Previous modeling of 3cl^{pro}

- Molecular dynamics simulations that suggest high flexibility [2]
- Molecular docking suggests that
  - HIV protease inhibitors including lopinavir can be repurposed against the COVID-19 enzyme [3, 4]
    - there are clinical trials of using Kaletra (lopinavir/ritonivir) against COVID-19
  - Natural products may inhibit the enzyme [3]
- Binding free energy calculations
  - can be used to refine docking hits to identify the most promising repurposing candidates
  - may inform dosing recommendations in clinical trials
  - can model fluctuations of the enzyme in the presence of different known inhibitors
- To start this demonstration, I used AutoDock Vina to dock the FDA approved drugs database and known inhibitors [1] against 3cl-pro. Then I prepared the some systems for YANK.

Running binding free energy calculations with YANK