Chemometric Trace Analysis and Spectral Imaging Approaches to Disease Diagnostics: Forays into Malaria and Cancer

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Extended Abstract

The levels and speciation alterations, as well as correlations of trace chemicals (elements, metabolites) in human body tissues and fluids can be used as biomarkers for spectral diagnosis of disease as diseases lead to chemical and structural changes that alter the characteristics of spectra and images obtained from tissue / fluid samples. A major challenge in trace quantitative spectroscopic and spectral imaging analysis is the determination of low analytes in the presence of interfering matrix components. We report the achievement of greater sensitivity, speed and accuracy in the trace analysis and spectral imaging approaches to cancer and malaria diagnostics when these techniques are combined with multivariate chemometrics. We are focused on cancer and malaria as there is a connection between Epstein-Barr virus, falciparum malaria, and some forms of cancer; it has also been observed that similar drugs are effective in curing both diseases. We develop methodologies exploiting X-ray fluorescence (EDXRF, TXRF) spectroscopy, laser induced breakdown spectroscopy (LIBS) spectral/imaging, LED-based multispectral imaging microscopy, and laser Raman spectromicroscopy. Chemometrics is relatively new disciplines for mining (management, analysis and visualization) of extensive data sets and for extracting relevant information from extensive and complex multivariate measurements. It affords multivariate data reduction in a graphical interface which permits visualization of relationships between samples characterized by multiple measured variables and also affords exploratory analyses. In this way chemometrics opens up possibilities for investigation of unknown aspects of analyzed samples and for investigating influences of multiple parameters on the results of spectroscopic and spectral imaging analyses.

Imaging spectrometry is spectroscopy pursued in the image domain as virtually every spectroscopic technique can be used to generate chemical images. In spectroscopy, the measured spectrum is directly related to the structure and composition of the material under examination, enabling to probe the structural, dynamical, and functional properties of materials. In spectral imaging (which is especially suited to the study of micro-samples where the sample material is limited and the maximum amount of information needs to be obtained), material properties can be probed more rapidly and reliably in two and three dimensions. Depending on the technique, mapping results may comprise a single value collected at each x and y location on a surface, or a range of data such as a full spectrum. For either outcome, the results can be arranged into a hyperspectral data cube where each position (x_n, y_m) has an associated spectrum, the intensity of which extends in the z direction. Since each z is a multivariate data set, information about the chemical composition of a sample can be obtained by multivariate chemometric analysis. Multivariate spectral image data are however characterized by measurement error variances that are highly heterogeneous, inherent in the measurements or as consequence of data pretreatment.