Screening docked ligands and viewing trajectories/ensembles

• Demo
  – ViewDock - facilitates screening of ligands output by the program DOCK
  – FindHBond - identifies hydrogen-bonding interactions based on atom types and geometrical relationships
  – MD Movie - tool for visualization/analysis of molecular dynamics trajectories and other structural ensembles

• Hands-on experience
  – ViewDock tutorial (the online version can be accessed from the Chimera Help menu)