

Lecture 2. Computer-Aided Drug Design

- Download course materials
<https://mulan.swmed.edu/lecture2.tar.gz>

To unpack the tar.gz ball, run the following command:

tar xvfz lecture2.tar.gz

A new directory, lecture2 will be created

- **Install the following software packages**
 1. Autodock
<http://autodock.scripps.edu/downloads/autodock-registration/autodock-4-2-download-page/>
 2. Autodock-vina
<http://vina.scripps.edu/download.html>
 3. MGL
<http://mgltools.scripps.edu/downloads>
 4. Openbabel
http://openbabel.org/wiki/Get_Open_Babel
- Read articles (Articles1-4) in molecular docking in lecture2/reading
- Perform autodock and autodock4-vina tutorials.
 1. The instruction of autodock tutorial is in lecture2/tutorial/autodock4/autodock4-tutorial.pdf
 2. The instruction of autodock-vina tutorial can be found from <http://vina.scripps.edu/tutorial.html>
 3. The related files are located in lecture2/tutorial/autodock4 and lecture2/tutorial/autodock4-vina