**CDAR Meeting:** 2015-10-02 JiYoung Lee (Bahar Lab)

# **ANM server: Global Motion of Proteins**

## http://anm.csb.pitt.edu/

- \* The Anisotropic Network Model web server at 2015 (ANM 2.0), Eyal E, Lum G, Bahar I. Bioinformatics **31**, 1487-1489 (2015)
- \* Anisotropic network model: systematic evaluation and a new web interface, Eyal E, Yang LW, Bahar I. Bioinformatics **22**, 2619-2627, (2006)

## **Anisotropic Network Model Web Server 2.0**

Go to http://anm.csb.pitt.edu/ Enter PDB id 1. Inputs & ANM calculation (Enter) Cutoff, etc. **Click** Calculate Automatically go to output page: eigenvalues, eigenvectors, movies, etc. **Accept** Java running Change movie and save snapshot (1) **Click** Download files 2. Outputs & Analyses **Click** Create PDB (motion) (3) **Click** Create PyMol script (4) **Click B-factors/mode fluctuations** (5) **Click** Correlations (6)

Additional options: custom PDB, ligands Click Submit your own protein

**Click** Proceed with advanced input options

## Input & ANM calculation & Output



## 1. Inputs & ANM calculation

#### Anisotropic Network Model Web Server 2.0 (2014)



## 2. Outputs & Analyses: (1) Change movie and save snapshot



## 2. Outputs & Analyses: (2) Download files



## 2. Outputs & Analyses: (3) Create PDB (motion)

Create your own PDB file for a selected vibration mode	mode <b>2</b>   cutoff: 15   number of frames: 20   scale: 15
mode: 2	
number of frames (define resolution of motion): 20	
scale (define the amplitude of the motion): 15	2 A NE
submit Click	sen y
	STREE C
VMD Constant of the second sec	95
	Note, the following options are for visualization only and will not alter the PDB file
	Animation Vibration frequency 5 Display backbone Color fluctuations
	Download pdb file of vibrational motion for mode 2
	Click

1xpa.pdb.15.2.15.20.pdb

## 2. Outputs & Analyses: (4) Create PyMol script

Create PyMol scripts to vizualise vibrations	
Define modes (you will get a script for each of the modes in the range). from 2 2 to 2	
number of frames (determine resolution of motion, must be integer, even number prefered): 20 奠	
scale (define the amplitude of the motion): 15	
number of arrows (vectors indicate size and direction of motion) per chain : 5	an N
submit Click	
To explore the dynamics of each mode using PyMol:	
<ul> <li>Download the 3 files below associated with the mode to one folder on your local computer</li> <li>Open PyMol</li> <li>From the main menu choose the "Run" option</li> <li>In the dialog box choose the script with the suffix ".pml" that you just downloaded</li> <li>You will now see that the molecule appear on the screen. To start the animation just press on the play (triangle) side of the session.</li> <li>Use the other buttons to stop the animation and go back and forth between the frames. You can also control the choosing the "Speed" option from the "Movie" manu in the upper tool bar in the consule page.</li> </ul>	bottun on the lower right e speed of the animation by
A zipped directory with all files for modes 2 - 2	
Mode 2:	
Ixpa_Mode_00002.pml	
1xpa_Mode_00002_Arrows.py	
xpa_Mode_00002.pdb	
A zipped directory with the 3 files above	



**PyMol movie** 

## 2. Outputs & Analyses: (5) B-factors/mode fluctuations



### 2. Outputs & Analyses: (6) Correlations

Check movie **Reset graphics** Mode: 2 🌲 Select range of modes for covariance analysis: Change High Low 2 2 options -Calculation of covariance based on all modes Click Help me with this submit page **Click for explanation** 



#### **Correlated Anti-correlated**

### **Additional options**

#### Anisotropic Network Model Web Server 2.0 (2014) 🛽 🔘

