

Metabolomics Pipeline Overview

Introduction

A basic analysis pipeline in R for untargeted LC-MS metabolomics, including quality control, normalization, PCA overview of sample behavior, and differential feature analysis with linear models. The data are panels of untargeted LC-MS features from positive and negative ionization mode runs, such as metabolites measured from tissue, stool samples, or microbial cultures. In this hypothetical scenario, the data have been structured to resemble samples belonging to control subjects, one of two treatments (tr1 or tr2), or a dual-treatment group (tr1+tr2). The pipeline demonstrates a conventional approach to characterizing metabolomic differences among these groups.

PCA

(testing PCA plotting in .qmd document. Will contain discussion of this method used on the data)

