

# **CSD Release and Installation Notes**

## **2019 CSD Release Update 3**

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# 1 CSD Release Package

The 2019 CSD Release Update 3 installer is supplied via download, or via USB stick, for Windows, Linux (64-bit) and macOS. The installer contains:

- The Cambridge Structural Database, Version 5.40
- ConQuest 2.0.3
- Mercury 4.2.0
- enCIFer 1.7.3
- IsoStar 2.3.3
- Mogul 1.8.3
- CSD Conformer Generator 1.3.3
- Hermes 1.10.3
- GOLD 5.7.3
- CSD Ligand Overlay 1.2.3
- SuperStar 2.2.3
- DASH 3.4.3 (Windows only)
- CSD Python API 2.3.0

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

- CSD-CrossMiner 1.5.3 (64-bit only)
- WebCSD (accessed via <https://webcsd.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, CSD Ligand Overlay, CSD-CrossMiner and Conformer Generator

## CSD-Enterprise

All of the above

## 2 Database Content and Information

- The 2019 CSD Release contains 957,868 unique structures and 973,630 entries (CSD version 5.40). In addition, in the first data update of 2019 (Feb19) there are 20,033 further unique structures and 20,809 further entries. The second data update (May19) contains 14,140 unique structures (14,702 new CSD entries). The third data update (Aug19) contains 14,139 unique structures (14,673 new CSD entries). Together this all makes a total in the CSD of 1,006,180 unique structures and 1,023,815 entries.

## 3 What's New

### The CSD Database

- The 2019 CSD Release contains 957,868 unique structures and 973,630 entries (CSD version 5.40) – an increase of more than 57,000 entries from the previous year
- Targeted enhancements have also been made to over 80,000 existing CSD entries, including:
  - Comprehensive review and enhancement of another 14,000 historical entries
  - Addition of a further 15,000 metal oxidation states, meaning the CSD now contains oxidation state information for almost 300,000 entries
  - Article DOI links added to over 8,000 more entries
- We have now completed work to revolutionise the underlying technologies in the CSD system enabling us to broaden the data available through the database. This year's release increases the number of entries with anisotropic displacement parameters (ADPs) and occupancy factors, with ADPs now available in >675,000 entries (~75% of CSD structures).

### CSD-System

- The search engine behind ConQuest has now been completely replaced by a shared, reusable C++ implementation meaning that the searching functionalities in ConQuest, Mercury, WebCSD and the CSD Python API are now fully aligned. This also enables much more flexible, dynamic and advanced searching of the CSD in the future.
- The rewriting of ConQuest's fundamental search engine means that:
  - Many complex 2D substructure searches are now much faster
  - Nearly all types of search are significantly faster than the previous version
  - Element and formula searches are more effective
  - Many text searches now give more accurate results, especially author searches which now properly handle international name conventions
- During 2018, targeted improvements were also been made to WebCSD based on user feedback including:
  - Ability to expand the 3D visualiser to full screen
  - New formula searching option
  - Additional templates for structure search
- A major new feature was added to Mercury in the 2019 CSD Release Update 1 - the polyhedral display style. This provides the ability to represent metal coordination centres as polyhedra, thus generating much more impactful graphics for metal-organic structures.
- In order to direct our software development more effectively in the future, a user opt-in product telemetry system has been added to the software portfolio in the 2019 CSD Release Update 2. This allows us to collect some basic, entirely anonymous, diagnostic data on which CSD applications and features are being used, if you would like to know more, see [CCDC Product Telemetry](#).
- The CSD Python API has also been extended to support all types of 3D query available in ConQuest.
- The Polymer Expansion functionality in Mercury has been significantly improved in the 2019 CSD Release Update 3 to provide much faster and more responsive exploration of polymeric, or networked, structures. Additional features to tailor the expansion approach and prune back the structural view have been added to make generating high impact graphics easier.

### CSD-Materials

- A new component has been introduced to CSD-Materials - the Solvate Analyser allows you to easily identify any number of unique solvents, co-formers or counter-ions and quickly visualise their packing as well as any relevant hydrogen bonds involving the solvents.
- We have also introduced three new classes to the CSD-Materials area of the CSD Python API:
  - A new class to handle and simulate crystal morphologies
  - A new class to calculate H-bond propensity predictions
  - A new class to calculate H-bond coordination predictions
- In the 2019 CSD Release Update 3, the CSD Python API has been extended to introduce a class for automated generation of molecular interaction maps (as available in the Full Interaction Maps component in Mercury)

## CSD-Discovery

- CSD-Discovery applications are now installed to a Discovery\_2019 folder, rather than the GoldSuite directory used in previous releases.
- Note that CSD-CrossMiner – an interactive and highly versatile pharmacophore query tool – is installed in a separate CSD\_CrossMiner\_1.5.0 folder. 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 and enhancements to CSD-CrossMiner to make it more memory efficient when storing large number of hits
  - Exposure of CSD-CrossMiner pharmacophoric searches in the CSD Python API
  - Ability in CSD-CrossMiner to filter down results to remove classes of hits, including filtering hits to remove or only include compounds that contain a particular substructure
  - Exposure in the CSD Python API of three different methodologies for cavity and pocket searching in proteins
- Further improvements have been made to the CSD-Discovery suite in the 2019 CSD Release Update 2. The CSD-CrossMiner database has been extended to include nucleic acid-containing structures from the PDB. The CSD Python API has also been augmented to provide better handling of proteins including:
  - Easier investigation of patterns of interactions between protein binding sites, waters, metals and small molecules
  - Understanding of geometric patterns within small molecules bound to proteins
  - Better representation of protein structures, including recognition of nucleotide structures
- Additional improvements have been made in the 2019 CSD Release Update 3 including:
  - The CSD Python API has been improved to provide much faster substructure searching across CSD and PDB data with a speed-up of between 30x and 200x
  - GOLD has been improved for high-throughput docking to provide simplified output for faster running on many platforms and easier results analysis
  - Further extension of the CSD Python API to introduce a class for automated generation of molecular interaction maps (as available in SuperStar)



## 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 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-System that use Python (specifically ConQuest, Mogul’s sketcher and the API script interface in Mercury and Hermes). 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'
```

For API scripts, we would recommend use of a Python 3 install of the API if you encounter this issue, as Python 3 has better support for non-ascii characters.

- **Use of the Aromatics Analyser component in Mercury on older platforms:**  
The Aromatics Analyser component in Mercury (available to Research Partners and CFC members) is not supported on RedHat Enterprise 6, CentOS 6 or Windows 32-bit operating systems due to the underlying machine learning libraries that this component is built on.
- **Use of the ‘View diagrams’ option in the ‘Results and analysis’ tab in Mogul results in a diagram that cannot be dismissed:**  
The ‘View diagrams’ button in the ‘Research and analysis’ tab of Mogul can cause a Diagram to be displayed incorrectly on Windows & Linux systems, whereby the diagram cannot be closed and overlays the Mogul interface permanently. Currently the only solution is to close and restart Mogul.

## 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](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 macOS Installation) and registering the software.
3. Install the IsoStar 2.3 server (Linux) (see IsoStar 2.3 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 and 10
- Linux - Intel compatible, 64-bit:
  - RedHat Enterprise 6 and 7
  - CentOS 6 and 7
  - Ubuntu 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 10.12, 10.13 and 10.14

If you choose to use a version other than those listed above we cannot guarantee that the 2019 CSD Release Update 3 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

As detailed with the 2018 CSDS Update 3 release, 32-bit linux executables are no longer available. With this and all future releases all linux executables will be 64-bit only and will not be compatible with 32-bit linux operating systems.

We also anticipate that the 2020 CSD Release will remove official support for 32-bit Windows systems. Note that this withdrawal of support does not necessarily mean that our future software releases will not work on 32-bit Windows operating systems, but that we cannot guarantee they will be able to do so from the 2020 release onwards. At this point

some or all of the CSD Release software will start to require a 64-bit Windows operating system.

The `cqbatch` and `mogulbatch` command line utilities will be deprecated from the 2020 release onwards. While these will still remain a part of the CSD System software during 2020, their use will no longer be recommended and we would instead encourage switching to use of the CSD Python API. We anticipate that `cqbatch` will be removed entirely in the 2021 release.

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

### 5.2.3 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.

### 5.2.4 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](mailto: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.

### 5.2.5 Disk Space Requirements

A complete installation of the 2019 CSD Release Update 3 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-2019-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\_2019' sub-directory, and Hermes, GOLD and SuperStar in a 'Discovery\_2019' sub-directory, and the CSD Python API in a 'Python\_API\_2019' 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 2019 -> Uninstall CSD System 2019

## 7 Linux Installation

### 7.1 Installation Procedure

Linux versions of the CSD software are provided for only 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 or `csds-2019-linux-x64.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 System, type:  

```
./csds-linux-x64.run
```
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 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 System, 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 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-2019-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\_2019\CSD\_540"

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\csds2019" --mode unattended --unattendedmodeui none --Licensing RegisterAfterInstall --site_id 1234 --conf_code ABCDEF --email user@company.com`
- Linux
  - `./csds-linux-x64.run --prefix /soft/ccdc/csds2019 --mode unattended --unattendedmodeui none --Licensing RegisterAfterInstall --site_id 1234 --conf_code ABCDEF --email user@company.com`
- macOS
  - `open csds-osx.app --prefix /Applications/CCDC/csds2019 --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\csds2019" --mode unattended --unattendedmodeui none --Licensing SelectLicenceFile --SelectLicenceFile "C:\my files\csd_licence.dat"`
- Linux
  - `./csds-linux-x64.run --prefix /soft/ccdc/csds2019 --mode unattended --unattendedmodeui none --Licensing SelectLicenceFile --SelectLicenceFile /home/user/csd_licence.dat`
- macOS
  - `open csds-osx.app --prefix /Applications/CCDC/csds2019 --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](mailto: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_540"
```

## 9.6 Uninstallation using the command line

In much the same way as the installer executable, the uninstaller that is created in the CSD\_2019 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](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](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 2019

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\_2019/bin (where <INSTALLDIR> is the path to your CSD\_2019 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\_2019/bin (where <INSTALLDIR> is the path to your Discovery\_2019 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 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.

### 12.4.1 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 and enCIFer 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 `as540be.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 `mogul540.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_2019/bin` and `<INSTALLDIR>/Discovery_2019/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_2019; export CSDHOME`  
where `<INSTALLDIR>` is the top level CCDC directory of your CSD System installation.

For example:

```
CSDHOME=/usr/local/CCDC/CSD_2019; export CSDHOME
```

Or

```
CSDHOME=/Applications/CCDC/CSD_2019
```

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

```
setenv CSDHOME <INSTALLDIR>/CSD_2019
```

For example:

```
setenv CSDHOME /usr/local/CCDC/CSD_2019
```

3. To add <INSTALLDIR>/CSD\_2019/bin and <INSTALLDIR>/Discovery\_2019/bin to your PATH for Bourne shell (sh) or Korn shell (ksh), type

```
PATH=<INSTALLDIR>/CSD_2019/bin:<INSTALLDIR>/Discovery_2019/bin:
$PATH; export PATH
```

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

```
setenv PATH
<INSTALLDIR>/CSD_2019/bin:<INSTALLDIR>/Discovery_2019/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\_2019/desktop and Discovery\_2019/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 mol2 files, 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 2019 CSD Release Update 2 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_2019` 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_2019\miniconda` directory and type 'python'.

#### 13.2.2 Using the CSD Python API on Linux

Start a terminal and navigate to the `Python_API_2019` 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 2.7.15.

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_2019` 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 2.7.15.

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.

Please refer to the CSD Python API forum at [https://www.ccdc.cam.ac.uk/forum/csd\\_python\\_api/](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 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):

CCDC Product Registration

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](mailto: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"/>

Register Online Register Offline Proxy Abort

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

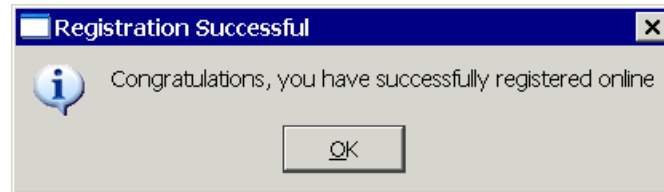
If you already have an existing *csd\_licence.dat* file, hit the **Locate file containing valid licence** button at the top of the *CCDC Product Registration* dialogue. From within the resultant

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](mailto: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:	, Confirm Code:	, Serial No:
----------	-----------------	--------------

Automated Email: [licence@ccdc.cam.ac.uk](mailto:licence@ccdc.cam.ac.uk)  
Other Licence Enquiries: [licence\\_help@ccdc.cam.ac.uk](mailto: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](mailto: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_2019\CSD V5.40` 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_2019\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_2019/DATA/CSD 540` 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](mailto: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\_2019/csd/csd\_licence.dat

### macOS:



```
<INSTALLDIR>\CSD_2019\DATA\CSD_540\csd_licence.dat  
where <INSTALLDIR> is, e.g., \Applications\CCDC
```

## Windows:

```
<INSTALLDIR>\CSD_2019\CSD V540\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_2019/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 either Mercury or Hermes. Specific updates for the CSD-CrossMiner installation, if you have one installed, can be obtained automatically via the equivalent option within CSD-CrossMiner.

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

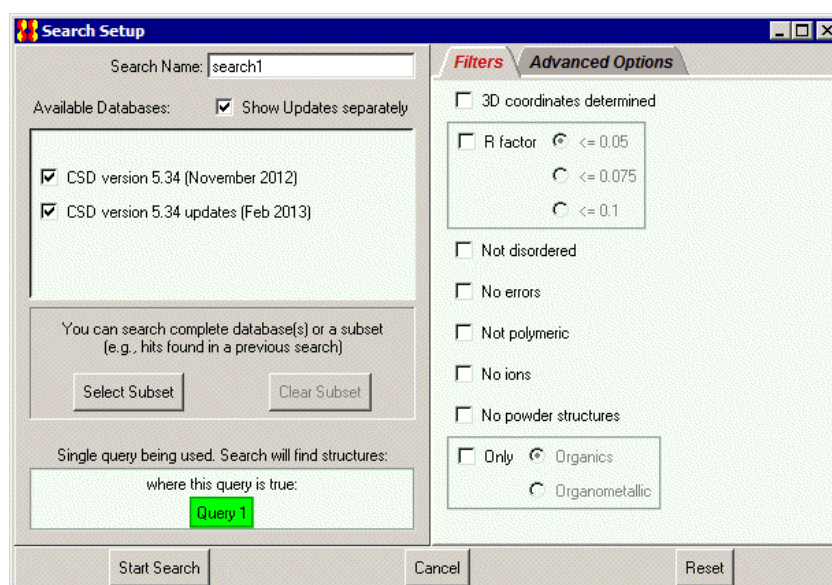
<https://www.ccdc.cam.ac.uk/support-and-resources/downloads/>

You will be required to enter your 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

With the 2019 release, ConQuest and the other CSD-System 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 V5.40 database files. On Linux this is typically:

```
<INSTALLDIR>/CSD_2019/csd
```

While on Windows, this is normally:

```
C:\Program Files (x86)\CCDC\CSD_2019\CSD_540
```

And on macOS:

```
/Applications/CCDC/CSD_2019/DATA/CSD_540
```

You must then run the Activate program.

1. For Linux, ensure that `<INSTALLDIR>/CSD_2019/bin` is in your `PATH` and type:  
`activate`

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

```
Programs -> CCDC -> CSD System Software 2019-> Activate in-house database
```

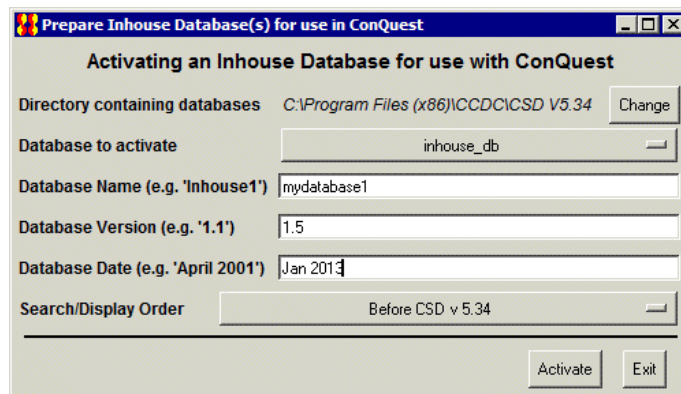
from the Windows Start menu.

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

```
/Applications/CCDC/CSD_2019/conquest.app/Contents/Resources/bin  
/activate
```

**Note:** Windows 7 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 v5.40**, 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
  - $\leq 0.05$
  - $\leq 0.075$
  - $\leq 0.1$
- Not disordered
- No errors
- Not polymeric
- No ions
- No powder structures
- Only
  - Organics
  - Organometallic