Multidimensional Coherent vibrational Spectroscopy of Peptides

- The response of complex molecules to sequences of femtosecond infrared pulses provides snapshots of structures and solvent dynamics.
- Extension of Multidimensional NMR to the optical regime: Cross peaks show couplings among localized vibrations, lineshapes reveal fluctuations.
- Recent experiments reveal tether-ring couplings in a molecular switch (Rotaxanes) (PNAS V102, 13378-13382, 2005. “Probing the structure of a rotaxane with two-dimensional infrared spectroscopy” and PNAS V102, 13717-13718, 2005 “Coherent femtosecond multidimensional probes of molecular vibrations”)

Fig: Sensitivity analysis is used to dissect the two dimensional Double quantum coherence spectrum of a 74 residue peptide into β sheet (red) and α helix (black) regions (PNAS. V102, 7443-7448, 2005, Zhuang W., Abramavicius D. and Mukamel S.)