Nancy J McMillan, Arriana Chavez, Nancy Chanover, David Voelz, Kyle Uckert, Rula Tawalbeh, John Gariano, Ivan Dragulin, Xifeng Xiao and Robert Hull, "Rapid and Portable Methods for Identification of Bacterially Influenced Calcite: Application of Laser-Induced Breakdown Spectroscopy and AOTF Reflectance Spectroscopy, Fort Stanton Cave, New Mexico", AGU Fall Meeting, Abstract #B33B-0171, San Fransisco, CA,

Rapid, in-situ methods for identification of biologic and non-biologic mineral precipitation sites permit mapping of biological hot spots. Two portable spectrometers, Laser-Induced Breakdown Spectroscopy (LIBS) and Acoustic-Optic Tunable Filter Reflectance Spectroscopy (AOTFRS) were used to differentiate between bacterially influenced and inorganically precipitated calcite specimens from Fort Stanton Cave, NM, USA. LIBS collects light emitted from the decay of excited electrons in a laser ablation plasma; the spectrum is a chemical fingerprint of the analyte. AOTFRS collects light reflected from the surface of a specimen and provides structural information about the material (i.e., the presence of O-H bonds). These orthogonal data sets provide a rigorous method to determine the origin of calcite in cave deposits. This study used a set of 48 calcite samples collected from Fort Stanton cave. Samples were examined in SEM for the presence of biologic markers; these data were used to separate the samples into biologic and non-biologic groups. Spectra were modeled using the multivariate technique Partial Least Squares Regression (PLSR). Half of the spectra were used to train a PLSR model, in which biologic samples were assigned to the independent variable "0" and non-biologic samples were assigned the variable "1". Values of the independent variable were calculated for each of the training samples, which were close to 0 for the biologic samples (-0.09 - 0.23) and close to 1 for the non-biologic samples (0.57 - 1.14). A Value of Apparent Distinction (VAD) of 0.55 was used to numerically distinguish between the two groups; any sample with an independent variable value < 0.55 was classified as having a biologic origin; a sample with a value > 0.55 was determined to be non-biologic in origin. After the model was trained, independent variable values for the remaining half of the samples were calculated. Biologic or non-biologic origin was assigned by comparison to the VAD. Using LIBS data alone, the model has a 92% success rate, correctly identifying 23 of 25 samples. Modeling of AOTFRS spectra and the combined LIBS-AOTFRS data set have similar success rates. This study demonstrates that rapid, portable LIBS and AOTFRS instruments can be used to map the spatial distribution of biologic precipitation in caves.