoStar-2.2.5-linux-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 system, 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-2018-osx.tar` file 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. Double click on `csds-osx` and follow the on-screen instructions to install the software and databases.

8.3 Troubleshooting

Operation of ConQuest and PreQuest on macOS requires an X server to be running in rootless mode such that X-Window applications can be successfully launched as separate windows on the console display. A suitable X11 server can be downloaded from <http://xquartz.macosforge.org>.

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 System, 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-System to your needs.

9.1 Installing the CSD data and CSD-System software separately

It is possible to install the CSD data and the CSD-System 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 System 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 install 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. This enables 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 (x86)\CCDC and /Applications/CCDC on macOS.
- **--uattendedmodeui** can take the values:
 - **none** for an unattended silent install
 - **minimal** for limited feedback
 - **minimalWithDialogs** for dialog driven feedback if possible
- **--Licensing** can take the values of:
 - **NotNow** to skip registration. Registration will need to be completed manually later
 - **RegisterAfterInstall** to attempt to register the software automatically immediately after the installation process. Will additionally require the site id, confirmation code and email to be specified (see below). This registration mode requires the machine to have access to the internet as it will contact the CCDC licensing server.
 - **SelectLicenseFile** will use a specified existing license file. Requires use of **--SelectLicenceFile** to identify the required licence file (see below)
- **--site_id <site id> --conf_code <confirmation code> --email <email>** are used to in conjunction with **--Licensing RegisterAfterInstall** to register the software during the installation process.

- **--SelectLicenceFile <license file>** is used in conjunction with **--Licensing SelectLicenceFile** to provide the location of the existing license file.
- **--enable-components** and **--disable-components** will enable and disable the installation of the data (datagroup) and the software (softwaregroup) components of the CSD-System. 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 (x86)\CCDC\CSD_2018\CSD_539"

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 (x86)".

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

- Windows
 - `csds-windows.exe --prefix "C:\Program Files (x86)\CCDC\csds2018" --mode unattended --unattendedmodeui none --Licensing RegisterAfterInstall --site_id 1234 --conf_code ABCDEF --email user@company.com`
- Linux
 - `./csds-linux-x64.run --prefix /soft/ccdc/csds2018 --mode unattended --unattendedmodeui none --Licensing RegisterAfterInstall --site_id 1234 --conf_code ABCDEF --email user@company.com`
- macOS
 - `open csds-osx.app --prefix /Applications/CCDC/csds2018 --mode unattended --unattendedmodeui none --Licensing RegisterAfterInstall --site_id 1234 --conf_code ABCDEF --email user@company.com`

or with an existing license file:

- Windows
 - `csds-windows.exe --prefix "C:\Program Files (x86)\CCDC\csds2018" --mode unattended --unattendedmodeui none --Licensing SelectLicenceFile --SelectLicenceFile "C:\my files\csd_licence.dat"`
- Linux
 - `./csds-linux-x64.run --prefix /soft/ccdc/csds2018 --mode unattended --unattendedmodeui none --Licensing SelectLicenceFile --SelectLicenceFile /home/user/csd_licence.dat`
- macOS
 - `open csds-osx.app --prefix /Applications/CCDC/csds2018 --mode unattended --unattendedmodeui none --Licensing`

```
SelectLicenceFile --SelectLicenceFile  
/home/user/csd_licence.dat
```

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.

9.6 Uninstallation using the command line

In much the same way as the installer executable, the uninstaller that is created in the CSD_2018 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 available as a separate download to the main CSD System installer and is available for 64-bit Windows, Linux and macOS systems only. Use of CSD-CrossMiner will require a CSD-Discovery or CSD-Enterprise level licence.

To install CSD-CrossMiner, download and follow the installation instructions provided with the download links from the CSDS download page on the CCDC website (https://www.ccdc.cam.ac.uk/csds_download).

11 WebCSD Access

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

`http://webcsd.ccdc.cam.ac.uk`

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 System Software

12.1 Windows

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

Programs -> CCDC -> CSD System Software 2018

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

12.2 Linux

Using a command line console, change directory to <INSTALLDIR>/CSD_2018/bin (where <INSTALLDIR> is the path to your CSD_2018 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 GoldSuite software, change directory to <INSTALLDIR>/GoldSuite_2018/bin (where <INSTALLDIR> is the path to your GoldSuite_2018 installation directory), or ensure that this is in your system PATH.

Then for Hermes, type:

```
hermes
```

For the GOLD interface in Hermes, type:

```
gold
```

12.3 macOS

To start any CSD system software component on macOS click on the appropriate icon in the Dock, or in the installation folder for ConQuest, Mercury, Mogul, IsoStar, enCIFer, Hermes 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 Ligand Overlay functionality. Access to these requires a CSD-Discovery enabled licence.

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

Hermes can also act as a client for viewing Relibase+ files. On Windows, your browser should be automatically configured by the CSD installer to open Relibase+ files. For Safari on macOS there is no helper mechanism to automatically open downloaded files with Hermes. Instead you will need to download the file, then open it in Hermes manually. On Linux, on downloading a rlbcoor or reliview file from Relibase+ ensure that you choose the Open With option and choose <INSTALLDIR>/GoldSuite_2018/bin/hermes.

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

12.4.1 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 in the examples sub-directories of each GOLD Suite product.

Tutorial 1 involves PDB entry 1ACM. This is aspartate carbamoyl transferase complexed with a phosphonated, polar peptide ligand.

To use GOLD to dock the peptide ligand into aspartate carbamoyl transferase perform the steps outlined in the GOLD documentation for Tutorial 1.

The top level of the HTML version of the documentation can be found in the docs subdirectories of each GOLD Suite product.

12.5 Registration of CSD System Components

The CSD System Installer will offer you the opportunity to register the CSD System as part of the installation process, either by accessing our online registration servers, or by entering details of an existing and valid licence file. Registration online will require your Site Code and Confirmation Code.

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

For more information about registration and licensing (see CSD System Software Licensing).

Mercury 3.10.1 and enCIFer 1.6.2 may be installed and used without requiring use of a CSD licence. Licensing Mercury will, however, allow access to additional features that are only available to CSD system users.

12.6 Configuration of CSD System Components

12.6.1 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 `as539be.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>

12.6.2 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 `mogul539.path` and will be found in the `data` subdirectory in the location where you installed the database files.

12.6.3 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 (see Registering the Different Mercury Components).

12.7 Setting up the CSD System 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_2018/bin` and `<INSTALLDIR>/GoldSuite_2018/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>; export CSDHOME`
where <INSTALLDIR> is the top level CCDC directory of your CSD System installation.

For example:

```
CSDHOME=/usr/local/CCDC/CSD_2018; export CSDHOME
```

Or

```
CSDHOME=/Applications/CCDC/CSD_2018
```

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

```
setenv CSDHOME <INSTALLDIR>
```

For example:

```
setenv CSDHOME /usr/local/CCDC/CSD_2018
```

3. To add <INSTALLDIR>/CSD_2018/bin and <INSTALLDIR>/GoldSuite_2018/bin to your PATH for Bourne shell (sh) or Korn shell (ksh), type

```
PATH=<INSTALLDIR>/CSD_2018/bin:<INSTALLDIR>/GoldSuite_2018/bin:
$PATH; export PATH
```

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

```
setenv PATH
<INSTALLDIR>/CSD_2018/bin:<INSTALLDIR>/GoldSuite_2018/bin:$PATH;
rehash
```

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

12.8 Unity desktop launchers for Ubuntu Linux

The CSD software now installs .desktop files suitable for use with the Unity desktop's launcher mechanism.

The files are installed into the CSD_2018/desktop and GoldSuite_2018/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 Unity 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 as a searchable application to launch in the Unity interface.

In order to allow the 'Open With' dialog in browsers on Ubuntu 16 to offer IsoStar or Hermes as options when viewing IsoStar scatterplots or Relibase entries, this step will be required with the isostar.desktop and hermes.desktop files respectively.

See <https://help.ubuntu.com/community/UnityLaunchersAndDesktopFiles> for more details.

13 CSD Python API

The 2018 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_2018` 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 System 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_2018\miniconda` directory and type 'python'.

13.2.2 Using the CSD Python API on Linux

Start a terminal and navigate to the `Python_API_2018` 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 2.7.12.

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_2018` 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 2.7.12.

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 Mac 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.

Please refer to the CSD Python API forum at https://www.ccdc.cam.ac.uk/forum/csd_python_api/ for details on how to obtain and install these packages.

14 CSD System Software Licensing

14.1 Licensing Overview

As more than one program requires access to the licence information, the licence file is preferentially stored in a centralised location, the directory which contains the main database files. When a product is registered the file *csd_licence.dat* is created in the CSD database directory or, if this is not possible, either a location will be requested or a *csd_licence.dat* file will be created in the home directory of the user.

When checking the licence information for a given machine, all the programs will proceed by checking one or more locations for licence data:

- If the environment variable `CCDC_CSD_LICENCE_FILE` is set to a valid filename, then this file will be checked.
- The contents of *csd_licence.redirect* in the database directory will then be examined; any line not starting with # will be checked to see if it is the name of a valid licence file that can be accessed. If any can be accessed, then these will be checked and the first one possible used.
- The file *csd_licence.dat* in the main database directory will then be checked.
- In the unlikely event that it is not possible to write to any of the possible licence file locations, some programs (Mogul or Mercury) may allow you to save and/or locate the licence data in a different location to the above. If this has been done, this location will be checked.
- If a *csd_licence.dat* file is located in the home directory of the user (/home/user on Linux /documents and /users/user on Windows 7/8 or 10), this will be checked last.

If a valid licence for the machine cannot be located, the machine will have to be licensed i.e. a component of the CSD System software will have to be registered on the machine (see Registration Overview).

The file *csd_licence.redirect* can be used in the event that the directory containing the database files is read-only, meaning it is not possible to write any licence information to the *csd_licence.dat* file. In this case, the filename(s) of one or more licence files (found in writable locations) should be added to the *csd_licence.redirect* file; these files can then be used instead of the *csd_licence.dat* file. Note that it is possible to include both Windows and Linux filenames in this file.

If any of the *csd_licence.redirect* and *csd_licence.dat* approaches do not work, the `CCDC_CSD_LICENCE_FILE` environment variable can be set to point all the applications to a different location. For example, to use a similar method to previous releases you could set `CCDC_CSD_LICENCE_FILE` to `<conquest_dir>/csd_licence.dat`.

This licensing system is particularly suitable for users with unlimited licences who can then take advantage of the IP licensing option (see IP-Based Licensing).

14.2 Registration Overview

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

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

Note: For those institutions with a site licence an IP-based licensing mechanism is available. This mechanism provides site-wide access to the CSD without the need to register individual machines (see IP-Based Licensing).

CSD System software registrations are machine specific. You must register a single CSD System component (i.e. ConQuest, Mogul, IsoStar client or Mercury) separately on each machine on which it is to be used. This results in a different Validation Number for each machine.

1. If you already have a current CSDS licence, hit the **Locate file containing valid licence** button (see Specifying an Existing Licence File).
2. Enter your Site Code and 6-digit Confirmation Code in the dialogue box shown below (the registration window shown is for ConQuest, however a similar window will appear if using Mogul or Mercury for the first time) as well as a valid email address. These codes are supplied in a communication accompanying this release (in some circumstances the Codes will already be displayed in the dialogue box):



3. Attempt to register online by hitting the **Register Online** button in the dialogue box (see Online Registration). If you access the internet via a proxy server, you can enter its details first via the proxy button.
4. If your machine is not connected to the internet or if online registration fails, you must register offline (see Offline Registration).

14.3 Specifying an Existing Licence File

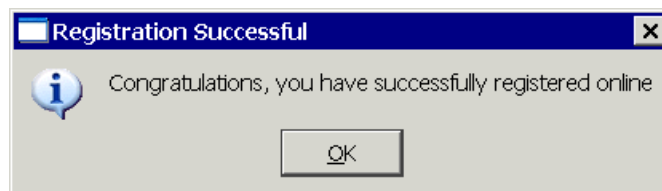
If you already have an existing *csd_licence.dat* file, hit the **Locate file containing valid licence** button at the top of the *CCDC Product Registration* dialogue. From within the resultant

Specify licence file location window, browse to the directory containing the licence file, select the *csd_licence.dat* file then hit the **Open** button.

14.4 Online Registration

To register online, hit the **Register Online** button.

If online registration is successful you will see the following dialogue box:



Note: When registering ConQuest, Mogul, or Mercury in this way it is possible to purchase additional licences online by clicking on the **Buy Additional Licences Online** button in the corresponding *Online Registration* window.

If the number of machines on which CSD System Software has been run at your site exceeds the number specified in your Licence of Access agreement, then you will be offered some or all of the following options:

- Register CSD System software on this machine as an evaluation.

This option is only available online.

- Purchase an additional CSD System software licence.

Valid provided that your basic CSD subscription does not lapse. In order to purchase additional CSD System software licences you must contact the CCDC using the phone, fax or email address displayed.

- Transfer an existing CSD System software licence from another machine.

This option is available online and enables you to reassign one of your existing CSD System software licences from another machine. This may be necessary if, for example, the original machine has been decommissioned or has suffered a system crash. The number of times that licences can be reassigned is limited so this option may not be available. If you wish to transfer a licence but you are not offered this option then please contact the CCDC using the phone, fax or email address displayed.

14.5 Offline Registration

If your machine is not connected to the internet, or if online registration fails, you must register offline. In order to do this, you will need to send the following information to the CCDC by email:

- Site Code
- Confirmation Code
- Serial Number

The Serial Number will be displayed in an extension to the original Registration dialogue box which appears after you hit the **Register Offline** button:

Locate file containing valid licence or register below.

You must register to be able to use ConQuest. This registration will also allow you to use certain other CSD Products.

Please enter your site number and confirmation code (found on your accompanying letter) and an email address, then select the '**Register Online**' button. If you are unable to register online please select '**Register Offline**' to activate the offline registration section.

We have asked for your email address to help us validate your registration and to enable us to support you in your use of this system. We may occasionally use this information to seek your feedback or to keep you updated on developments related to the CSD. Please be assured that we will not pass your details on to anyone outside the CCDC without your explicit permission at the time.

Use of this software is governed by an Agreement between the CCDC and your organisation. A copy of the standard Licence Agreement can be found [here](#) and if you have any questions, please contact admin@ccdc.cam.ac.uk

Click [here](#) for more information about licencing.

Site Number	Confirm Code	Email Address
<input type="text"/>	CC <input type="text"/>	<input type="text"/>

To **Register Offline**, please contact CCDC with the following information:

Site No: <input type="text"/>	, Confirm Code: <input type="text"/>	, Serial No: <input type="text"/>
-------------------------------	--------------------------------------	-----------------------------------

Automated Email: licence@ccdc.cam.ac.uk
Other Licence Enquiries: licence_help@ccdc.cam.ac.uk
Fax: +44 1223 336033 Phone: +44 1223 336394

After your information has been checked you will be given a **validation code**. This code should be entered below either now or next time you try to start this program.

Note that copy/paste of the validation code into any of the boxes below should work.

<input type="text"/>	-	<input type="text"/>	-	<input type="text"/>	-	<input type="text"/>	-	<input type="text"/>
<input type="text"/>	-	<input type="text"/>	-	<input type="text"/>	-	<input type="text"/>	-	<input type="text"/>

The Site Code, Confirmation Code and Serial Number can be copied and pasted from the Registration dialogue box and sent by email to: licence@ccdc.cam.ac.uk

You should automatically receive a Validation Number by return email.

To complete your registration, you must enter this Validation Number in the space provided at the bottom of the Registration dialogue box as it appears after the **Register Offline** button has been hit.

If you are unable to obtain a Validation Number by automated email then contact the CCDC with your Site Code, Confirmation Code and Serial Number using:

Email: licence_help@ccdc.cam.ac.uk
Phone: +44 1223 336408

and a Validation Number will be issued to you.

14.6 Batch registration tool

The CSD Software installation now includes a batch registration tool that can be used to attempt on-line registration via the command line. This tool can assist in registration on servers where no display is present, or in automating the registration of installations across a site.

The batch registration tool will attempt to register the current machine online and append the resultant licence to `csd_licence.dat` in your current working directory. It is therefore advised to run the tool from the main CSD database directory, where it will be automatically picked up by all users. You will require write permission to the current working directory and `csd_licence.dat` file if one already exists.

The instructions below assume the database is installed in the default location – if located elsewhere then the command line instruction will require the correct path to the `batch_register` tool.

14.6.1 Windows

From the `CSD_2018\CSD V5.39` directory run:

```
..\Mercury\batch_register.exe -current_machine -site_id XXXX -  
conf_code YYYYY -email me@domain.com -auto_accept_licence
```

14.6.2 Linux

From the `CSD_2018\csd` directory run:

```
../bin/batch_register -current_machine -site_id XXXX -conf_code YYYYY  
-email me@domain.com -auto_accept_licence
```

14.6.3 macOS

From the `CSD_2018/DATA/CSD 539` directory run:

```
../../mercury.app/Contents/MacOS/batch_register -current_machine -  
site_id XXXX -conf_code YYYYY -email me@domain.com -  
auto_accept_licence
```

14.6.4 Advanced Use of the batch registration tool

The batch registration tool may also be used in various other modes to facilitate registration on systems where online registration is not possible. For example, the tool can collect serial numbers of individual systems and store these in files in a single location. These files can then be used on a system that does have internet access to create a single licence file valid for all the systems where serial number data was collected.

To view the various options for the batch registration tool, run it with the `-help` argument. For help with batch registration please contact support@ccdc.cam.ac.uk.

14.7 Registering the Different Mercury Components

Accessing CSDS features:

- If Mercury is started before the CSD software is registered, only a base level version of Mercury will be available. A small CCDC icon will be shown against all the menu items and main-window widgets that are unavailable in this version. You will need to register Mercury to access CSDS features. Registration can be done in one of three ways:
 - Mercury will prompt you for a site code and confirm code when it is first started if ConQuest or Mogul has not already been registered.
 - A pop-up will appear if any of the registered features are selected. Follow the on-screen instructions.
 - Go to **Help, Register Mercury** and follow the instructions.

Accessing the CSD-Materials and CSD-Discovery menus:

- Licensing of the CSD-Materials functionality of Mercury is handled through the existing CSD licensing system and the *csd_licence.dat* file. To register CSD-Materials in a copy of Mercury where it is currently not activated, select the **Register CSD-Materials...** option from the *Help* menu. Registration can be completed both online and offline as described above for the CSD System.
- Licensing of the CSD-Discovery accessible components of Mercury is handled in much the same manner. To register CSD-Discovery in a copy of Mercury where it is currently not activated, select the **Register CSD-Discovery...** option from the *Help* menu.
- A CSD-Enterprise licence will allow access to both CSD-Materials and CSD-Discovery components.

The **Help, About Mercury...** menu option will display details about your current licensing status, including CSD-Materials and CSD-Discovery.

14.8 IP-Based Licensing

An IP-based licensing mechanism is available to institutions with site licences. This mechanism enables site-wide access to the CSD without the registration of individual machines.

The licensee should nominate a number of individual IP addresses, or ranges, which are authorized to access the CSD System. IP addresses should be provided in an email and sent to:

licence_help@ccdc.cam.ac.uk

The addresses provided will then be encrypted into a licence key (*csd_licence.dat*) that will allow ConQuest to operate on those machines. The *csd_licence.dat* file can either be distributed from a central location or copied to each local client installation. The *csd_licence.dat* file should be copied to the following central locations:

Linux:

```
<INSTALLDIR>/CSD_2018/csd/csd_licence.dat
```

macOS:

```
<INSTALLDIR>\CSD_2018\DATA\CSD_539\csd_licence.dat  
where <INSTALLDIR> is, e.g., \Applications\CCDC
```

Windows:

```
<INSTALLDIR>\CSD_2018\CSD_V539\csd_licence.dat  
where <INSTALLDIR> is, e.g., C:\Program Files (x86)\CCDC
```

The licensing system is particularly suitable for use with IP licensing. We will be able to provide you with IP licence data that can be stored in the central *csd_licence.dat*. The whole directory can then be set as read only for safety and every program will be able to retrieve and use the licence data.

14.9 Registration Problems

Under some circumstances ConQuest may have problems saving the registration information. This is most likely to happen when the ConQuest files are located on a different machine and mounted in such a way that the machine being registered is not able to write to the central licence file: (e.g. `<INSTALLDIR>/CSD_2018/csd/csd_licence.dat`).

If this happens ConQuest will produce a pop-up listing the Serial Number and the Validation Number for that machine. The following action should be taken in order to complete the registration procedure on this machine.

Either:

- Log into a user account on a machine which does have write access to the validation file and register ConQuest as that user.

Or:

- On a different machine that can write to the validation file, edit `csd_licence.dat` and add a line similar to the one shown below. You will need to make sure that the hyphens in the serial numbers are represented as underscores:

```
SN_1111_2222_3333_4444 = ('hostname', '1111-2222-3333-4444-5555-6666-  
7777-8888-9999')
```

Where the digits after `SN_` are the Serial Number given in the pop-up, `hostname` is the name of the machine and the final set of digits are the Validation Number given in the pop-up.

We are aware that some sites may have difficulty registering online due to the use of a local proxy server. In such cases, it is necessary to set the proxy server information via the **proxy** button on the CCDC product registration dialog prior to clicking on **Register Online**.

14.10 Current Licence Information

It is possible to look at your current licence usage and allowances via the **Help, Current Licence Information** option in ConQuest.

The resultant page is divided into 2 sections:

- Basic site information
- Licence summary and any details of individual licences used, such as serial number, validation code, registration method (including IP-address if registered online) and time of registration

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 release of the CSD System.

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

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

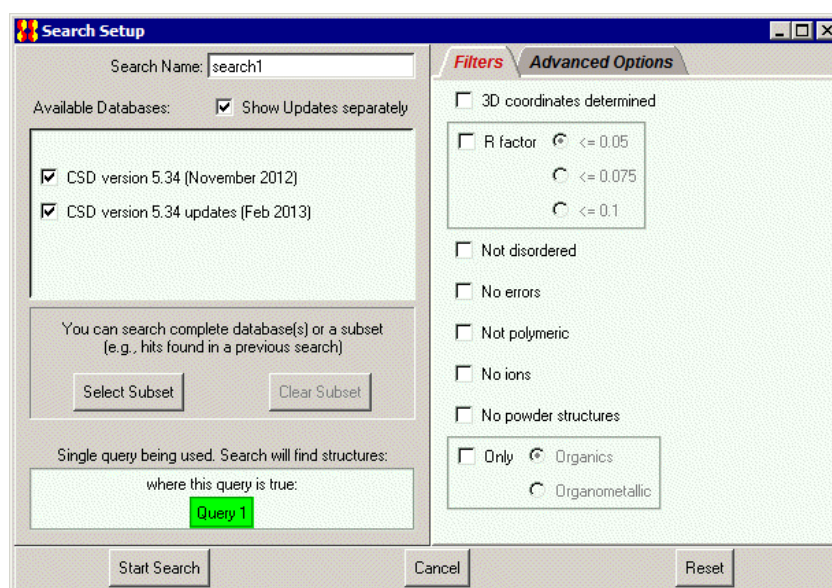
<https://www.ccdc.cam.ac.uk/support-and-resources/downloads/>

You will be required to enter your Site Code and Confirmation Code 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

ConQuest can search in-house databases in addition to the main CSD. These databases are created using the PreQuest program. 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 three in-house database files (*.ind*, *.msk* and *.tcd*) to the same directory as the CSD V5.39 database files. On Linux this is typically:

```
<INSTALLDIR>/CSD_2018/csd
```

While on Windows, this is normally:

```
C:\Program Files (x86)\CCDC\CSD_2018\CSD V539
```

And on macOS:

```
/Applications/CCDC/CSD_2018/DATA/CSD_539
```

You must then run the Activate program.

1. For Linux, ensure that `<INSTALLDIR>/CSD_2018/bin` is in your `PATH` and type:
`activate`

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

Programs -> CCDC -> CSD System Software 2018-> Activate in-house database

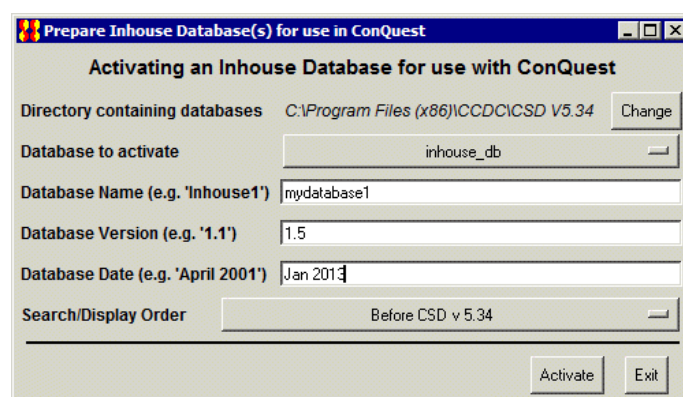
from the Windows Start menu.

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

```
/Applications/CCDC/CSD_2018/conquest.app/Contents/Resources/bin  
/activate
```

Note: Windows 7, 8 and 10 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 v5.39**, 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.

18 Classroom ConQuest

Classroom ConQuest is a version of ConQuest which has been designed for group teaching activities.

- Anyone with at least one normal ConQuest licence can install as many copies of Classroom ConQuest as they require.
- It has all the functionality of *normal* ConQuest with the limitation that searches can only be done on a subset of entries.
- The subset of entries can either be the default selection supplied with Classroom ConQuest or one derived by the user from the main CSD.

Note: Classroom ConQuest licences do not allow access to Mogul or additional functionality in Mercury.

18.1 Installing Classroom ConQuest

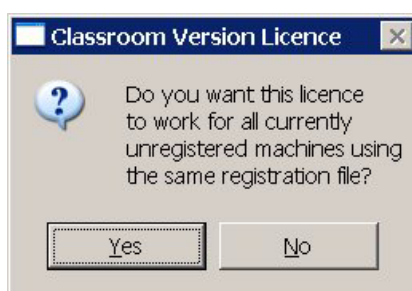
It is possible to register ConQuest as a Classroom version. In order to install Classroom ConQuest, you must first obtain a Classroom ConQuest Validation Number from the CCDC.

To obtain a Classroom ConQuest Validation Number please contact the CCDC with your Site Code and Confirmation Code using:

Email: licence_help@ccdc.cam.ac.uk
Phone: +44 1223 336394

and a Classroom ConQuest Validation Number will be issued to you.

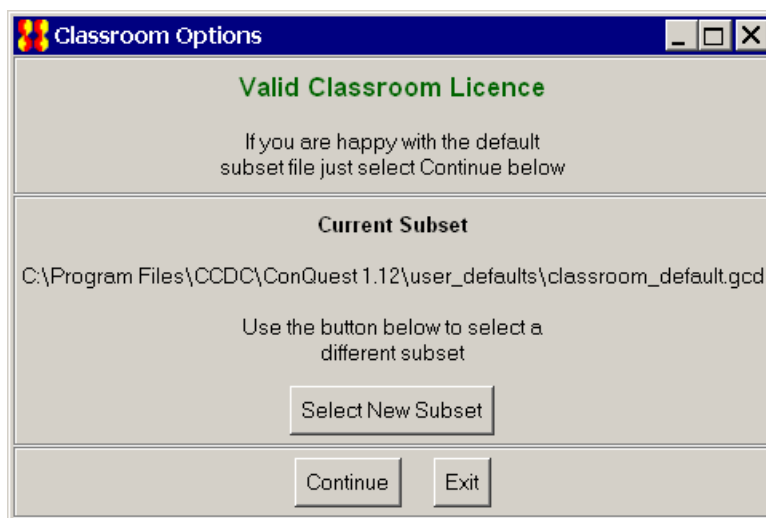
Once you have obtained your Classroom ConQuest Validation Number proceed as for a *normal* ConQuest installation up to the point of registration. At registration select **Register Offline** and enter your Classroom ConQuest Validation Number in the boxes at the bottom of the dialogue box. Provided that the number that you have entered is valid the following pop-up will appear:



- If you select **No** then the Validation Number will be linked only to the machine on which you are registering Classroom ConQuest. This is similar to standard registration procedure.
- If you select **Yes** then ConQuest will run on any machine that shares the same Validation file as the machine on which you registered. Selecting yes can be useful when you wish to install Classroom ConQuest on a cluster of machines as in this case you need only enter the Classroom ConQuest Validation Number once. This will not affect versions of ConQuest that have been registered in the normal way.

18.2 Basics of Using Classroom ConQuest

Each time a *Classroom registered* version of ConQuest is started it will produce a dialogue box similar to the following:

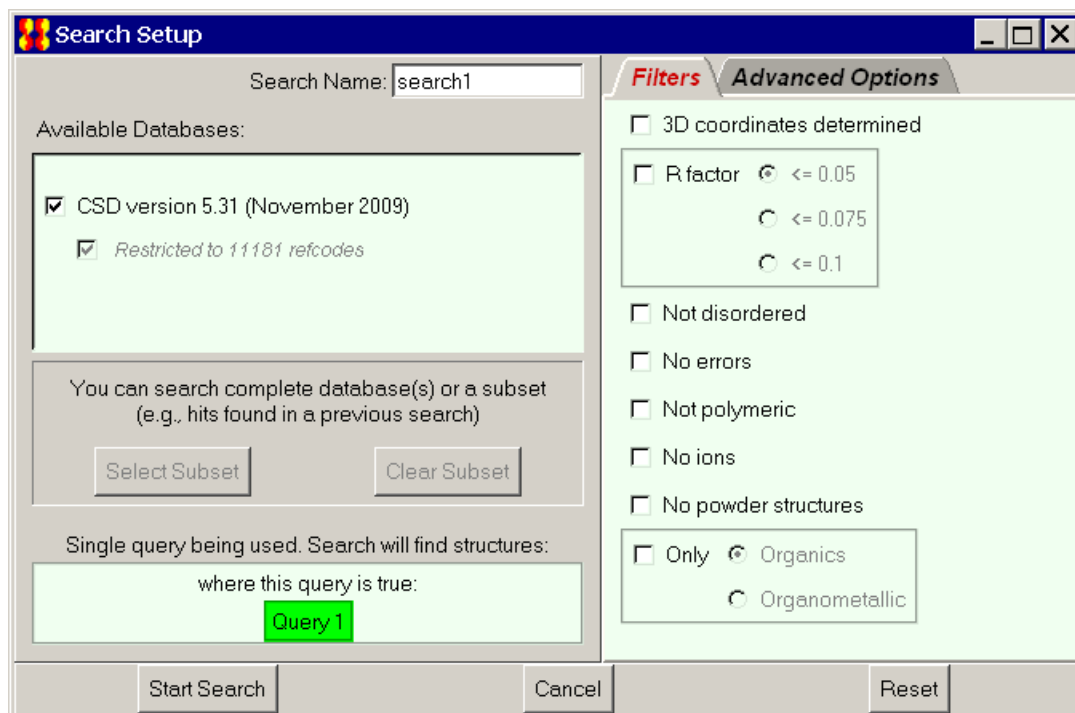


The aim of this dialogue box is to:

- Tell you if the Classroom licence has expired.
- Allow the selection of a different subset for the duration of the session (see Choosing a Subset).

Within ConQuest everything is normal except for the *Search Setup* dialogue box, which indicates that:

- Only the main CSD is available.
- Searches are restricted to a subset of refcodes (the associated check-button is disabled so that it cannot be changed).
- The **Set Subset** and **Clear Subset** buttons are inactive.



18.3 Choosing a Subset

The subset used by Classroom ConQuest is specified by a file containing a list of CSD refcodes.

The default refcode list is `classroom_default.gcd` which is located in the `user_defaults` directory.

You can elect to use a different subset of up to one fifth of the number of entries in the current version of the CSD. This can be done by:

- Replacing the default file with a new one that has the same name.
- Editing `user_defaults/conquest_options` so that the line beginning `classroom_refcode_list = ...` indicates the location of the refcode list to be used (specify the full path). For Windows use forward slashes (/) in the path instead of back slashes (\).
- Selecting a different subset using the **Select New Subset** button to select a different refcode list. This button is displayed when each Classroom ConQuest session is started (see Basics of Using Classroom ConQuest).

Although Classroom ConQuest will start if your refcode list is too big, it will issue an error message when you attempt to start a search.