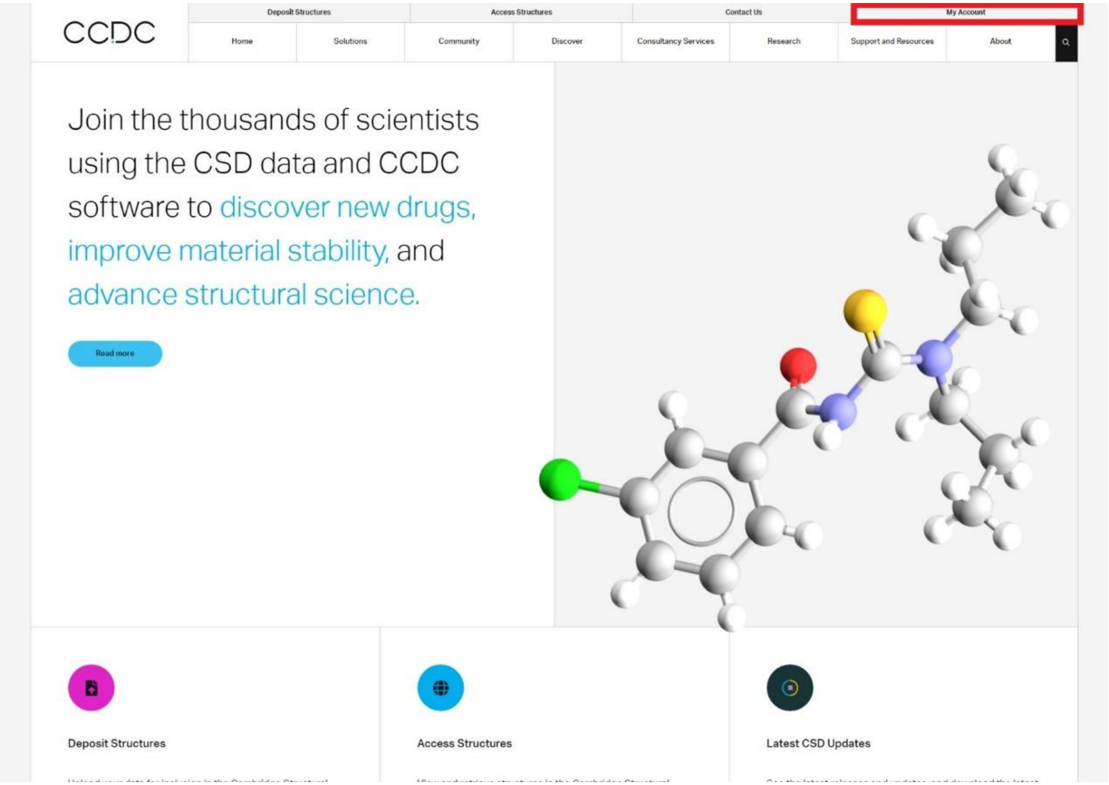
1.打开 CCDC 官网：https://www.ccdc.cam.ac.uk/

2.注册并登录 CCDC 账户



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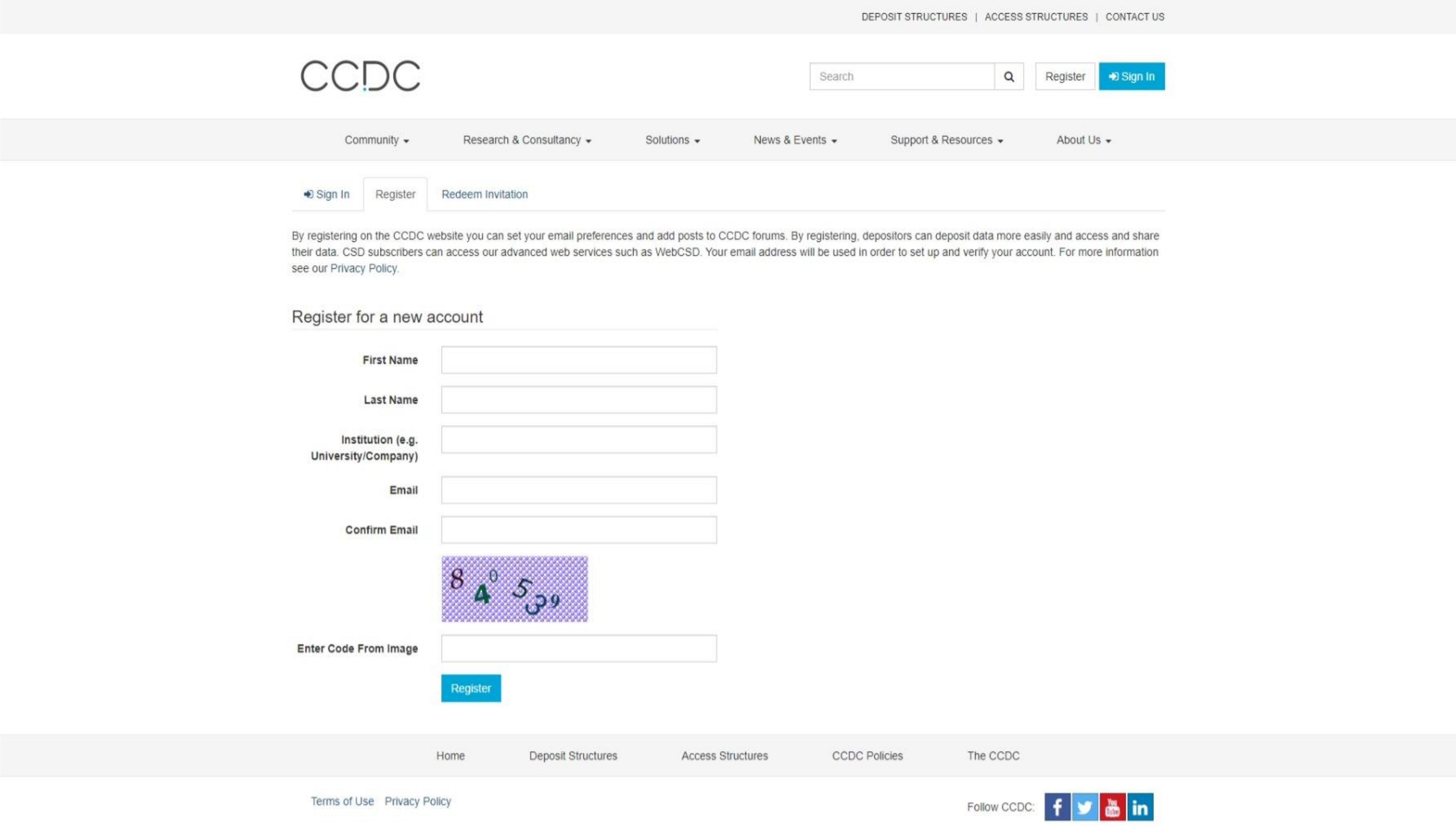
Latest CSD Updates

Join the thousands of scientists using the CSD data and CCDC software to discover new drugs, improve material stability, and advance structural science.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Sign In
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Redeem Invitation

By registering on the CCDC website you can set your email preferences and add posts to CCDC forums. By registering, depositors can deposit data more easily and access and share their data. CSD subscribers can access our advanced web services such as WebCSD. Your email address will be used in order to set up and verify your account. For more information see our Privacy Policy.

Register for a new account

First Name
Last Name
Institution (e.g. University/Company)
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Enter Code From Image

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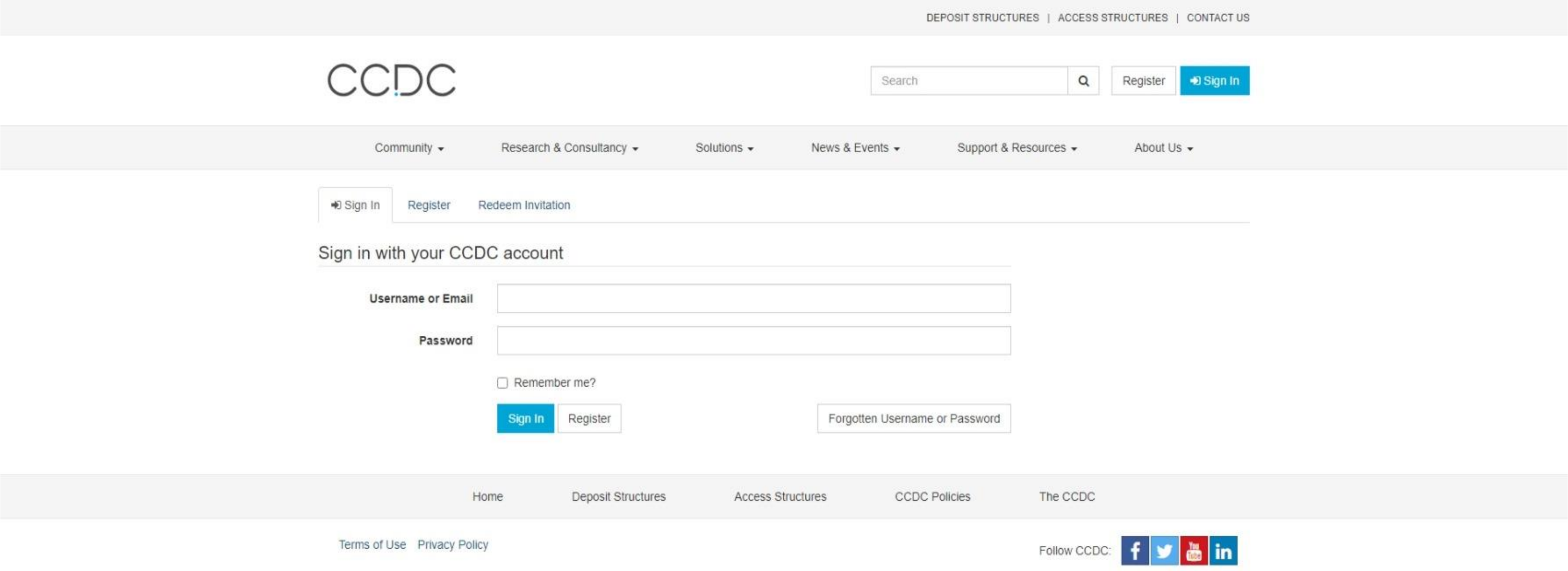
3. 完成注册，登录账户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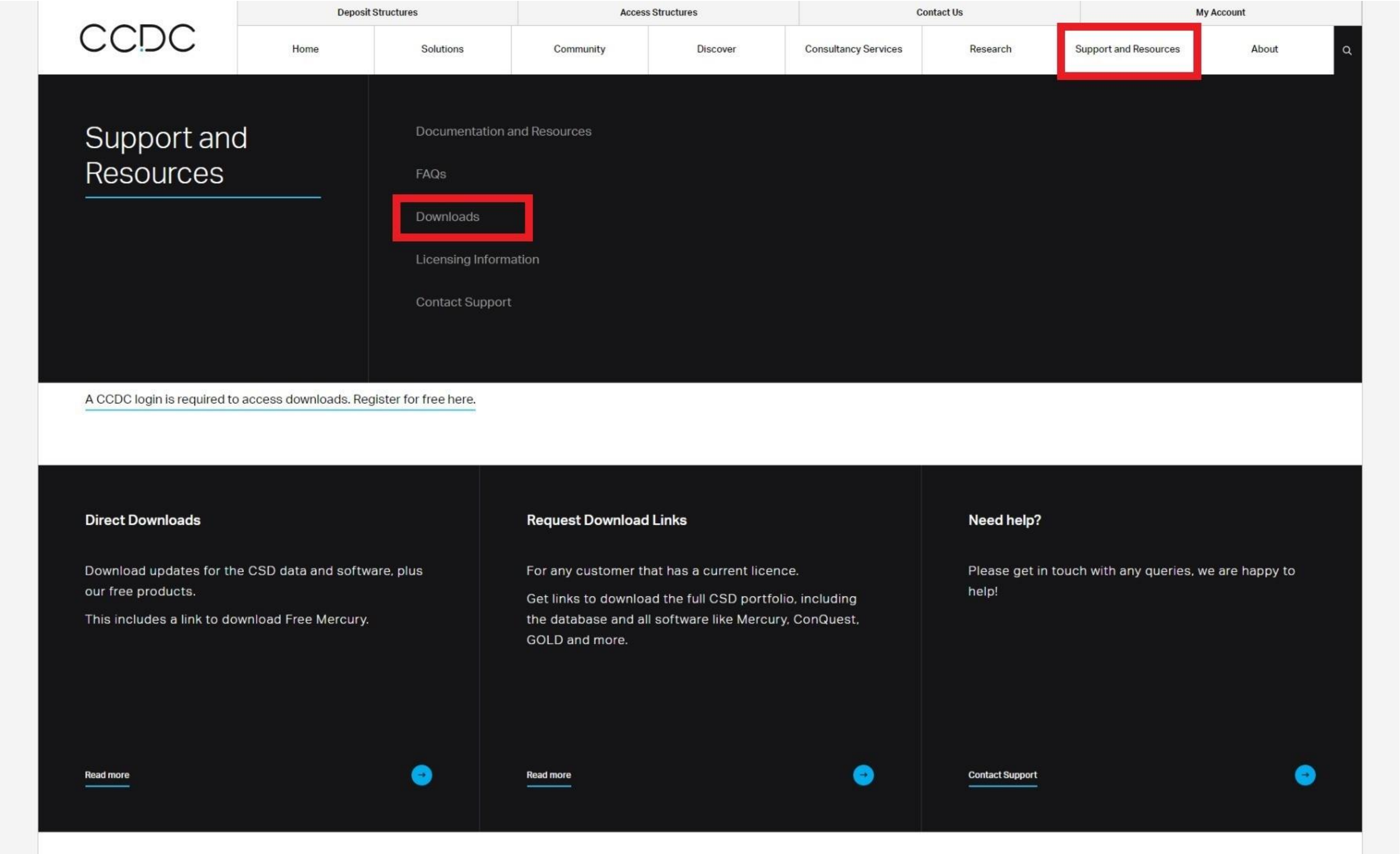
4. 登录成功，下载 CSD 客户端软件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A CCDC login is required to access downloads. Register for free here.

Direct Downloads

Download updates for the CSD data and software, plus our free products.

This includes a link to download Free Mercury.

Read more

Request Download Links

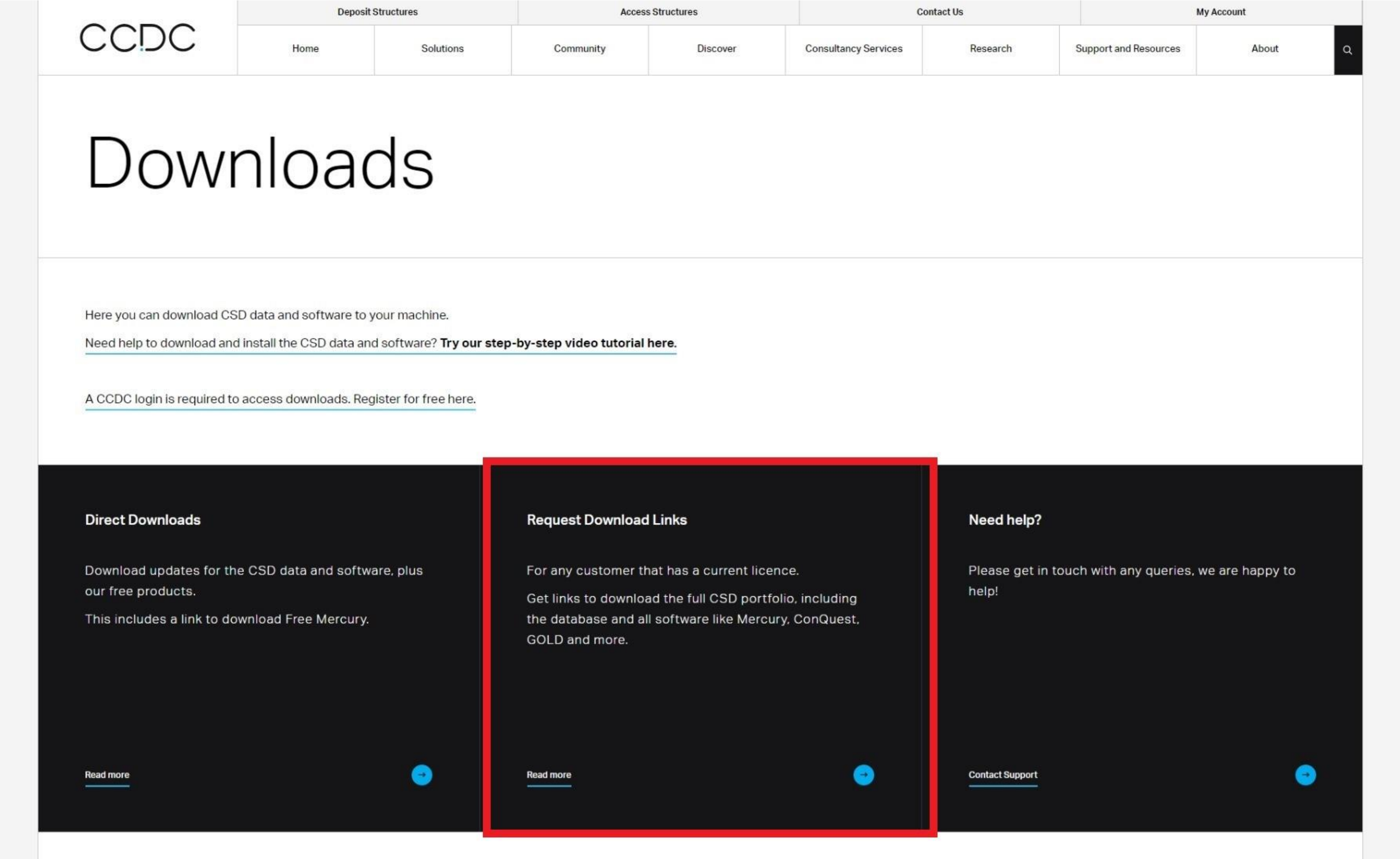
For any customer that has a current licence.

Get links to download the full CSD portfolio, including the database and all software like Mercury, ConQuest, GOLD and more.

Need help?

Please get in touch with any queries, we are happy to help!

Contact Support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Downloads

Here you can download CSD data and software to your machine.

Need help to download and install the CSD data and software? **Try our step-by-step video tutorial here**.

A CCDC login is required to access downloads. Register for free here.

Direct Downloads

Download updates for the CSD data and software, plus our free products.

This includes a link to download Free Mercury.

Read more

Request Download Links

For any customer that has a current licence.

Get links to download the full CSD portfolio, including the database and all software like Mercury, ConQuest, GOLD and more.

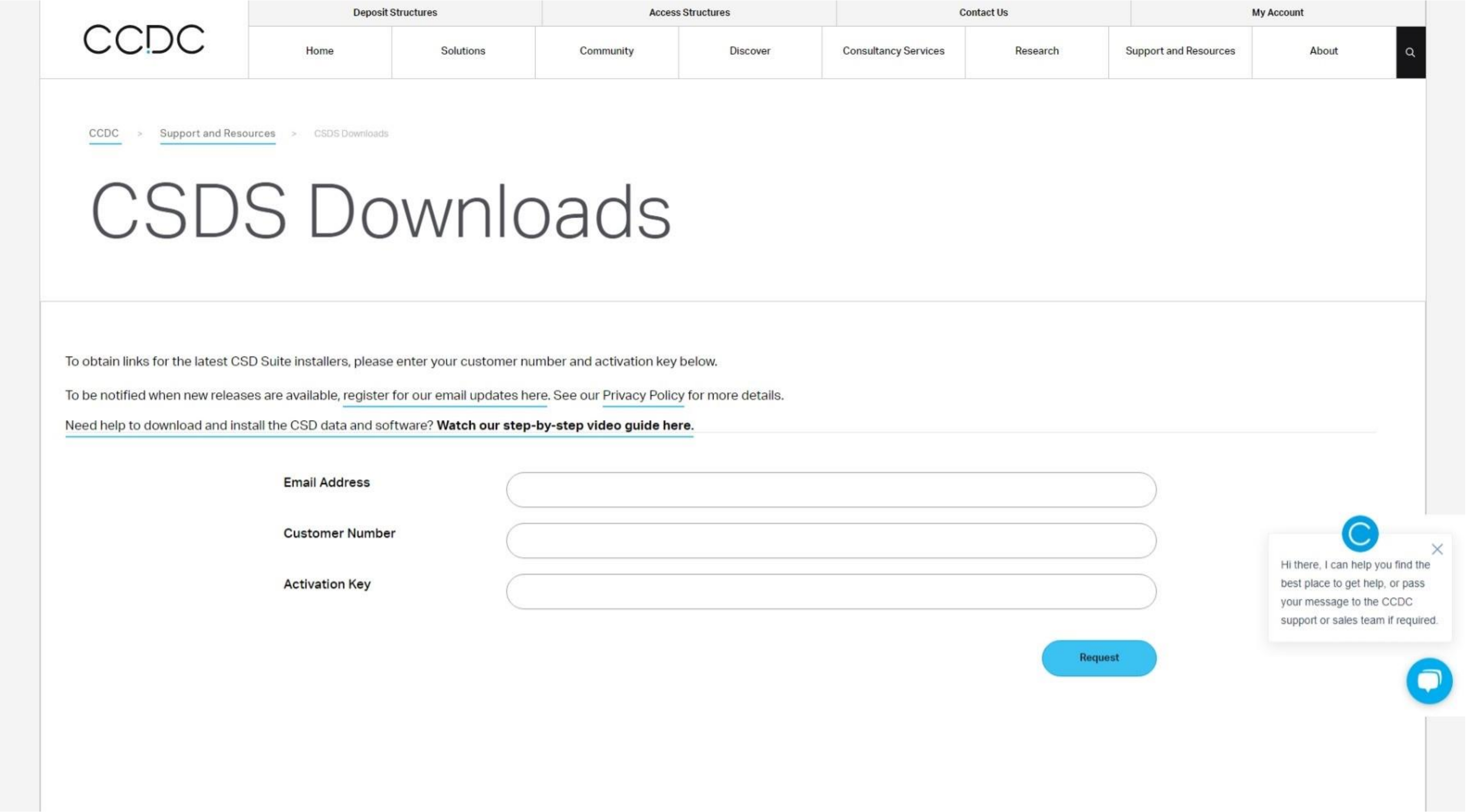
Read more

Need help?

Please get in touch with any queries, we are happy to help!

Contact Support

5.输入注册账户的邮箱以及 Customer Number & Activation Key(即为 licences)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CCDC > Support and Resources > CSDS Downloads

CSDS Downloads

To obtain links for the latest CSD Suite installers, please enter your customer number and activation key below.

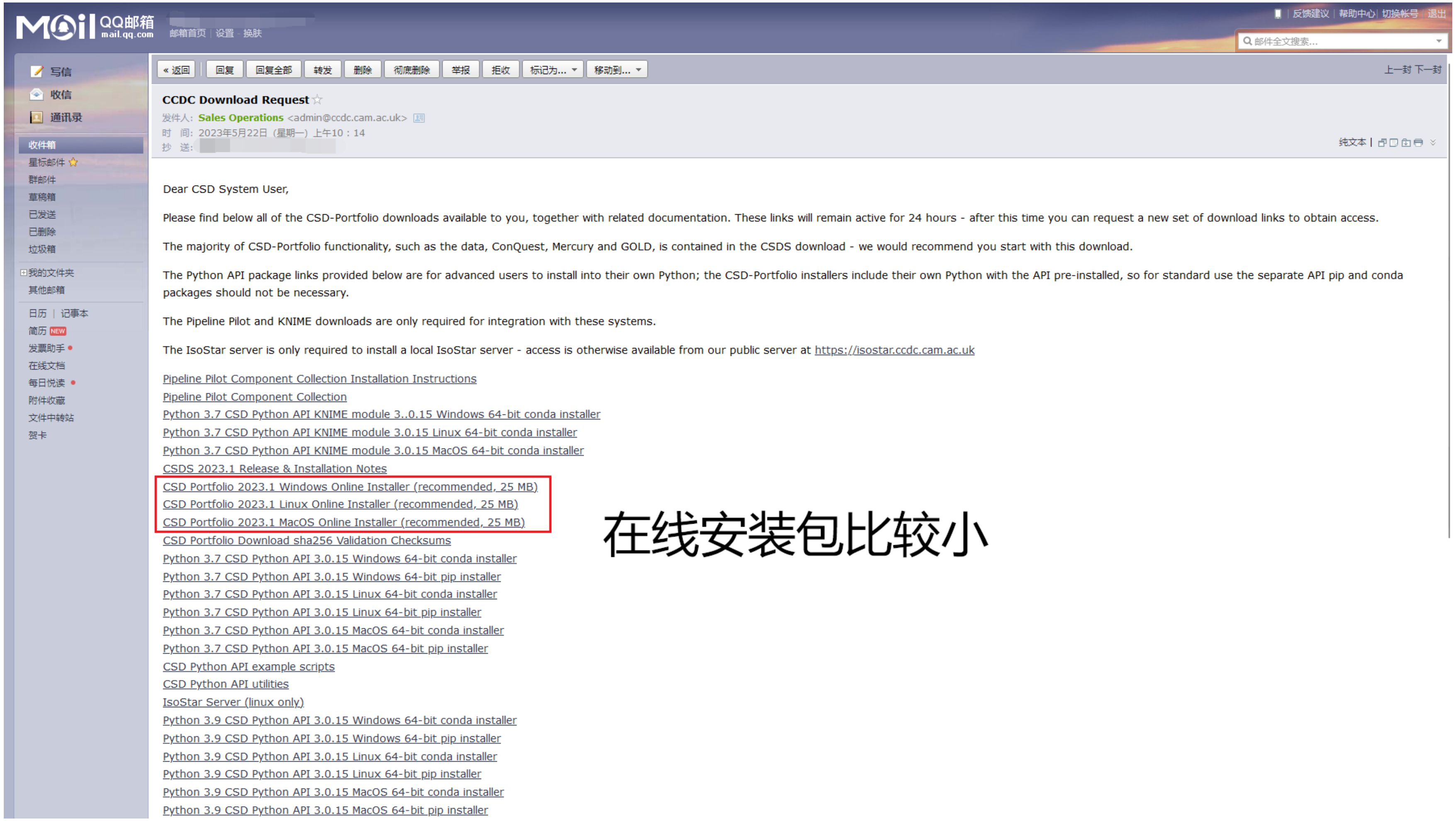
To be notified when new releases are available, register for our email updates here. See our Privacy Policy for more details.

Need help to download and install the CSD data and software? **Watch our step-by-step video guide here.**

Email Address
Customer Number
Activation Key
Request

Hi there, I can help you find the best place to get help, or pass your message to the CCDC support or sales team if required.

6. 注册邮箱会收到下载链接，点击所需的版本完成下载(链接只有 24 小时有效，请及时下载)



CCDC Download Request

发件人: **Sales Operations** <admin@ccdc.cam.ac.uk>
时　间: 2023年5月22日（星期一）上午10：14
抄　送: [redacted]

Dear CSD System User,

Please find below all of the CSD-Portfolio downloads available to you, together with related documentation. These links will remain active for 24 hours - after this time you can request a new set of download links to obtain access.

The majority of CSD-Portfolio functionality, such as the data, ConQuest, Mercury and GOLD, is contained in the CSDS download - we would recommend you start with this download.

The Python API package links provided below are for advanced users to install into their own Python; the CSD-Portfolio installers include their own Python with the API pre-installed, so for standard use the separate API pip and conda packages should not be necessary.

The Pipeline Pilot and KNIME downloads are only required for integration with these systems.

The IsoStar server is only required to install a local IsoStar server - access is otherwise available from our public server at https://isostar.ccdc.cam.ac.uk

Pipeline Pilot Component Collection Installation Instructions
Pipeline Pilot Component Collection
Python 3.7 CSD Python API KNIME module 3..0.15 Windows 64-bit conda installer
Python 3.7 CSD Python API KNIME module 3.0.15 Linux 64-bit conda installer
Python 3.7 CSD Python API KNIME module 3.0.15 MacOS 64-bit conda installer
CSDS 2023.1 Release & Installation Notes
CSD Portfolio 2023.1 Windows Online Installer (recommended, 25 MB)
CSD Portfolio 2023.1 Linux Online Installer (recommended, 25 MB)
CSD Portfolio 2023.1 MacOS Online Installer (recommended, 25 MB)
CSD Portfolio Download sha256 Validation Checksums
Python 3.7 CSD Python API 3.0.15 Windows 64-bit conda installer
Python 3.7 CSD Python API 3.0.15 Windows 64-bit pip installer
Python 3.7 CSD Python API 3.0.15 Linux 64-bit conda installer
Python 3.7 CSD Python API 3.0.15 Linux 64-bit pip installer
Python 3.7 CSD Python API 3.0.15 MacOS 64-bit conda installer
Python 3.7 CSD Python API 3.0.15 MacOS 64-bit pip installer
CSD Python API example scripts
CSD Python API utilities
IsoStar Server (linux only)
Python 3.9 CSD Python API 3.0.15 Windows 64-bit conda installer
Python 3.9 CSD Python API 3.0.15 Windows 64-bit pip installer
Python 3.9 CSD Python API 3.0.15 Linux 64-bit conda installer
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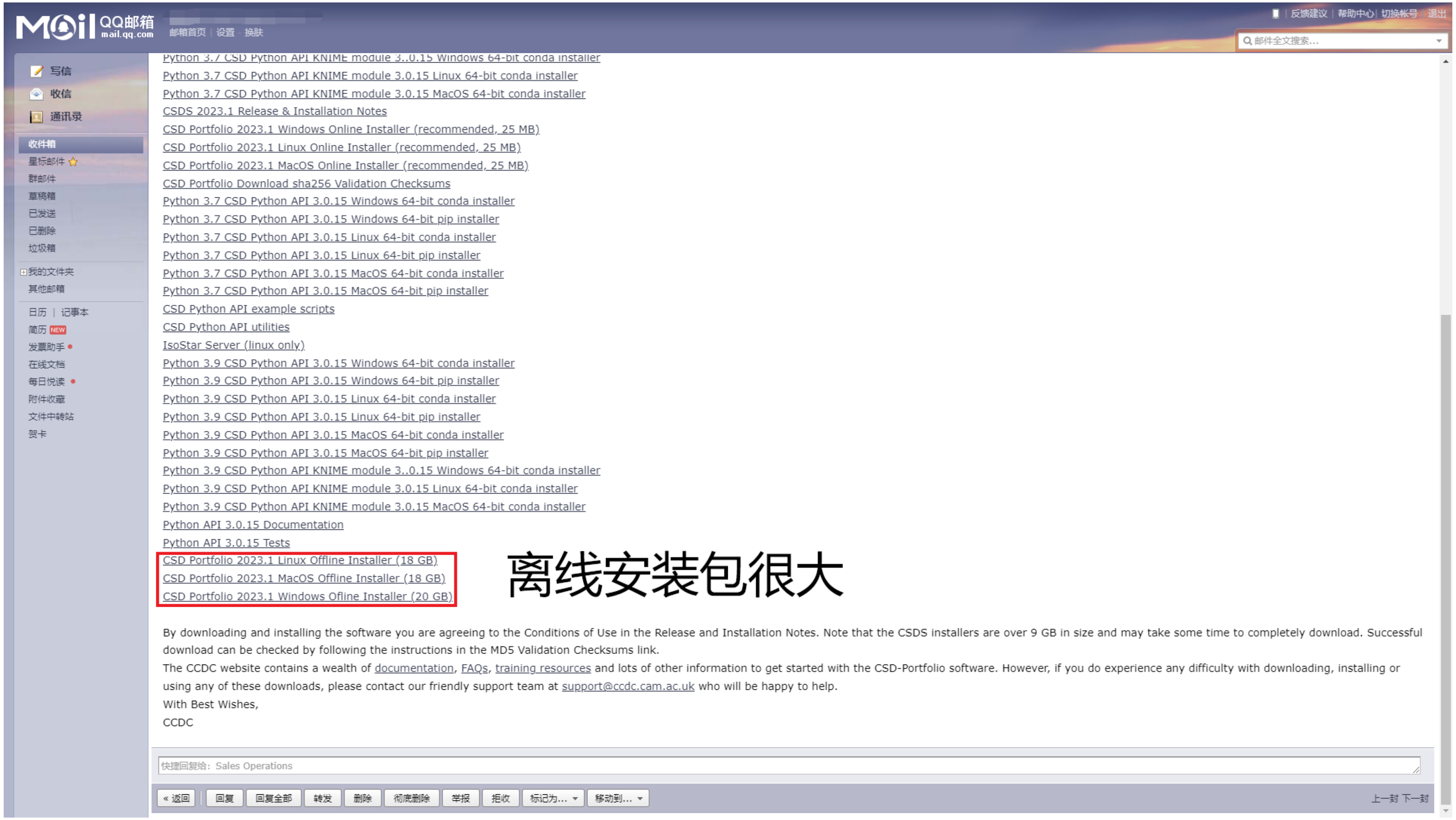
Python 3.9 CSD Python API 3.0.15 MacOS 64-bit conda installer
Python 3.9 CSD Python API 3.0.15 MacOS 64-bit pip installer

在线安装包比较小



Python 3.7 CSD Python API KNIME module 3..0.15 Windows 64-bit conda installer
Python 3.7 CSD Python API KNIME module 3.0.15 Linux 64-bit conda installer
Python 3.7 CSD Python API KNIME module 3.0.15 MacOS 64-bit conda installer
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Python 3.7 CSD Python API 3.0.15 Linux 64-bit pip installer
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Python 3.9 CSD Python API KNIME module 3..0.15 Windows 64-bit conda installer
Python 3.9 CSD Python API KNIME module 3.0.15 Linux 64-bit conda installer
Python 3.9 CSD Python API KNIME module 3.0.15 MacOS 64-bit conda installer
Python API 3.0.15 Documentation
Python API 3.0.15 Tests
CSD Portfolio 2023.1 Linux Offline Installer (18 GB)
CSD Portfolio 2023.1 MacOS Offline Installer (18 GB)
CSD Portfolio 2023.1 Windows Offline Installer (20 GB)

离线安装包很大

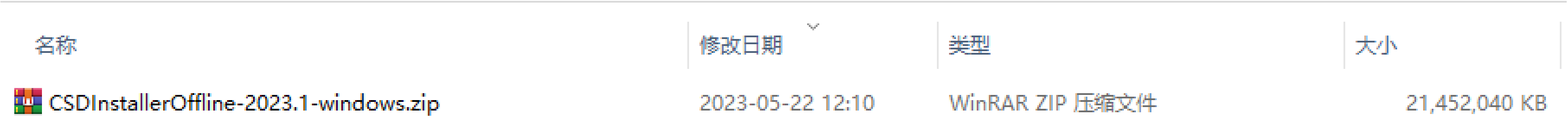
By downloading and installing the software you are agreeing to the Conditions of Use in the Release and Installation Notes. Note that the CSDS installers are over 9 GB in size and may take some time to completely download. Successful download can be checked by following the instructions in the MD5 Validation Checksums link.

The CCDC website contains a wealth of documentation, FAQs, training resources and lots of other information to get started with the CSD-Portfolio software. However, if you do experience any difficulty with downloading, installing or using any of these downloads, please contact our friendly support team at support@ccdc.cam.ac.uk who will be happy to help.

With Best Wishes,
CCDC

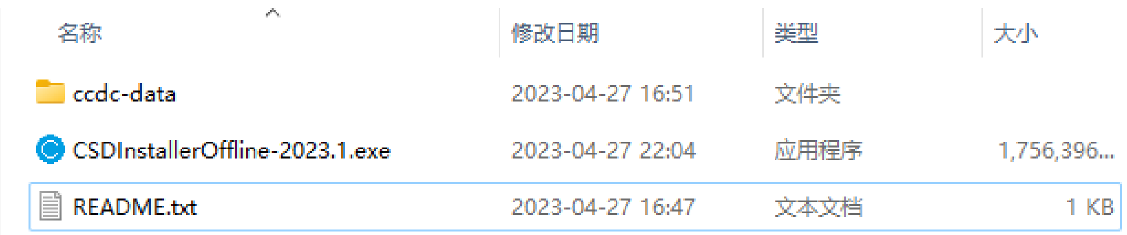
推荐下载离线安装包

7. 完成下载，离线包大约 20GB

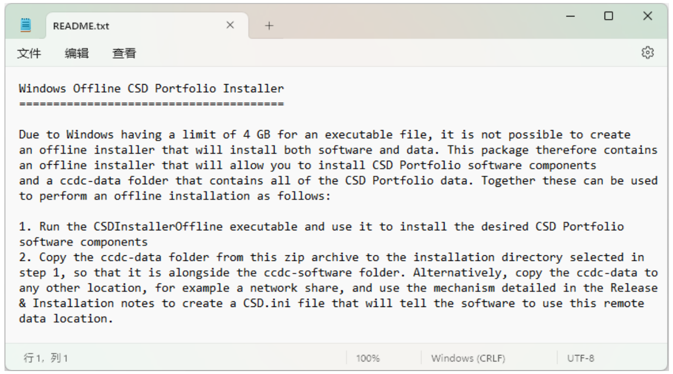


名称	修改日期	类型	大小
CSDInstallerOffline-2023.1-windows.zip	2023-05-22 12:10	WinRAR ZIP 压缩文件	21,452,040 KB

解压后打开文件夹，选择 Readme 先进行安装前阅读



名称	修改日期	类型	大小
ccdc-data	2023-04-27 16:51	文件夹	
CSDInstallerOffline-2023.1.exe	2023-04-27 22:04	应用程序	1,756,396...
README.txt	2023-04-27 16:47	文本文档	1 KB



```
Windows Offline CSD Portfolio Installer
=======================================

Due to Windows having a limit of 4 GB for an executable file, it is not possible to create
an offline installer that will install both software and data. This package therefore contains
an offline installer that will allow you to install CSD Portfolio software components
and a ccdc-data folder that contains all of the CSD Portfolio data. Together these can be used
to perform an offline installation as follows:

1. Run the CSDInstallerOffline executable and use it to install the desired CSD Portfolio
software components
2. Copy the ccdc-data folder from this zip archive to the installation directory selected in
step 1, so that it is alongside the ccdc-software folder. Alternatively, copy the ccdc-data to
any other location, for example a network share, and use the mechanism detailed in the Release
& Installation notes to create a CSD.ini file that will tell the software to use this remote
data location.
```

由于 Windows 的可执行文件限制为 4 GB，因此无法创建将同时安装软件和数据的脱机安装程序。因此，此软件包包含一个脱机安装程序，允许您安装 CSD Portfolio 软件组件和一个 ccdc-data 文件夹，其中包含所有 CSD Portfolio 数据。这些一起可用于执行脱机安装，如下所示：

1. 运行 CSD Installer Offline 可执行文件并使用它安装所需的 CSD Portfolio 软件组件
2. 将此 zip 归档文件中的 ccdc-data 文件夹复制到步骤 1 中选择的安装目录中，使其位于 ccdc-software 文件夹旁边。或者，将 ccdc-data 复制到任何其他位置（例如网络共享），并使用 Release & Installation 注解中详细介绍的机制创建 CSD. ini 文件，该文件将告诉软件使用此远程数据位置。

运行系统要求：

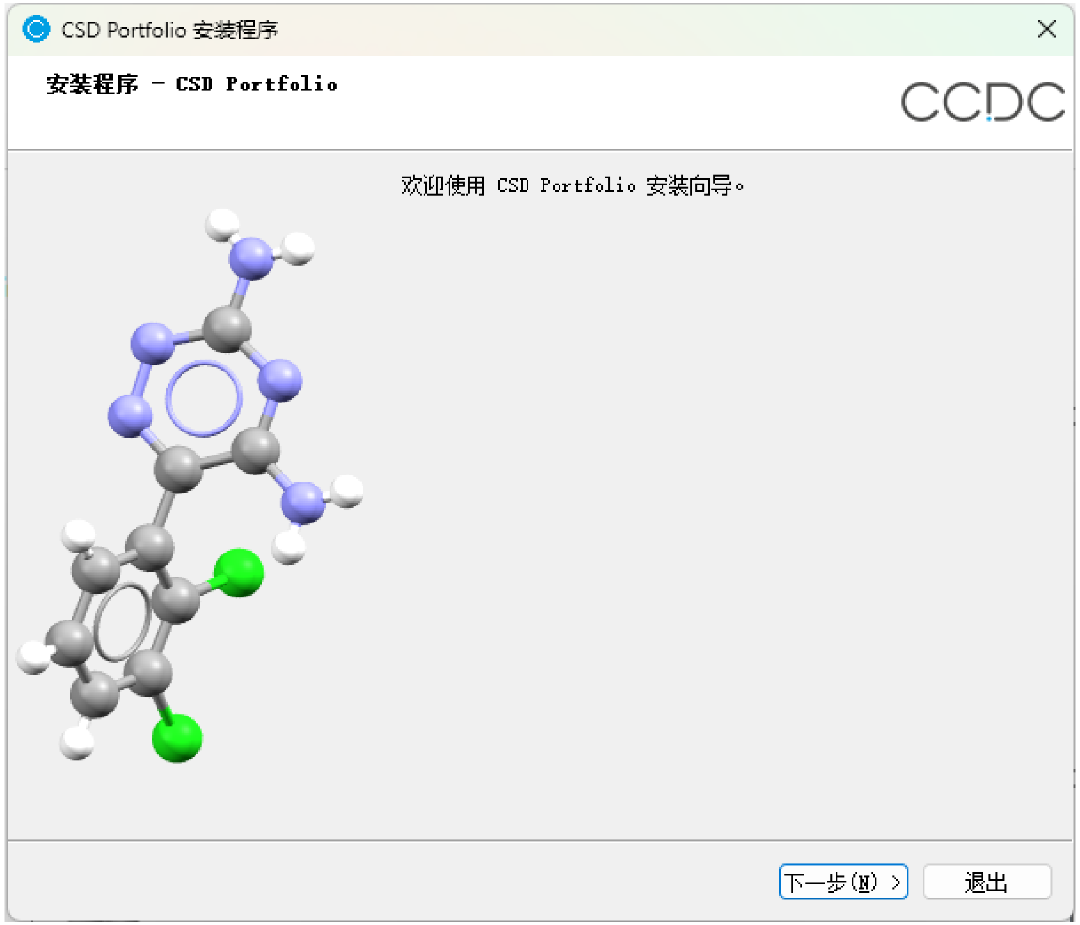
- Windows - Intel compatible, 64-bit:
    - Windows 10 and 11
- Linux - Intel compatible, 64-bit:
    - RedHat Enterprise 7.6 or higher, and 8
    - CentOS 7.6 or higher
    - CentOS Stream 8
    - Ubuntu LTS 20 and 22
- macOS - Intel compatible or Apple ARM (via Rosetta 2 emulation)*, 64-bit:
    - macOS 11, 12 and 13

- Disk Space:
    - A complete install requires 37GB (7GB software, 30GB data)

  - Approximately 50GB free disk space will be required during installation to allow for the cache
  - By default the software will be installed in your home directory - if you have a quota you will probably need to install it elsewhere and change the location of the cache too
- Minimum recommended RAM: 8 GB
  - Minimum recommended RAM for use of CSD-CrossMiner: 32 GB
- Graphics card and drivers that support OpenGL version 2 (see this support database entry for more details)

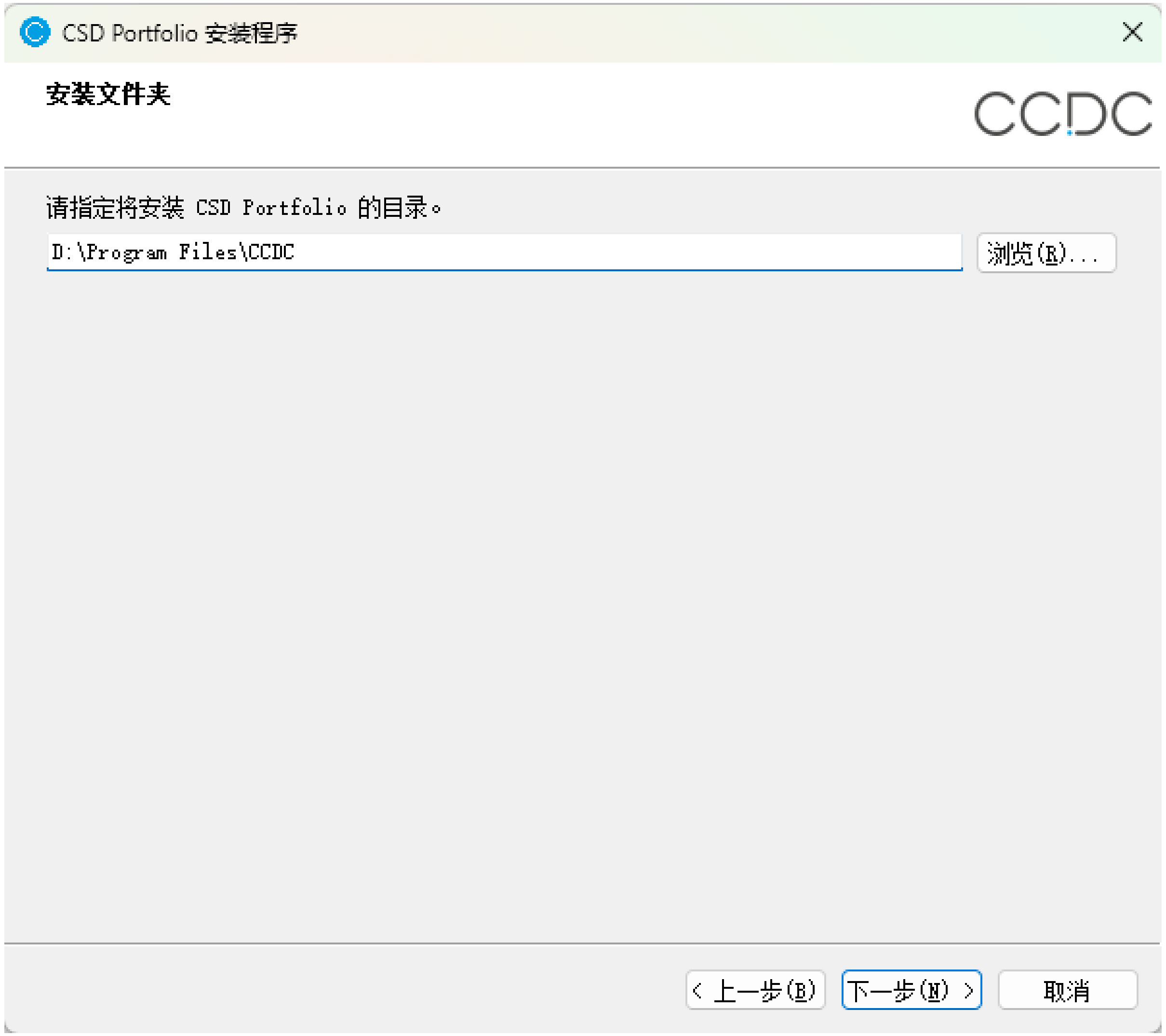
同时建议先行下载Microsoft Visual C Runtime运行库合集保证运行环境完整，网上搜索最新版VC运行库合集自行选择下载安装即可。

8. 选择安装程序，开始安装



CSD Portfolio 安装程序
安装程序 – CSD Portfolio
CCDC
下一步(N) >
退出

欢迎使用 CSD Portfolio 安装向导。

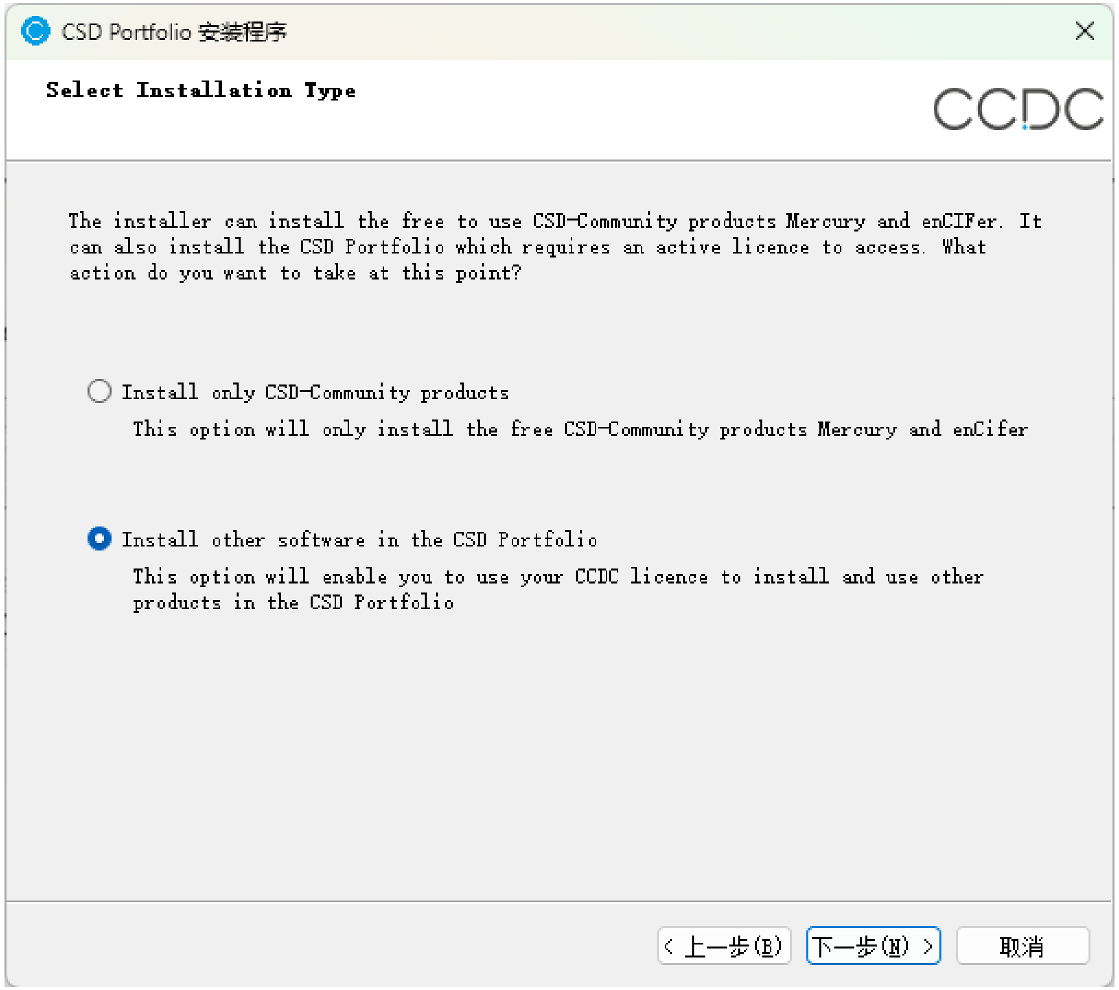

CSD Portfolio 安装程序
CCDC

安装文件夹

请指定将安装 CSD Portfolio 的目录。

D:\Program Files\CCDC

浏览(R)...
< 上一步(B)
下一步(N) >
取消



Select Installation Type

The installer can install the free to use CSD-Community products Mercury and enCIFer. It can also install the CSD Portfolio which requires an active licence to access. What action do you want to take at this point?

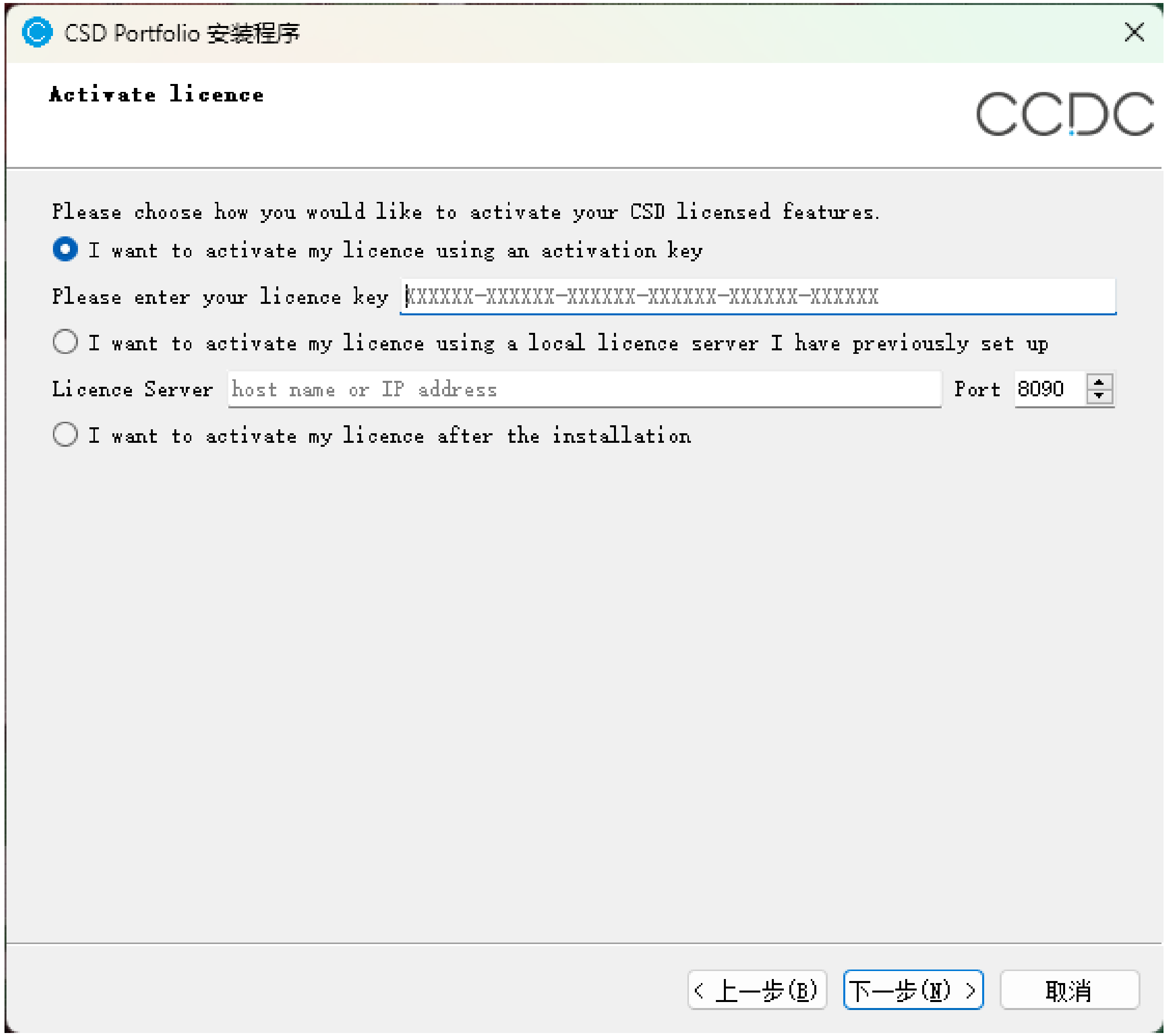
○ Install only CSD-Community products

This option will only install the free CSD-Community products Mercury and enCifer

● Install other software in the CSD Portfolio

This option will enable you to use your CCDC licence to install and use other products in the CSD Portfolio

正式用户勾选第二个安装完整版 CSD



Activate licence

Please choose how you would like to activate your CSD licensed features.

● I want to activate my licence using an activation key

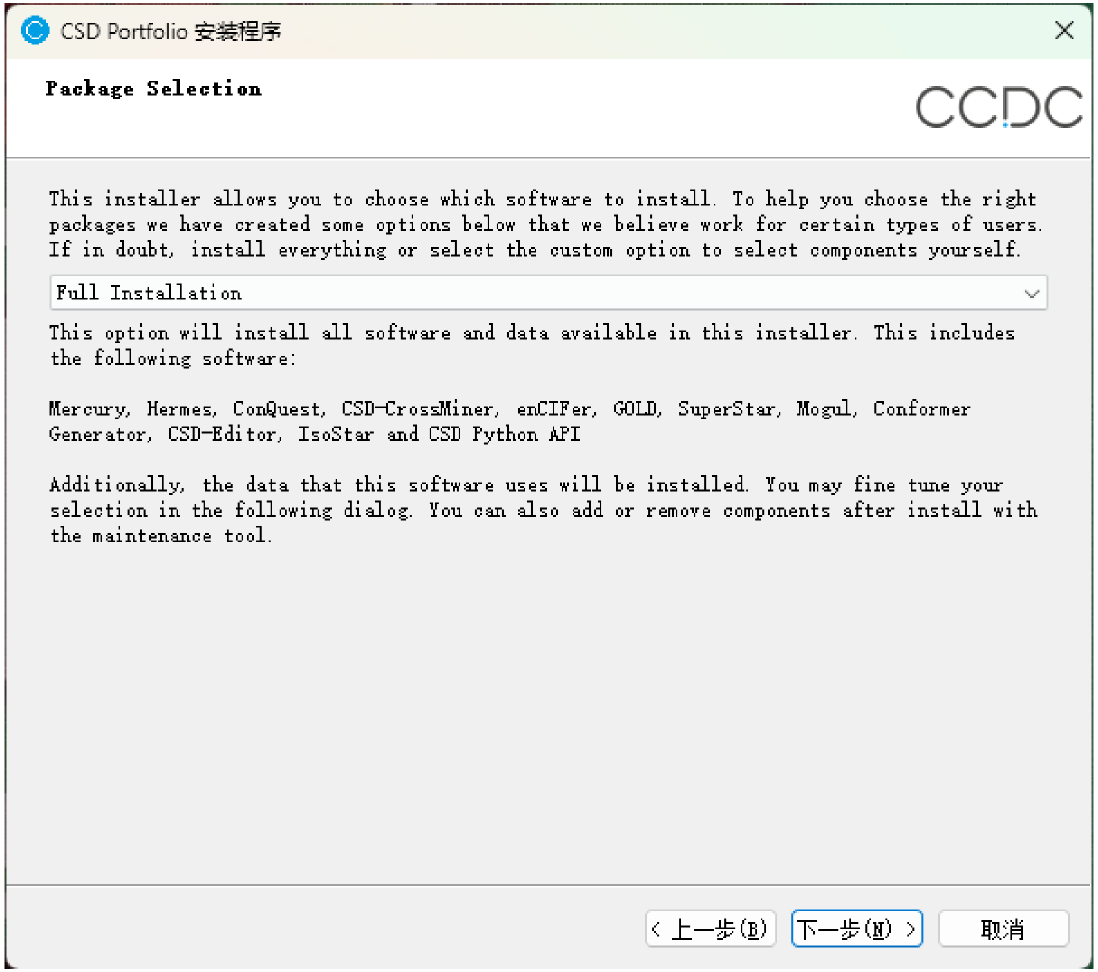
Please enter your licence key XXXXXX-XXXXXX-XXXXXX-XXXXXX-XXXXXX-XXXXXX

○ I want to activate my licence using a local licence server I have previously set up

Licence Server host name or IP address Port 8090

○ I want to activate my licence after the installation

首次安装选择第一项，输入本单位专属激活码进行激活



Package Selection

This installer allows you to choose which software to install. To help you choose the right packages we have created some options below that we believe work for certain types of users. If in doubt, install everything or select the custom option to select components yourself.

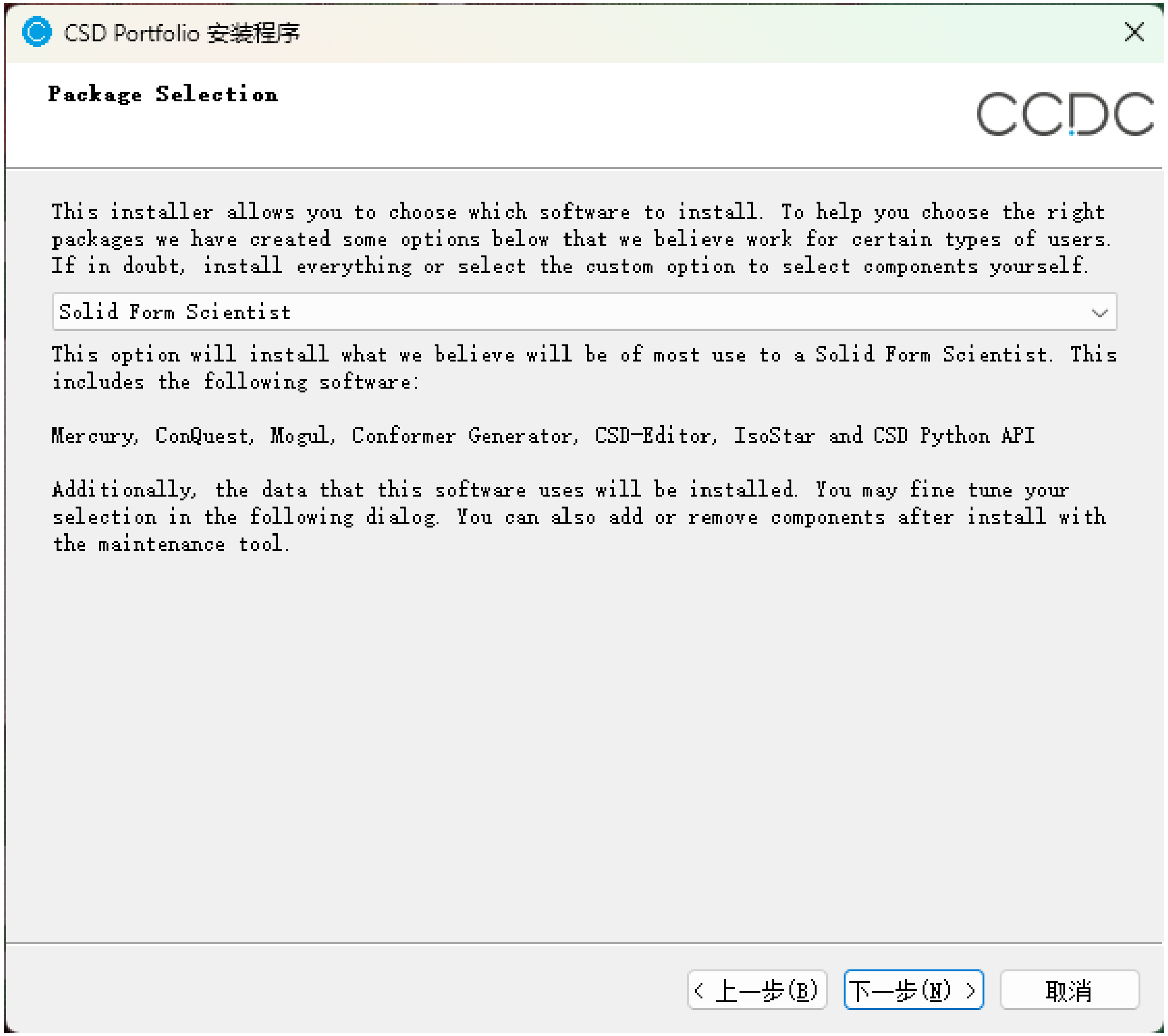
Full Installation

This option will install all software and data available in this installer. This includes the following software:

Mercury, Hermes, ConQuest, CSD-CrossMiner, enCIFer, GOLD, SuperStar, Mogul, Conformer Generator, CSD-Editor, IsoStar and CSD Python API

Additionally, the data that this software uses will be installed. You may fine tune your selection in the following dialog. You can also add or remove components after install with the maintenance tool.

此处可选择安装哪些模块，并且提供了几种推荐组合供特定研究方向使用，亦可自定义选择



Package Selection

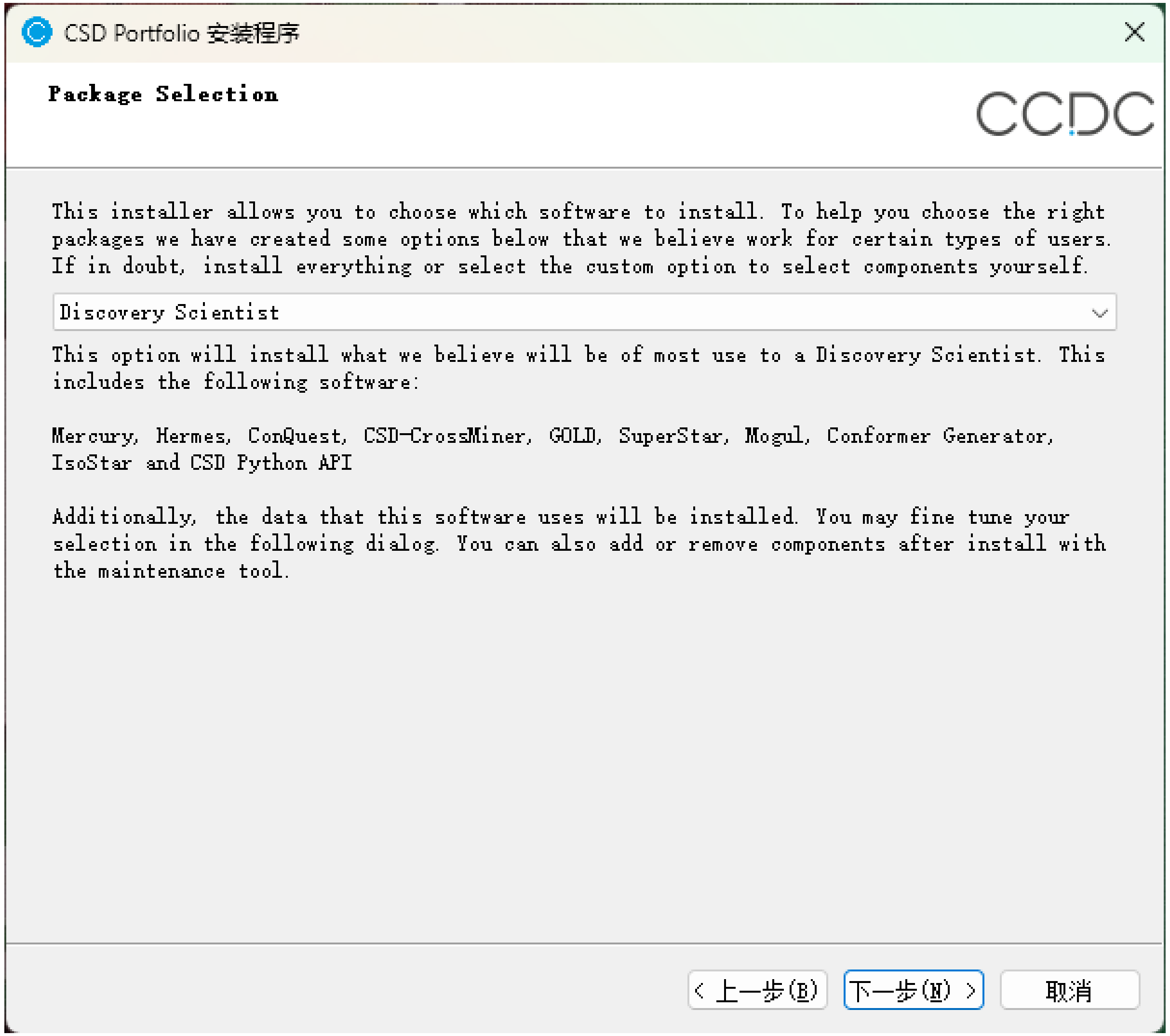
This installer allows you to choose which software to install. To help you choose the right packages we have created some options below that we believe work for certain types of users. If in doubt, install everything or select the custom option to select components yourself.

Solid Form Scientist

This option will install what we believe will be of most use to a Solid Form Scientist. This includes the following software:

Mercury, ConQuest, Mogul, Conformer Generator, CSD-Editor, IsoStar and CSD Python API

Additionally, the data that this software uses will be installed. You may fine tune your selection in the following dialog. You can also add or remove components after install with the maintenance tool.



Package Selection

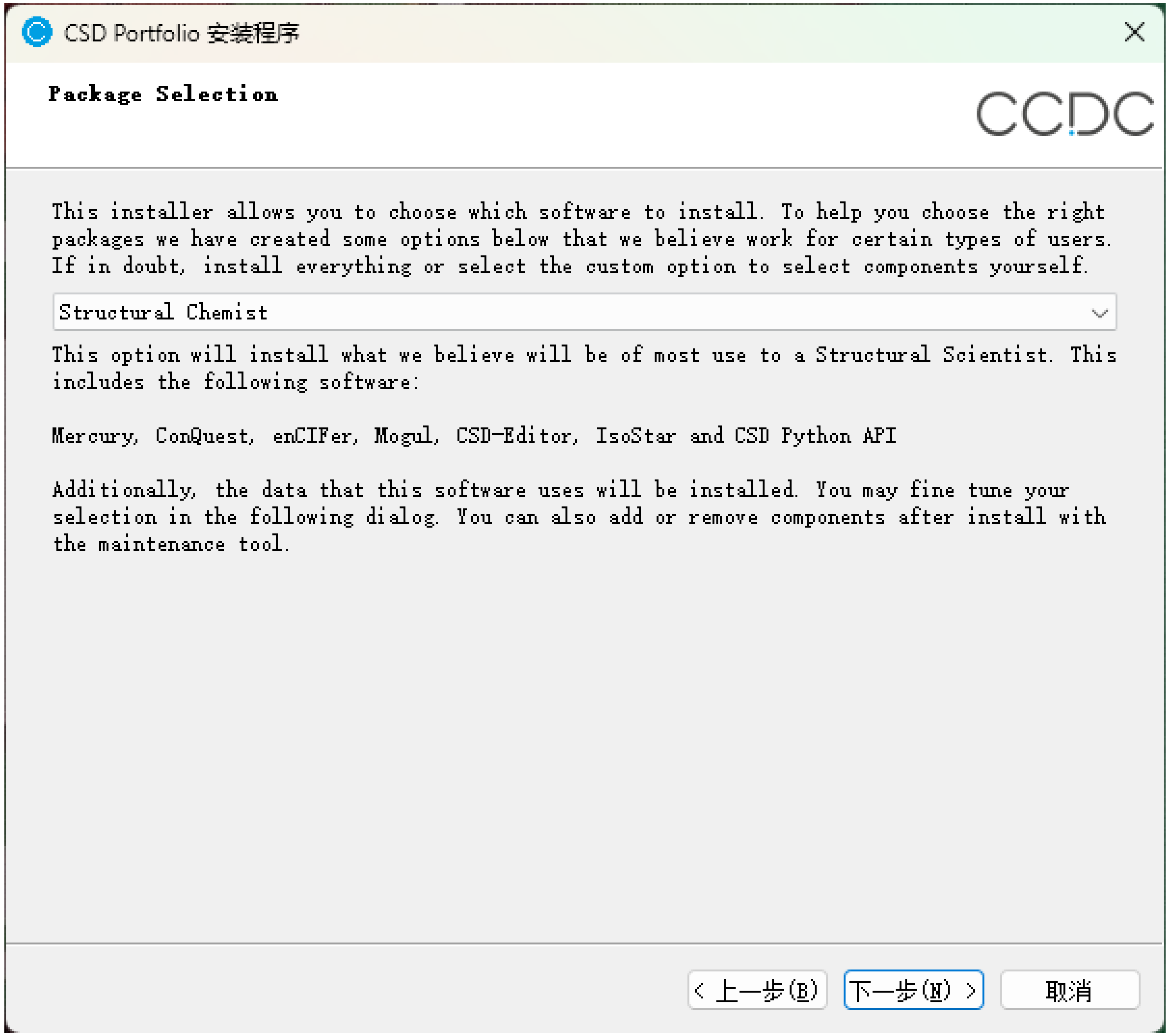
This installer allows you to choose which software to install. To help you choose the right packages we have created some options below that we believe work for certain types of users. If in doubt, install everything or select the custom option to select components yourself.

Discovery Scientist

This option will install what we believe will be of most use to a Discovery Scientist. This includes the following software:

Mercury, Hermes, ConQuest, CSD-CrossMiner, GOLD, SuperStar, Mogul, Conformer Generator, IsoStar and CSD Python API

Additionally, the data that this software uses will be installed. You may fine tune your selection in the following dialog. You can also add or remove components after install with the maintenance tool.



Package Selection

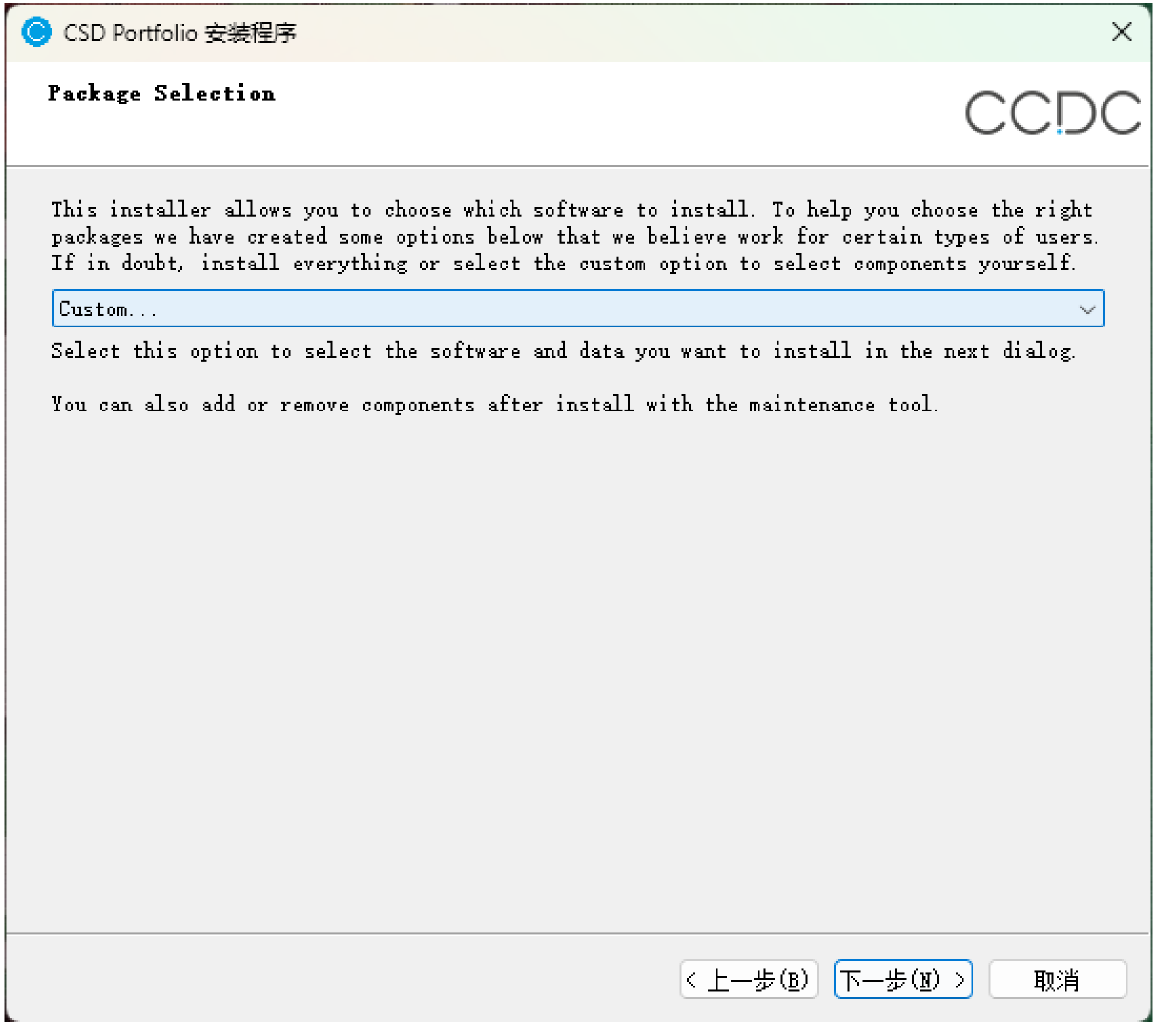
This installer allows you to choose which software to install. To help you choose the right packages we have created some options below that we believe work for certain types of users. If in doubt, install everything or select the custom option to select components yourself.

Structural Chemist

This option will install what we believe will be of most use to a Structural Scientist. This includes the following software:

Mercury, ConQuest, enCIFer, Mogul, CSD-Editor, IsoStar and CSD Python API

Additionally, the data that this software uses will be installed. You may fine tune your selection in the following dialog. You can also add or remove components after install with the maintenance tool.



Package Selection

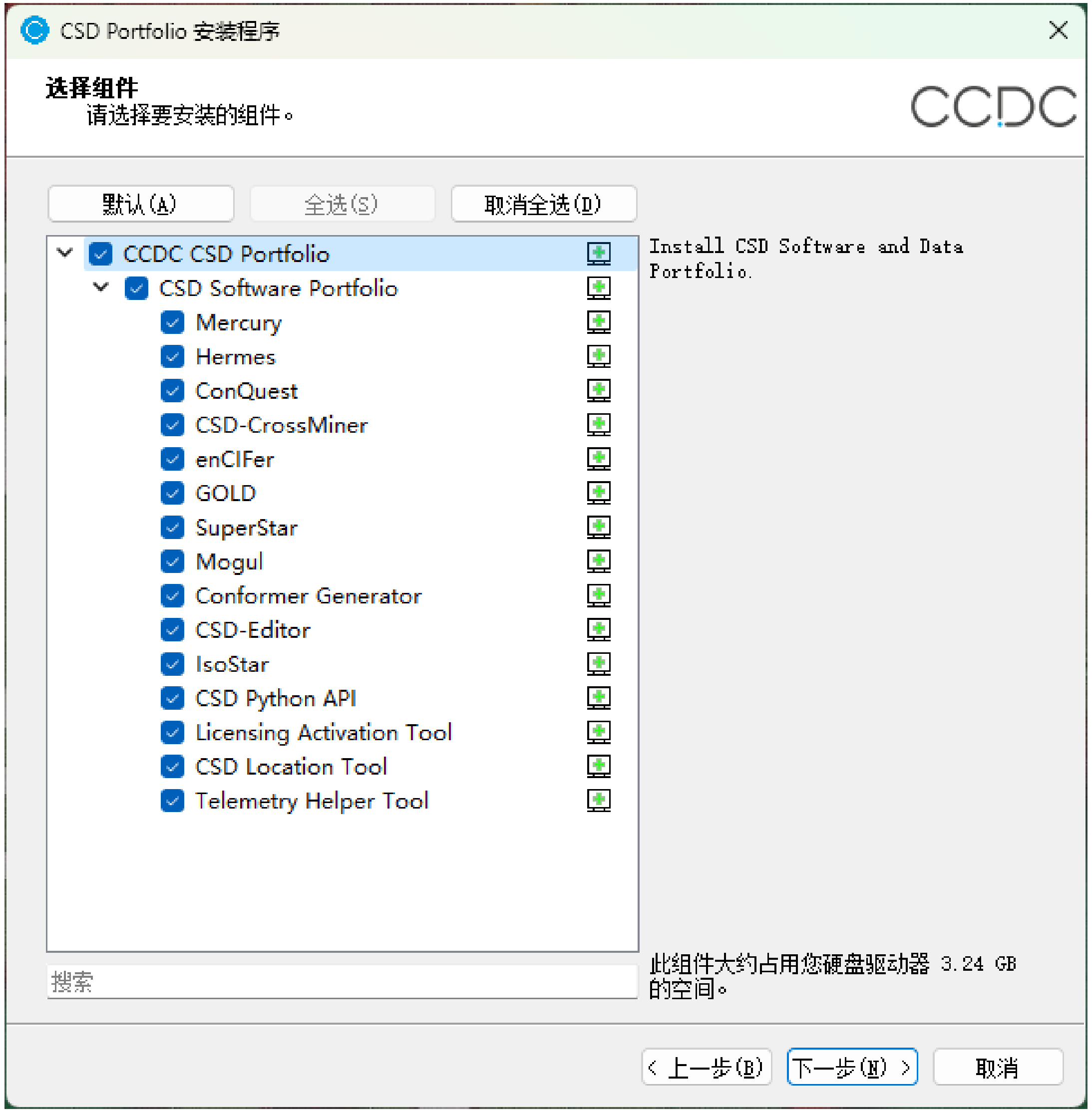
This installer allows you to choose which software to install. To help you choose the right packages we have created some options below that we believe work for certain types of users. If in doubt, install everything or select the custom option to select components yourself.

Custom...

Select this option to select the software and data you want to install in the next dialog.

You can also add or remove components after install with the maintenance tool.

自定义选择

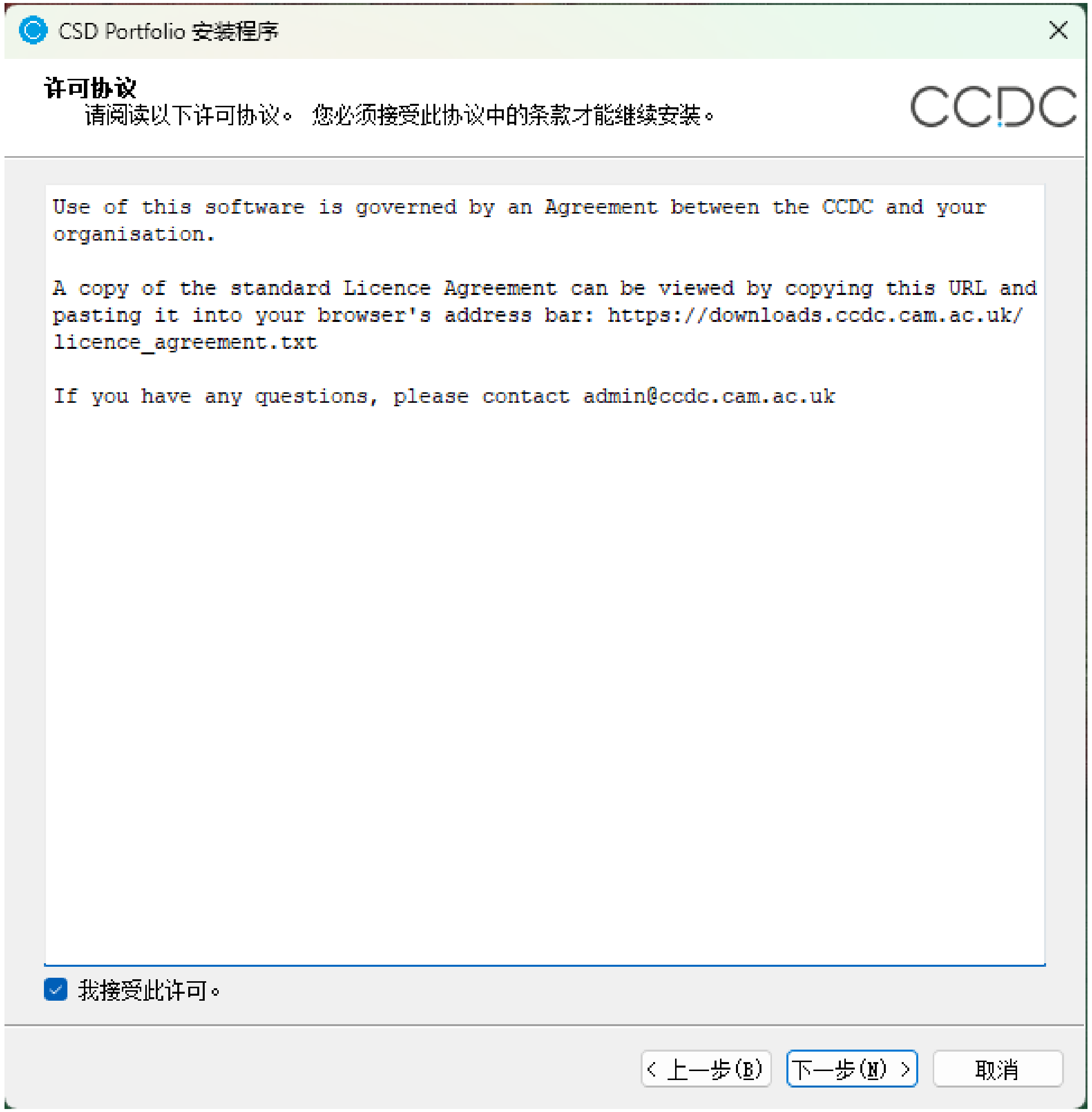

CSD Portfolio 安装程序
CCDC
默认(A)
全选(S)
取消全选(D)
搜索
< 上一步(B)
下一步(N) >
取消

选择组件
请选择要安装的组件。

- ☑ CCDC CSD Portfolio
  - ☑ CSD Software Portfolio
    - ☑ Mercury
    - ☑ Hermes
    - ☑ ConQuest
    - ☑ CSD-CrossMiner
    - ☑ enCIFer
    - ☑ GOLD
    - ☑ SuperStar
    - ☑ Mogul
    - ☑ Conformer Generator
    - ☑ CSD-Editor
    - ☑ IsoStar
    - ☑ CSD Python API
    - ☑ Licensing Activation Tool
    - ☑ CSD Location Tool
    - ☑ Telemetry Helper Tool

Install CSD Software and Data Portfolio.

此组件大约占用您硬盘驱动器 3.24 GB 的空间。



许可协议

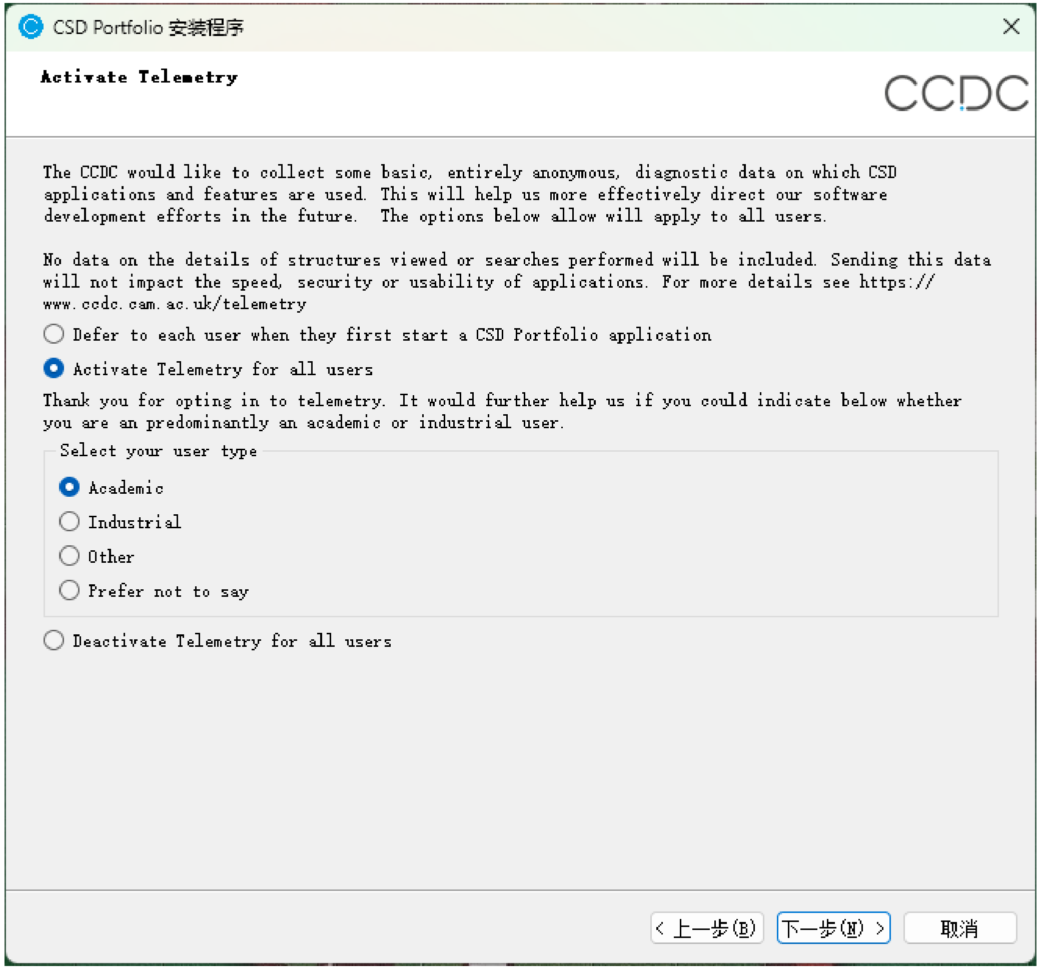
请阅读以下许可协议。 您必须接受此协议中的条款才能继续安装。

Use of this software is governed by an Agreement between the CCDC and your organisation.

A copy of the standard Licence Agreement can be viewed by copying this URL and pasting it into your browser's address bar: https://downloads.ccdc.cam.ac.uk/licence_agreement.txt

If you have any questions, please contact admin@ccdc.cam.ac.uk

☑ 我接受此许可。



Activate Telemetry

The CCDC would like to collect some basic, entirely anonymous, diagnostic data on which CSD applications and features are used. This will help us more effectively direct our software development efforts in the future. The options below allow will apply to all users.

No data on the details of structures viewed or searches performed will be included. Sending this data will not impact the speed, security or usability of applications. For more details see https://www.ccdc.cam.ac.uk/telemetry

○ Defer to each user when they first start a CSD Portfolio application

● Activate Telemetry for all users

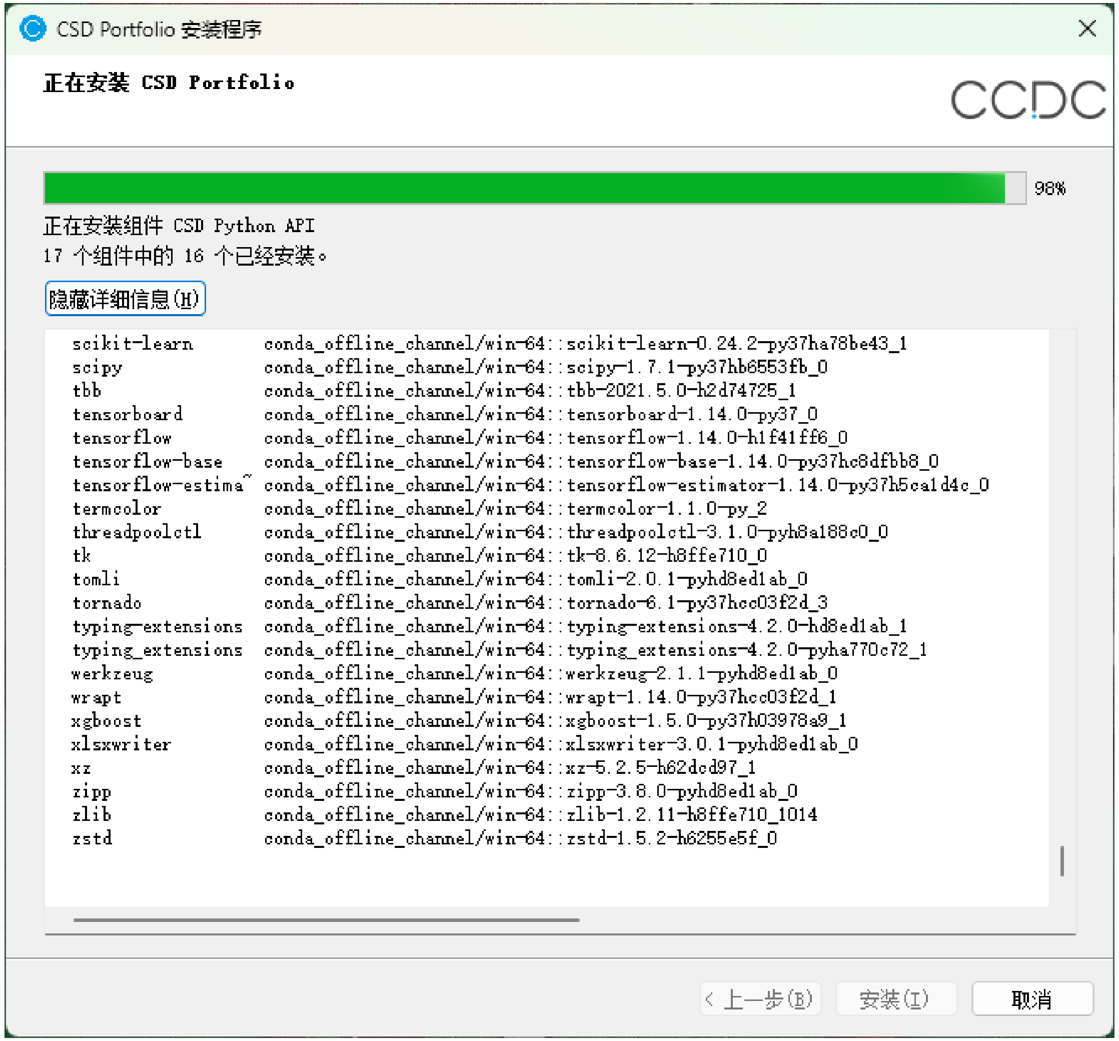
Thank you for opting in to telemetry. It would further help us if you could indicate below whether you are an predominantly an academic or industrial user.

Select your user type

● Academic
○ Industrial
○ Other
○ Prefer not to say

○ Deactivate Telemetry for all users

选择是否接受使用数据收集以及用户类型调查，若不接受收集数据则勾选最后一项



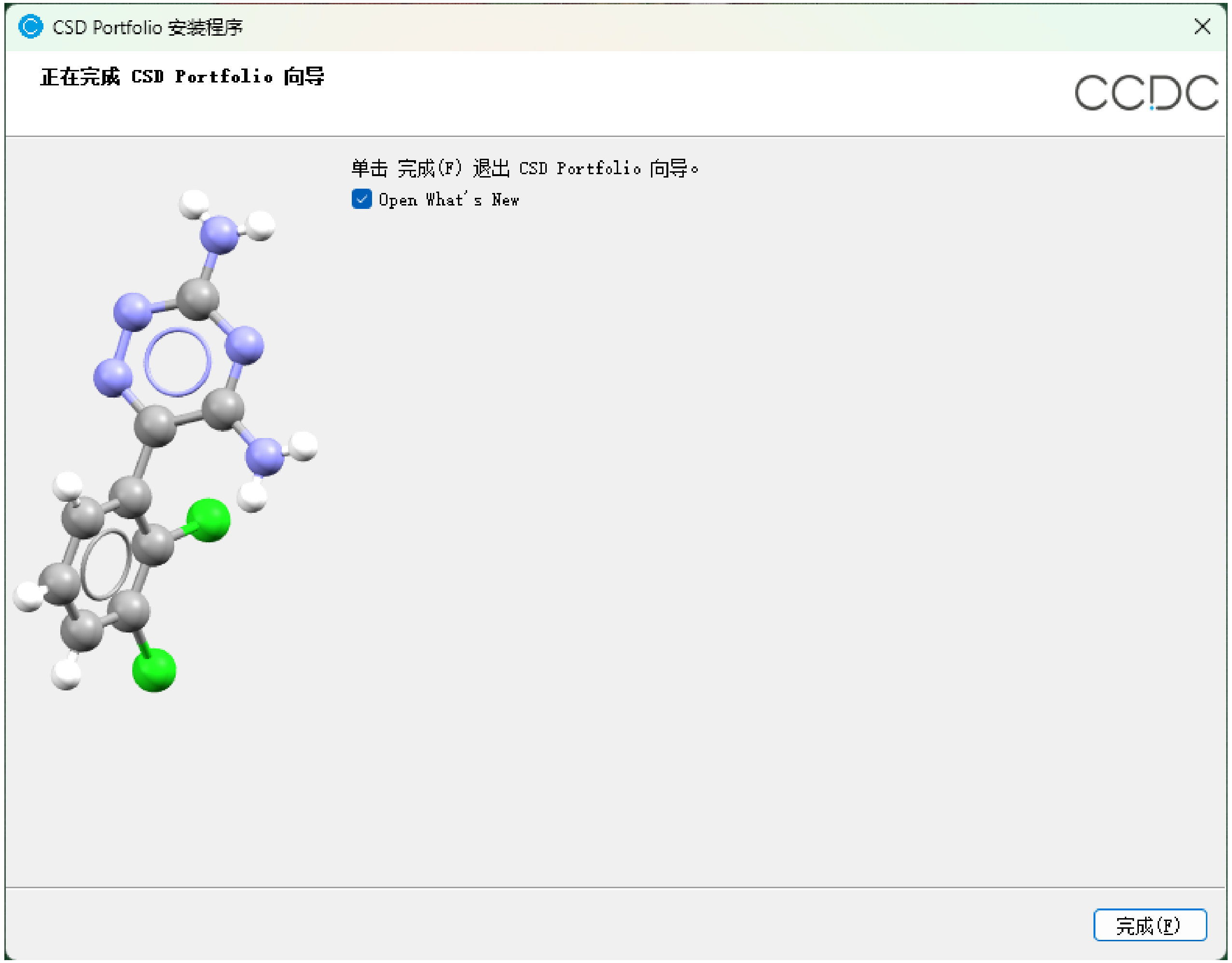
正在安装 CSD Portfolio

正在安装组件 CSD Python API

17 个组件中的 16 个已经安装。

```
scikit-learn       conda_offline_channel/win-64::scikit-learn-0.24.2-py37ha78be43_1
scipy              conda_offline_channel/win-64::scipy-1.7.1-py37hb6553fb_0
tbb                conda_offline_channel/win-64::tbb-2021.5.0-h2d74725_1
tensorboard        conda_offline_channel/win-64::tensorboard-1.14.0-py37_0
tensorflow         conda_offline_channel/win-64::tensorflow-1.14.0-h1f41ff6_0
tensorflow-base    conda_offline_channel/win-64::tensorflow-base-1.14.0-py37hc8dfbb8_0
tensorflow-estima~ conda_offline_channel/win-64::tensorflow-estimator-1.14.0-py37h5ca1d4c_0
termcolor          conda_offline_channel/win-64::termcolor-1.1.0-py_2
threadpoolctl      conda_offline_channel/win-64::threadpoolctl-3.1.0-pyh8a188c0_0
tk                 conda_offline_channel/win-64::tk-8.6.12-h8ffe710_0
tomli              conda_offline_channel/win-64::tomli-2.0.1-pyhd8ed1ab_0
tornado            conda_offline_channel/win-64::tornado-6.1-py37hcc03f2d_3
typing-extensions  conda_offline_channel/win-64::typing-extensions-4.2.0-hd8ed1ab_1
typing_extensions  conda_offline_channel/win-64::typing_extensions-4.2.0-pyha770c72_1
werkzeug           conda_offline_channel/win-64::werkzeug-2.1.1-pyhd8ed1ab_0
wrapt              conda_offline_channel/win-64::wrapt-1.14.0-py37hcc03f2d_1
xgboost            conda_offline_channel/win-64::xgboost-1.5.0-py37h03978a9_1
xlsxwriter         conda_offline_channel/win-64::xlsxwriter-3.0.1-pyhd8ed1ab_0
xz                 conda_offline_channel/win-64::xz-5.2.5-h62dcd97_1
zipp               conda_offline_channel/win-64::zipp-3.8.0-pyhd8ed1ab_0
zlib               conda_offline_channel/win-64::zlib-1.2.11-h8ffe710_1014
zstd               conda_offline_channel/win-64::zstd-1.5.2-h6255e5f_0
```

进行安装

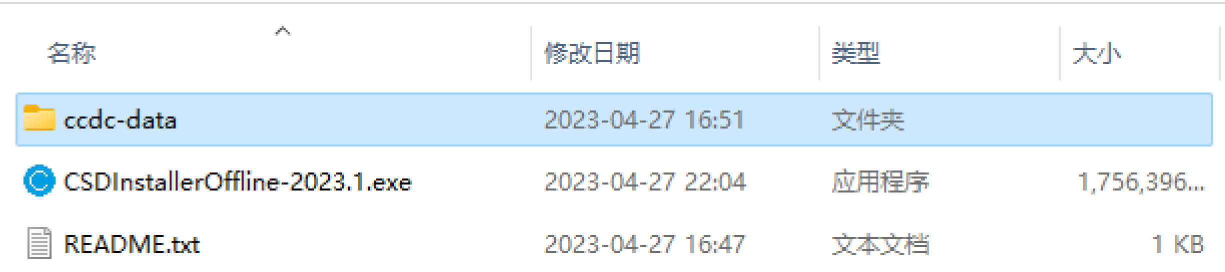

CSD Portfolio 安装程序
CCDC
完成(F)

正在完成 CSD Portfolio 向导

单击 完成(F) 退出 CSD Portfolio 向导。

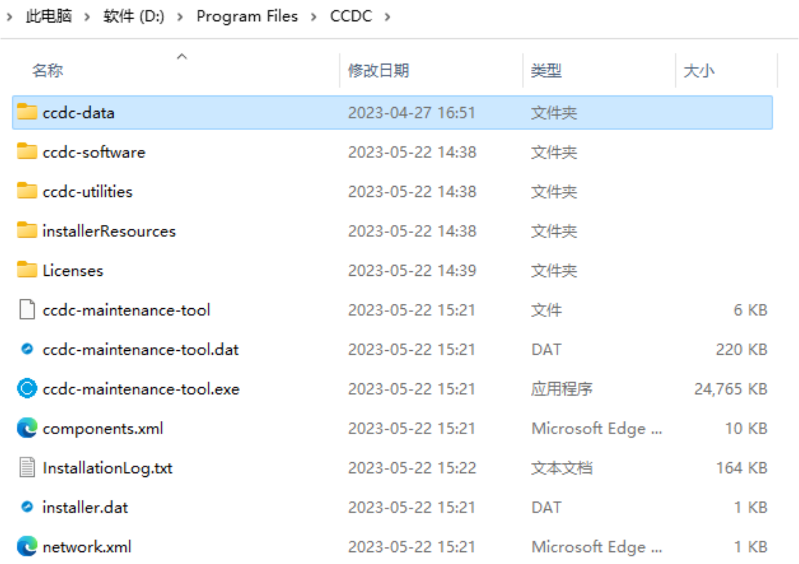
☑ Open What's New

完成安装



名称	修改日期	类型	大小
ccdc-data	2023-04-27 16:51	文件夹	
CSDInstallerOffline-2023.1.exe	2023-04-27 22:04	应用程序	1,756,396...
README.txt	2023-04-27 16:47	文本文档	1 KB

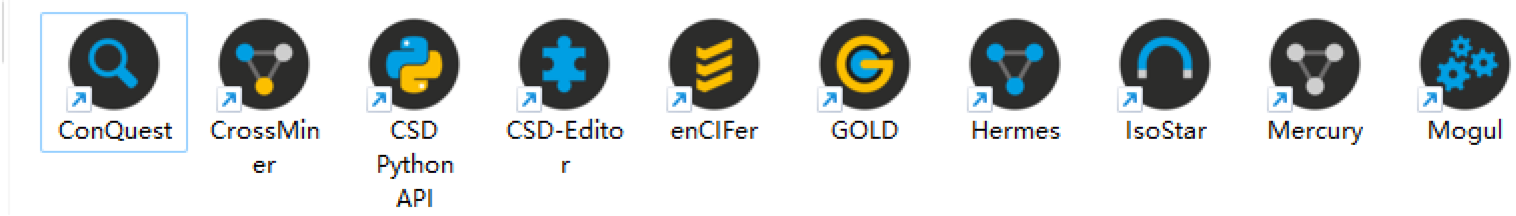
复制 ccdc-data 文件夹到安装目录下，复制完成后方可使用



› 此电脑 › 软件 (D:) › Program Files › CCDC ›

名称	修改日期	类型	大小
ccdc-data	2023-04-27 16:51	文件夹	
ccdc-software	2023-05-22 14:38	文件夹	
ccdc-utilities	2023-05-22 14:38	文件夹	
installerResources	2023-05-22 14:38	文件夹	
Licenses	2023-05-22 14:39	文件夹	
ccdc-maintenance-tool	2023-05-22 15:21	文件	6 KB
ccdc-maintenance-tool.dat	2023-05-22 15:21	DAT	220 KB
ccdc-maintenance-tool.exe	2023-05-22 15:21	应用程序	24,765 KB
components.xml	2023-05-22 15:21	Microsoft Edge ...	10 KB
InstallationLog.txt	2023-05-22 15:22	文本文档	164 KB
installer.dat	2023-05-22 15:21	DAT	1 KB
network.xml	2023-05-22 15:21	Microsoft Edge ...	1 KB

9. 将散落在桌面的快捷方式整理到文件夹中方便查看，选择对应模块，开始使用


ConQuest
CrossMiner
CSD Python API
CSD-Editor
enCIFer
GOLD
Hermes
IsoStar
Mercury
Mogul

各模块使用方法可参考链接中的讲解视频：

https://www.labtube.tv/channel/MTY2MA/videos

10. 更多问题，请点击首页的 Support and Resources 中的 FAQs 查询。

若软件出现闪退，请尝试更新显卡驱动；

若需下载最新结构数据，可在此链接中获取：

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