

*下载与使用仅限上科大校园内网

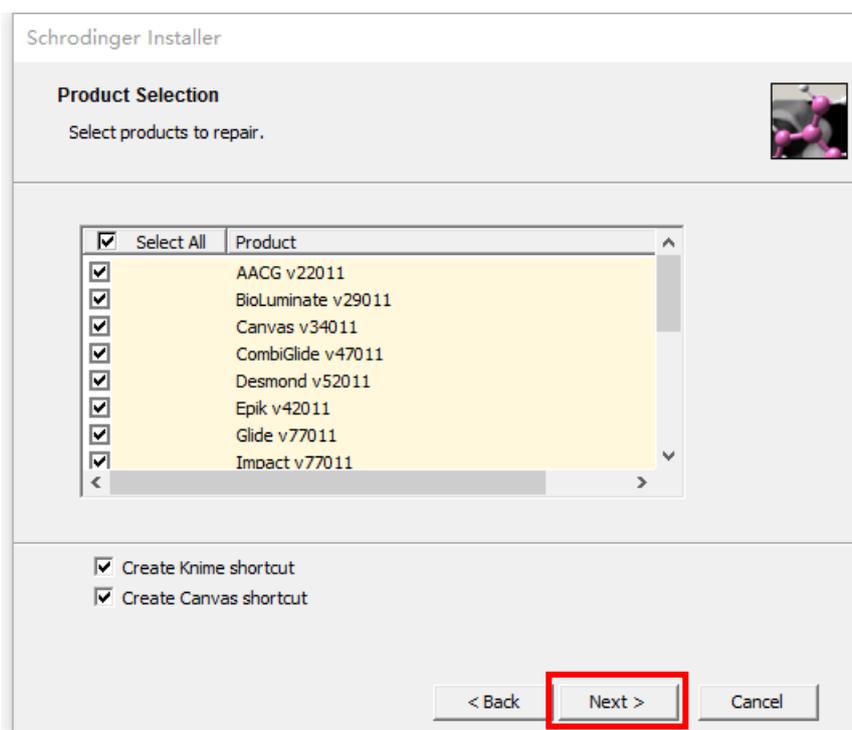
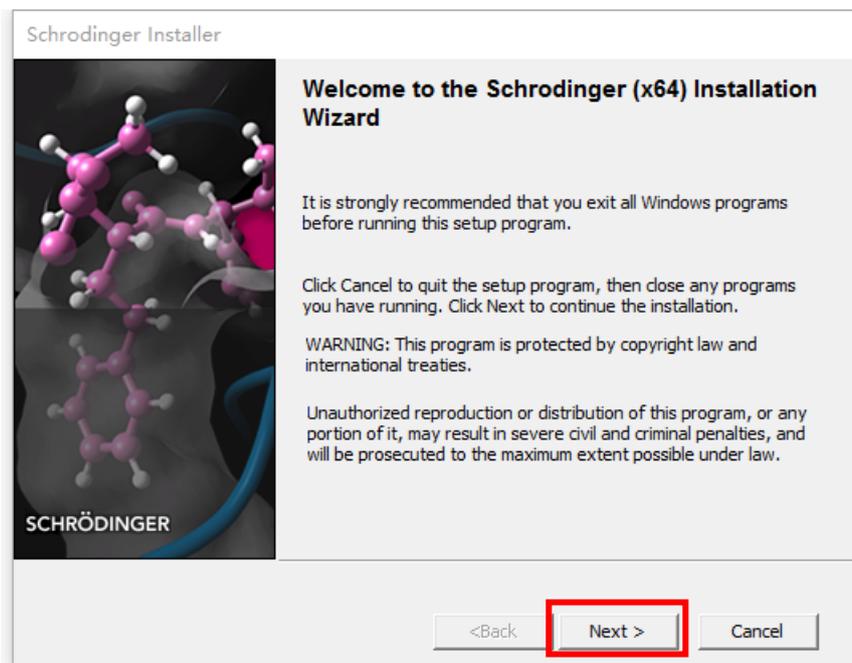
Windows 操作系统：

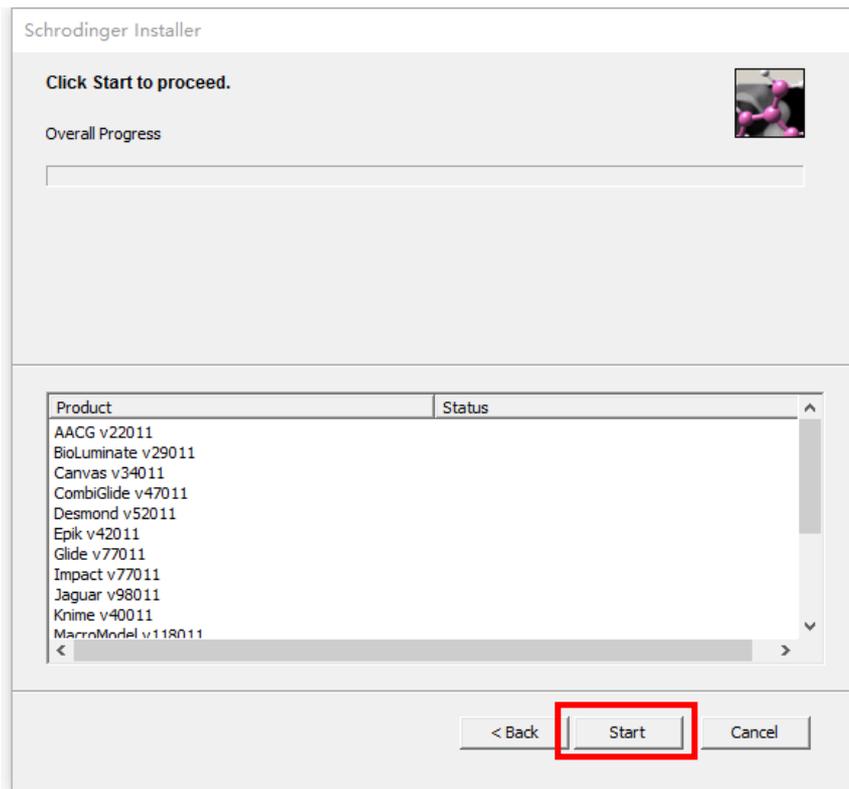
软件下载地址：

<http://zhaolab.shanghaitech.edu.cn/software/>

[Schrodinger_Suites_2017-4_Advanced_Windows-x64.zip](#)

安装：





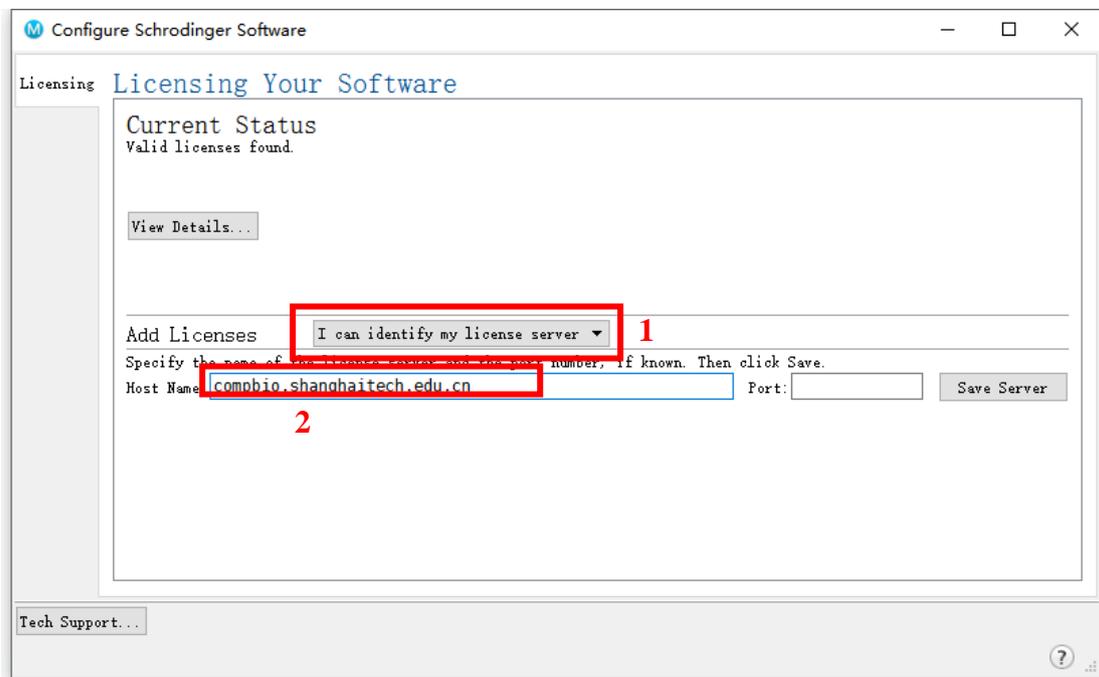
安装完成后，在 Windows 系统栏找到安装目录



点击 Configure Software，等待程序弹出：

Add License 选择 *I can identify my license server*

Host Name: *combio.shanghaitech.edu.cn*



Save Server, 完成。

Linux 操作系统

软件下载地址：

http://zhaolab.shanghaitech.edu.cn/software/Schrodinger_Suites_2017-4_Advanced_Linux-x86_64.tar

下载完成后，解压：

```
[root@hpc2 Schrodinger]# ls
Schrodinger_Suites_2017-4_Linux-x86_64.tar
[root@hpc2 Schrodinger]# tar -xvf Schrodinger_Suites_2017-4_Linux-x86_64.tar
Schrodinger_Suites_2017-4_Linux-x86_64/combiglide-v4.7-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/aacg-v2.2-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/canvas-v3.4-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/mcpro-v4.8-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/EULA_standard.rtf
Schrodinger_Suites_2017-4_Linux-x86_64/psp-v5.0-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/phase-v5.3-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/glide-v7.7-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/epik-v4.2-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/jaguar-v9.8-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/impact-v7.7-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/bioluminate-v2.9-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/desmond-v5.2-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/psp-hmmerpfamdb-thirdparty-database.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/mmshare-v4.0-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/knime-v4.0-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/INSTALL
Schrodinger_Suites_2017-4_Linux-x86_64/macromodel-v11.8-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/SchrodingerKNIMEFreeUpdateSite_4.0.11.201711131631.zip
Schrodinger_Suites_2017-4_Linux-x86_64/qikprop-v5.4-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/SchrodingerKNIMEUpdateSite_4.0.11.201711131631.zip
Schrodinger_Suites_2017-4_Linux-x86_64/alldocs-v4.0-docs.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/maestro-v11.4-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/psp-blastwebdb-thirdparty-database.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/pldb-v4.0-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/psp-hmmerpfam-thirdparty-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/psp-blast-thirdparty-Linux-x86_64.tar.gz
Schrodinger_Suites_2017-4_Linux-x86_64/CHECKSUM.md5
```

进入至解压目录，运行命令./INSTALL

```
aacg-v2.2-Linux-x86_64.tar.gz          impact-v7.7-Linux-x86_64.tar.gz      psp-blast-thirdparty-Linux-x86_64.tar.gz
alldocs-v4.0-docs.tar.gz              INSTALL                               psp-blastwebdb-thirdparty-database.tar.gz
bioluminate-v2.9-Linux-x86_64.tar.gz  jaguar-v9.8-Linux-x86_64.tar.gz     psp-hmmerpfamdb-thirdparty-database.tar.gz
canvas-v3.4-Linux-x86_64.tar.gz       knime-v4.0-Linux-x86_64.tar.gz      psp-hmmerpfam-thirdparty-Linux-x86_64.tar.gz
CHECKSUM.md5                          macromodel-v11.8-Linux-x86_64.tar.gz psp-v5.0-Linux-x86_64.tar.gz
combiglide-v4.7-Linux-x86_64.tar.gz    maestro-v11.4-Linux-x86_64.tar.gz    qikprop-v5.4-Linux-x86_64.tar.gz
desmond-v5.2-Linux-x86_64.tar.gz      mcpro-v4.8-Linux-x86_64.tar.gz      SchrodingerKNIMEFreeUpdateSite_4.0.11.201711131631.zip
EULA_standard.rtf                     mmshare-v4.0-Linux-x86_64.tar.gz    SchrodingerKNIMEUpdateSite_4.0.11.201711131631.zip
glide-v7.7-Linux-x86_64.tar.gz        phase-v5.3-Linux-x86_64.tar.gz
[root@hpc2 Schrodinger_Suites_2017-4_Linux-x86_64]# ./INSTALL
```

按 Enter 以继续

```
Schrodinger Software Installer

Please respond to each question by entering the appropriate response
or pressing ENTER to accept the default (shown in parentheses).

You will be given a chance to review all of your installation choices
before any files are actually installed.

You can quit the installation at any time by pressing CTRL+C.

For more information, see the Installation Guide, which is in the file
"install_guide.pdf", in the same directory as this INSTALL script.

Proceed to Schrodinger Suite2017-4 installation...

[Press ENTER to continue]
█
```

此处需要输入安装的路径：以 `/share/install/Schrodinger`（**安装目录**）为例

```
1) SCHRODINGER directory

Select the directory where you want to install this software.

This directory will hold a script to launch each installed product,
a subdirectory for each release of each product, and documentation.
To run the software, you must set the SCHRODINGER variable to this
directory.

It is necessary to install the software for each major release in
a separate SCHRODINGER directory. If you are installing additional
products for a release, or upgrading a product to a new version with
the same major version number, you can install into the same
SCHRODINGER as the existing software from that release, but software
from different major releases should never be mixed.

Current SCHRODINGER directory: /share/install/schrodinger2017-4
SCHRODINGER directory: (/share/install/schrodinger2017-4) /share/install/Schrodinger█
```

确认安装 (y):

```
Your installation choices were:

SCHRODINGER directory:      /share/install/Schrodinger
SCHRODINGER_THIRDPARTY directory: /share/install/Schrodinger/thirdparty
Scratch directory:          /usr/tmp

product      version  platform      status      compatible  action
-----
glide        7.7     Linux-x86_64  NEW        yes        INSTALL
pldb         4.0     Linux-x86_64  NEW        yes        INSTALL
bioluminate  2.9     Linux-x86_64  NEW        yes        INSTALL
aacg         2.2     Linux-x86_64  NEW        yes        INSTALL
hmmerpfamdb <database>  NEW        yes        INSTALL
blastwebdb  <database>  NEW        yes        INSTALL
alldocs      4.0     <docs>        NEW        yes        INSTALL
canvas       3.4     Linux-x86_64  NEW        yes        INSTALL
desmond      5.2     Linux-x86_64  NEW        yes        INSTALL
mcpro        4.8     Linux-x86_64  NEW        yes        INSTALL
psp          5.0     Linux-x86_64  NEW        yes        INSTALL
blast        Linux-x86_64  NEW        yes        INSTALL
hmmerpfam    Linux-x86_64  NEW        yes        INSTALL
impact       7.7     Linux-x86_64  NEW        yes        INSTALL
jaguar       9.8     Linux-x86_64  NEW        yes        INSTALL
macromodel   11.8    Linux-x86_64  NEW        yes        INSTALL
maestro      11.4    Linux-x86_64  NEW        yes        INSTALL
qikprop      5.4     Linux-x86_64  NEW        yes        INSTALL
combiglide   4.7     Linux-x86_64  NEW        yes        INSTALL
phase        5.3     Linux-x86_64  NEW        yes        INSTALL
epik         4.2     Linux-x86_64  NEW        yes        INSTALL
knime        4.0     Linux-x86_64  NEW        yes        INSTALL
mmshare      4.0     Linux-x86_64  NEW        yes        INSTALL

Note: The mmshare module provides common resources for all products.
      It is installed automatically when necessary.

Are these choices correct? [y/n] ( ) █
```

完成安装

```
*) Configuring your installation

If you need to request licenses, install or transfer licenses, or configure
remote machines for calculations, run the the Schrodinger software
configuration tool on a machine with a display.

The tool can be launched directly via $SCHRODINGER/utilities/configure
or by choosing the Configure Software item under the Help menu in Maestro.
If the current machine has a display, you can also launch it from this screen.

Launch the configuration GUI now? [y/n] ( ) n

***** Schrodinger software installation is complete. *****

[root@hpc2 Schrodinger_Suites_2017-4_Linux-x86_64]# █
```

待完成安装后，在命令行中输入 `vi ~/.bashrc`

导入软件的安装路径（此处为 `/share/install/Schrodinger`）及 `license` 授权，将下面三行输入 `.bashrc` 文件中，保存并退出。

```
export PATH=/share/install/Schrodinger:/share/install/Schrodinger/utilities:$PATH
export LM_LICENSE_FILE=27008@compbio.shanghaitech.edu.cn
export SCHRODINGER=/share/install/Schrodinger
```

安装完成。