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

Olivia Yang
Osaka University
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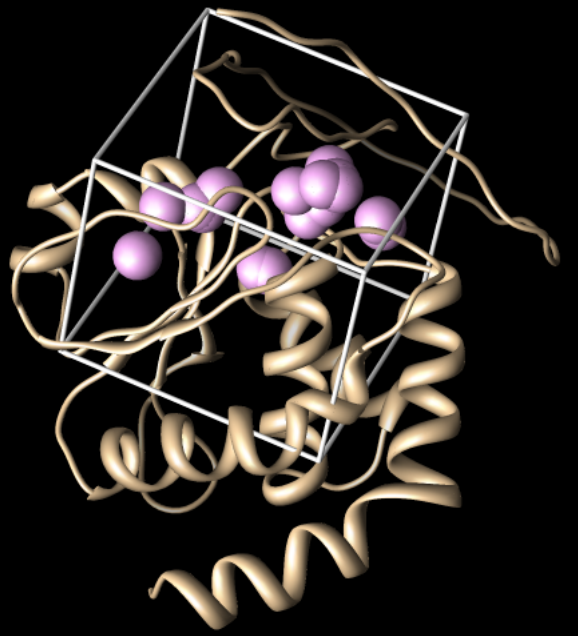

Proposed Research

- **Using virtual screening methods to find a specific inhibitor for SSH-2**
- Because proteins in the DSP family have a highly conserved active site, compounds must be screened for affinity across the entire family
- Proteins in the family without x-ray crystallography structures had 3D structures generated by homology comparison program MODELLER
- 3D structures must be refined in order to get more accurate results from docking
  - Energy refinement with UCSF Chimera
  - Loop refinement with MODELLER
  - Compound screening with DOCK6

Week 1 Progress

- List of MODELLER protein structures compiled from last year's PRIME project
  - Prioritized proteins based on structure
- Finished energy minimization steps of priority proteins
- Loop refinement started for most priority proteins
- Finished preparation steps for DUSP19, started docking

Next Week's Goals

- Fix loop refining script so script will stop running once finished modeling
- Find way to get DOPE scores for each loop refined model for better determination of best model
- Test MODELLER and docking scripts on milk cluster
- Find out how to best use SSH-1 and SSH-3 models

Clockwise, from top left:
-Simultaneous butter/jam squeeze packet
-Pizza+sushi welcome party
-Arrival picture
-Airplane playground structure
-Cat!

Culture!