

Article

# New Insights into the Multivariate Analysis of SER Spectra Collected on Blood Samples for Prostate Cancer Detection: Towards a Better Understanding of the Role Played by Different Biomolecules on Cancer Screening. A Preliminary Study

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**Simple Summary:** In recent years, research on biofluids using Raman and SERS has expanded dramatically, indicating the enormous promise of this technology as a high-throughput tool for identifying cancer and other disorders. In the investigations thus far, researchers have concentrated on a specific illness or condition, but the techniques employed to acquire experimental spectra prevent direct comparison of the data. This necessitates comparative research of a variety of diseases and an increase in scientific cooperation to standardize experimental conditions. In our study, positive results were reached by applying a combined SERS multivariate analysis (MVA) to the urgent problem of prostate cancer diagnosis that was directly linked to real-world settings in healthcare. Moreover, in comparison to the prostate-specific antigen (PSA) test, which has a high sensitivity but limited specificity, our combined SERS-MVA method has greater specificity, which may assist in preventing the overtreatment of patients.

**Abstract:** It is possible to obtain diagnostically relevant data on the changes in biochemical elements brought on by cancer via the use of multivariate analysis of vibrational spectra recorded on biological fluids. Prostate cancer and control groups included in this research generated almost similar SERS spectra, which means that the values of peak intensities present in SERS spectra can only give unspecific and limited information for distinguishing between the two groups. Our diagnostic algorithm for prostate cancer (PCa) differentiation was built using principal component analysis and linear discriminant analysis (PCA-LDA) analysis of spectral data, which has been widely used in spectral data management in many studies and has shown promising results so far. In order to fully utilize the entire SERS spectrum and automatically determine the most meaningful spectral features that can be used to differentiate PCa from healthy patients, we perform a multivariate analysis on both the entire and specific spectral intervals. Using the PCA-LDA model, the prostate cancer and control groups are clearly distinguished in our investigation. The separability of the following two