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## **POSTER - Signal Optimization and Chemometric Analysis of Laser-Induced Breakdown Spectroscopy Bacterial Spectra to Quantify Detection Limits and Improve Classification Accuracy**

*Monday 8 June 2020 15:00 (15 minutes)*

Our lab has been investigating the use of laser-induced breakdown spectroscopy (LIBS) for the rapid identification of bacteria in simulated clinical specimens. LIBS is a laser-based spectrochemical technique that allows a near-instantaneous measurement of the elemental composition of a target. Subtle yet reproducible differences in the concentration of inorganic elements like phosphorous, magnesium, calcium, and sodium in the bacterial cell allow a differentiation of the bacteria on the basis of their atomic emission spectrum alone. This can be used for the rapid identification of unknown specimens.

The current testing protocol involves the collection of bacteria using disposable pathology swabs, shaking off the cells into a water suspension, and centrifuging the suspension through a custom-fabricated cone device that concentrates the cells into a 1 mm diameter circular area on a nitrocellulose filter medium. A 10 ns 1064 nm laser pulse focused onto the deposition creates a high-temperature microplasma allowing a measurement of the elemental composition of the cells after dispersion and recording of the atomic emission spectrum with an Echelle spectrometer.

Currently, the construction of a spectral library database containing the LIBS emission spectra from hundreds of spectra obtained from 5 different bacterial species and sterile water control specimens is ongoing. The spectra are analyzed using discriminant function analysis and partial least-squares discriminant analysis to classify unknown samples and to determine the method's sensitivity and specificity. The limit of identification is also being investigated by improving the external validation accuracy of highly diluted specimens.

Manipulation of the library with outlier elimination techniques, reduction of elemental contaminants contributing to extraneous background signals, and the addition of silver microparticles to enhance signal intensities are all being investigated to produce a standardized protocol that minimizes the bacterial limit of detection while maximizing classification accuracy.

**Authors:** BLANCHETTE, Emma (University of Windsor); Ms SLEIMAN, Sydney (University of Windsor)

**Co-authors:** MARVIN, Jeremy (University of Windsor); ARAIN, Haiqa (University of Windsor); MARTINEZ, Archie (University of Windsor); Ms TIEU, Alayna (University of Windsor); REHSE, Steven (University of Windsor)

**Presenters:** BLANCHETTE, Emma (University of Windsor); Ms SLEIMAN, Sydney (University of Windsor)

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