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(U*) POS-D17 – Quantification of Sensitivity and Specificity in a Laser-Induced Breakdown Spectroscopy Diagnostic Assay for Pathogenic Bacteria Detection and Classification

Wednesday 9 June 2021 13:45 (2 minutes)

Laser-induced breakdown spectroscopy (LIBS) is a laser-based spectrochemical technique that allows a near-instantaneous measurement of the elemental composition of a target by making time-resolved spectroscopic analyses of laser-induced ablation plasmas. Utilizing nanosecond laser pulses and a broadband high-resolution Echelle spectrometer, high signal-to-noise optical emission spectra can be obtained from almost any desired target.

When the ablation target contains bacterial cells, the inorganic elements present in the bacterial cells (phosphorous, magnesium, calcium, and sodium) can be used to discriminate the bacteria on the basis of their atomic emission spectrum alone. Currently, we deposit bacterial cells onto a nitrocellulose filtration medium by centrifuging very low titer liquid specimens through a custom-fabricated centrifuge tube insert device. Prior to centrifugation, the bacteria cells are obtained by swabbing abiotic surfaces upon which a known number of bacteria cells have been deposited. The cells are then shaken off the disposable pathology swabs into a water suspension in a vortex mixing instrument.

Spectra from five different bacterial pathogens and pathogen surrogates (Staphylococcus epidermidis, Escherichia coli, Mycobacterium smegmatis, Pseudomonas aeruginosa, and Enterococcus faecalis) and sterile water control specimens have been obtained along with spectra from sterile deionized water control specimens.

This presentation will detail our efforts to identify and optimize chemometric algorithms for the autonomous classification of unknown spectra. Algorithms such as principal component analysis (PCA), discriminant function analysis (DFA), partial least squares discriminant analysis (PLSDA), and artificial neural networks (ANN) have been investigated. Rates of sensitivity and specificity have been determined and will be presented for the various techniques. Efforts to use chemometric algorithms to discriminate low-titer suspensions from blank water specimens and thus calculate limits of detection and limits of identification will also be discussed.

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