Instructions for preparing a separate python for running HullRad on Mac Intel machines. This procedure will install a self-contained version of Python with all necessary libraries in a sub-directory (folder) in your home directory (personal user folder). It will not change any system files and can be removed in the future by simply deleting the sub-directory.

This installation and running of HullRad uses a terminal window. If you are not familiar with this, just click on the Terminal icon in the Utilities folder on your Mac. A window will appear in which you can type commands. The following assumes you are using zsh shell which is the default for MacOS. (If you don't know what that means ignore it.)

Miniconda is a minimalist version of Anaconda, the popular software package manager.
Download miniconda from: https://docs.anaconda.com/miniconda/

Choose macOS
and this - Miniconda3 macOS Intel x86 64-bit bash

This file will usually go into your Downloads directory. Now launch a Terminal window and type the following commands on the command line prompt to copy the downloaded file to your home directory (or just copy and paste the `Courier` font following the `%`).
`% cd` (Automatically changes to your home directory in case you are not already there)
`% cp Downloads/Miniconda3-latest-MacOSX-x86_64.sh .` (Note the dot at the end.)

Unpack the distribution
```
% source Miniconda3-latest-MacOSX-x86_64.sh -b -p $HOME/miniconda
```
Answer y when prompted
This will take a minute

Activate it,
```
% zsh miniconda/bin/activate
```

Initialize everything,
```
% miniconda/bin/conda init --all
```

You may get the following,
==> For changes to take effect, close and re-open your current shell. <==
Do it.
You should have a new command line prompt with (base) in it.

Create a python environment for HullRad.
This will also install needed libraries (numpy scipy biopython)
```
% conda create --name HullRadPython python=3 numpy scipy biopython
```
Answer `y` when prompted.

Done with installation

Now when you want to use HullRad in a terminal window.

Make a sub-directory (folder) and put your PDB files there.
You can make a new folder using the Finder (as an example, I'll name it PDBs). Then highlight the folder, chose View | Show Path Bar. The full path will be displayed at the bottom. For example, it may look something like,

Macintosh HD > Users > pat > Documents > PDBs

Where pat is my home directory.

In a Terminal window change to the sub-directory with the PDB files. For example, for a newly launched Terminal window that, by default, puts you in your home directory,

```
% cd Documents/PDBs
```

Then go to the HullRad website (www.jhu.edu), download the latest version of HullRad (currently HullRadV10.py or HullRadSASV3.py), copy it to the sub-directory with your PDB files.

```
% cp ~/Downloads/HullRadV10.py .
```
(Note the leading tilde and trailing dot)

In the Terminal window you want to use for HullRad activate the environment (this tells the computer to use the special HullRad python installation).

```
% conda activate HullRadPython
```

You should have a new Terminal line prompt with "(HullRadPython)" in it. If this is not the case, HullRad won't work.

Type, e.g.,

```
% python HullRadV10.py 7rsa.pdb
```

The first time will take a while because all the libraries have to be loaded in RAM, subsequent will be faster.

When done with HullRad if you want to exit the special HullRad python environment,

```
% conda deactivate
```

Or just close the terminal window.

To permanently remove the special Python installation just delete the miniconda directory.

Notes on PDB files. Many PDB files (or mmCIF) files from the RCSB have multiple copies of the protein of interest. It's likely this is not the oligomer state in solution. For HullRad to give you an accurate analysis the PDB file should represent exactly what you have in solution. You should always look at a PDB file using a molecular graphics program before using the file for anything else (e.g., PyMOL, Chimera, VMD, Jmol, etc.). You can edit the PDB file to contain only the copy (chains) as it exists in solution.

Many PDB files also have missing residues. HullRad may not notice this and the calculated hydrodynamic properties will not reflect the solution structure. Sometimes the crystallographers will include only the backbone atoms but not the side chain. HullRad needs at least the CB atom and will not work if the entire side chain is missing. A solution to the above for proteins is to use the AlphaFold structure. For a folded protein it will be an accurate model. Note that if your protein has flexible loops, or an IDR, the single structure will likely not represent what exists in solution. But the AlphaFold structure will be a good start for modeling an ensemble of conformations.

Beware that the AlphaFold structure has all the amino acids in the open reading frame of the DNA. If your protein is processed by the cell, the actual protein you are studying in solution will be different from the AlphaFold one.

To find both the AlphaFold structure and the sequence of the mature, processed protein go to UniProt (https://www.uniprot.org/). Find your protein in this database, and on the protein's Entry page, you will find links to the AlphaFold structure and the sequence of the mature form.