

This movie is our first work using Molecular Dynamics simulation data, where a major fraction of the motion observed is due to vibration. The dataset was kindly provided by Shaw *et al.* (Science, 15 October 2010, Vol. 330, pp. 341-346), and represent 250 nanoseconds of simulated motion, sampled every 0.25 nanosec.

The protein in Basic Pancreatic Trypsin Inhibitor (BPTI), and it is seen in the transition between two known conformations, with a 1.97 Å RMSD between them.

This first work is an attempt to see the major motion (transition between conformations), while keeping the background vibrations present, but not so much as to distract from the 'useful' movement.

We have used BioBlender to import the relevant sequence, after alignment. Atoms are displayed with their VdW spheres, and their colour is a level of grey proportional to their lipophilic value, as calculated by pyMLP. The movie is then rendered and motion blur is applied (a visual effect necessary for blending subsequent frames and providing a sense of continuity and speed of motion). The movie is finally recorded (and played) at 80 frames per seconds.

If you will have the patience to look at the movie for a minute or two (play as loop), this is what you should see.

At first most attention is grabbed by vibrations; after some seconds, once the eyes 'learn' to filter out the vibration noise, you'll notice the change of conformation; after a minute or so, you'll distinguish not only the change of general shape, but also the surface features (a change in the distribution of hydrophobic patches).

Comments are welcome.