INNOVATING CROSS-DOMAIN SOLUTIONS TO DETECT EMERGING BIOLOGICAL THREATS

Machine Learning-enabled Development Of Sers Sensors For The Detection Of Trace Analytes

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Field detection of trace analytes faces challenges with reliability, cost-effectiveness, swiftness, and portability. Handheld Raman spectroscopy coupled with surface-enhanced Raman scattering (SERS) substrates offer portability and reasonable acquisition times, but there is a lack of reproducible, cost-effective SERS sensors and reliable spectral classification of trace analytes. Here we describe an important first step towards this end by using machine learning (multi-objective Bayesian optimization) to expedite the development of SERS sensors using plasmonic nanoparticles. We optimized input variables across several common fabrication methods (spin coating, flow coating, and printing) and evaluated their SERS performance for enhancement and substrate uniformity using dyes as well as trace analytes of interest. The use of machine learning in sensor development expedites the time required to develop this technology in comparison to traditional research methods. Ultimately, we hope this technology will allow for cost-effective routine monitoring of trace analytes in the field.