

OpenSpectro: An Open-Source Spectroscopic Profiling Platform

Haoran Zhang*, Elizabeth C. Courtney*, Kyle C. Quinn+ and Amanda Watson*

* Department of Electrical and Computer Engineering, University of Virginia
+ Department of Anesthesiology, University of Virginia

Research Overview

Creating the open-source platform OpenSpectro for spectroscopic profiling can:

- Systematically map molecular signatures to optimize wavelength selection for multi-wavelength PPG sensors.
- Improve wearable health-monitoring accuracy using customized wavelength attention weights for 17 key biomarkers.

Open-Source Profiling Platform

OpenSpectro: An Open-Source 3D Spectroscopic Profiling Platform



spectroscopic Profiling for Biomedical Analysis

Abstract

Spectroscopic analysis is essential for identifying optical-based molecular signatures—distinct patterns observed across various wavelengths. Understanding these signatures provides critical insights for designing wearable health-monitoring devices. In particular, constructing three-dimensional (3D) spectroscopic graphs of molecular spectra enables the optimization of multi-wavelength photoplethysmography (PPG) sensors, improving their accuracy and performance. However, no prior work has systematically mapped spectroscopic signatures to optimize wavelength combinations, slowing advancements in multi-wavelength PPG sensor deployment. To address this gap, we introduce OpenSpectro, an open-source spectroscopic profiling platform for visualizing and sharing molecular spectral data, particularly human physiological biomarkers. OpenSpectro features a preliminary spectroscopic database containing 17 biomarkers and a spectral attention optimization model that identifies customized wavelength attention weights for each biomarker.

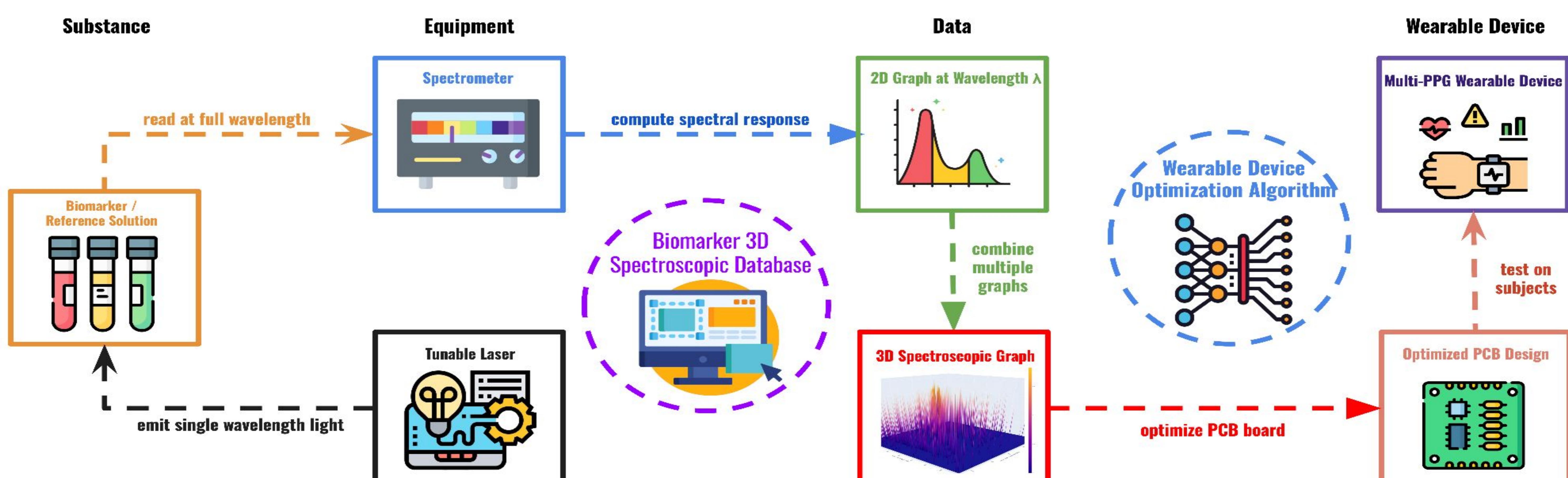
3D Visualization
Interactive 3D molecular signature analysis with real-time manipulation

Wavelength Optimization
Multi-PPG wavelength optimization given target biomarker signature

Collaborative Platform
Share and compare spectroscopic profiles with researchers worldwide

 GitHub

System Architecture



Wavelength Optimization

A. 2D Spectroscopic Optimization

- Input: $A \in \mathbb{R}^{N \times M}$ (Rows = Biomarkers, columns = absorbance across wavelengths)
- Attention vector (weights per wavelength): $w_i = (w_{(i,1)}, \dots, w_{(i,M)}) \in [0, 1]^M$
- Objective function:

$$\mathcal{L}_i(w) = \alpha \sum_{m=1}^M w_{(i,m)} A_{(i,m)} - \beta \sum_{\substack{j=1 \\ j \neq i}}^N \sum_{m=1}^M w_{(j,m)} A_{(j,m)}$$

$\alpha > 0$: emphasize target biomarker
 $\beta > 0$: penalize overlap with others

- Optimization goal:

$$\max_{w \in [0,1]^M} \sum_i \mathcal{L}_i(w)$$

B. 3D Spectroscopic Optimization

- Input: $S \in \mathbb{R}^{N \times M_1 \times M_2}$ (excitation \times detection wavelengths)
- Attention matrix: $W_i \in [0, 1]^{M_1 \times M_2}$
- Objective function:

$$\mathcal{L}_i(W) = \alpha \sum_{u=1}^{M_1} \sum_{v=1}^{M_2} W_{(i,u,v)} S_{(i,u,v)} - \beta \sum_{\substack{j=1 \\ j \neq i}}^N \sum_{u=1}^{M_1} \sum_{v=1}^{M_2} W_{(j,u,v)} S_{(j,u,v)}$$

→ Incorporates fluorescence and absorbance for enhanced discrimination.

C. Key Notes:

- α, β are tunable hyperparameters
- Optimization performed under constraints: $w \in [0, 1]$
- Results guide multi-wavelength sensor design

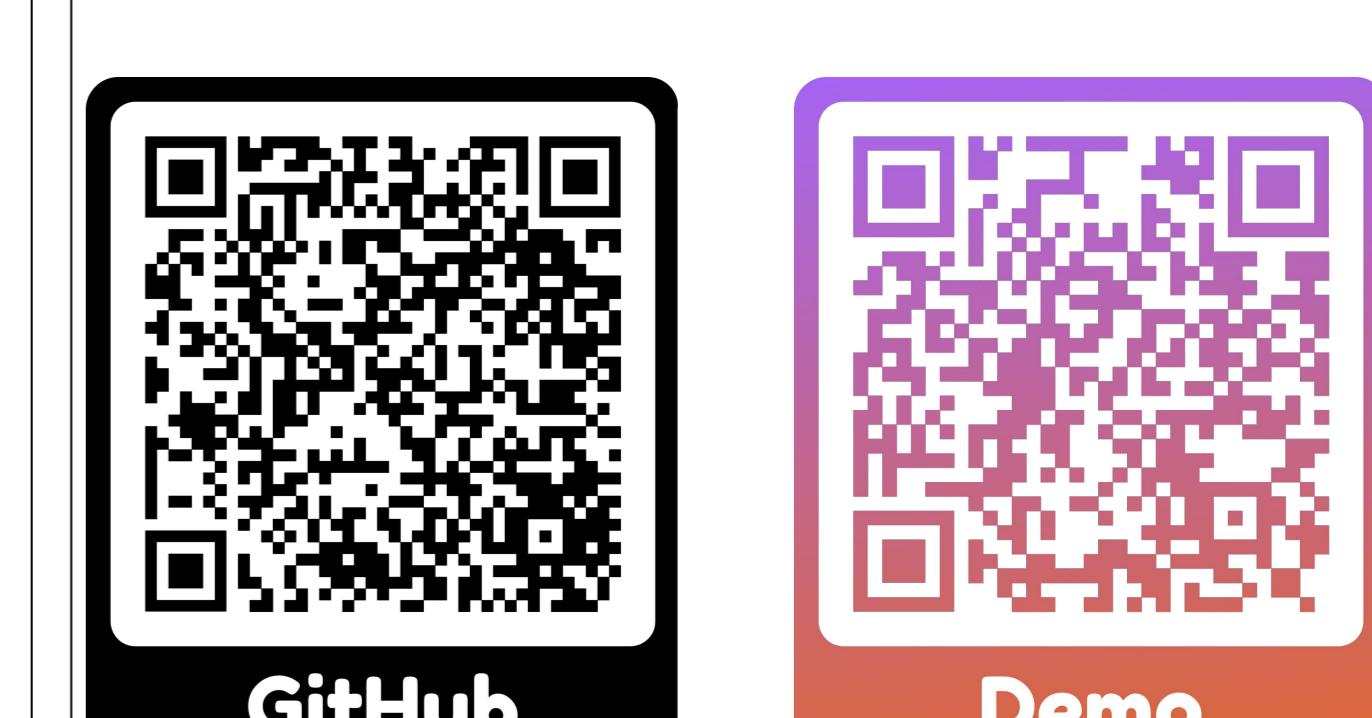
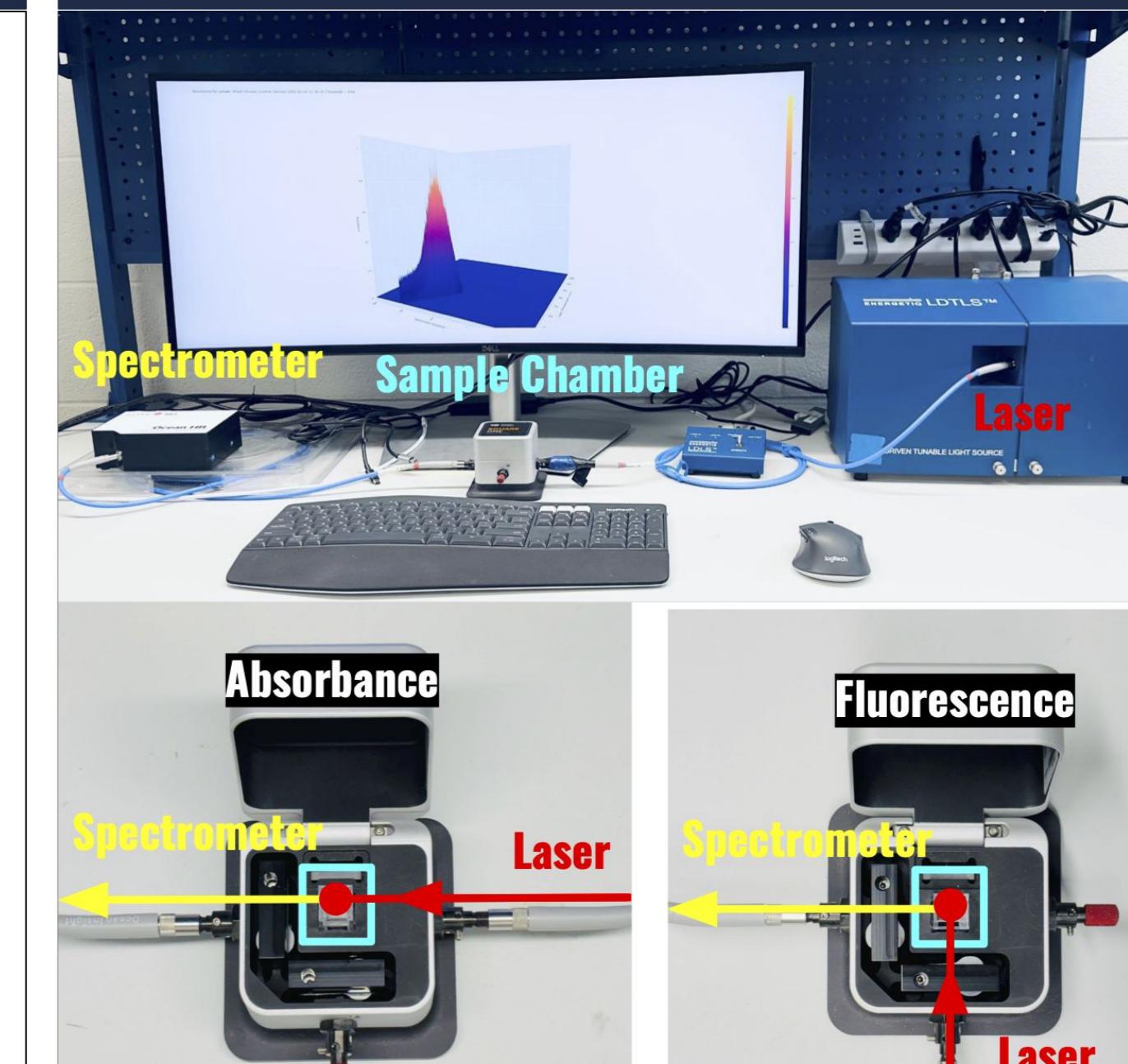
Detection Effectiveness (DE)

$$DE(w_i) = \frac{\text{Target}}{\sqrt{\text{Interference}}} = \frac{\sum_{m=1}^M w_{(i,m)} A_{(i,m)}}{\sqrt{\sum_{\substack{j=1 \\ j \neq i}}^N \sum_{m=1}^M w_{(j,m)} A_{(j,m)}}}$$

- Quantify alignment between attention weights and target biomarker absorbance.
- Minimize spectral overlap with non-target biomarkers for better sensing specificity.

ID	Biomarker Name	Target	Interference	DE
1	Bilirubin	2.53	42.60	0.39
2	C-Reactive Protein	2.48	41.90	0.38
3	Collagen	1.25	21.10	0.27
4	Creatinine	1.43	24.21	0.29
5	Ghrelin	0.00	0.00	NA
6	Glucose	5.11	86.39	0.55
7	HDL	2.07	35.08	0.35
8	Hemoglobin A_e	4.15	70.00	0.50
9	Hemoglobin Human	6.41	108.2	0.62
10	Human Leptin	2.46	41.65	0.38
11	Insulin	1.06	17.94	0.25
12	Melatonin	1.82	30.76	0.33
13	Sodium Lactate	3.57	60.32	0.46
14	Tryptophan	3.50	59.32	0.45
15	Tyrosine	0.72	12.22	0.21
16	Urea	0.90	15.12	0.23
17	VLDL	7.84	89.61	0.83

Equipment



Find more of our work at the lab website:
www.watsonresearchlab.org