Recent technological advances in mass spectrometry, development of richer mass spectral libraries and data processing tools have enabled large scale metabolic profiling that provides a direct functional readout of cellular activity and physiological status. However, biological interpretation of metabolomics studies heavily relies on knowledge-based tools that contain information about metabolic pathways. Incomplete coverage of different areas of limits metabolism and lack of information about non-canonical connections between metabolites the scope of applications of such tools. Data driven approaches for building interactions networks from metabolomics data have proved useful.

In this talk, we propose an integrative framework based on Gaussian graphical models for joint estimation of such interaction networks from metabolomics profiles across multiple experimental conditions or disease subtypes. We discuss in detail modeling, estimation and statistical inference aspects, and provide extensions of the framework for integrating metabolomics data with other Omics modalities (e.g. transcriptomics data, etc.). We further show how these interaction networks can be used in combination with topology based pathway enrichment methods to identify differentially enriched subnetworks across disease subtypes. The methodology is illustrated on three different independent cohorts of patients with early and late stage chronic kidney disease.

Refreshments will be served following the seminar in 1181 Comstock Hall.