Toward an Optical Digital Twin: AI-Enabled Raman Spectroscopy for Longitudinal Immune Profiling and Translational Diagnostics

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Abstract

Raman spectroscopy has matured into a powerful, label-free tool for molecular phenotyping of cells and tissues. A central direction of our current research is high-throughput Raman immune cell profiling from small volumes of peripheral blood. By capturing subtle molecular fingerprints of neutrophils, lymphocytes, and monocytes, Raman spectroscopy enables not only immune cell identification but also the characterization of functional activation states and host-response signatures.

In combination with advanced machine learning, multidimensional spectral datasets allow robust classification of infection and inflammatory conditions. Importantly, the methodology is non-destructive, requires minimal sample preparation, and is suitable for repeated measurements. This capability opens the possibility of longitudinal monitoring rather than single time-point diagnostics.

Building on these established Raman immune profiling platforms, we propose the concept of an Optical Digital Twin as a future translational framework. The Optical Digaital Twin does not yet exist as a fully implemented system; instead, it represents a next logical step: the systematic use of repeated Raman-based immune phenotyping to establish individualized molecular baselines. Such personalized reference states would enable early detection of deviations from an individual’s normal immune phenotype, potentially allowing earlier intervention before clinical symptoms fully manifest.

In a broader perspective, this future Optical Digaital Twin could integrate Raman-derived molecular information with complementary optical diagnostics and contextual physiological data streams. However, its foundation lies in the already established capability of Raman spectroscopy to reproducibly capture immune cell phenotypes at high information density.

Thus, rather than presenting a completed digital infrastructure, we outline a translational roadmap: from validated Raman immune cell prototyping toward

longitudinal baseline modeling and, ultimately, the development of an individualized Optical Digaital Twin framework for predictive and personalized medicine.
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