

# Caveat: YANK is still under development and may not work

- See a [github issue](#) that I raised for problems with both pipelines
- If a system doesn't work, for the purposes of this class
  - just try another system
  - I want you to
    - get familiar with the ideas and programs of binding free energy calculations
    - not beat your head against a wall trying to solve research-level problems

# References on M<sup>Pro</sup>

- [1] Jin, Z.; Du, X.; Xu, Y.; Deng, Y.; Liu, M.; Zhao, Y.; Zhang, B.; Li, X.; Zhang, L.; Peng, C.; Duan, Y.; Yu, J.; Wang, L.; Yang, K.; Liu, F.; Jiang, R.; Yang, X.; You, T.; Liu, X.; Yang, X.; Bai, F.; Liu, H.; Liu, X.; Guddat, L. W.; Xu, W.; Xiao, G.; Qin, C.; Shi, Z.; Jiang, H.; Rao, Z.; Yang, H. Structure of Mpro from COVID-19 Virus and Discovery of Its Inhibitors; preprint; Biochemistry, 2020. <https://doi.org/10.1101/2020.02.26.964882>.
- [2] Bzówka, M.; Mitusińska, K.; Raczyńska, A.; Samol, A.; Tuszyński, J.; Góra, A. Molecular Dynamics Simulations Indicate the COVID-19 Mpro Is Not a Viable Target for Small-Molecule Inhibitors Design; preprint; Molecular Biology, 2020. <https://doi.org/10.1101/2020.02.27.968008>.
- [3] Khaerunnisa, S.; Kurniawan, H.; Awaluddin, R.; Suhartati, S.; Soetjipto, S. Potential Inhibitor of COVID-19 Main Protease (Mpro) From Several Medicinal Plant Compounds by Molecular Docking Study; preprint; MEDICINE & PHARMACOLOGY, 2020. <https://doi.org/10.20944/preprints202003.0226.v1>.
- [4] Contini, A. Virtual Screening of an FDA Approved Drugs Database on Two COVID-19 Coronavirus Proteins; preprint; 2020. <https://doi.org/10.26434/chemrxiv.11847381>.