Vibrational Circular Dichroism of Proteins in H_2O Solution.

Baumruk, V.; Keiderling, T. A. *J. Am. Chem. Soc.* **1993**, *115*, 6939-6942.

IR-Topic: Vibrational CD

Chem Topic: Protein Structure, Amide I region

VCD is a hybrid of the more established electronic CD and infrared absorption spectroscopy. VCD can sense differently spectrally resolved transitions involving different localized vibrations of the molecule. References to detailed descriptions of the method are given in the paper.

The spectra shown below indicate that the VCD signals are related to the secondary structure of the protein. Once this relation is established, it can be used to determine qualitatively the secondary structure of other proteins. This is usually done in connection with other data (e.g. X-ray constraints, NMR constraints, etc.).

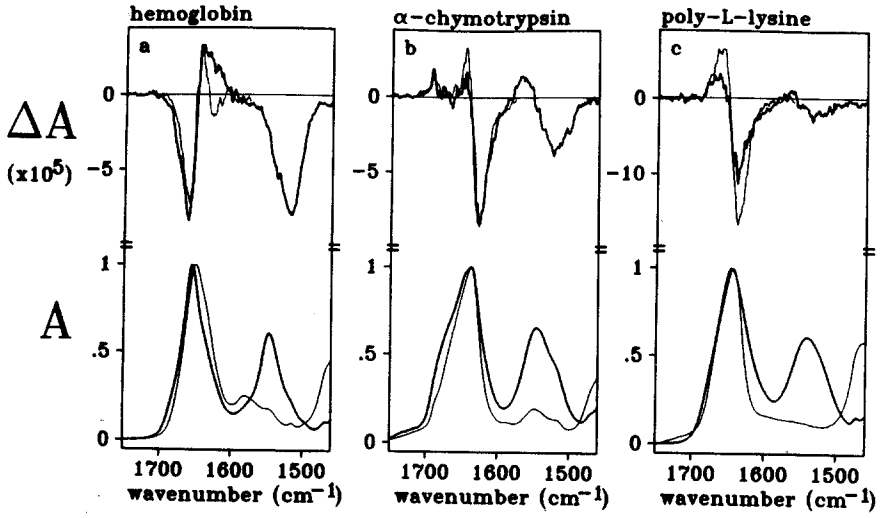

Figure 2. FTIR absorption and dispersive IR VCD spectra of (a) hemoglobin (high α), (b) α-chymotrypsin (high β), and (c) poly-L-lysine at pH 7 (random coil form) in the amide I and II regions. Both absorbance and VCD spectra are normalized to $A_{max} = 1$ for the amide I. Actual peak absorbance of the sample in the maximum of the amide I band was ~0.2-0.4. For comparison, the amide I′ VCD spectra and corresponding FTIR absorption (in D_2O) are overplotted (thin line).

Hemoglobin	α-Chymotrypsin	poly-L-lysine
α-helical	β-sheet	random coil
intense positive VCD	intense negative VCD	neg.VCD, least band shape