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Differentiation and classification of bacterial endotoxins based on surface enhanced Raman scattering and advanced machine learning

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Abstract

Bacterial endotoxin, a major component of the Gram-negative bacterial outer membrane leaflet, is a lipopolysaccharide shed from bacteria during their growth and infection and can be utilized as a biomarker for bacterial detection. Here, the surface enhanced Raman scattering (SERS) spectra of eleven bacterial endotoxins with an average detection amount of 8.75 pg per measurement have been obtained based on silver nanorod array substrates, and the characteristic SERS peaks have been identified. With appropriate spectral pre-processing procedures, different classical machine learning algorithms, including support vector machine, k-nearest neighbor, random forest, *etc*., and a modified deep learning algorithm, RamanNet, have been applied to differentiate and classify these endotoxins. It has been found that most conventional machine learning algorithms can attain a differentiation accuracy of >99%, while RamanNet can achieve 100% accuracy. Such an approach has the potential for precise classification of endotoxins and could be used for rapid medical diagnoses and therapeutic decisions for pathogenic infections.

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