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
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