

Drug Docking with Schrodinger HPRC Short Course Series

Supplements to the reminder email:

For better hands-on experience during the short course, it is highly recommended that you make sure the Schrodinger software loads properly in your account on Grace before attending the short course. Please see the information and instructions below. If you are not familiar with the HPRC Grace Portal, please watch the following short instructional videos:

Using OpenOnDemand: Intro <https://youtu.be/dqa2ZzsEmQs>

Using OpenOnDemand: How to Run a VNC Job <https://youtu.be/ORxFJVSZSyc>

1) Connect to the HPRC Grace Portal: <https://portal-grace.hprc.tamu.edu>

2) Launch a VNC Session. Under Interactive Apps, choose VNC, request a session with:

Number of hours: **3**

Number of cores: **4**

Total Memory (GB): **8**

Node type: **ANY**

and then click **Launch**. When the desktop is ready, click the launch **VNC** button, which will open VNC in a new browser tab..

3) Load the modules required to run the Schrodinger software.

Type in the terminal:

ml purge

ml Schrodinger/2021-3

4) Run the Schrodinger software (maestro).

Type in the terminal: **maestro**

It may take a few minutes for Maestro to show up, please be patient. If it loads properly, you can close Maestro and log out from the session by typing exit in the terminal.

If you experience any problems, please contact help@hprc.tamu.edu