Chimera introduction

Our group

- Structural Bioinformatics group in TAU
- Led by Prof. Haim Wolfson
- Focused on developing algorithms to solve major computational tasks in 3D bioinformatics
- Just search for “BioInfo3D” in Google

Chimera

- Developed by UCSF
- Based on Python code with a C++ infrastructure
- Open source and free to use
- Highly extensible
- Active support forum
- Just search for “UCSF Chimera” in Google

UCSF CHIMERA

an Extensible Molecular Modeling System

Starting with Chimera

- Open a terminal
- Type in : chimera
- Loading a structure : File -> Open , File -> Fetch
- Fetch from the internet :
  - **File -> Fetch**
  - Make sure **“pdb”** is chosen
  - Insert an identifier : **1ea3** (Influenza matrix protein)
  - Click **“Fetch”**
- Set download directory will cache the results

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Playing with the protein

- Use the 3 mouse buttons to rotate, move and zoom
- Use Control + Left click to choose
- Control + Left click outside the structure to cancel
- Hold Control + drag to choose a group of elements
- Use up/down to extend/limit a chosen group

- Use **Presets->Interactive 1** to color automatically
- Choose a unit on the red monomer and extend it
- Go **Actions->Atoms->delete**

Playing with the protein

- To show/hide atoms/ribbons/surface etc. go to Actions->Atoms/Ribbons/Surface->Show

- Do :
- **Actions->Atoms->Show**
- **Actions->Atoms->Ball and stick**
- **Actions->Ribbon->Hide**

Using the command line

- Favorites->Command line
- ***select #0:65-67.A*** – selects AA 65-67 from chain A of model 0
- Get Help : ***help select***

Viewing models

- **Favorites->Model Panel**
- Each model can be **“Active”** – moved with the mouse or not “active” – not movable with the mouse
- Each model can be **“Shown”** – currently visible
- Models can be easily merged with **“copy/combine”** , saved to a pdb file with **“write PDB”** etc.
- Models can be closed through **“close”**
- **Close the model menus**
- Clear the session - **File->Close session**

Matching models

- Compare E.coli thioredoxin reductase in two conformations : 1f6m, 1tde
- **File->Fetch->1f6m**
- **Present->Interactive 1 (ribbons)**
- We want to leave only chain A so :
- **Select->Chain->A**
- **Select->Invert (all models)**
- **Actions->Atoms->delete**

Matching models

- **File->Fetch->1tde**
- In order to see their secondary structure:
- **Present->Interactive 1 (ribbons)**
- **Select->Chain->A->1f6m (#0)**
- **Actions->Color->red**

Matching models

- **Tools->Structure Comparison->Matchmaker**
- Choose as “Reference structure” one of the structures and the other one as “Structure to match”
- Press OK
- Matchmaker performs sequence alignment and based on it tries to minimize RMSD between aligned residues
- You get the RMSD in the lowest part of the window
- To retrieve it you can do **Favorites->Replay Log**

Morph between the models

- **Tools->Structure Comparison->Morph Conformations**
- Press **Add..** And add the two structures
- Press **Create**
- You now have a new model which is in fact the morph movie
- Go to **Favorites->Model** panel
- Choose the two models and close them
- Enjoy the movie
- Clear the session : **File->Close session**