

Raman optical activity (ROA) represents a modern spectroscopic technique that can be applied to a wide range of chiral molecules starting from small organic molecules up to complex biomolecular systems. Among other things ROA provides information about solution structure of peptides and proteins. The aim of the thesis was to determine the relationship between three-dimensional structure and Raman optical activity of disulphide and amide groups in peptides. Characteristic band patterns of the polyproline II conformation (left-handed 3₁-helix) were found in the ROA spectra of poly(Pro-Gly-Pro), oxytocin and hinge peptide linked to the antigen sequence. ROA signal in the S-S and C-S stretching region was observed in ROA spectra of model cyclodextrin compounds connected with disulphide bonds. Positive ROA band in the S-S stretching region was found in the ROA spectrum of oxytocin (the peptide with one S-S bridge). According to the theoretical studies of model disulphides, positive ROA signal in this region indicates positive dihedral angle C-S-S-C. This result is in agreement with the crystal structure. We have also worked on extension of ROA measurements to the hydrogen stretching region (2500–3200 cm⁻¹).