

Intro to Rosetta

Part 2

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Attendance
tinyurl.com/y33jhcxr

De Novo Structure Prediction

- Needs 4 files:
 - Fasta sequence
 - 9mer and 3mer fragment files
 - Options file
- Can generate fragment files from Robetta
- Do Novo program found in main/source/bin/
 - Called AbinitioRelax.default.linuxgccrelease

```
-ln~  
    -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~
```

Run with

`./AbinitioRelax.default.linuxgccrelease @options`

Generates `S_0001.pdb` and `score.sc`

Open with

`pymol S_0001.pdb`