Current research in the Macklin laboratory involves spectrometric studies to obtain structural information about intermolecularly associated molecules and ions in solution and adsorbed, self-assembled interfacial aggregates. Such structural indications lead to improved understanding of structure-function relationships for numerous important chemical processes. Micro-Raman spectrometry is the primary tool used for structural characterization of dissolved and adsorbed substances. The micro-Raman measurements are generally complemented or corroborated by ultra-violet visible (uv-vis), Fourier transform infrared (FTIR) and/or nuclear magnetic resonance (NMR) spectrometric measurements.

In one such effort, uv-vis and Raman spectrometry are used to study aggregation of various dyes in solution. The dyes of interest are the photo-active cyanine dyes and others that are useful in photographic, photovoltaic and other photochemical and electrical applications. The measurements are carried out as a function of dye concentration, the concentration of an added electrolyte and temperature in order to gain information about thermodynamics and structure of the associated species. The resulting interpretations will be further established by FTIR and NMR measurements.

Another example of ongoing research activity involves the development of ultra-sensitive chemical sensing capabilities based on micro-Raman spectroelectrochemical indications. The approach chosen in this case is to begin with chromophores that adsorb strongly from solution onto a silver surface and by resonance and surface enhancement show extremely high Raman intensities. We have obtained Raman measurements of attogram quantities of some chromophoric substances adsorbed onto a silver surface with a diameter of about 50 microns by this method. These molecules are then chemically altered so as to interact in an expected manner with specific target molecules. Changes in the enhanced Raman spectrum of the surface adsorbed substance due to the presence of a target molecule can be taken as indicative of the expected chemical interaction. The goal is to discover changes that are capable of indicating chosen biochemical interactions and/or the presence of small concentrations of environmental contaminants.