

Recovery of Characteristic Thiabendazole Raman Peaks from Ethanol-Dominated Spectra Toward Microfluidic SERS-Based Pesticide Sensing

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Summary:

We present a reference-guided Raman analysis workflow developed as a signal processing module for a microfluidic SERS sensor targeting pesticide detection. A two-component linear model based on ethanol and dry thiabendazole (TBZ) reference spectra was used to recover analyte contributions from ethanol-dominated spectral data. The recovered TBZ component preserved key diagnostic peaks and enabled automated peak identification. The current results are based on measurements of a sample of 2 µL and serve as a proof-of-concept for future flow-through sensing systems.

Keywords: thiabendazole, Raman spectroscopy, SERS, microfluidics, spectral unmixing

Background, Motivation and Objective

Thiabendazole (TBZ) is a benzimidazole fungicide relevant for residue monitoring in environmental and food-related samples. Raman and surface-enhanced Raman spectroscopy (SERS) provide molecular specificity; however, in liquid-phase measurements the analyte signal is often obscured by strong solvent contributions. This limitation persists even when using advanced plasmonic substrates engineered for efficient excitation at near-infrared wavelengths [1].

In this work, we develop a compact spectral unmixing workflow intended as a signal processing component of a microfluidic SERS sensor, where analyte-containing solutions will flow over an active sensing substrate. As an intermediate step, we evaluate the recovery of TBZ Raman features from spectra dominated by ethanol using a controlled static measurement configuration.

Description of the New Method or System

Corrected spectra measured on SERS substrates - Au-based nanostructures fabricated via electron-beam lithography and designed to achieve plasmonic resonance in the 800–900 nm range, matching 785 nm excitation—were analyzed in the 300–1800 cm⁻¹ spectral range.

Each measured spectrum was modeled as a linear combination of reference spectra [2]:

$$I_{mix} = \alpha \cdot I_{ethanol} + \beta \cdot I_{TBZ}$$

where $I_{ethanol}$ and I_{TBZ} correspond to ethanol and dry TBZ references, respectively. To improve robustness, the dominant ethanol band region (850–910 cm⁻¹) was excluded from fitting.

The recovered analyte contribution ($\beta \cdot I_{TBZ}$) was further processed using prominence-based peak detection to identify characteristic Raman bands. The approach is computationally lightweight and compatible with real-time data processing in flow-through sensing configurations. SERS measurements were performed using a fiber-optic probe coupled to a 785 nm excitation source, consistent with the substrate design.

The overall sensing concept is illustrated in Fig. 1a, where a microfluidic SERS platform is envisioned. In this system, analyte-containing solution flows over a nanostructured Au substrate, and the Raman signal is collected via a fiber-optic probe. The proposed spectral unmixing approach is intended as a signal processing module within this architecture.

Results

The proposed decomposition successfully isolated a TBZ-like spectral component even when the raw spectra were strongly dominated by ethanol. As shown in Fig. 1b, the measured spectra exhibit a dominant ethanol contribution, particularly in the 850–910 cm^{-1} region, which obscures direct identification of analyte features. Following spectral unmixing, the recovered TBZ component (Fig. 1c) preserves characteristic Raman bands near 782, 1009, 1275, 1377, 1450, and 1592 cm^{-1} , enabling reliable peak identification. The averaging of the reconstructed TBZ spectra across concentrations further enhances the visibility of diagnostic features.

The concentration dependence of the unmixing coefficient β is presented in Fig. 1d. Despite inter-series variability, a monotonic trend is observed for most measurement series, supporting the use of β as a semi-quantitative indicator of TBZ concentration.

References

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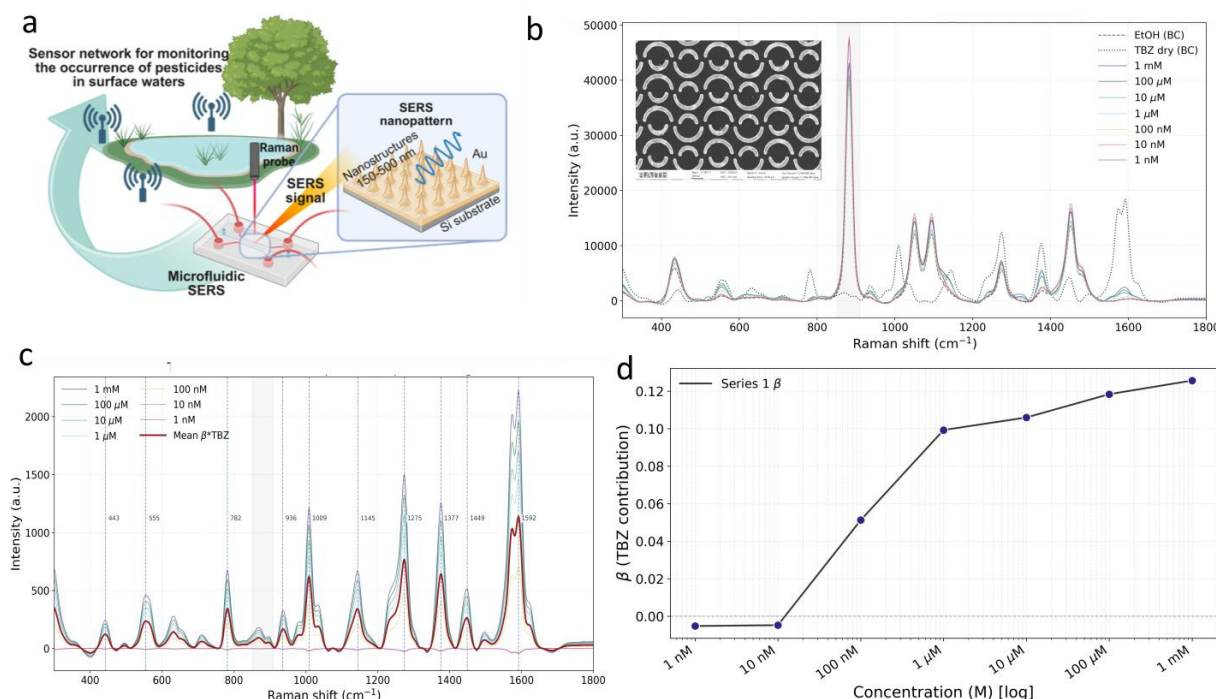


Fig. 1. (a) Concept of a microfluidic SERS sensing platform for pesticide detection, where analyte-containing solution flows over a nanostructured Au substrate and Raman signal is collected using a fiber-optic probe. (b) Raw Raman spectra of TBZ in ethanol at different concentrations, dominated by solvent contribution; inset: SEM image of the SERS substrates showing Au nanostructures. (c) Recovered TBZ spectral component obtained by two-component unmixing, showing enhanced visibility of characteristic Raman bands. (d) Dependence of the unmixing coefficient β (TBZ contribution) on concentration.