Instructions for preparing a separate python for running HullRad on Windows with Powershell. 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.

You may already have PowerShell on your machine (It may be called Terminal in the dock). If not follow the instructions here,
https://learn.microsoft.com/en-us/powershell/scripting/install/installing-powershell-on-windows

Miniconda is a minimalist version of Anaconda, the popular software package manager.
Download miniconda from: https://docs.anaconda.com/miniconda/
Choose Miniconda3 Windows 64-bit

This will usually go into your Downloads directory. Double click on the downloaded
Miniconda3-latest-Windows-x86_64.exe
Follow the instructions on the screen.

From the Start menu open the Anaconda Powershell Prompt (miniconda3)
You should have a new command line prompt with (base) in it.

In the PowerShell window create a python environment for HullRad.
This will also install needed libraries (numpy scipy biopython)

```
> conda create --name HullRadPython python=3 numpy scipy biopython
```

Done with installation.
(You can close the Anaconda Powershell Prompt window if wanted, you will need to re-launch it when you want to use HullRad).

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Now when you want to use HullRad, make a sub-directory (folder) and put your PDB files there. For example, make a folder called PDBs inside your home directory (folder).

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.

From the Start menu open the Anaconda Powershell Prompt (miniconda3)

Activate the environment (this tells computer to use the special HullRad python installation). Type (or copy paste) the following in the PowerShell command line.

```
> conda activate HullRadPython
```

You should have a new line prompt with "(HullRadPython)" in it

In the PowerShell window that now knows about HullRad, change to the directory where both HullRadV10.py (or HullRadSASV3.py) and PDB files are. For example,
`> cd PDBs` (Assuming you made the PDBs folder inside your home directory (folder)).

Then type for example:
```
> python HullRadV10.py 7rsa.pdb
```

When done with HullRad just close the Anaconda Powershell window.

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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.