Recent advances in ion cyclotron resonance mass spectrometry (ICR-MS) have dramatically increased the quantity and quality of data obtained from complex mixtures. The goal of ICR-MS is to identify the molecular formula for each constituent in a complex mixture of chemicals. However, more compositional information results in a severe data processing "bottleneck", because the data process workflow is an interdisciplinary, highly complex, and time-consuming process. Clearly one of the major research challenges in this area is how to strategize data reduction techniques and molecular formula attribution for a wide variety of mixtures, including natural organic matter (NOM), petroleum, biofuels, lipids, and metabolites.

MagLab-developed software packages (PetroOrg and EnviroOrg) simplify and automate complex chemical mixture data analysis to provide high-throughput, accurate, and customizable data visualization. The software is offered commercially and has grown to support • ion mobility mass spectrometry, • lipids analysis, • automated multivariate analysis (principal component analysis and hierarchical cluster analysis), • liquid chromatography mass spectrometry (LC-MS), and • batch processing of analyses.

Facilities: Ion Cyclotron Resonance