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Dynamics of Small Peptides: Comparison of NMR Relaxation Experiments with Molecular Dynamics Simulations[1] DAVID TORRES, ELIZABETH GONZALEZ, MICHELLE STEIGER, JAMES CLARAGE, University of St. Thomas — Understanding biological molecules from differing perspectives and obtaining results which concur with one another has been a goal of researchers for years. We applied both theoretical and experimental approaches to study the biophysics and dynamics of a small biological molecule, the dipeptide Alaninephenylalanine (Ala-Phe). For our theoretical approach we used the computer programs NAMD and VMD to place the dipeptide in a box of water and simulate atomic motions for every atom in the system for 100 nanoseconds. From these simulations we can predict correlation times for the atomic movements. Experimentally, relaxation times (T1, T2) were collected using Nuclear Magnetic Resonance (NMR). Comparing theory with experiment, we found similarities in the trends of correlation times for various atoms in the molecule.

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