

About Spin Label Modeling Tutorial

This zip archive contains a tutorial that parallels the Molecular Modeling of Spin Labels Chapter in Biological Magnetic Resonance, eds. M.A. Hemminga and L.J. Berliner.

The tutorial directory contains a sub-directory for each section within this tutorial. Each subdirectory contains the input and output files for the corresponding section. These files are often copied from the output of previous sections, and we note where these files existed before we copied them to the current section's directory. The output files (in Output directory) are for comparison when troubleshooting potential problems. Note that deviations between your output and our output will occur where a random variable seed is used.

System Requirements

The software used for simulation and analysis includes the commercial software CHARMM (v. 27). An academic license for CHARMM can be obtained from <http://www.charmm.org/> and requires a LINUX/UNIX operating system. Other programs include the freeware NAMD, PSFgen and VMD and are available at <http://www.ks.uiuc.edu/> for all popular operating systems. The tutorial assumes that all manipulations are executed in a LINUX/UNIX environment.