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

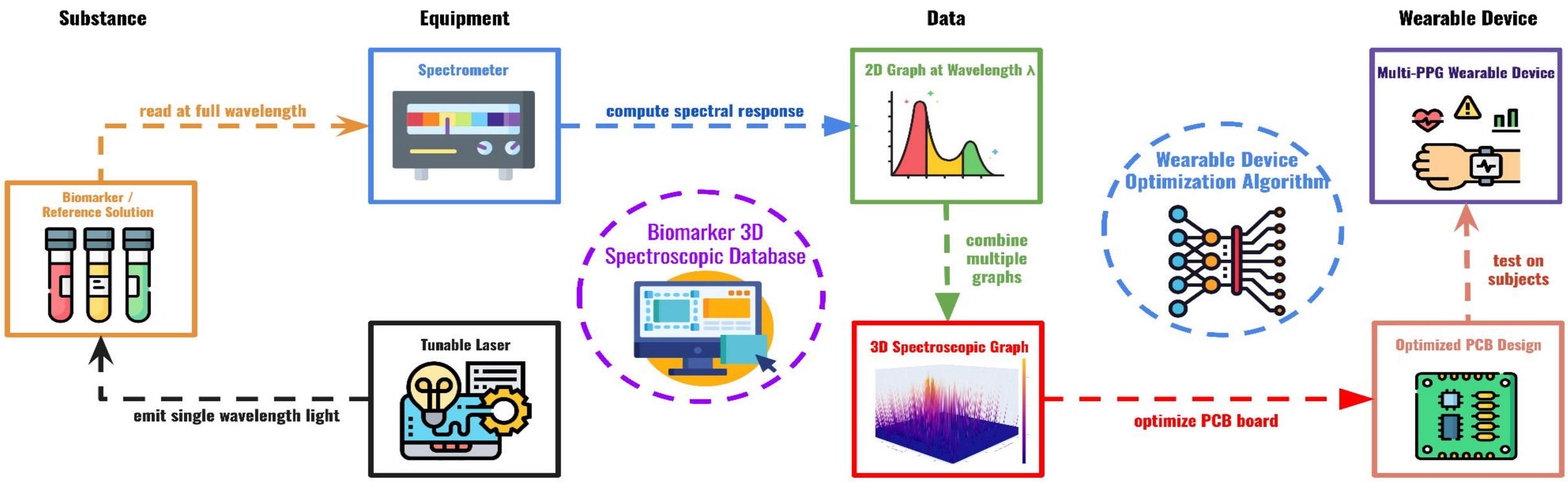
Research Overview

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

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):** $\mathbf{w}_i = (w_{(i,1)}, \ldots, w_{(i,M)}) \in [0,1]^M$
- **Objective function:**

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

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

- **Optimization goal:**

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

B. 3D Spectroscopic Optimization

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

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

→ 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

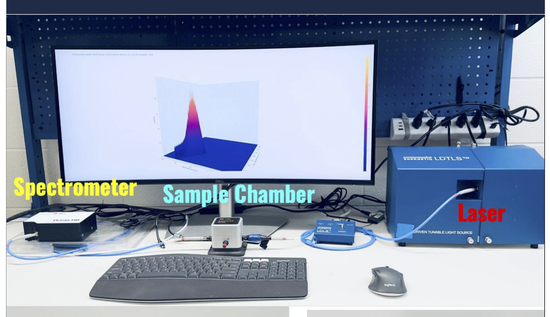
Detection Effectiveness (DE)

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

- 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



GitHub

Demo

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