Lecture 1. Introduction to Molecular Modeling And Molecular Simulations

- Download materials
  https://mulan.swmed.edu/lecture1.tar.gz

  To unpack the tar.gz ball, run the following command:
  tar xvfz lecture1.tar.gz
  A new directory, lecture1 will be created

- BioHPC account setup
  If you already have an account, please specify your login name, otherwise specify a user name you would like to use

  Please email me your login name/user name to me

- Read two papers in the lecture1/readings subdirectory

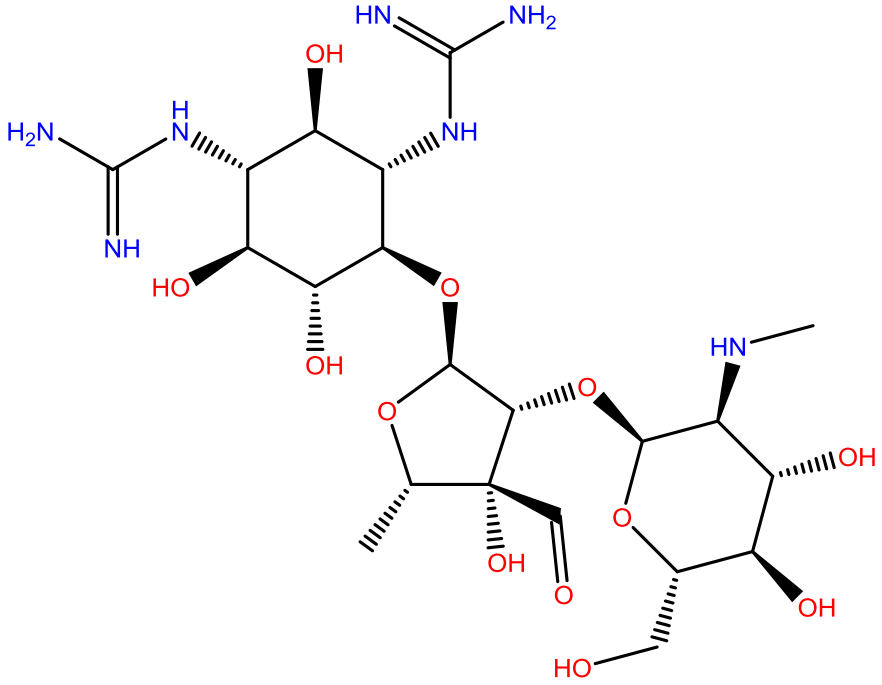
- Learn how to use most common Linux/Unix commands
  vi
  Grep
  Awk
  Sed
  C-shell programming

  (Wait if you cannot access a Linux system, I will email you an instruction on how to log into BioHPC)

- Lear how to use PyMOL
  1. Install PyMOL when necessary (select an proper version from lecture1/software/pymol)
  2. Go through the tutorial (IntroPyMOL.pdf) using the provided pdb files (1BE9, 4S0V) or download your own PDB files from www.pdb.org

- Use online tools
  1. Go to https://mulan.swmed.edu/mmfft/ select “Sign in As A Guest”, Go to “Antechamber” pulldown menu, select “Graphic Antechamber”, then draw a streptomycin structure (shown below), convert it to 3D, and save it as a mol2 file (“Charge method” set to “AM1BCC”, “Atom

Type" set to "sybyl"). What is the SMILES string of this molecule?



2. Go to Molinspiration website (http://www.molinspiration.com/), draw a suvorexant structure (shown below), and then calculate the basic molecular properties and bioactivities.