

# Plan to Finish

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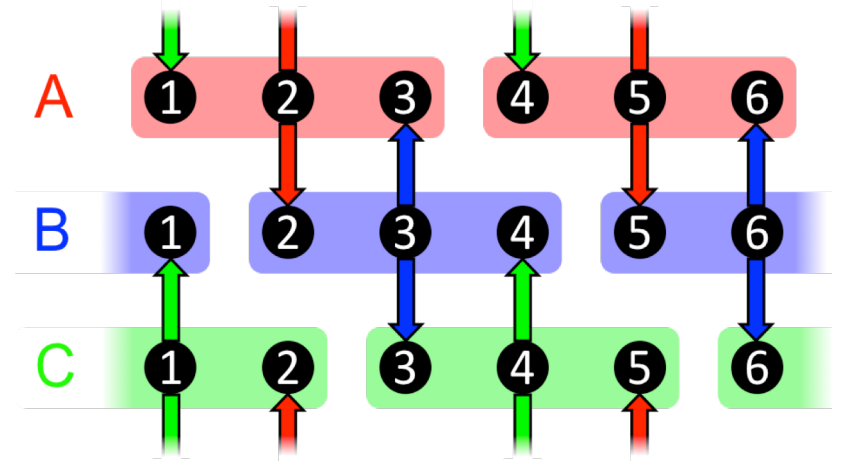
# HFB-DMET

Research Goals:

- Write Fock-space FCI Code
- Implement Hartree-Fock Bogoliubov Theory with Bootstrap Embedding

Project Goals:

- Summarize performance of HFB-BET in a journal article



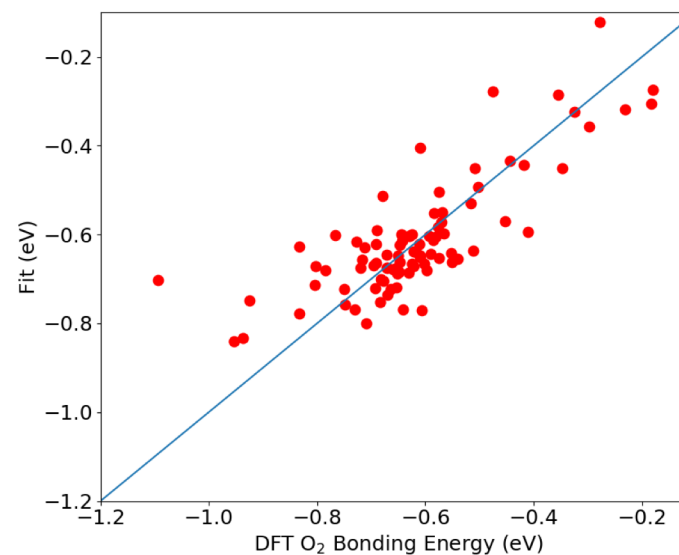
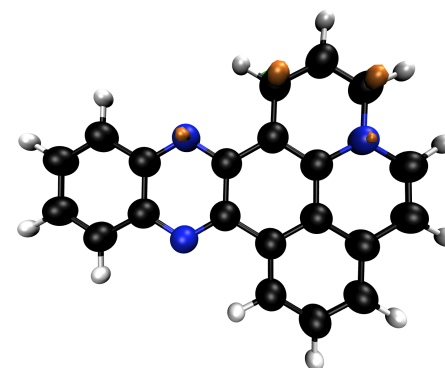
# Catalysis

## Research Goals:

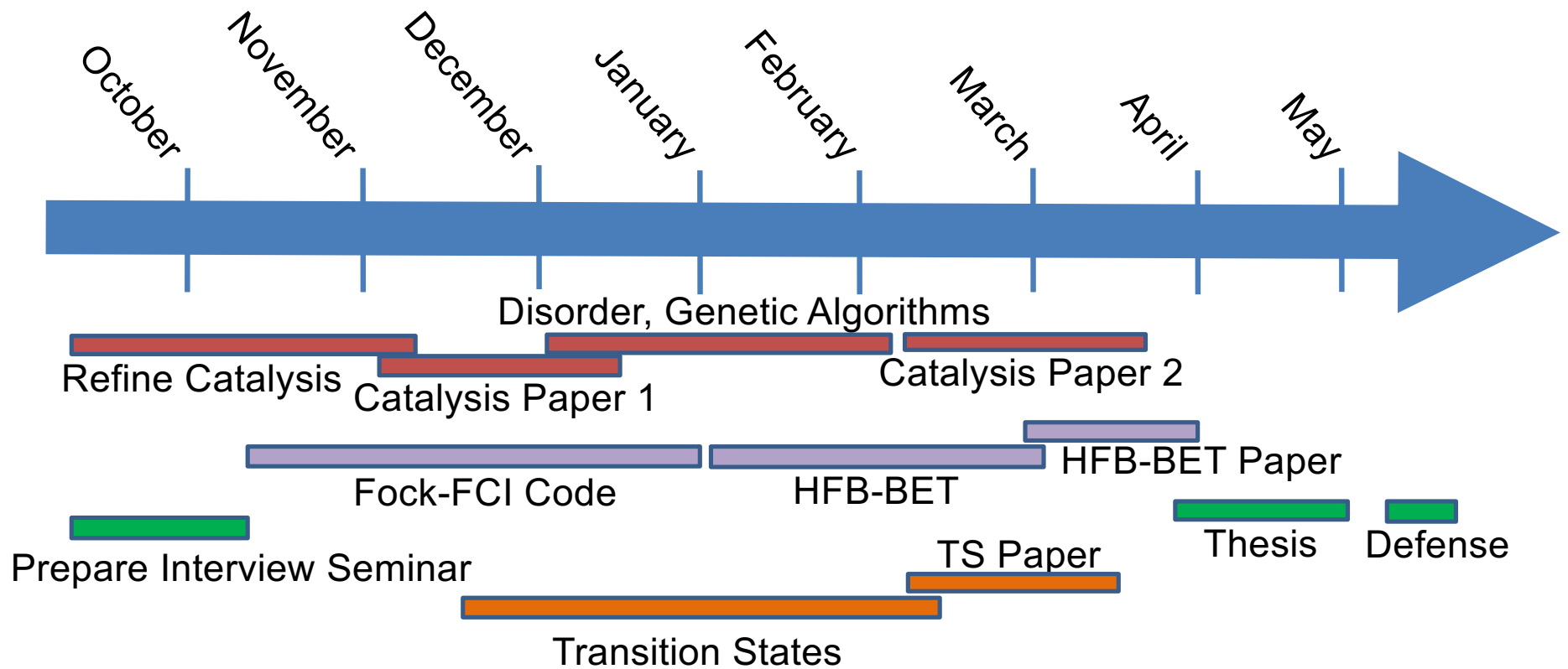
- Refine model for predicting intermediate energies
- Create classifier for identifying active sites
- Incorporate transition state information into screening process

## Project Goals:

- Summarize automated catalysis discovery in 1-2 papers
- Summarize transition state predictions in 1 paper



# Timeline



# Plan to Finish

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**Friday, October 18, 2018**

Anthony Quartararo

Pentelute Lab

# Plan to finish: Milestones

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## Milestone 1: Validate putative binders identified from solution screens

- Perform Bio-Layer Interferometry and fluorescence polarization to determine affinities of each interaction

## Milestone 2: Investigate the practical limit of library sizes

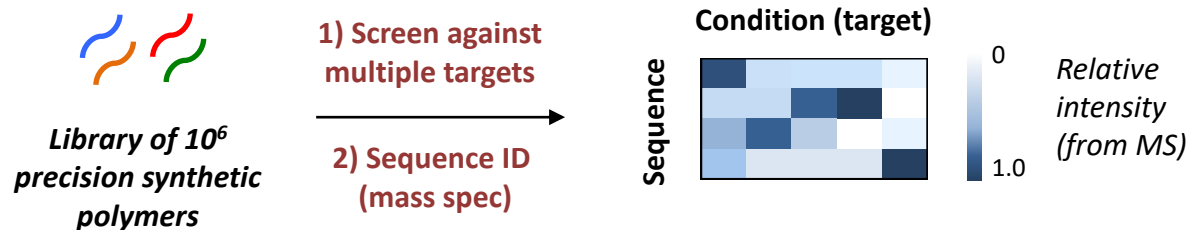
- Expand library sizes to  $10^8$ , approaching diversities of molecular biology-based screening approaches
  - Demonstrate successful isolation and sequencing of positive controls

## Milestone 3: Extend screening platform to whole cells/whole cell lysates

- Identify binders to whole RBCs as proof-of-concept
- Identify binders to proteins isolated from native environments

## Milestone 4: Multiplex screening to pan against multiple targets in parallel

- Demonstrate parallel screening against of up to 10 protein targets at once



# Plan to finish: timeline

