

# ProtCool

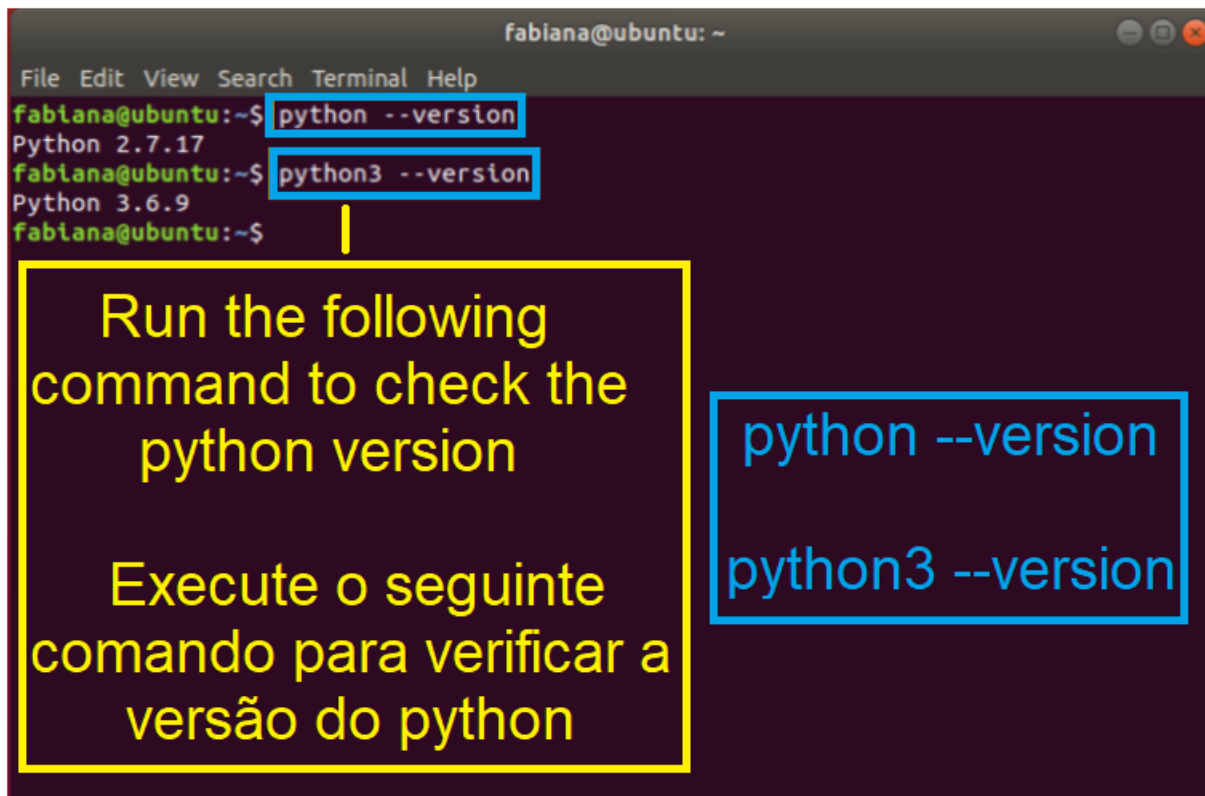
## Install ProtCool Tutorial

### STEP 1 - Checking the installed PYTHON Version:

Before running the installer, the researcher must ensure that python is properly installed and configured.

```
python --version  
python3 --version
```

The first command informs the version of python2 and the second command informs the version of python3, as shown in the image:



The image shows a terminal window titled 'fabiana@ubuntu: ~'. The terminal output is as follows:

```
fabiana@ubuntu:~$ python --version  
Python 2.7.17  
fabiana@ubuntu:~$ python3 --version  
Python 3.6.9  
fabiana@ubuntu:~$
```

Two blue boxes highlight the commands 'python --version' and 'python3 --version'. A yellow box on the left contains the text: 'Run the following command to check the python version' and 'Execute o seguinte comando para verificar a versão do python'. A blue box on the right contains the commands 'python --version' and 'python3 --version'.

As seen in the image above, this computer has both python installed, so you can move on to STEP 3 directly.

If any of the versions of python 2 or python3 is not found, STEP 2 must be followed.

### STEP 2 - Installing the PYTHON:

To install python 2, run the following command:

# ProtCool

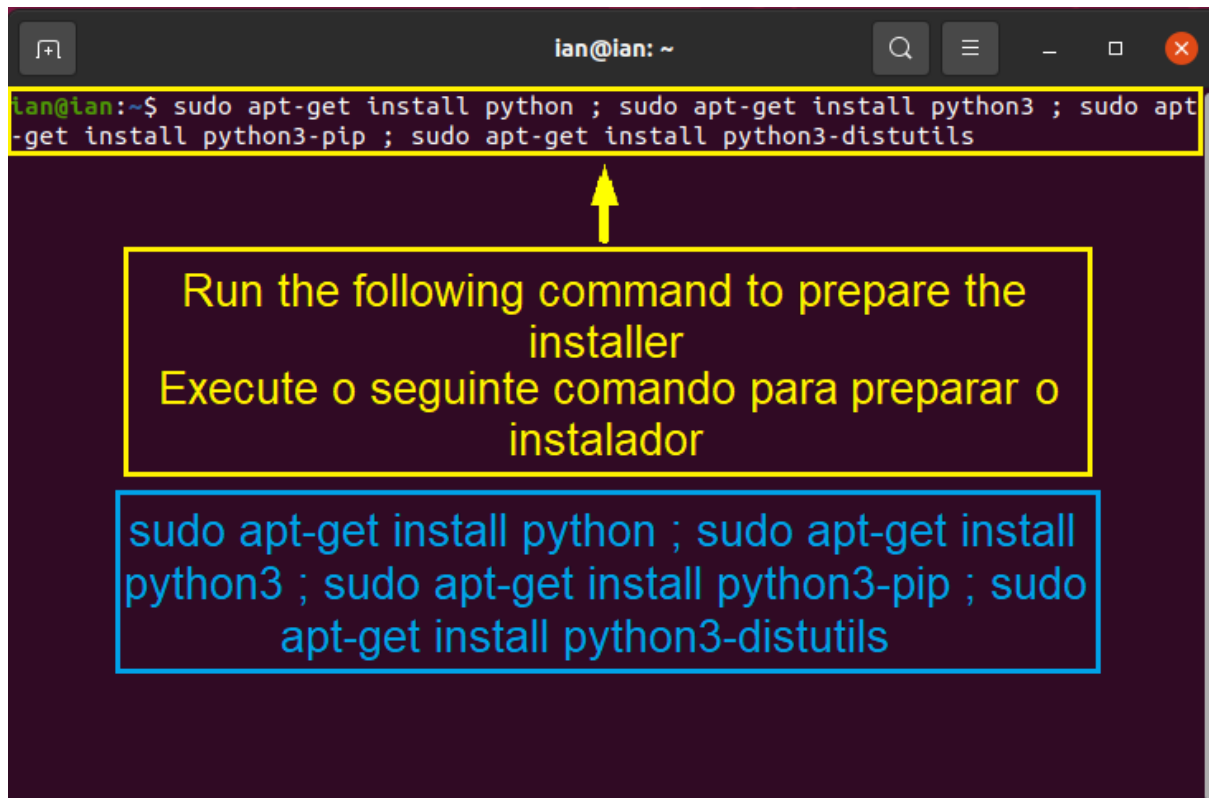
## Install ProtCool Tutorial

```
sudo apt-get install python
```

To install python 3, run the following command:

```
sudo apt-get install python3  
sudo apt-get install python3-pip  
sudo apt-get install python3-distutils
```

You can run all commands at once, as shown in the image, so that both systems are installed at once.



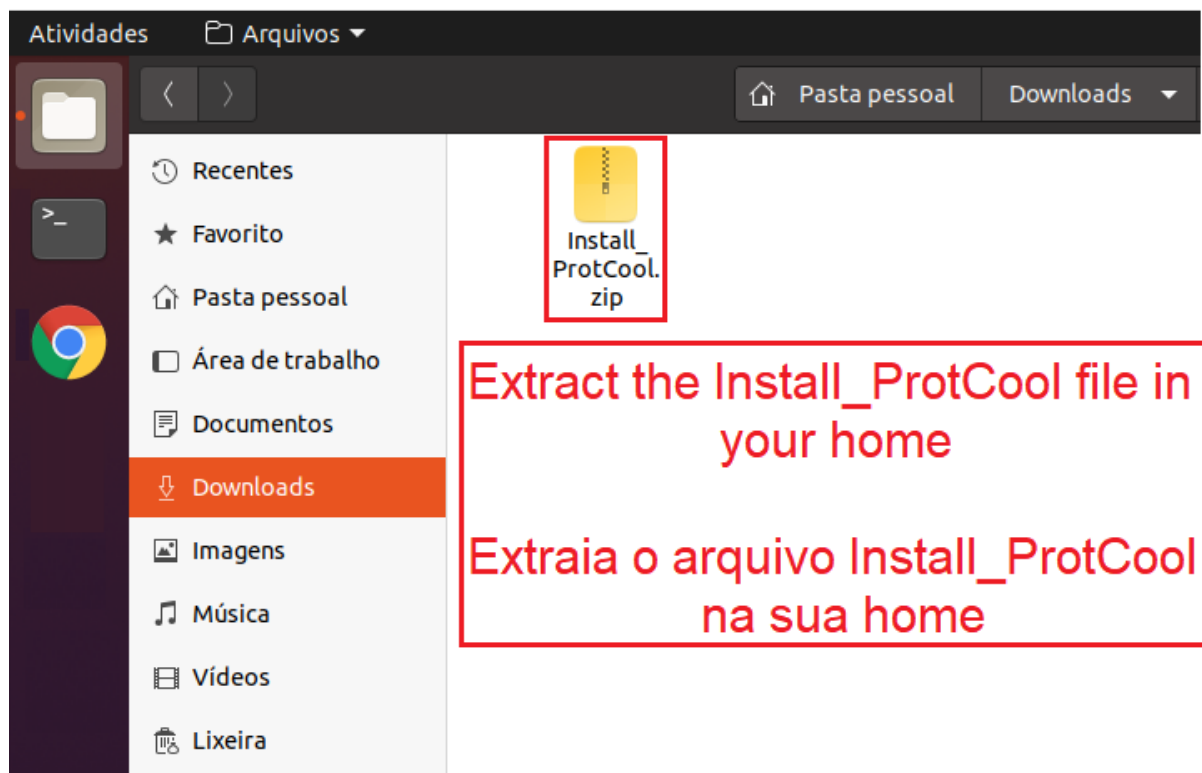
When we run the commands, we are installing both python 2, python 3 and the pip3 and distutils add-ons on the computer.

# W ProtCool

## Install ProtCool Tutorial

### PASSO 3 – Instalação do ProtCool

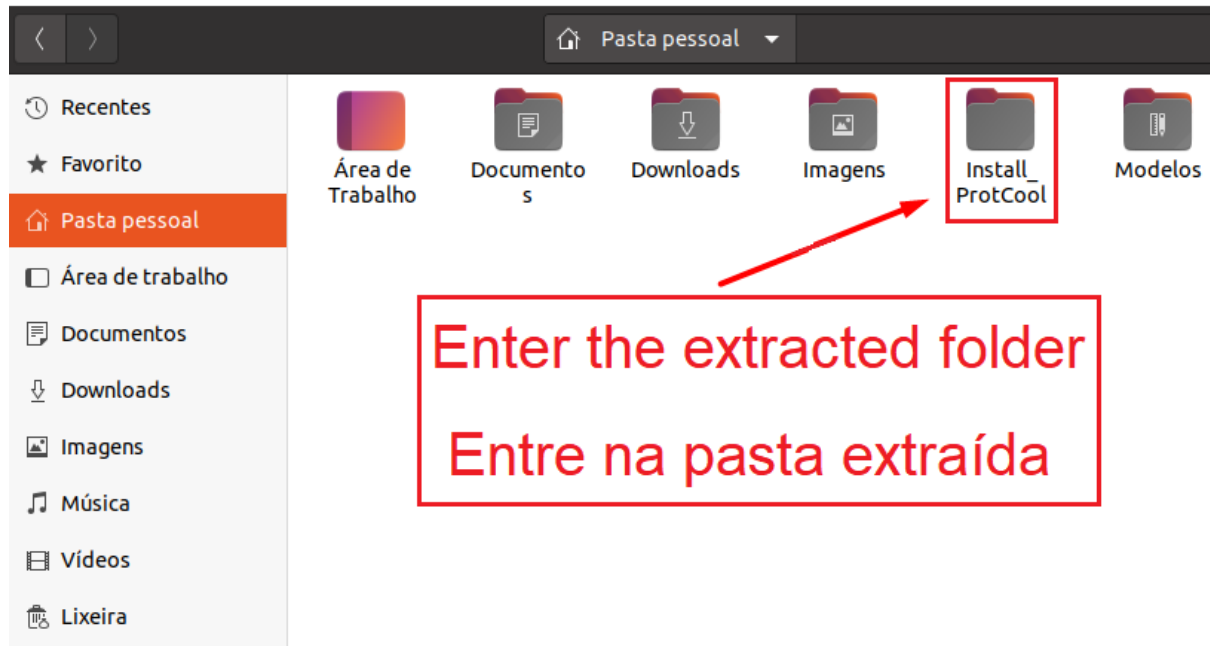
The researcher must go to the place where he downloaded Install\_ProtCool.zip and extract it in the folder on at home, if it is extracted in another folder, the installer will not run properly.



Inside the searcher's home folder, there will be the installer with all the files needed for installation. The researcher must enter at folder to proceed with the installation.

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Inside the installer folder there are 3 files: ProtCool, Install\_ProtCool.py and ReadMe folder:

- ProtCool - folder with ProtCool system files;
- Install\_ProtCool.py - installer that will make all settings for the researcher to work;
- ReadMe - Contains instructions on the installer itself, a tutorial on how to use the interface, and guidance to verify the PathUser.



## Install ProtCool Tutorial

```
ReadMe.txt
#### To run the installer it is necessary to have python and python3 installed on the machine - Para executar o instalador é necessário ter o python e python3 instalados na máquina ####

sudo apt-get install python
sudo apt-get install python3
sudo apt-get install python3-pip
sudo apt-get install python3-distutils

#### Extract the Install_ProtCool.zip file in your home - Extraia o arquivo Install_ProtCool.zip na sua home ####

#### Inside the extracted folder, run the following command - Dentro da pasta extraída, execute o seguinte comando ####

python3 Install_ProtCool.py

#### After following the installation, the system is ready for use - Após seguir a instalação, o sistema está pronto para o uso ####

#### Check the videos and tutorials for using ProtCool - Verifique os vídeos e tutoriais para utilização do ProtCool ####

#####

#### Tutorial for using the interface - Tutorial para usar a interface ####

Open the terminal inside the folder - Abra o terminal dentro da pasta
"home + "/ProtCool/ProtCool.Interface"

Run the following command - Rode o comando a seguir
python3 run.py localhost

In the browser enter the following link - No navegador entre com o seguinte link
http://127.0.0.1:5000/

After that the interface is ready for use - Após isso a interface está pronta para o uso

#####

#### List of installed systems/libraries - Lista de sistemas/bibliotecas instalados ####

PIP3, VMD, Requests, pygdb, Autodock, Vina, Smina, Selenium, Modeller, Geckodriver, Amber, MGLTools

#####

#### PathUser.txt check - Verificar PathUser ####

Please check the PathUser file in the ProtCool / path and ProtCool / ProtCool.Docking directories. This file must contain 4 lines, being:
Favor verificar o arquivo PathUser, que está nos diretórios ProtCool/path e ProtCool/ProtCool.Docking. Esse Arquivo deve contar 4 linhas, sendo:

Line 1 = Amber path
Line 2 = MGLTools autodock path
Line 3 = MGLTools bin path
Line 4 = END

File example:
/home/user/amber18
/home/user/MGLTools-1.5.6/MGLToolsPkgs/AutoDockTools
/home/user/MGLTools-1.5.6/bin
END

If it is not in this format, please modify the paths to the correct directory of your machine
Caso não esteja nesse formato, favor modificar os caminhos para o diretório correto da sua máquina
```

The following is a brief description of what each part of the ReadMe file is:

Instructions for the installer - Describes what must be installed previously, moreover, shows step by step how to run the installer.

Tutorial on how to access the interface - Step by step instructions on how to access the interface.

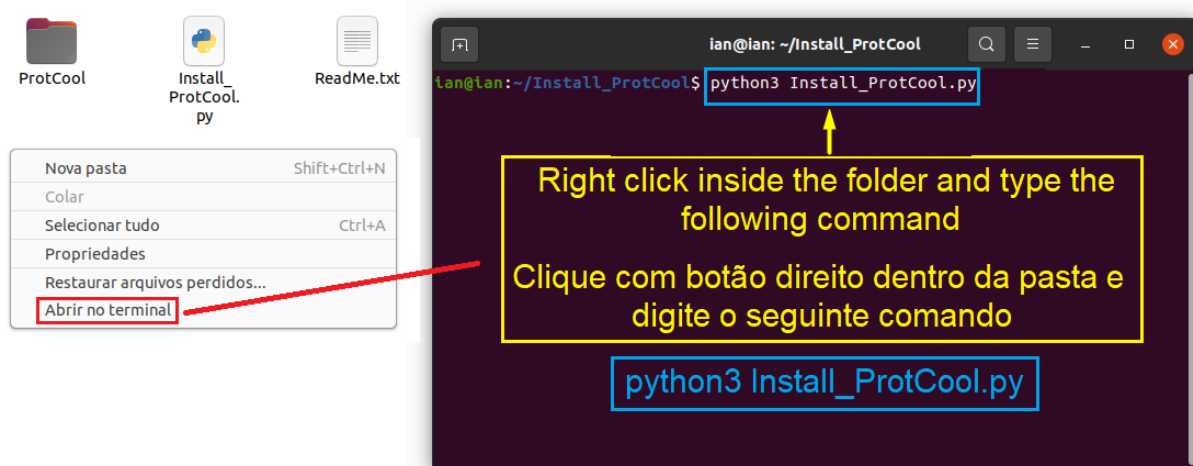
Direction to check the PathUser - If the researcher already has Amber or MGLTools installed, there may be problems with the tools. This part of the ReadMe describes the step by step of what should be done.

The researcher must open the terminal inside the folder and execute the following command:

```
python3 Install_ProtCool.py
```

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When executing the above command, the system will be executed, as shown in the screen below:

```
ian@ian: ~/Install_ProtCool
ian@ian:~/Install_ProtCool$ python3 Install_ProtCool.py

ProtCool

Welcome to the ProtCool installer!
To run the tool you will need to install the following dependencies:

Bem vindo ao instalador ProtCool!
Para executar a ferramenta sera necessaria a instalacao das seguintes dependencias:

PIP3, VMD, Requests, pypdb, Autodock, Vina, Smina, Selenium, Modeller, Gecko driver, Amber, MGLTools

#####
```

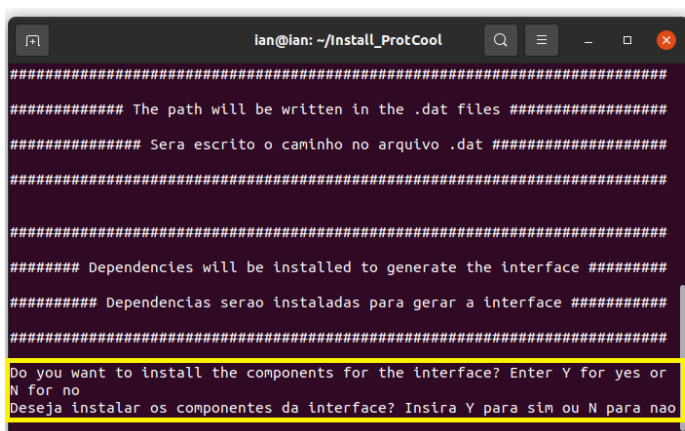
The installer will configure and install everything that will be necessary for the researcher to be able to work, but it will be the researcher who will allow each installation, answering “Y” or “N” for each system. This ensures that the researcher only installs what is needed on his equipment.

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## Install ProtCool Tutorial

Programs to be configured and installed:

PIP3, VMD, Requests, pypdb, Autodock, Vina, Smina, Selenium, Modeller, Geckodriver, Amber, MGLTools

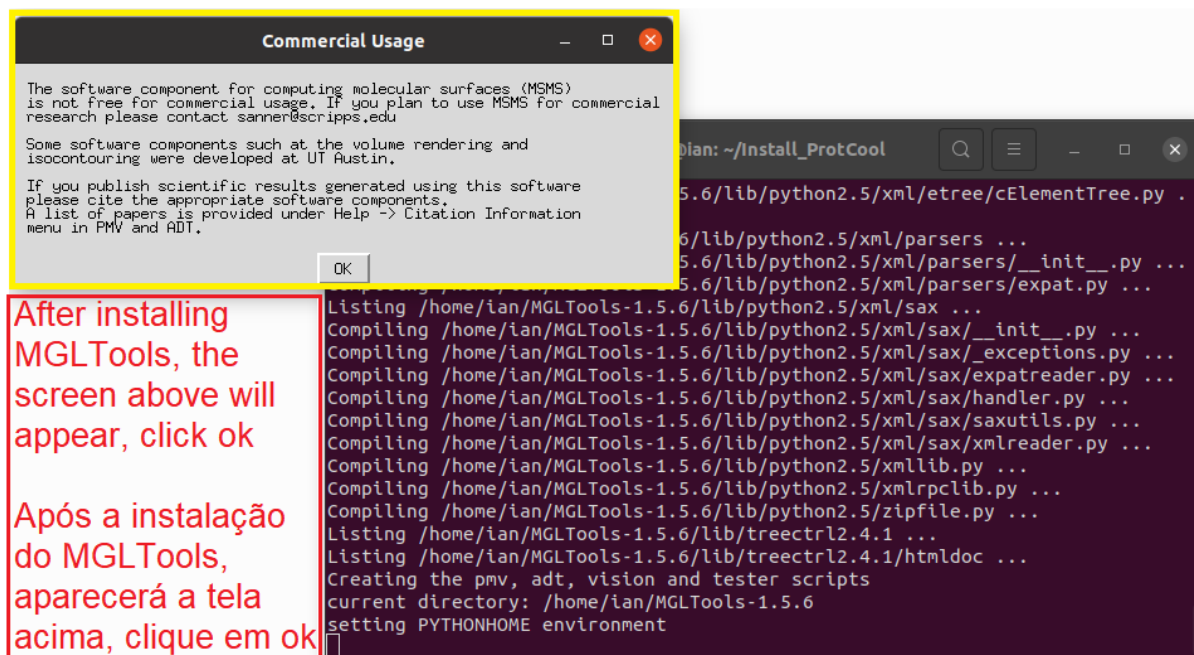


```
ian@ian: ~/Install_ProtCool
#####
##### The path will be written in the .dat files #####
##### Sera escrito o caminho no arquivo .dat #####
#####
##### Dependencies will be installed to generate the interface #####
##### Dependências serão instaladas para gerar a interface #####
#####
Do you want to install the components for the interface? Enter Y for yes or
N for no
Deseja instalar os componentes da interface? Insira Y para sim ou N para nao
```

The researcher will choose to choose which files to install

O pesquisador optará por escolher quais arquivos deseja instalar

After MGLTools is installed, a warning about commercial use will appear, click "ok" to finish the installation.



```
Commercial Usage
The software component for computing molecular surfaces (MSMS)
is not free for commercial usage. If you plan to use MSMS for commercial
research please contact sanner@scripps.edu

Some software components such as the volume rendering and
isocontouring were developed at UT Austin.

If you publish scientific results generated using this software
please cite the appropriate software components.
A list of papers is provided under Help -> Citation Information
menu in PMV and ADT.

[OK]

ian@ian: ~/Install_ProtCool
5.6/lib/python2.5/xml/etree/cElementTree.py .
5.6/lib/python2.5/xml/parsers/_init_.py ...
5.6/lib/python2.5/xml/parsers/expat.py ...
Listing /home/ian/MGLTools-1.5.6/lib/python2.5/xml/sax ...
Compiling /home/ian/MGLTools-1.5.6/lib/python2.5/xml/sax/_init_.py ...
Compiling /home/ian/MGLTools-1.5.6/lib/python2.5/xml/sax/_exceptions.py ...
Compiling /home/ian/MGLTools-1.5.6/lib/python2.5/xml/sax/expatreader.py ...
Compiling /home/ian/MGLTools-1.5.6/lib/python2.5/xml/sax/handler.py ...
Compiling /home/ian/MGLTools-1.5.6/lib/python2.5/xml/sax/saxutils.py ...
Compiling /home/ian/MGLTools-1.5.6/lib/python2.5/xml/sax/xmlreader.py ...
Compiling /home/ian/MGLTools-1.5.6/lib/python2.5/xmllib.py ...
Compiling /home/ian/MGLTools-1.5.6/lib/python2.5/xmlrpclib.py ...
Compiling /home/ian/MGLTools-1.5.6/lib/python2.5/zipfile.py ...
Listing /home/ian/MGLTools-1.5.6/lib/treectrl2.4.1 ...
Listing /home/ian/MGLTools-1.5.6/lib/treectrl2.4.1/html doc ...
Creating the pmv, adt, vision and tester scripts
current directory: /home/ian/MGLTools-1.5.6
setting PYTHONHOME environment
```

After installing MGLTools, the screen above will appear, click ok

Após a instalação do MGLTools, aparecerá a tela acima, clique em ok



## Install ProtCool Tutorial

After installation, a message will appear confirming that everything went well, and that the system is ready for use.

```
ian@ian: ~/Install_ProtCool
-- source ./initMGLtools.sh (bash) or ./initMGLtools.csh (c-shell)

Please have a look at README file for more information about
licenses, tutorials, documentations and mailing lists for the different
packages enclosed in this distribution
If you have any problems please visit our FAQ page (http://mgltools.scripps.edu
/documentation/faq).

find: '/run/user/1000/gvfs': Permissão negada
MGLTools path added to PathUser - Caminho do MGLTools adicionado ao PathUser
MGLTools path already registered - Caminho do MGLTools ja registrado
MGLTools path added to PathUser - Caminho do MGLTools adicionado ao PathUser

#####
# All dependencies have been finalized. Thank you for doing the installation! #
# Todas as dependencias foram finalizadas. Obrigado por fazer a instalacao! #
#####

ian@ian:~/Install_ProtCool$
```

After installation, at home folder will be the ProtCool folder where the researcher will work. In addition, there will be folders created by the installer that will be needed to run the tools.

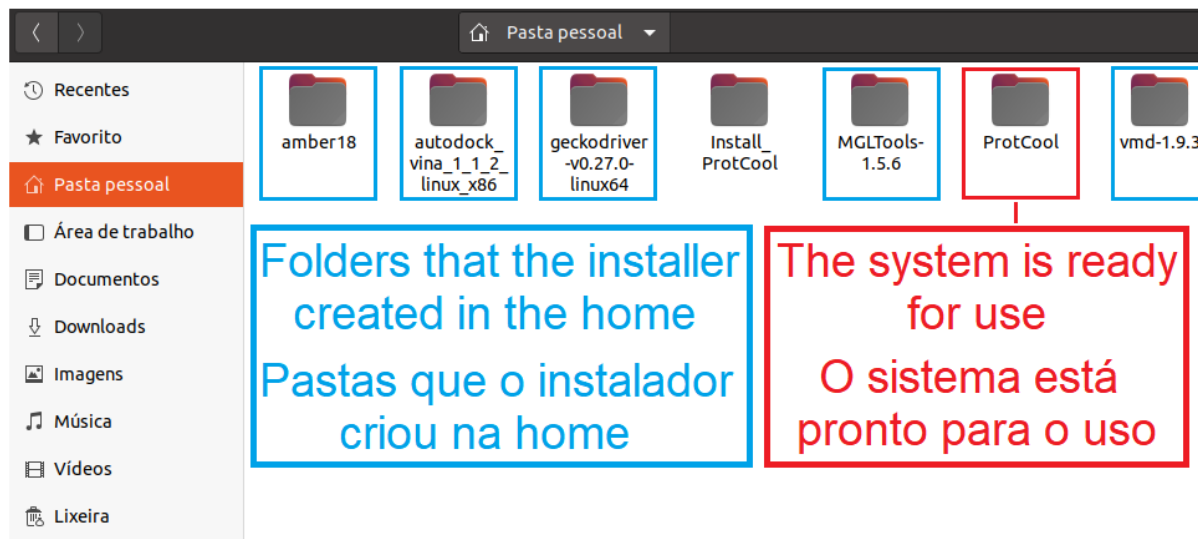
Folders that were created at home:

```
amber18, autodock_vina_1_1_2_linux_x86,
geckodriver-v0.27.0-linux64, MGLTools-1.5.6, ProtCool, vmd-1.9.3
```



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The researcher can delete the computer so the system installation folder, as the ZIP folder that was lowered by the researcher.

If the researcher wishes, there is a step-by-step video that reproduces this material.

For the execution of the systems, the researcher can check both the videos and the tutorials of each of the systems.