3 things: free up space, explain ans demonstrate binding event and what a docking software does, hands-on demo

* conda clean -a
* Double-click shortcut for pymol: find executable, drag to dock/COPY to desktop or elsewhere
* Create a folder to store all the project files
* Validate path to ob and smina installation
* place scripts in appropriate location and chmod +x
* PDB entry web view: missing, mutated, chains, binders
* Induced fit and binding mode: 7l6t vs 6w4h, alignment in pymol, catalytic site
* Preparing specific chain of 6w4h as pdb
* Save pymol sessions frequently
* Pdb2pqr server
* Get pqr file, open in pymol, check H
* Copy ligand from original to new object and add H
* Combine protonated ligand and receptor in a new object and rename the object
* Fix receptor position
* Remove clashes of new Hs with sculpting
* (Reason of using rigid receptor here): mimic certain substrate, inaccuracies in the sculpting model
* Extract ligand
* Save ligand as sdf in a "ligand" folder
* bash optimize or double-click
* Recombine the receptor and ligand
* Copy the object complex, rename object, modify ligand
* Extract ligand and optimize geometry
* Recombine receptor-ligand complex
* Create a new folder named complex
* save the complexes in the complex folder. No space in filename!
* Download the scripts provided in unix/box-local to the directory containing the complex folder
* In the chemtools conda env, cd to working dir, execute the docking script
* Note on the speed of flexible docking
* Output score and poses (lig only for rigid docking, united atom ff)
* Distance between hbond donor-acceptor
* Optional check interaction with binana server
* Producing molecular graphics in pymol: distance, residues labels, show only residues 4A from ligand plus KDKE, hide non-polar hydrogens for clarity, ray-tracing images
* CSV file with docking score