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

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Week 2 Progress

• DOCK running on both rocks-200 and milk clusters
• Jobs can be sent between clusters
• DOCK jobs for DUSP19 and DUSP21 complete
  – May have some errors in some slices with DUSP19
• Loop modelling and energy minimization complete for most modelled proteins
Next Week’s Goals

• Check and resend problematic slices of DUSP19
• Check results of DUSP21, rerank, and prepare for AMBER screening
• Find way to get DOPE scores for each loop refined model for better determination of best model
• Start DOCK preparation and DOCK for other proteins
Clockwise, from top left:
-Kinkakuji (金閣寺, Temple of the Golden Pavilion)
-Monjayaki with lab members after 6 hours of karaoke
-Hands-on instant ramen making experience
-Shrine in Kinkakuji park area
-School cafeteria food!
-Okonomiyaki
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