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

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Week 7 Progress

• Script for finding and removing AMBER errors completed

• AMBER screening of SSH1 completed, preparing for rerank, grabtop, and consensus

• AMBER screening of SSH3 continuing
  – Cluster resources of milk reallocated to Vicky for faster screening
Next Week’s Goals

- Finish up screening and clean up results of SSH1 and SSH3
- Learn how to script across multiple clusters
- Start AMBER screen for proteins that have finished with DOCK scoring (DUSP21)
- Get AMBER screening working across multiple clusters without issues
**Major Successes**

- Wrote scripts to automate installation for clusters and find and remove AMBER error molecules
- 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:
- Make your own soba experience success
- Sukiyaki with special red konnyaku noodles
- View of Lake Biwa (琵琶湖) from the top floor of Hikone castle (彦根城)
- Converyer belt sushi
- Traditional boat ride (水郷めぐり)
- Styrofoam river rafting, a popular new sport on the water systems (かばた) of Takashima (高島市)
Shimojo lab tour group picture! (Taken at Hikone castle)
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