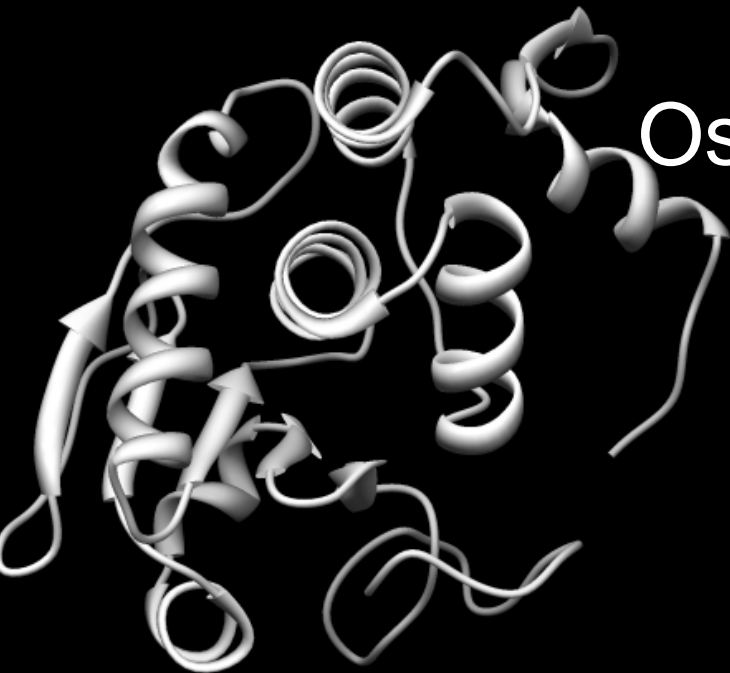


Virtual screening and 3D protein structure model optimization of the DSP family

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Week 6 Progress

- Learning perl
- Working on script to find and remove error causing molecules in AMBER
- Got access to NCHC cluster
- Vicky running AMBER slices with error molecules removed for SSH1 on milk
- Josh continuing AMBER for SSH3 on milk and DOCK for PRL2 on rocks-200

Next Week's Goals

- Get AMBER screening working across multiple clusters without issues
- Check to see if other clusters can be used
 - ocikbpra currently seems to be under maintenance
- Get AMBER error finding script working
- Finish up screening and clean up results of SSH1 and SSH3

Major Successes

- Wrote script that automates installation for clusters
- Making progress on screening priority proteins in DSP family, SSH1 and SSH3
- Learning basics and application of computer programming

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:

-World's largest bronze statue of the Buddha Vairocana (大仏)

-Great Buddha Hall (大仏殿) of Todaiji (東大寺). It is the largest wooden structure in the world.

-Statue of Agyo (阿形), one of two guardians of Buddha (known as Nio, 仁王)

-Nandaimon (南大門), where the Nio are found

-Herd of deer in a field near Kasuga taisha

-South gate (南門) of Kasuga taisha

Culture!



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