PÔSTER - RESUMO - SENSORES E BIOSSENSORES

SERS-BASED DETECTION OF THE PESTICIDE THIRAM IN STRAWBERRY SAMPLES

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Despite its high sensitivity, surface-enhanced Raman spectroscopy (SERS) still lacks robust methodologies for analytical applications. In this context, this study aims to evaluate the feasibility of using SERS as an analytical tool for detecting the pesticide thiram in real samples, such as strawberries. Silver nanoparticles (AgNPs) were synthesized and employed as a SERS platform, and aliquots of thiram (diluted in ethanol) were added to the colloidal suspension for spectral acquisition. For measurements in real samples, SERS spectra were collected according to the following procedure: an aliquot of thiram (10 µL) at the desired concentration was deposited onto the sample surface and, after drying, a nanoparticle dispersion (20 µL) was added. The Raman and SERS spectra of thiram show considerable differences, mainly attributed to molecular cleavage upon adsorption onto the metallic surface. Although the SERS spectral profile does not change significantly with decreasing thiram concentration, new bands appear at higher pH values, likely due to the formation of byproducts. The extinction spectra of the nanoparticles in the presence of thiram indicate that

different aggregates are formed depending on the pesticide concentration. These findings are consistent with transmission electron microscopy (TEM) images. At low concentrations, more elongated aggregates are observed, whereas at higher concentrations, more globular aggregates predominate. Dynamic light scattering (DLS) measurements show that aggregate size increases at higher concentrations. Static contact angle measurements indicate that the nanoparticles exhibit a superhydrophilic surface, resulting in high surface energy. This may explain the strong affinity of the pesticide for adsorption onto the nanoparticle surface and the subsequent formation of aggregates. Quantitative analysis under ideal conditions was performed over a thiram concentration range from 1.0 × 10-5 to 8.0 × 10-8 mol L^{-1}, achieving a limit of detection of 5.84 × 10-8 mol L^{-1}. In real samples, 30 spectra were collected at each concentration within the range of 8.0 × 10-6 to 1.0 × 10-4 mol L^{-1}. The mean and standard deviation of the spectral intensities were then calculated and plotted as a function of concentration. High variability in the measurements was observed, along with the absence of a linear response region, hindering the determination of a limit of detection. This behavior is likely due to the non-uniform distribution of both the pesticide and the nanoparticles on the surface, or alternatively, to morphological irregularities of the strawberry.

Acknowledgements: INEO (FAPESP - processo nº 2025/27044-5 and CNPq - processo: 408449/2024-1 and 313211/2023-0), FAPESC (2024TR002330) and CAPES.

Palavras-chave: sers; silver nanoparticles; thiram; food safety.