Installing YANK

- If you want to run YANK on Bridges, you need to install it in your directory
- For detailed instructions, see http://getyank.org/latest/installation.html
- In short, once you have anaconda/miniconda installed, you can type
  - conda config --add channels omnia --add channels conda-forge
  - conda create --name yank yank
  - conda update --all

Receptor setup

- The YANK workflow requests a PDB file for the receptor
- You have already done similar steps
- I prepared the receptor file by
  - submitting the structure 6LU7 to the PDB2PQR server
  - removing the ligand and water from the main result, 6LU7.pqr
    - results of these first steps are here: 3cl-pro/YANK/receptor
  - copying 6LU7.pqr to 6LU7.pdb to have a file name accepted by the YANK workflow