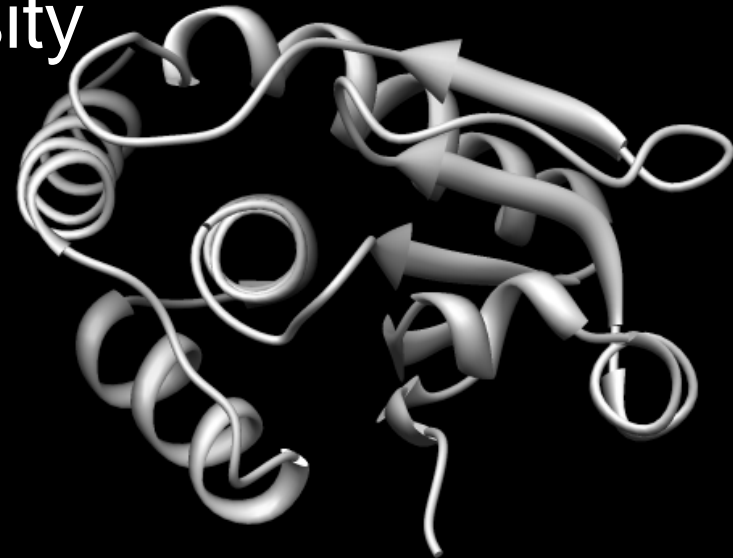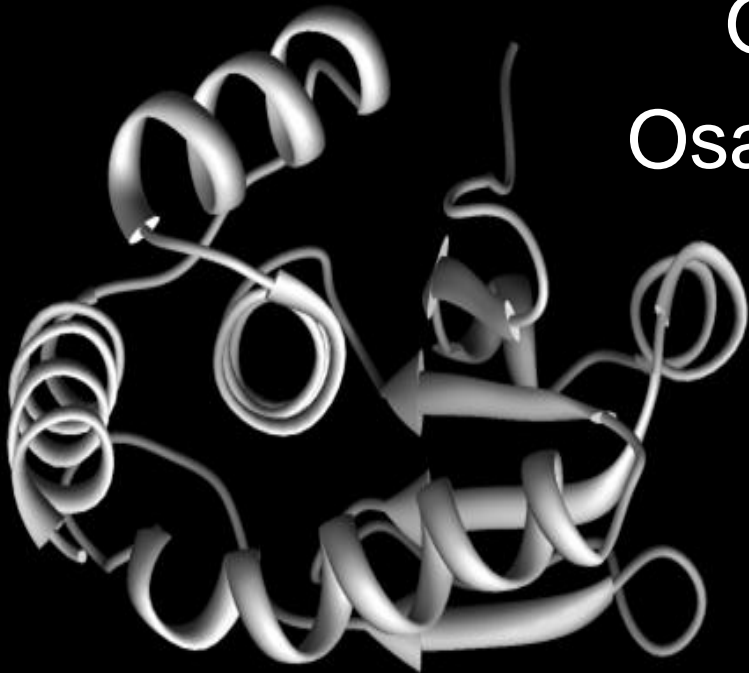# Virtual screening and 3D protein structure model optimization of the DSP family

Olivia Yang

Osaka University

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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 automates 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)

-Conveyer 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)

Culture!

Shimojo lab tour group picture! (Taken at Hikone castle)

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