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Accurate diagnosis of thyroid cancer using a combination of surface-enhanced Raman spectroscopy of exosome on MXene-coated gold@silver core@shell nanoparticle substrate and deep learning

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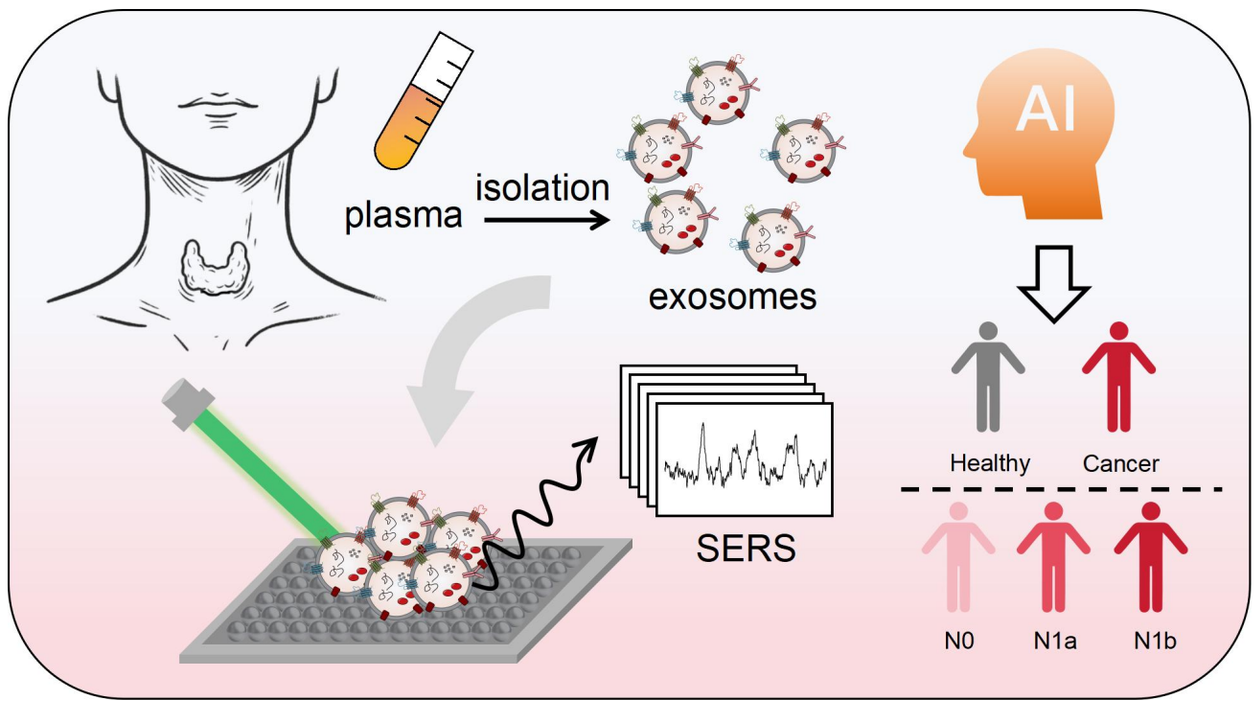
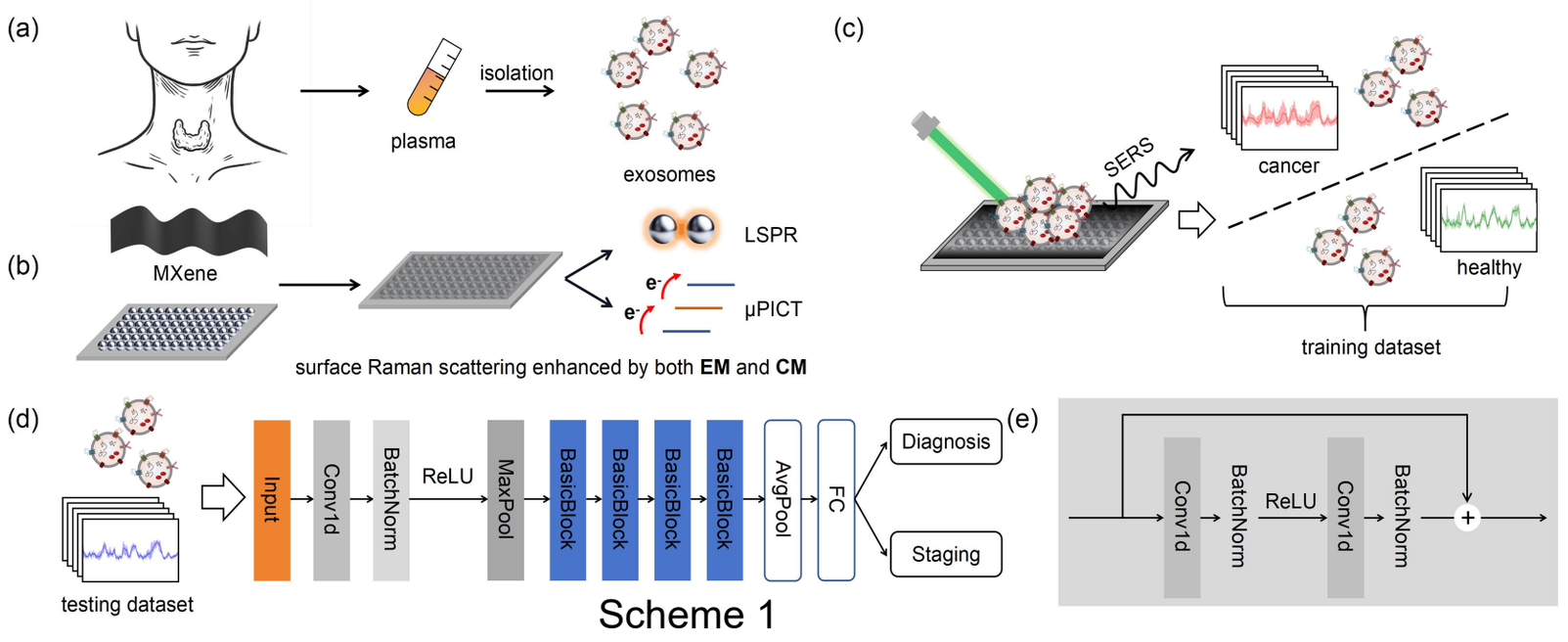
Introduction

As the most widespread endocrine cancer globally, the incidence rate of thyroid cancer continues to rise annually. Currently, ultrasound image-guided fine needle aspiration biopsy is gold standard for diagnosis of thyroid cancer. However, this method relies heavily on the experience of clinical physicians and cannot identify small cancers or lesions with atypical morphology. For improving the diagnosis accuracy of thyroid cancer, a label-free Raman profiling of exosomes has been employed for facilitating accurate diagnosis and staging of thyroid cancer through a combination of EM/CM dual-enhanced MXene-coated gold@silver core@shell nanoparticle (Au@Ag NP) SERS platform with a residual neural networks-based deep learning model (as shown in Scheme 1). Due to synergistic effect of EM mechanism provided by Au@Ag NP and the charge transfer between the MXene layer with probe molecules, the MXene-coated Au@Ag NP substrate shows a Raman analytical enhancement factor (AEF) as high as 2.10×10^{10}, which can label-free Raman profiling of exosomes as low as 1.7×10^{9} EVs mL^{-1}. Moreover, the acquired SERS spectra of exosomes from clinical samples were subsequently utilized to train the deep residual network, resulting in a diagnostic accuracy of 96.0% and a staging accuracy of 86.6% for thyroid cancer.



Graphical Abstract



Scheme 1

Materials and methods

Reagents and instruments:$HAuCl_4\cdot3H_2O$, $AgNO_3$, ascorbic acid , LiF (99.9%), HCl (36.5-38.0%), HF (40%), n-hexane (99.9%), Rhodamine B (99.9%) . Methods:Fabrication and characterization of the SERS substrates, Exosome extraction and characterization, SERS measurement of RhB, SERS measurement of exosomes from clinical samples, FDTDsimulations,DFT calculations, Statistical analysis based on deep learning

Results

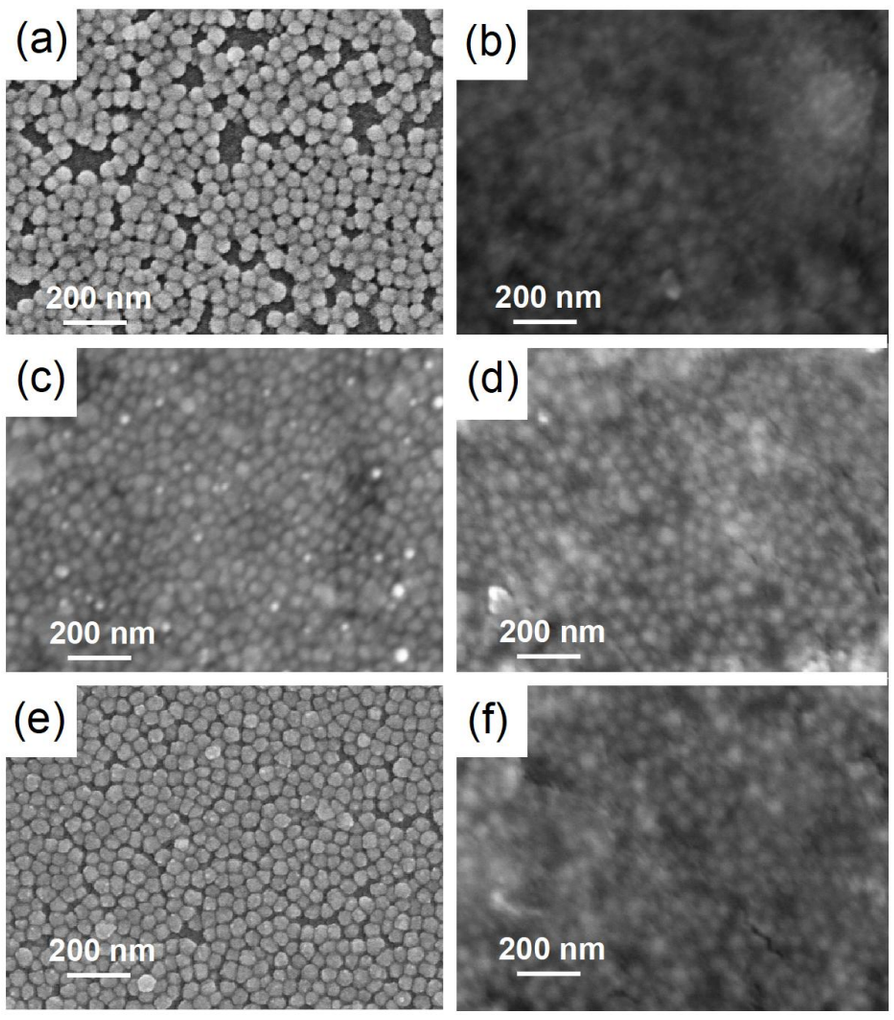


Figure 1

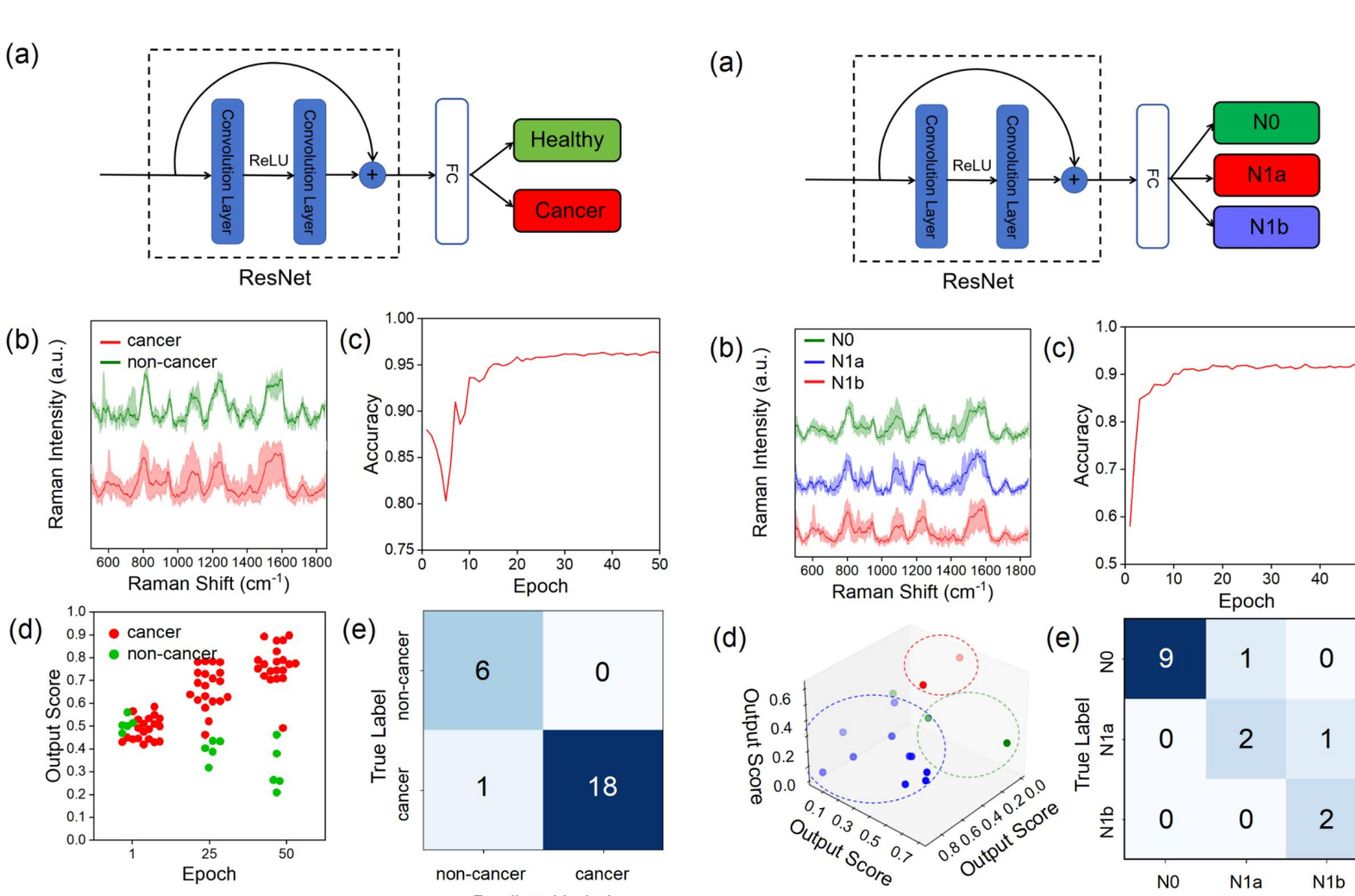


Figure 3

Figure 4

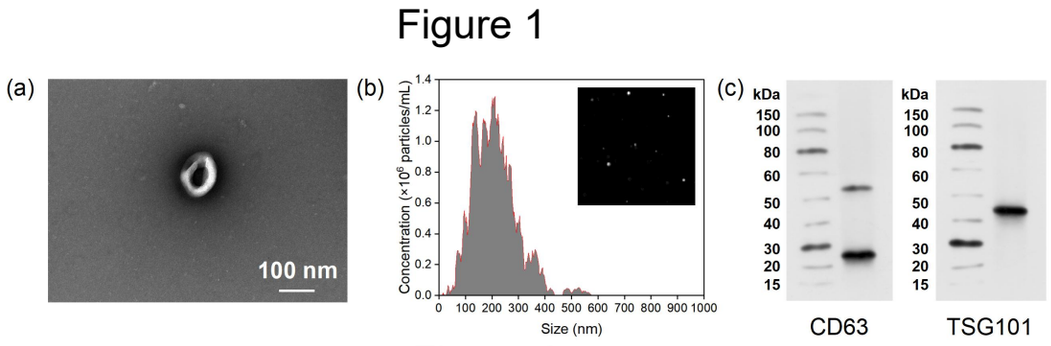


Figure 2

Discussion / Conclusion

In summary, this study demonstrates the great potential of label-free profiling of exosomes from plasma for facilitating accurate diagnosis and staging of thyroid cancer through combination of EM/CM dual-enhanced MXene-coated Au@Ag NP SERS platform with a residual neural networks-based deep learning model. The acquired SERS spectra of exosomes from clinical samples on the MXene-coated Au@Ag NP SERS platform, which has a LOD of 1.7×109 EVs mL-1 for exosomes, are employed to train the diagnosis and staging models, enabling thyroid cancer diagnosis with an accuracy of 96.0% and staging classification with an accuracy of 86.6%, respectively. The results demonstrate the feasibility and power of this integrated approach for accurate SERS analysis of exosomes toward improved cancer management, and augment current understanding of the potential diagnostic applications of exosome analysis. Larger datasets, inclusion of additional subgroups or histological types, and integration with clinical information in the future may enable more robust predictive models with broader clinical implications.