

Running YANK

- YANK parameters are described in YAML scripts, e.g. [3cl-pro/YANK_GAFF/yaml/MPro_ZINC0000001542916.yaml](#)
- Running ``yank script -y MPro_ZINC0000001542916.yaml'` will execute the code, but you shouldn't do it on the login node on Bridges
- On Bridges you can enter ``python submit_YANK.py --type shared --yaml MPro_ZINC0000001542916.yaml'`, which will create a script and submit it to the queue.

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