

## **Infrared molecular fingerprinting – a new technological platform for cancer screening and diagnostics**

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### **Abstract**

The concentrations, chemical modifications, and relative abundance of organic molecules in systemic biofluids can serve as direct indicators of human physiological health, including cancer. Despite a significant medical need for time- and cost-effective non-invasive diagnostic alternatives, a key challenge for modern omics technologies remains in reproducible and robust multi-molecular detection and interpretation.

Infrared fingerprinting presents an alternative approach based on optical vibrational profiling, which captures spectroscopic patterns across the entire molecular landscape. Specifically, we develop and investigate the application of infrared molecular fingerprinting for high-throughput in vitro cancer diagnostics of human blood serum and plasma, integrated with machine learning. Technological developments are evaluated in clinical studies encompassing several thousands of individuals - forming a critical foundation for potential in vitro cancer diagnostics.

Leveraging broadband optics and large-scale clinical studies, we provide evidence indicating that the spectral information of blood plasma and serum contains infrared spectroscopic signatures specific to four common cancer entities - lung, breast, bladder and prostate cancer. The effectiveness of disease detection correlates with stage of cancer progression. Additionally, we highlight the potential of infrared molecular fingerprinting to predict mortality outcomes. Furthermore, we demonstrate that infrared spectra have the capacity to also detect commonly occurring health deviations. Interestingly, we identified further potential of infrared fingerprinting to distinguish between various cooccurring non-communicable diseases, enabling screening for a variety of conditions and enhancing risk stratification.

Infrared molecular fingerprinting presents an analytical framework of molecular profiling - a versatile platform offering multi-phenotyping capabilities with insights into explainable molecular analytics. We underscore its potential for cancer diagnostics, health monitoring and risk stratification in naturally heterogeneous populations, while also serving as a tool for analyzing intact post-transcriptional molecular modifications. We address the challenges of multi-molecular spectral analyses and provide evidence-based examples demonstrating how infrared spectroscopy opens new avenues for high-throughput in vitro diagnostics - a powerful gateway to assessing health and disease in a molecule- and disease-agnostic manner.

### **Do you have any conflicts of interest?**

No, I do not have a conflict of interest.