Biomolecules form a class of complex systems that are fundamental to the existence of life. The function of biomolecules can be controlled by very small length scale fluctuations, vibrations, and the “spin” associated with metal ions, all of which involve quantum effects that are associated with the emerging field of “Quantum Biology”. We develop theoretical models to help explain our experimental studies of biomolecular structure and dynamics. We use ultrafast laser-based techniques such as vibrational coherence and impulsive Raman spectroscopy as well as broadband pump-probe kinetics that span femtosecond to millisecond timescales. We also use more traditional techniques such as infrared spectroscopy and resonance Raman scattering. These approaches have excellent time and frequency resolution and can be used as spectroscopic probes not only for biomolecules in solution but also for imaging biological tissue and cells. Ultrafast kinetic studies have recently uncovered important sub-nanosecond proton tunneling processes that are taking place in biomolecules at room temperature.

Time-resolved dynamic information helps us to probe biochemical reaction coordinates and unstable catalytic intermediates that involve enzyme-substrate complexes. The vibrational coherence measurements are designed to probe very low frequency motions within a protein active site, which have energies that can be thermally excited. Such motions are used by biomolecules to extract energy from the environment to implement chemical reactions and to do useful biochemical work. The kinetic studies characterize processes taking place over a wide dynamic range of timescales. These processes involve proton tunneling, diatomic ligand binding, rapid (local) structural relaxations, and more global protein conformational interconversions. Many of our studies have involved heme containing proteins and enzymes, which have roles in oxygen storage, electron and proton transport, signaling and catalysis. Photoactive molecules, such as the green fluorescent protein (GFP) shown in the figure, have also been intensively investigated to better understand the fundamental aspects of proton transport and tunneling in both the electronically excited and ground states of biological systems.