Virtual screening and 3D protein structure model optimization of the DSP family

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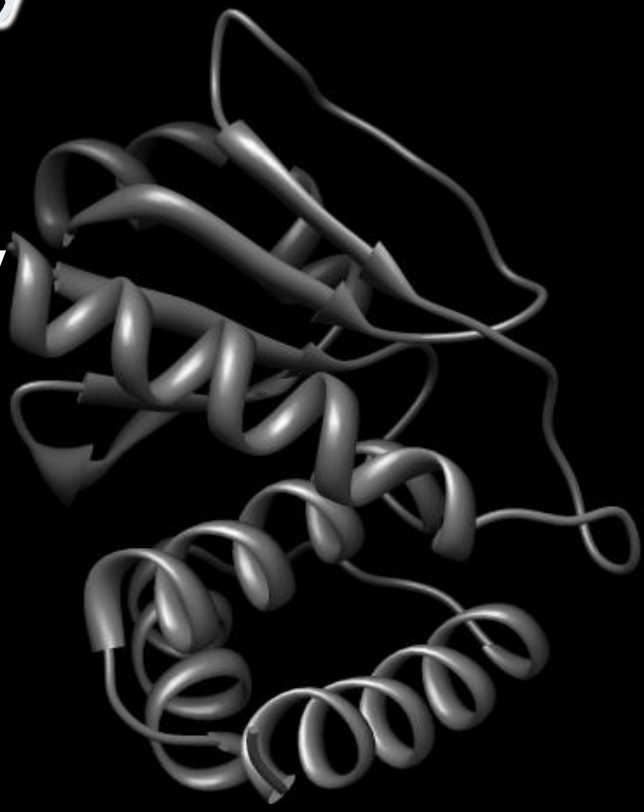

Week 5 Progress

- Reranked results of SSH3 DOCK screening
- Vicky continuing AMBER screening of SSH1 on milk
- Josh continuing AMBER screening of SSH3 on milk
- Working on fixing issues with DOCK on milk and ocikbpra
  - Reinstalled DOCK and open-mpi on milk
  - Cleaned out ocikbpra cluster and reinstalled

Next Week's Goals

- Get AMBER screening working across multiple clusters without issues
- Start AMBER screening of DUSP21
- Organize and compile results of DOCK and AMBER screenings of SSH1, SSH3
- Read about Open MPI and DOCK6 software functionality to better understand problems that are coming up and figure out how to fix problems
- Learn more about scripting

Major Successes

- Wrote script that automates installation for clusters
- Making progress on screening priority proteins in DSP family, SSH1 and SSH3

Road Blocks

- Installation issues leading to problems in screening
  - Working on pinpointing issues
  - Discussing issues with teammates and dividing tasks
- Sharing processor space
  - Processors used for priority proteins first

Clockwise, from top left:
-Making friends with the Toyonaka campus cat
-Path to Kasiga Grand Shrine (春日大社) in Nara
-Fireworks at the Tenjin festival (天神祭)
-Making friends with deer in Nara
-Okonomiyaki! (お好み焼き)
-Bamboo forest in Arashiyama (嵐山)

Culture!




Before and after:
(Traditional Japanese style buffet in Arashiyama)

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