FISHER FELLOWSHIP AWARD for 2009-2010

Bryan Hanson, Professor of Chemistry and Biochemistry – (Fall) "Development of an R Software Package for the Chemometric Analysis of Spectra"

Abstract

The objective of this project is to develop an R software package for the chemometric analysis of spectra. "R" is an open-source computing environment designed primarily for graphical analysis and statistics. Chemometrics is the science of interpreting complex sets of chemical measurements, such as collections of NMR and IR spectra, which are obtained from instruments typically found in chemistry laboratories. During my recent sabbatical, which focused on plant metabolomics, I developed proficiency in R and wrote functions to analyze data I was collecting. During my Fisher Fellowship, I will take this nucleus of functions, add features and options, and implement a number of new capabilities. I will also learn the necessary supporting skills of making R packages, version control, and I will extend my statistical background. The final product will be a complete software package for plotting and analyzing sets of spectra such as are typically encountered in metabolomic studies. I will use this package in my metabolomics research and it will be made available to the R community.