

Raman Spectral Analysis of Therapeutic Efficacy of Galectin-3 Inhibitor in Prostate Cancer with Machine Learning

Alexander Khmaladze, University at Albany, SUNY, Albany, NY, USA

Abstract

Raman micro-spectroscopy is widely used for chemical composition mapping within live biological samples, such as cells, organoids, and tissues. It permits non-invasive and non-destructive measurements that do not require special sample preparation processes, such as dye labelling or staining. While conventional spectral analysis techniques have been employed to extract useful patterns from Raman data, emerging developments in machine learning offer new opportunities to advance the field. Through examination of spectral features in the Raman data, we detected distinct molecular bond signatures indicative of changes in key biomolecules, including proteins, lipids, and nucleic acids. We applied supervised machine learning models (Random Forest, Support Vector Machine), as well as Singular Value Decomposition to classify Raman spectra and capture patterns in the spectral data, enabling accurate differentiation between treated and control groups.

In this study, Raman spectroscopy (RS) was used to examine the effects of the potent Gal-3 inhibitor GB1107 on CaP cell lines with varying metastatic potential, specifically PC-3, DU-145, and LNCaP. Glycoproteins such as Galectin-3 (Gal-3) and prostate-specific membrane antigen (PSMA) play important roles in numerous biological processes, including cell apoptosis, angiogenesis, and inflammation. Downregulation of these glycoproteins in the highly metastatic human prostate cancer (CaP) cell line PC-3 has been shown to reduce tumor growth.

Comparison of Raman spectra from GB1107-treated PC-3, DU-145, and LNCaP cells with untreated control cells revealed significant spectral differences. These differences corresponded to changes in phosphatidylinositol (596 cm^{-1}), O-P-O stretching of DNA (786 cm^{-1}), lipid/phospholipid DNA backbone vibrations ($1090\text{--}1100\text{ cm}^{-1}$), nucleic acids, lipids, and proteins associated with the amide III band ($1296\text{--}1305\text{ cm}^{-1}$), fatty acids (1440 cm^{-1}), and proteins associated with the amide I band (1655 cm^{-1}). These observations suggest that the DNA phosphate backbone may become destabilized during cancer progression, potentially facilitating metastasis in prostate cancer cells.

In this presentation, I will also discuss additional applications of Raman spectroscopy, including studies of brain tissue sections, tissue engineering samples, and cells exposed to iron.