

Abstract:

The aim of the thesis is to utilize Raman optical activity (ROA) to get unique information on peptide/protein conformation, which is otherwise difficult or even impossible to obtain. We have focused on investigation of amide and disulfide groups. Utilizing tailor-made model structures (rigid tricyclic spirodilactams with two interacting nonplanar amide groups), special model peptides and even biologically active molecules (neurohypophyseal hormones and their agonistic and antagonistic analogs, antimicrobial peptide lasiocepsin and its analogs having different disulfide pattern) we have traced specific spectral manifestation of nonplanar amides and disulfides. ROA results were supplemented by data obtained by complementary chiroptical methods – electronic (including vacuum UV – SRCO) and vibrational circular dichroism. When used in a concerted fashion, these techniques provide complex information on peptide/protein secondary structure. Where possible, experimental chiroptical data were compared to *ab initio* calculations. In chiroptical spectra we have found and interpreted signals reflecting nonplanarity of the amide group. Moreover, in ROA spectra we have identified signals due to S–S stretching vibrations which seem to reflect sense of the disulfide group torsion.