IOCN 2025 Conference

The 5th International Online Conference on Nanomaterials

22–24 September 2025 | Online

MDPI

Nanostructure-Driven SERS and AI for Selective Identification of Bacterial Biomarkers

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INTRODUCTION & AIM

- Global challenge: Bacterial infections and antimicrobial resistance (AMR) cause **millions of deaths** and **massive economic loss**.
- Current methods (**culture, PCR, ELISA**): Accurate but **slow**, **costly**, and **not field-deployable**
- SERS advantage: **Single-molecule sensitivity**, **real-time** and **multiplex detection**.
- Two strategies:
  - Direct detection of whole bacteria: **low signal**, **complex backgrounds** and **overlapping** spectra.
  - Indirect detection of biomarkers: better sensitivity but **weak affinity** and **reproducibility** issues.
- Key challenges: **Highly complex spectra** + **non-monotonic calibration curves** hinder reliable quantification.

OBJECTIVE:

- Benchmark against six bacterial biomarkers (**2,3-DHBA, 2,5-DHBA, Pyocyanin, LTA, Enterobactin, β-carotene)**.
- Collect spectra on bare AgNR arrays (**no affinity modifications**).
- Classification and quantification of biomarkers with **convolutional neural networks (CNNs)** models.
- **Feature interpretation** using **Grad-CAM** and **SHAP** to identify spectral regions critical for classification and quantification.
- Demonstrate a robust, **AI-driven biosensing strategy** for **weak** or **inconsistent** SERS signals

METHOD

AgNR Fabrication

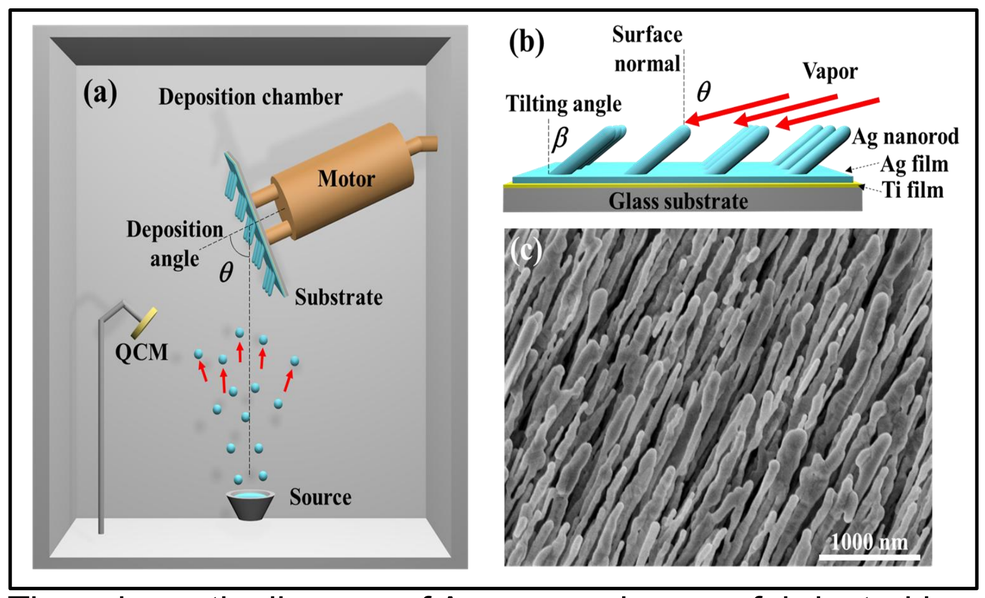


Figure 1. (a) The schematic diagram of Ag nanorod arrays fabricated by oblique angle deposition; (b) the definition of deposition angle θ and Ag nanorod tilting angle β; and (c) a representative SEM image of the AgNR

Detection Strategy

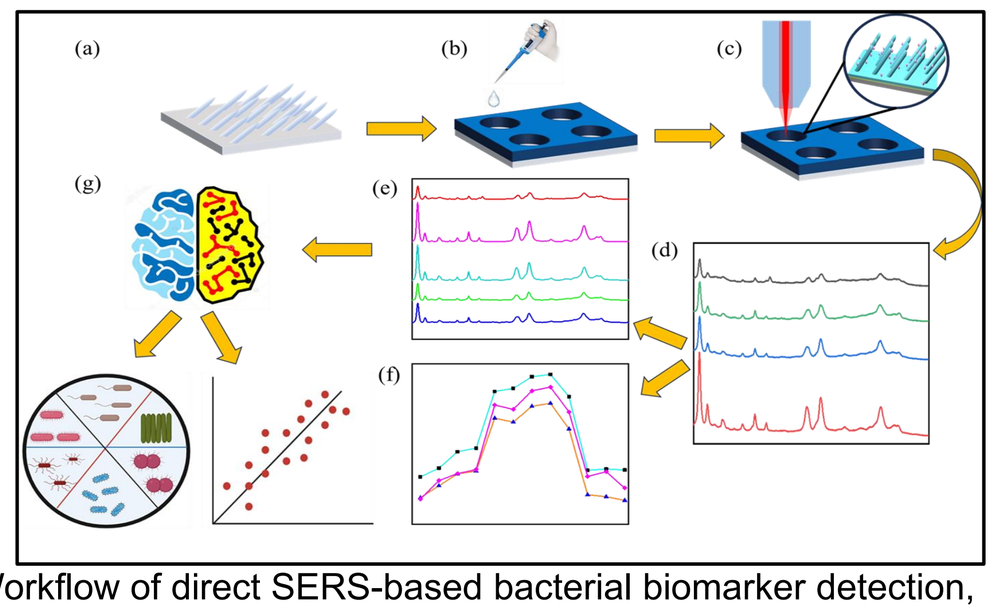
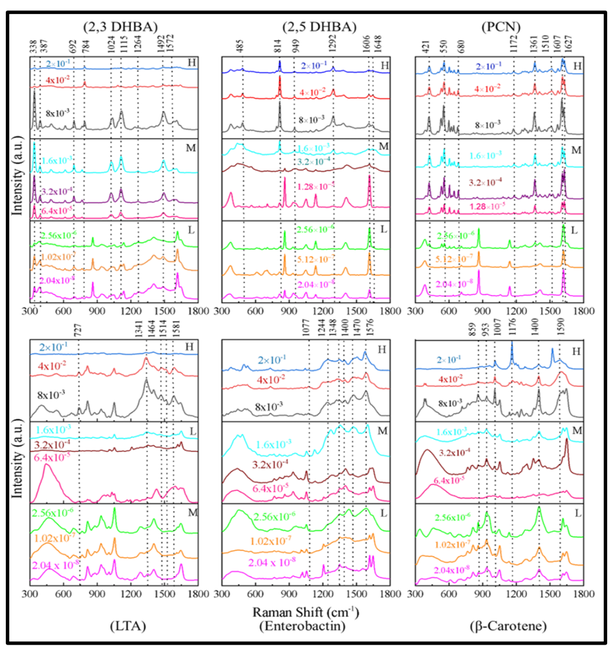


Figure 2. Workflow of direct SERS-based bacterial biomarker detection, AgNR substrates are integrated with PDMS wells for sample drop-casting, followed by Raman spectral acquisition. The resulting spectral fingerprints are analyzed through machine learning to enable biomarker classification and quantitative evaluation.

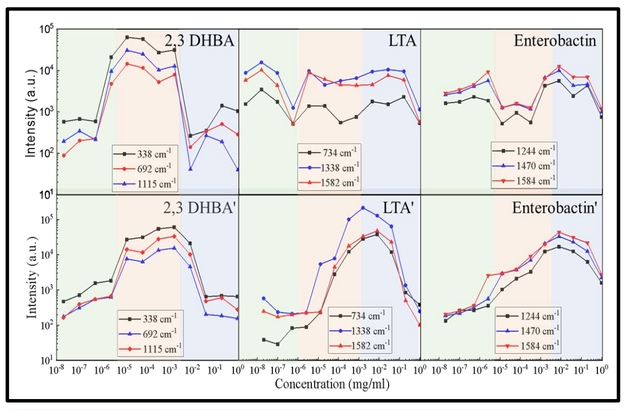
RESULTS & DISCUSSION

BIOMARKER SPECTRA



- Low affinity, background, and noise make direct identification difficult
- Calibration curve: intensity does not increase smoothly with concentration complicates quantification

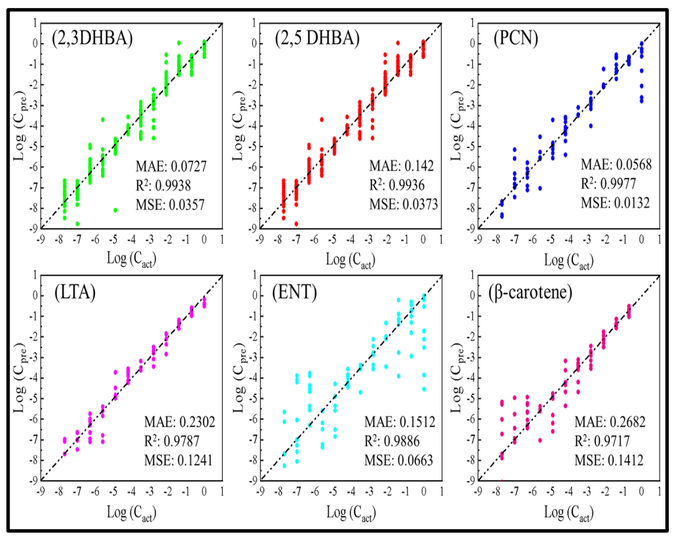
CALIBRATION CURVE

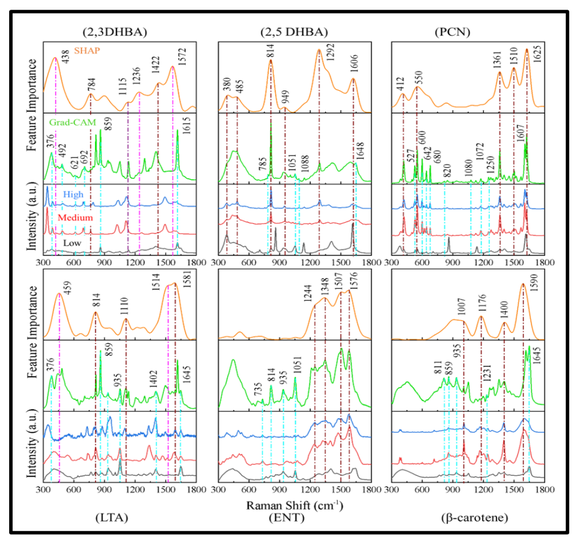


CNN CLASSIFICATION

	2,3-DHBA	2,5-DHBA	Pyocyanin	LTA	Enterobactin	β-carotene	Reference
2,3-DHBA	100	0	0	0	0	0	0
2,5-DHBA	0	97.3	2.7	0	0	0	0
Pyocyanin	0	0	100	0	0	0	0
LTA	0	0	0	100	0	0	0
Enterobactin	0	0	0	0	100	0	0
β-carotene	0	0	0	0	0	100	0
Reference	0	0	0	0	0	0	100

REGRESSION AND FEATURE OF IMPOTRANCE





- To identify the most important spectral features driving CNN classification and regression, Grad-CAM and SHAP analyses were applied.
- Both methods revealed that key spectral features consistently align with characteristic SERS peaks of each bacterial biomarker, confirming their role in model decisions.

CONCLUSION

- CNNs achieved >99.9% classification accuracy across all six biomarkers, even for weakly binding molecules.
- Regression performance was strong ($R^2 > 0.97$, MAE < 0.27),.
- Deep learning compensates for low analyte–substrate affinity, revealing hidden spectral patterns.

FUTURE WORK

- Enhancing affinity: Apply external voltage to modulate analyte adsorption on AgNR Electrochemical-SERS: Develop integrated platforms combining AgNR arrays with electrochemical control.

Reference

Kumar et al. (2024) *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, *320*, 124627.

Acknowledgement

Project Supported by USDA: NIFA 2023-67015-39237

Qatar National Research Fund: NPRP12S-0224-190144