Summary

The Thesis deals with MD simulations of solutions of chiral solutes in chiral solvents. These solutions consist of 2,2,2-trifluoro-1-phenylethanol, 1-phenylethanol and 1-phenyl-ethanamine.The differences in NMR properties between different combnations of solvent and solute absolute configuration were modeled. Indeed, differences in radial distribution functions and conformer abundances of solute calculated by the WHAM method were found. These results correlated with experimental differences in NMR shifts. Additionally, a method of cluster preselection was developed. It significantly decreased the amount of clusters needed for computations of NMR shieldings and hence the computer time.

Keywords: chirality, molecular dynamic, nuclear magnetic resonance