

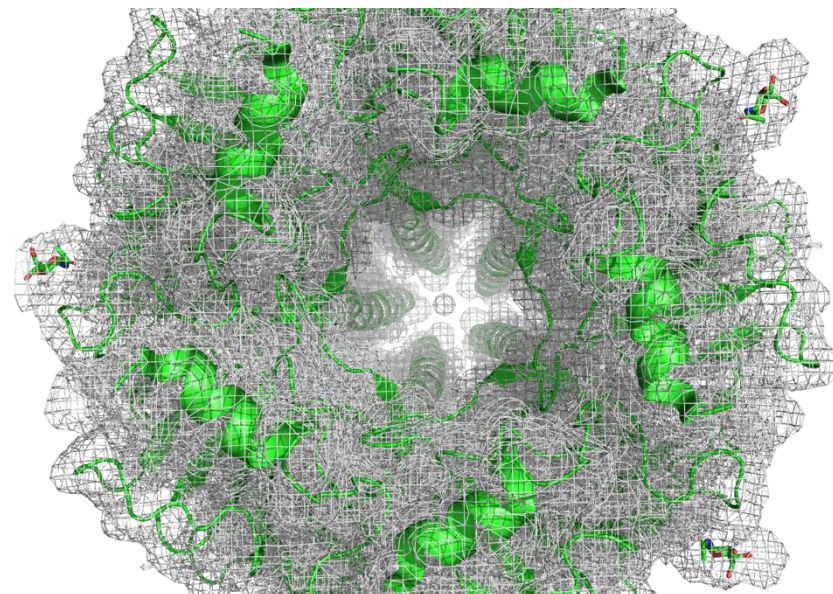
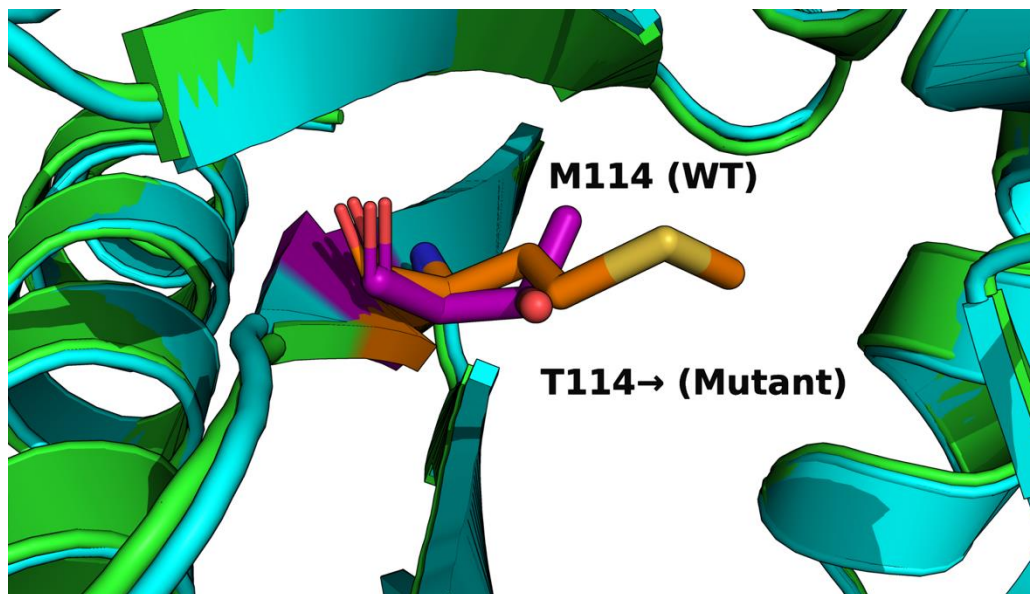
RECITATION 2

Figure Review · Cluster Access

Modern Methods in Drug Design — COBB2035

Recitation 1 - PyMol

Installed the open-source PyMol



1. Labels:
 1. Residue or ligand name plus number.
 2. Nothing overlapping.
2. Color sticks by element. N blue, O red.
3. Show the atoms that carry the claim and Frame the claim
4. Make the molecules distinguishable. One colour per chain or protein. Do not use a confusing color palette.
5. Write a caption a reader can understand the full figure from.
6. Show only what the caption talks about.

Recitation 2

Getting onto the cluster

WINDOWS ONLY

A bash shell first

```
# PowerShell, running as Administrator
wsl --install    # installs Ubuntu by default
wsl --list --online  # other distributions
wsl    # drop into the Linux shell
```

STEP 1

Log in, change your password

```
ssh username@cluster.csb.pitt.edu # username is all lowercase
passwd # change the temporary password
```

STEP 2

SSH key

Run these on your laptop

```
ssh-keygen -t ed25519 # accept the default path;
ssh-copy-id username@cluster.csb.pitt.edu
ssh username@cluster.csb.pitt.edu # should not prompt now
```

WHAT YOU JUST MADE

~/.ssh/id_ed25519

Private key.

~/.ssh/id_ed25519.pub

Public key. This is the half that gets copied to the cluster.

~/.ssh/authorized_keys

On the cluster. ssh-copy-id appends your public key to it.

permissions

700 on ~/.ssh, 600 on authorized_keys. Wrong modes = silent fallback to password.

BEFORE YOU RUN ANYTHING

PARTITIONS

`dept_cpu` Nodes without a GPU. Your default.

`dept_gpu` GPU nodes. Request the card with `--gres=gpu:1`

headnode01:~\$ think_before_you_type
headnode01:~\$ be_kind_to_your_fellow_users

THIS IS A SHARED RESOURCE

STOP

RUNNING VSCODE ON THE HEAD NODE

YOUR EDITOR. YOUR JOB. EVERYONE PAYS.

- ✗ SLOW LOGINS
- ✗ QUEUE DELAYS
- ✗ LAGGY NFS
- ✗ ANGRY USERS
- ✗ CRYING ADMINS

DON'T BE THAT PERSON.

HEAD NODE IS NOT A WORKSTATION

- NO GUI APPS
- NO IDES
- NO EXCUSES

RESPECT THE CLUSTER.

WARNING

Running VSCode on the head node can consume CPU, memory, and I/O resources needed by everyone.

EDIT LOCALLY. SUBMIT JOBS. LET OTHERS WORK. BE CONSIDERATE. BE AWESOME.

I'M A PENGUIN, NOT YOUR PERSONAL DESKTOP.

SHARE RESPECT. SHARE COMPUTE.

```
[user@login01 ~]$ qstat
```

Job ID	Name	User	ST	Time	Nodes
1234567	md_sim	alice	R	12:34:56	64
1234568	dft_run	bob	R	05:23:11	128
1234569	training	carol	R	02:11:07	32
1234570	assembly	dave	Q	01:02:45	64
1234571	analysis	erin	R	00:45:21	16
1234572	genomics	frank	Q	00:10:03	128
1234573	weather	grace	R	03:33:19	256

```
[user@login01 ~]$
```

STEP 3

miniconda and the struct environment

```
srun --pty -p dept_cpu /bin/bash
```

```
# from the VS Code terminal - already on a compute node
```

```
cd ~
```

```
wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
```

```
bash Miniconda3-latest-Linux-x86_64.sh # accept the licence, allow conda init
```

```
exec bash # reload the shell so conda is on PATH
```

```
conda create -n struct python=3.12
```

```
conda activate struct
```

```
conda install -c conda-forge openff-toolkit-examples dill mdanalysis pdbfixer
```

```
(struct) mag1037@n001:~$ python
Python 3.12.14 | packaged by conda-forge | (main, Sep 1 2026, 15:55:32) [GCC 14.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import openmm
>>>
```

1. Let us know when you are done
2. Upload a screenshot to Gradescope to get graded

Basic = done

VS Code, use a Tunnel

```
cd ~      # the job script hardcodes ~/VSCode-linux-x64
wget --content-disposition -E -c \
  "https://code.visualstudio.com/sha/download?build=stable&os=linux-x64"
tar -xzf code-stable-x64-*.tar.gz    # extracts into ./VSCode-linux-x64
ls ~/VSCode-linux-x64/bin/code      # confirm this path exists
```

Install VS code extension: Remote – Tunnels

EXTRA ✓+

Launch it as a SLURM job

```
#!/bin/bash
#SBATCH --job-name=vscode
#SBATCH -p dept_cpu
#SBATCH -t 8:00:00
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=4
#SBATCH --output sbatch.stdout    # remember this filename

~/VSCode-linux-x64/bin/code tunnel \
    --accept-server-license-terms --name "slurm-${SLURM_JOB_ID}"
    or
    --accept-server-license-terms --name "cluster"
```

SUBMIT AND WATCH

```
sbatch tunnel.slurm
queue -me    # wait for ST to read R, not PD

more sbatch.stdout
```

WHAT YOU'RE LOOKING FOR

To grant access to the server, please log into <https://github.com/login/device> and use code XXXX-XXXX

