Sequence-structure relationships and molecular dynamics of small peptides

Teacher Installation Guide

QwikMD setup

QwikMD is a plugin for VMD that enables easy setup and run of MD simulations of biomolecules. Currently, QwikMD is only distributed in the beta release of VMD 1.9.3. You can install this beta release of VMD alongside VMD 1.9.2 if you want to maintain both versions. VMD 1.9.3 beta 1 is available for all platforms at the official VMD downloads page (http://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD).

Downloading files from the webpage requires a free account. Download the appropriate version for your platform. Mac users should download and open the .dmg file, then drag the application "VMD 1.9.3.app" into the Applications folder (an administrator password is required). Windows users should download and run the installer (administrator password required).

QwikMD is a plugin and does not perform any MD itself; it simply creates the necessary files to run a simulation and submits that simulation to a program capable of running it. The MD program used with QwikMD is called NAMD. You must have an appropriate version of NAMD installed on your computer in order to run any simulation. Download NAMD for your computer from the official NAMD downloads page (http://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=NAMD).

You will need to download the correct version for your platform. Once you download NAMD, you should extract the archive (usually by double clicking it) and move the files inside to any location on your computer. When using QwikMD, you will be asked to locate the "namd2" ("namd2.exe" on Windows) executable file that you have downloaded in order to run the simulation.

Additional steps for Windows users

QwikMD relies on establishing a connection to NAMD in order for it to work. The Windows Firewall blocks this connection by default. The first time you run a simulation with QwikMD, a Windows Firewall warning may appear. Follow the instructions to grant access to `namd2.exe` to communicate. You will need an administrator password. After

you do this once, you should be able to run simulations without typing an administrator password.