Attenuated Total Reflectance-Fourier Transform Infrared spectroscopy for monitoring biochemical changes in breast cancer serum across tumor stages

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Abstract

Spectral Bio-Markers (SBMs) play a vital role in modern biomedical research by capturing small biochemical alteration that reflect disease detection and progression. Infrared (IR) spectroscopy offers a nondestructive, label-free method to probe molecular vibrations. This study applies Attenuated Total Reflectance-Fourier Transform Infrared (ATR-FTIR)spectroscopy to blood serum as a label-free, minimally invasive technique to track biochemical changes linked to disease detection and progression in Breast Cancer (BC). This minimally invasive approach reveals statistically significant variations in SBMs corresponding to disease progression, underscoring its strong potential as a diagnostic and monitoring tool for breast cancer detection and disease tracking.

▪ Objectives

To evaluate ATR-FTIR spectral biomarkers in blood serum for distinguishing between healthy individuals and BC patients at different stages, and to assess their potential for monitoring disease progression.

Methods and Materials

▪ Principle of IR Absorption

- Molecules absorb infrared light matching their vibrational frequencies.
- Absorption spectra patterns can reveal biomolecules changes linked to disease.

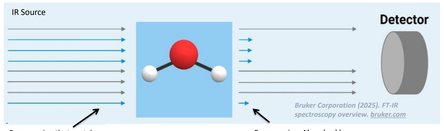


Figure 1: IR Absorption explained with molecule.

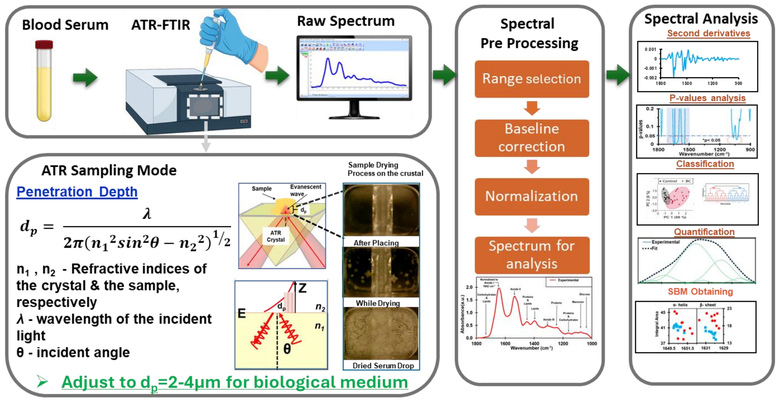


Figure 2:Sampling technique & Process of SBM obtaining from raw spectra.

Results

▪ Principal Component Analysis (PCA)

- PCA classified spectra of BC and Healthy Controls (HC), showing clear group separation.
- Corresponding loadings plots highlight key wavenumbers contributing to the variance responsible for the observed discrimination among BC and HC groups

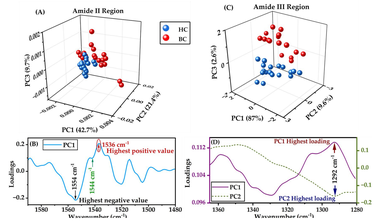


Figure 3: PCA 3D Score plots of selected bands (A) Amide 11 (C) Amide III showing group separation. (B) &(D) Corresponding Loading plots.

▪ Spectral Feature Quantification

Integral areas of Gaussian Function Energy Bands (GFEBs) derived from curve fitting show statistically significant differences between BC and HC, indicating their potential as SBMs.

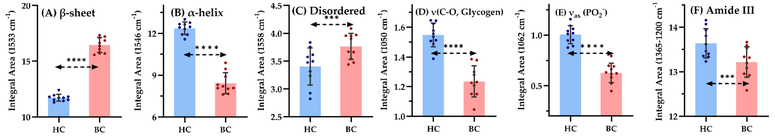
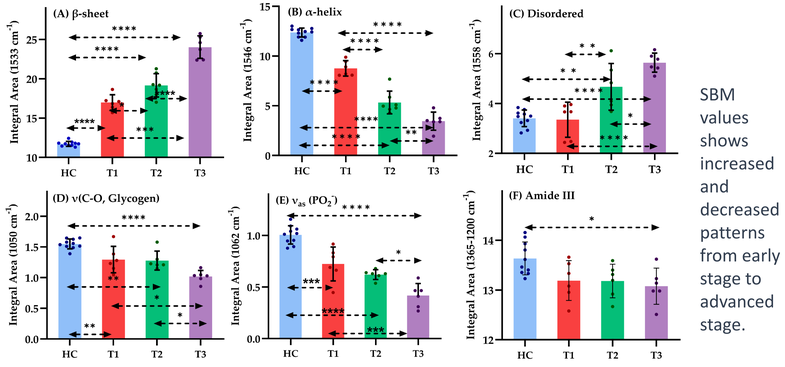


Figure 4: Representation of identified SBMs: Integral Area of the GFEBs fat(A) 1533 cm^{-1}, (B) 1546 cm^{-1}, (C) 1558 cm^{-1}, (D) 1050 cm^{-1}, (E) 1062 cm^{-1}, and GFEBs and (F) Integral area of 1365-1200 cm^{-1} region.

▪ Tumor Progression Analysis

To assess disease progression, samples were stratified by tumor size according to the T stage of TNM classification



SBM values shows increased and decreased patterns from early stage to advanced stage.

Figure 5: SBM variation across different tumor sizes.

Discussion

Table 1: Observed SBMs which are statistically significantly changing as the tumor size changes.

SBM	Wavenumber (±4) cm^{-1}	Trend
β-sheet	1536	↑ Increased
α-helix	1547	↓ Decreased
Disordered proteins	1558	↑ Increased
C–O glycogen stretch	1050	↓ Decreased
PO_2^- asymmetric stretching	1062	↓ Decreased
Amide III IS	1365-1200	↓ Decreased

Long Term Goal

Future work involves,

- Develop a portable diagnostic device integrated with a user-friendly desktop unit.
- Enable automated, end-to-end data analysis for rapid interpretation.
- Provide instant display of laboratory test reports.
- Operate using only 1–2 µL of patient blood, making the process highly minimally invasive.

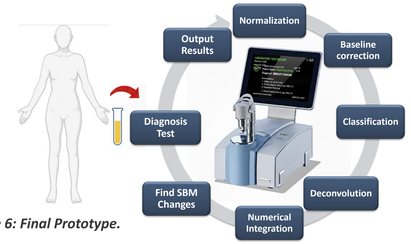


Figure 6: Final Prototype.

Conclusion

- ATR-FTIR spectroscopy effectively identifies serum-based spectral biomarkers that reflect molecular changes in breast cancer.
- Key protein structural changes reflect tumor-induced misfolding and aggregation.
- Identified spectral biomarkers show distinct increasing or decreasing trends with tumor size.
- These biomarker patterns demonstrate strong potential for tracking breast cancer progression.

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