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Direct Antimicrobial Resistance Prediction from Surface-Enhanced Raman Scattering Spectra Using Artificial Intelligence

WEN-LING LIN[1], TSAI-WEN WAN[2], WEI-CHENG CHANG[3], NAI-SHUN LIAO[3], CHUN-YI HSU[3], YU-HUI LIAO[3], YU-TSUNG HUANG[4], HAO-CHIEH CHIU[1,4]

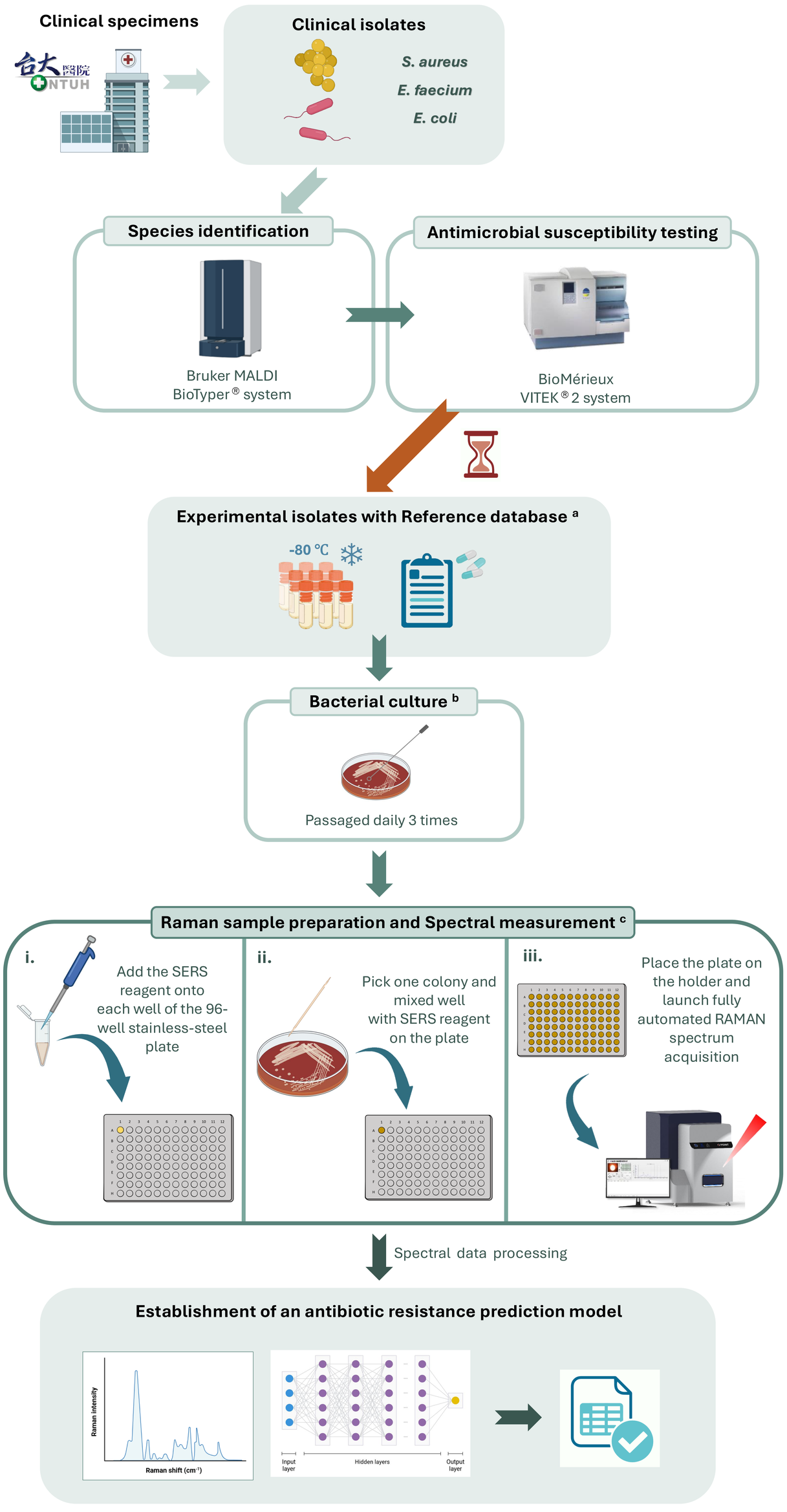
1. Department of Clinical Laboratory Sciences and Medical Biotechnology, College of Medicine, National Taiwan University.
2. Department of Microbiology and Immunology, Kaohsiung Medical University.
3. ITRUST MedTech.
4. Department of Laboratory Medicine, National Taiwan University Hospital.

Background

Infectious diseases are the third leading cause of death globally, with bacterial infections accounting for nearly half of the cases. The increasing prevalence of antibiotic-resistant bacteria presents a major public health challenge. While accurate antibiotic selection is essential, conventional culture-based antibiotic susceptibility testing (AST) typically requires up to 72 hours. To address this limitation, we partnered with ITRUST MedTech Inc. to develop a rapid, AI-driven antibiotic resistance prediction system based on Raman spectroscopy.

Methods

Clinical isolates of three key drug-resistant bacterial species—methicillin-resistant *Staphylococcus aureus* (MRSA), vancomycin-resistant *Enterococcus faecium* (VRE), and carbapenem-resistant *Escherichia coli* (CREC)—were obtained from the Department of Laboratory Medicine at National Taiwan University Hospital. Species identification and AST were validated using MALDI Biotyper® and the VITEK® 2 system, respectively. Raman spectra were acquired using ITRUST's fully automated high-throughput Raman spectroscope.



[a] **Clinical isolate source.** Clinical isolates were obtained from NTUH, cryopreserved at –80 °C with glycerol, and accompanied by validated species identification and antimicrobial susceptibility profiles to build the reference database.

[b] **Bacterial culture.** Bacteria were incubated on TSA II agar supplemented with 5% sheep blood at 37 °C for 16–18 h.

[c] **Sample preparation and Raman spectra measurement.** SERS reagents containing silver nanoparticle colloids and a 96-well stainless-steel plate were provided by ITRUST MedTech Inc. Bacterial colonies were mixed with the SERS reagent and air-dried before Raman measurement. A 735 nm laser was used to collect 10 Raman spectra per sample, with acquisition times ranging from 30s to 60s.

Results

A total of 408 *S. aureus*, 200 *E. faecium*, and 123 *E. coli* clinical isolates were collected. Of these, 100 *S. aureus*, 140 *E. faecium*, and 86 *E. coli* strains were used to construct a spectral database and train the AI model, while the remaining isolates were used for validation. Compared with VITEK 2 results, the AI system achieved prediction accuracies and AUCs of 85% (AUC 0.92) for MRSA, 90% (AUC 0.96) for VRE, and 81% (AUC 0.89) for CREC.

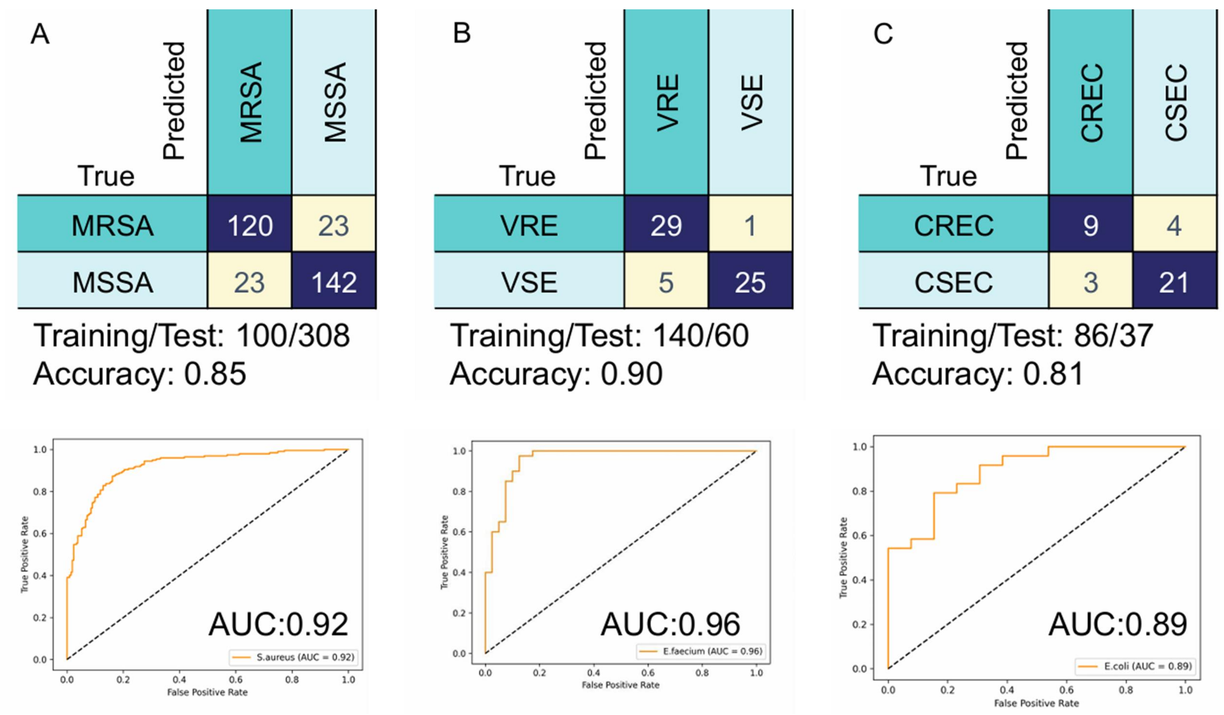


Fig. 1 Antibiotic resistance prediction via the artificial intelligence system

The figure displays antibiotic resistance prediction results for three bacterial species, with MRSA in 1A, VRE in 1B, and CREC in 1C. In these panels, true indicates the actual antimicrobial susceptibility profile determined by standard laboratory testing, while predict represents the resistance phenotype predicted by the model based on Raman spectral data. The training dataset consists of Raman spectra used to build the AI model, and the test dataset was used to evaluate model predictions.
Below, ROC curves for each antibiotic illustrate model performance, with the area under the curve (AUC) indicating accuracy (1.0 = perfect prediction, 0.5 = random chance).

Conclusion

This study demonstrates the feasibility of an AI-assisted Raman spectroscopy platform for rapid antimicrobial resistance prediction, with potential to reduce diagnostic delays, support targeted therapy, and improve clinical outcomes.