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



## Week 2 Progress

- Reranked results of SSH1 DOCK screening
- Finished DOCK of DUSP21
  - Error on one of the slices needs to be checked
  - Preparing for AMBER screening of DUSP21
- Learned new Linux commands

- Found DOCK issues on ocikbpra and rocks-200
  - Checked paths used; reinstalled DOCK, opal, and jakarta

### Next Week's Goals

 Get AMBER screening working across multiple clusters

Get DOCK working on all clusters without issues

Clean up results of DUSP21 DOCK

AMBER screen SSH1 (high priority)

 Find way to get DOPE scores for each loop refined model for better determination of best model

#### Clockwise, from top left:

- -Shijo street (四条通), pedestrian only for the Gion festival (祇園祭)
- -Float (鶏鉾, niwatori boko). One of many lining Shijo street
- -Food stand selling Kobe beef skewers

- -Inside the shrine (八坂神社, Yasaka shrine)
- -Green tea shaved ice
- -Outside the shrine



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