

# 安装PyRosetta和Rosetta

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## What is the relationship between PyRosetta, Rosetta, and Robetta?

PyRosetta is a Python-script based front-end to the Rosetta molecular modeling suite. Rosetta, which is a collaborative project between more than 15 labs world-wide, requires users to have substantial experience in C++ and Rosetta software development to write custom algorithms. Through the use of Python-bindings to Rosetta C++ source code, PyRosetta allows the end-user to have access to the same Rosetta functions available to Rosetta developers, through an easy-to-use Python script based interface. Robetta is a server available online for non-commercial use of Rosetta applications. Rosetta algorithms cited in literature are the same (or similar) to the code implemented by Robetta and PyRosetta.

## PyRosetta4

### 下载安装包

[在下载页面](#)搜索“Latest PyRosetta Versions”可以找到对应系统的预编译安装包。

### 编译

1. 安装Python和Pip

```
sudo apt install python3 python3-pip
```

2. 下载源代码、解压、访问

```
sudo -H tar -xjf PyRosetta4.Release.*.tar.bz2
cd PyRosetta4.Release*
cd setup
sudo -H python3 setup.py install
```

3. 运行测试

```
cd ..
sudo -H python3 self-test.py
```

## Rosetta

### 预编译

预编译二进制文件位于文件夹中，可将其加入\$PATH便于调用

```
./main/source/bin/
```

## 编译

### 1. 安装库

```
sudo apt install build-essential python2 python-is-python2 openmpi-bin  
openmpi-common openmpi-doc libopenmpi3 libopenmpi-dev  
sudo -H pip3 install SCons
```

### 2. 下载源码、解压、访问

```
tar -xzvf rosetta_*.tgz  
cd rosetta_*  
cd main/source
```

### 3. 编译

```
./scons.py -j<number_of_processors_to_use> mode=release bin  
./scons.py bin mode=release extras=mpi  
./scons.py -j<number_of_processors_to_use> mode=release cat=test
```

### 4. 运行测试

```
python test/run.py
```

## Reference

Rosetta

```
Username: Academic_User  
Password: Xry3x4
```

PyRosetta:

```
Username: levinthal  
Password: paradox
```

- [PyRosetta Build Guide](#)
- [Rosetta Build Guide](#)