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# Quantitative analysis of HIV/AIDS serum metabolites using 1H HRMAS-NMR spectroscopy

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## Abstract

Chemometric metabolomics analysis of nuclear magnetic resonance (NMR) spectra of human serum can distinguish normal serum (HIV-) from serum infected with the human immunodeficiency virus (HIV+) and serum from HIV+ patients on antiretroviral therapy (ART). However, the relationship between serum metabolite concentrations and disease severity has not been determined. We performed high-resolution magic angle spinning (HRMAS) NMR spectroscopy on HIV- (n=10), HIV+ (n=10), and ART (n=10) serum. We then analyzed the spectra with both a chemometric method and a quantitative method. For the chemometric analysis, the spectra were binned into 146 segments and used in a linear discriminant analysis (LDA) classification model. For the quantitative analysis, the high-resolution quantum estimation (HR-QUEST) method was used to determine the concentrations of 12 metabolites in the spectra. Metabolites with resonance peaks that contributed to the LDA classification were compared with viral load and CD4 count. The LDA model classified the three groups with 100% accuracy, with spectral segments contributing to glucose and glutamine having large coefficients. The HR-QUEST analysis showed a trend toward lower concentrations of alanine in HIV- versus HIV+ ($p = 0.07$) and ART ($p = 0.10$) sera. CD4 count was associated with alanine ($p < 0.01$), glutamine ($p = 0.02$), and glucose ($p = 0.02$) and a multivariate model with all three metabolites was predictive of CD4 count ($p = 0.04$). The combined chemometric and quantitative analysis revealed associations between specific metabolites and disease severity that would not have been noted with either analytical method on its own.

## Biography

Tracy Richmond McKnight is an Associate Professor in the Department of Radiology and Biomedical Imaging at the University of California, San Francisco (UCSF). Dr. McKnight earned a BS in physics from Spelman College in Atlanta, GA, an MS in physics from Polytechnic University in Brooklyn, NY, and a PhD in Bioengineering from the University of California, Davis. She joined UCSF as a postdoctoral fellow and built a research program using magnetic resonance techniques to study cancer and HIV. She is a member of the UCSF Brain Tumor Research Center, the UCSF Comprehensive Cancer Center, and the UCSF/UCB Bioengineering Graduate Group.