

MD627 893 Seminar in Medical Microbiology

Department of Microbiology, Faculty of Medicine, Khon Khean University

Title: Innovative Clinical Diagnosis: Utilizing SERS Sensors and Machine Learning for Biomolecular Detection

Student: Miss. Kingkan Jaisiri **Student ID:** 665070018-5

Advisor: Assist. Prof. Dr. Wisitsak Phoksawat

Date: 30 July 2024

Abstract

Surface-enhanced Raman spectroscopy (SERS) and Raman spectroscopy (RS) are professional techniques for biomolecule detection that can investigate the conformational changes in complex biological molecules with enhanced Raman scattering. The enhancement of Raman scattering involves two mechanisms: typically, the strong electromagnetic enhancement, and the chemical enhancement. Hopefully, the SERS method will be a promising tool for future routine clinical tests due to its speed, cost-effectiveness, and high accuracy.

For diabetic nephropathy, excessive proteins in human urine serve as early and sensitive markers, as well as primary and secondary renal diseases. Developing an efficient, expressive, and low-cost method for protein determination is needed. SERS technique is one of potential candidate tools to meet these criteria. Herein, researchers therefore developed SERS method by using gold nanoparticles (AuNPs) with diameters of 60 nm and 100 nm to distinguish between patients with proteinuria (Abnormal protein concentration in their urine) and healthy individuals (Normal protein concentration). Results showed that the PCA-LDA algorithm and ROC curves can provide diagnostic results for 78 samples. Sensitivity, specificity, accuracy, and AUC were 0.79, 0.89, 0.85, and 0.90 for the set with 60 nm AuNPs, respectively. Moreover, the set with 100 nm AuNPs, sensitivity, specificity, accuracy, and AUC were 0.79, 0.98, 0.90, and 0.91, respectively (Aitekenov et al., 2022). The results demonstrate the potential of SERS with 100 nm AuNPs as an optimal combination providing the best balance between sensitivity and specificity in this SERS-based method of proteinuria diagnostics.

For tuberculosis (TB), TB still be a major global public health problem that is caused by *Mycobacterium tuberculosis (Mtb)* infection and is airborne transmission. TB is divided into two types: latent TB (LTBI), in which bacteria hide in the host without causing symptoms (but sometimes it can develop into ATB), and active TB (ATB) is symptomatic. In the case of LTBI, screening in the community leading to prophylactic treatment will accelerate the elimination of TB. However, effective diagnostic tools for screening are poorly developed. In previous studies, the SERS technique can distinguish for four categories relative to TB infection (ATB, LTBI, early clearance, and healthy controls). In this research, the researchers aimed to investigate the performance of LTBI diagnostic approaches by combining the SERS analysis system with machine learning. They found that the SERS sensors provided 81% accuracy according to train-test split analysis and 75% for LOOCV analysis from all samples. The accuracy increased to 93 % when the logistic regression model was used for analysis following optimization of the sample collection, SERS chips, and database (Eiamchai et al., 2024). Therefore, this study summarized that SERS analysis with machine learning was potentially available diagnostic tool for LTBI screening.

References

- Aitekenov, S., Sultangaziyev, A., Ilyas, A., Dyussupova, A., Boranova, A., Gaipov, A., & Bukasov, R. (2022). Surface-enhanced Raman spectroscopy (SERS) for protein determination in human urine. *Sensing and Bio-Sensing Research*, 38, 100535. <https://doi.org/10.1016/j.sbsr.2022.100535>
- Eiamchai, P., Juntagan, C., Somboonsaksri, P., Waiwijit, U., Eisiri, J., Samarnjit, J., Kaewseekhao, B., Limwichean, S., Horprathum, M., Reechaipichitkul, W., Nuntawong, N., & Faksri, K. (2024). Determination of latent tuberculosis infection from plasma samples via label-free SERS sensors and machine learning. *Biosensors and Bioelectronics*, 250. <https://doi.org/10.1016/j.bios.2024.116063>