Bridging the Gap: *In-Silico* Guided Analytical Approaches for Enhancing the Cancer Detection

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The invention of the laser has revolutionized spectroscopy techniques, leading to groundbreaking applications across various fields. Its unique properties have empowered sensitive and precise tools for research from fundamental research to practical application in medicine, environment, industry, and defense. By combining cutting-edge spectroscopy with high-performance computational modeling, we can extend our understanding beyond transitional experimental limits. Our research group utilizes a combination of multi-scale *in-silico* modeling techniques, aptamer/antibody-based affinity purification with micro- and nano-particle technology, and data-driven spectroscopy to detect cancer biomarkers sensitively. Our current research focus area include:

1. Exploring Cell Signaling Aberrations in Cancer Cells. Mutations in cell signaling pathways are known drivers of cancer initiation and progression. We're investigating these alterations in specific cancers like Epithelial Ovarian Cancer (EOC), targeting key proteins like KRAS and p53. Our goal is to develop affordable, user-friendly methods for diagnosing signaling disruptions by simultaneously detecting multiple protein biomarkers with exceptional sensitivity and specificity. We envision using a combination of computational modeling (Fig-1) and Raman and Laser-induced Breakdown Spectroscopy (LIBS) to achieve this, ultimately paving the way for personalized treatment strategies and non-invasive diagnostic tools.

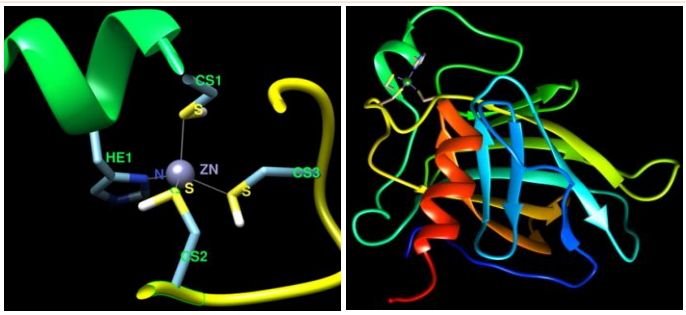

Fig-1. (a) QM optimized Zn region of p53 DBD, and (b) p53 DBD with Zn after energy minimization with Molecular Dynamics.

2. Biomarkers and Early Cancer Detection: Going Beyond. Early detection of cancer is crucial for successful treatment, but it can be difficult for cancers like ovarian cancer with subtle initial symptoms. We're developing non-invasive methods (Fig-2) that not only detect biomarkers with high accuracy but also provide deeper insights into cancer biology. One promising candidate is HE4, a protein linked to cancer cell proliferation and other processes. We're exploring its interactions with other proteins like ANXA2 using aptamer-based affinity purification and Raman spectroscopy. This combined approach aims to not only detect HE4 at early stages but also reveal hidden information about its interactions, potentially leading to novel diagnostic tools.

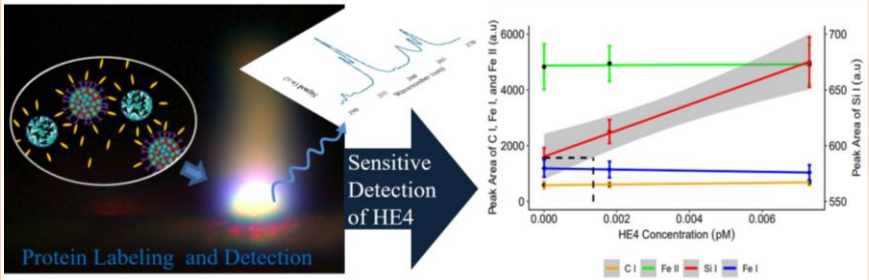

Fig-2. Sensitive detection of HE4 in human fluid with elemental encoded immunoassay with LIBS.

3. Aptamer-Based Tools for Precise Cancer Detection. Precision medicine requires tools that can detect genetic mutations and their links to epigenetic changes with high sensitivity and reliability. Spectroscopy techniques are gaining traction in this area, particularly label-free Raman biosensors, which hold promise for real-time cancer detection during surgery. Our project focuses on computational screening of aptamers, molecules that bind to specific targets, for use with Raman spectroscopy. This approach allows for simultaneous detection of multiple biomarkers in cancer cells, potentially even in vivo. By refining this method, we aim to minimize false detections and unlock the true potential of Raman spectroscopy for non-invasive, label-free tumor detection.

Participating REU students will engage in active research using cutting-edge biophysics techniques. They will learn to model biomolecular structures, dynamics, and interactions using both computational and hands-on methods. Our lab offers experience with immunoassays, LIBS, Raman spectroscopy, and mass spectrometry. We start with beginner-friendly modules and gradually introduce you to advanced spectral data analysis using machine learning and Python programming. The participant will gain valuable experience while contributing to research with the potential to revolutionize cancer diagnostics and treatment!