

Mass spectrometry (MS) is an extraordinarily powerful analytical tool for identification, structure determination, and (in favorable cases) quantitation of both pure materials and components of mixtures. These features have made MS virtually indispensable in support of research in fields ranging from organic and inorganic synthesis to forensics, environmental monitoring, medicine, and ion chemistry. Exciting advances in ionization capabilities continue to extend the range of materials and problems amenable to analysis by MS. One of the most important of these advances has been the development of electrospray (ES) MS, which relies on solution chemistry to overcome the strong interactions between large molecules, then solvent evaporation from sprayed droplets to remove ions from solution. The efficiency of sampling depends sensitively on detailed solution chemistry. Gaps in understanding of this complex chemistry introduce possible artifacts and can make optimization a largely empirical process - significant problems in applications where a few micrograms of material represent the world's supply!

Our research seeks improved understanding of the chemical factors which affect modern MS ionization techniques, and on using that understanding to enable new applications. Current applications include a new collaboration with DuPont to devise means of characterizing reactive heterogeneous slurries - important and very complex reaction matrices often encountered in the chemicals and pharmaceuticals industries. We are also seeking to develop methodology for assessing the composition of synthetic and natural co-polymers, including "proteomics" studies aimed at enhancing the viability of biofuels as energy alternatives. Much of this work relies on comparative measurements with other spectroscopic probes, and determinations of physical properties for correlation with mass spectrometric sensitivity. Collaborators working for at least a year can learn and perform the MS methodology. Students with more short-term involvement are likely to focus on corroborative studies while working closely with other mass spectrometrists in the group.