

# Master's Thesis Abstract

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Understanding molecular structure of biochemically relevant molecules is of fundamental interest for these molecules ultimately determine all functions of living organisms. Raman optical activity (ROA) is a chiroptical spectroscopic technique highly sensitive to molecular structure. This thesis presents an introduction to important concepts of ROA and two independent projects aiming to extend the possibilities of ROA, both from theoretical and experimental points of view. The first project is a conformational analysis of dialanine, an important model peptide. A combined quantum mechanics / molecular dynamics approach was used in spectral simulations and resulted in spectra with an unprecedented agreement with experiment. To obtain information about conformer equilibria, a decomposition procedure of an experimental spectrum into calculated individual conformer spectra was coded and tested, and proved to be a viable approach. The second project was an attempt to carry out pioneering ROA measurements of amyloid fibrils, which are difficult to measure due to their inhomogeneous nature (insolubility, birefringence). Within this project, the preparation protocol for such samples was improved. The performance of an all new rotational cuvette was examined and found to suffer from fluorescence problems. Also, ROA measurement in various polarization modes was tested, preliminary results suggest the SCP mode to be least prone to false signals. Although some progress was made, the ultimate goal of obtaining faithful, reproducible ROA spectra of amyloid fibrils has not been achieved.