

*“Digesting the Alphabet Soup of Multivariate Analysis”*

**Daniel J. Graham**

NESAC/BIO, University of Washington, Seattle, WA

[djgraham@uw.edu](mailto:djgraham@uw.edu)

Secondary Ion Mass Spectrometry data is complicated. Even a spectrum from a “simple” surface can contain hundreds if not a few thousand peaks. The relative intensity of these peaks can be influenced by the composition, structure and arrangement of the surface molecules. The challenge then becomes being able to extract information from the spectra that can answer the questions being asked about the samples under investigation. This challenge is further complicated because one can easily generate very large sets of data. A 2D SIMS image can easily contain tens of thousands of pixels and a 3D depth profile can contain millions, each with a full mass spectrum. Sifting through this data manually would be time consuming and inefficient. Fortunately, there are tools available to aid in processing these large data sets. This tutorial will explore the use of multivariate analysis (MVA) methods as tools to help understand and interpret SIMS data. The course material will present practical guidelines on how properly analyze SIMS data using MVA and other advanced data processing methods.

For each topic in the tutorial, examples will be presented that demonstrate how to apply and interpret the results generated from various MVA methods. Best practices for pre-processing data and presenting MVA results will be discussed. The tutorial will be concluded with an interactive discussion to address current needs, questions and strategies for approaching complex data sets.

**Topics:** Planning for MVA (What and how much data do I need to collect?); Data pre-processing (What pre-processing should I use?); MVA methods (What are they and what do they do?); Interpreting the results of MVA (What does it mean?); Resources for MVA (Where can I get help?).

**Requirements:** There are no special requirements for this course.