Rosetta
Tips and Tricks

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Attendance
tinyurl.com/y33jhcxr

Rosetta Tips

- Always try Googling the error message
- Need to be aware of relative paths
- To extract need to have enough space for both the archive and expanded folder, then for compiled files
- Run bin files from source folder
  - ./bin/AbinitoRelax
- Add **&** to end of command to run in the background
- Take advantage of Tab complete and arrows

main/source – Main folder to put files

main/source/bin – Executables to run

main/database – Chemical properties

demos/tutorials – Useful tutorials

tools – Handy automation scripts

```
-in¬
        -file¬
                -fasta input_nanobody/nanobody.fasta¬
                -frag3 input_nanobody/aat000_03_05.200_v1_3¬
                -frag9 input_nanobody/aat000_09_05.200_v1_3¬
-abinitio¬
        -relax¬
        -increase_cycles 10¬
        -rg_reweight 0.5¬
        -rsd_wt_helix 0.5¬
        -rsd_wt_loop 0.5¬
-relax¬
        -fast¬
-out¬
        -pdb¬
        -nstruct 300¬
        -file¬
                -scorefile score.sc¬
-overwrite¬
```

- Linux terminal text editor
- Run with 'vim file.txt'
- Modal text editor
  - To type text, press 'i' first
  - To get back to default mode, press ESC
- Useful for editing files for Rosetta
- See my Vim slides for more details
- Use vimtutor to learn through doing
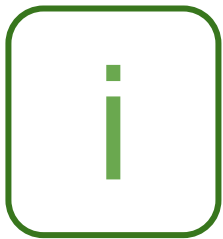
i	Enter insert mode
ESC	Go back to normal mode
ZZ	Save and exit file
p	Paste from clipboard
v	Enter visual mode select text
:	Enter command prompt

:w – Save file

:wq – Save and Quit

:sort – Sort selected lines

:set ff=unix – Use Unix line endings

Linux Tricks

- Use /mnt/c/ to access Windows from Linux subsystem
  - mv /mnt/c/Downloads/rosetta ~
    - C:\Users\NAME\AppData\Local\Packages\DISTRO_FOLDER\LocalState\rootfs
- Install things with
  - sudo apt install PROGRAM
  - Use 'search' to find program
  - Tab complete program

PyMOL

- Different from PyRosetta

- **Left click** Pan/Rotate
- **Right click** Zoom in/out
- **Middle click** Move
- **Scroll** Change visual depth
- Align all structures with one
    - align S_000X, all