Metabolomics Workshop Outline:

With a growing attention to the discovery of new natural products and understanding their role in mitigation organismal interactions, MS based metabolomics has received growing attention as a tool for understanding these complex chemical-ecology systems. The collection and analysis of community (ecosystem) wide data and the integration of MS variables with ecological and genomics datasets presents significant challenges that must be addressed in order to apply these tools. The Hitchcock Center for Chemical-Ecology at UNR has developed new approaches to using LC-MS datasets for addressing long-standing questions in chemical-ecology and natural products chemistry. This workshop will focus on the application of LC-MS based metabolomics from experimental design, data collection, and analysis. An overview of various approaches to LC-MS data analysis, including diversity measures, de-replication, and automated approaches to the annotation of LC-MS datasets will be presented.

Requirements:

- Metabolomic Data Set (maybe we can provide an example data set if people don't have one)
- Computer (*all freeware are available* for both Windows and Mac with the exception of ProteoWizard) or computer lab
- Smart Classroom

Software Platforms:

Spreadsheet software	LC-MS processing freeware	R data processing packages	R statistical packages
• Excel (or other spreadsheet software)	• mzMine • OpenChrom • ProteoWizard	• XCMS • MSnbase • CAMERA • metaMS	• Adegenet • Igraph • Mclust • Vegan • WGCNA

PROPOSED OUTLINE

Part I: Experimental design	*Part II:* Data Extraction and Alignment
- Randomization - Using Standards - Quantitative - Semi-quantitative - Qualitative - GLP - Grinding - Weighing - Extraction	- File formats - ProteoWizard - Openchrom - mzMine - XCMS and wrappers - XCMS - MSnbase - CAMERA - metaMS - Standards Post-analysis - Internal - External

Part III: Data Analysis
- Diversity   - Richness   - Shannon Diversity   - Simpson Diversity   - Correction methods   - Ordination Techniques   - PCA   - Factor analysis   - Cluster Techniques   - Hierarchical Cluster Analysis   - Gaussian Mixed Model Clustering   - DAPC   - Network Techniques   - WGCNA   - Compound activity mapping   - Dereplication   - Similarity Networking   - LC-MS compound classification   - Database searching