Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Probing the β-hairpin local structure by FTIR, 2D IR and ab initio calculations[1] JIANPING WANG, Department of Chemistry, University of Pennsylvania, PA 19104, JIANXIN CHEN, ROBIN M. HOCHSTRASSER — Small peptides form vibrational exciton systems that can be examined by means of recently developed two-dimensional infrared (2D IR) correlation techniques. We used these methods to examine a 12-residue β-hairpin (trpzip2) and its two ^{13}C-isotopomers in the 6-μm region. Different frequency shifts are seen when ^{13}C=^{16}O substitution is in the terminal or turn region of the hairpin. The difference is believed to be due to the localization of the amide-I modes, which is supported by molecular dynamics simulations. In addition, ^{13}C-substitution perturbs the amide-I vibrational exciton band, providing a spectroscopic probe for peptide local conformation. Peptide global and local structural information were derived from the diagonal and the cross peaks of the 2D IR correlation spectra. The measured intermode vibration coupling constants were compared with those predicted by ab initio DFT computations and transition charge coupling calculations.

[1]This research was supported by grants from NIH (GM12592 and RR01348) and NSF to R.M.H.

Jianping Wang
Department of Chemistry, University of Pennsylvania

Date submitted: 04 Jan 2006 Electronic form version 1.4