

# The interactions between DnaK, GrpE, and HtpG

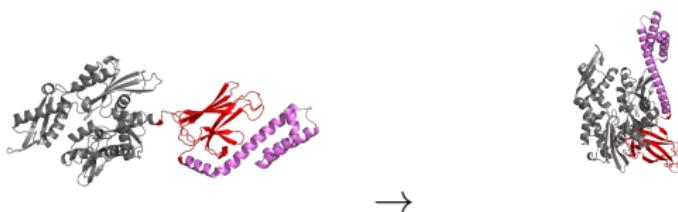
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21 Jan 2021

# Introduction

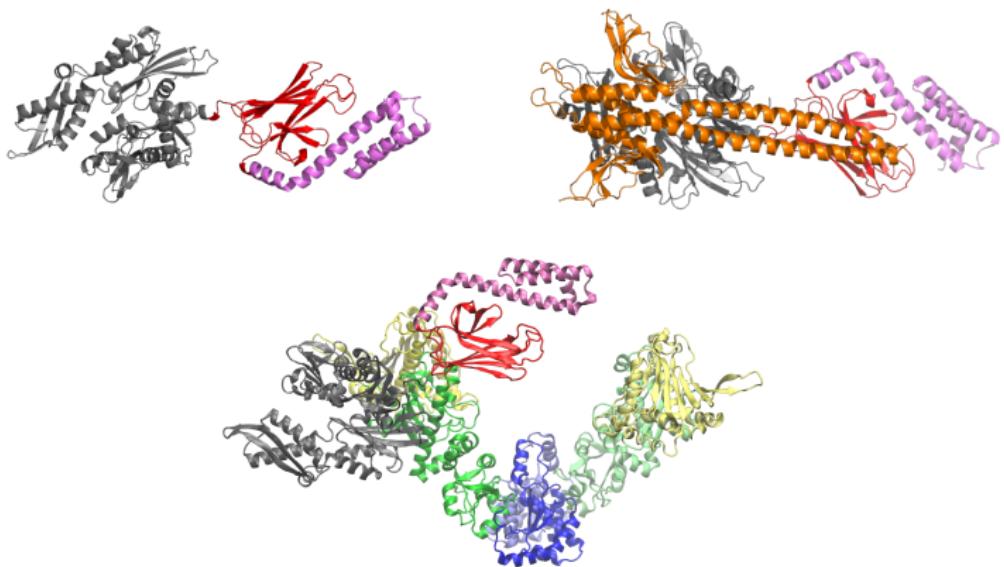
- ▶ DnaK is a molecular chaperone within E. Coli that is known to interact with several cochaperones to refold substrate
- ▶ Interactions in the same binding site indicate that there may be crossover in the actions that occur when binding GrpE and HtpG
- ▶ Observing the interactions that occur between DnaK, Grpe, and HtpG could lead to an explanation of the mechanism of ADP-ATP exchange in the DnaK system



## Normal Mode Analysis of Elastic Network Model

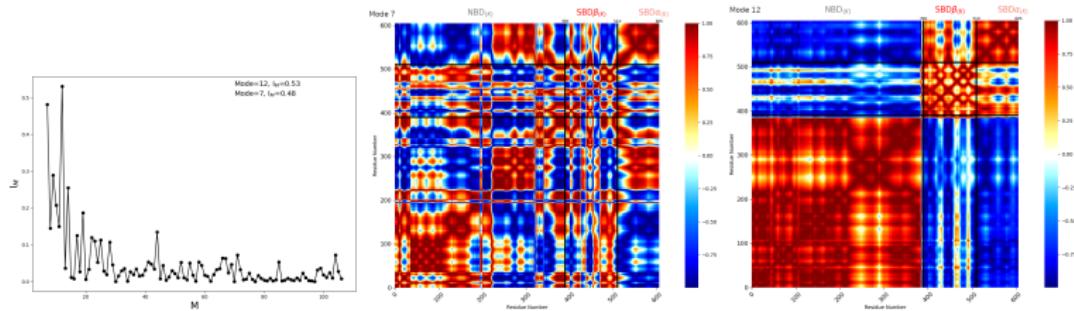
- ▶ Models are collected from PDB (DnaK alone, DnaK-GrpE, and DnaK-HtpG)
- ▶ Interaction models are optimized by using analysis tools such as Itasser, ZRANK
- ▶ Models are simplified from all-atoms to coarse grain, single node at Carbon- $\alpha$  position
- ▶ Springs are placed between any nodes that are within 9 Å, then calculations are performed to produce vibrational modes
- ▶ Vibrational modes are compared to biological conformations to ensure high overlap between one conformation and another

# Binding of DnaK, GrpE, and HtpG

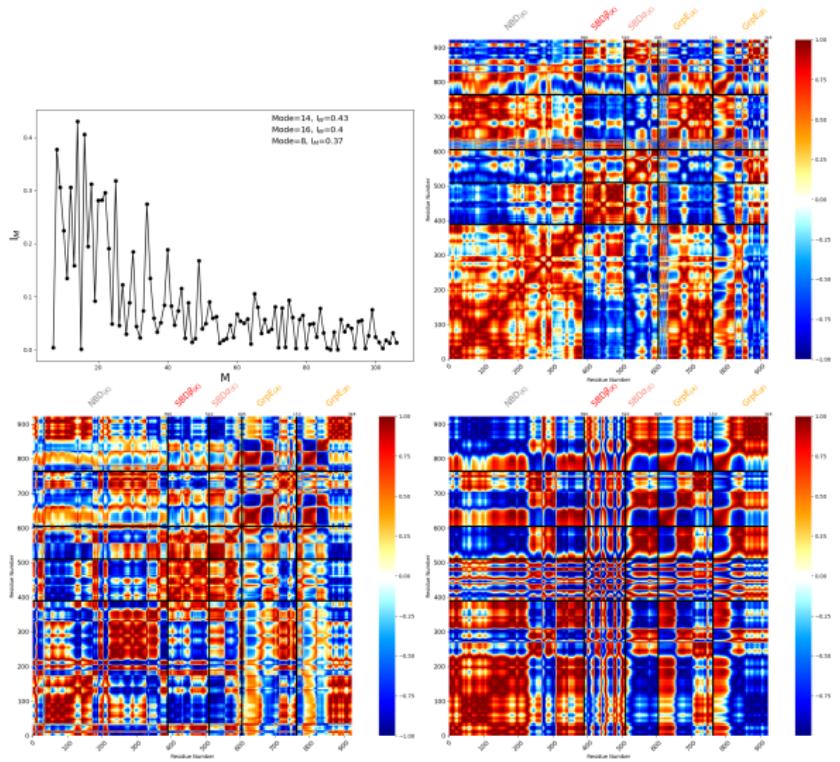


# DnaK ADP Conformation Correlations

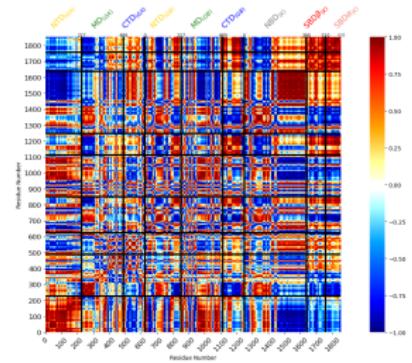
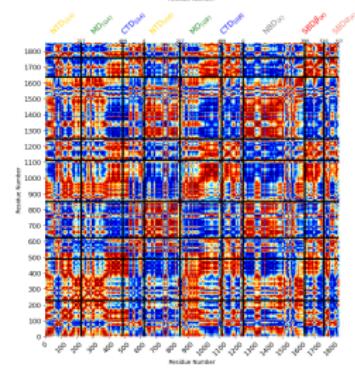
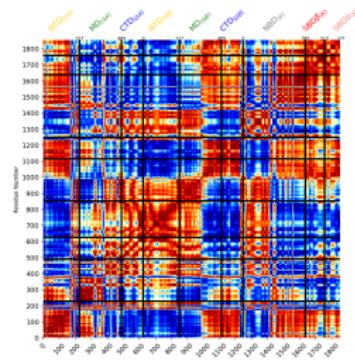
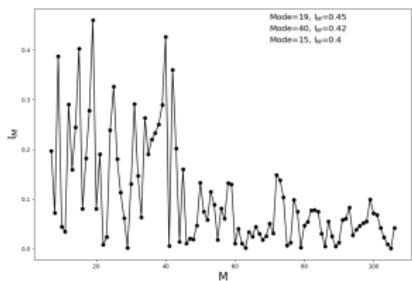
- ▶ Correlation matrices show which sections of the proteins are moving in conjunction with each other
- ▶ Each of the models appear different within their correlations



## DnaK GrpE-bound Correlations



# DnaK HtpG-bound Correlations



## DnaK ADP Conformation Correlations

- ▶ Correlation matrices show which sections of the proteins are moving in conjunction with each other
- ▶ Each of the models appear different within their correlations
- ▶ DnaK-GrpE model has similar rigid-body communications to DnaK alone
- ▶ DnaK-HtpG model has more intramolecular rigid-body communications than DnaK alone model

## Next Steps

- ▶ Hoping to publish the manuscript on HtpG-DnaK soon
- ▶ Much more work must be done analyzing the data from this experiment
- ▶ Another project comparing the HtpG-DnaK interaction to ER homologs is being set up for this semester