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Explainable Raman classification of toxic cyanobacterial species using a multichannel 1D-CNN with raw, baseline and preprocessed spectra as independent inputs

Harmful cyanobacterial blooms threaten freshwater resources, making rapid identification of toxic species critical for water quality management. Raman spectroscopy offers a label-free alternative to microscopy and molecular assays. However, preprocessing steps may attenuate subtle spectral information needed to accurately distinguish highly similar samples. We present a framework in which a multichannel one-dimensional convolutional neural network (1D-CNN) receives three inputs per measurement: raw spectra, baseline estimations and preprocessed spectra. Confocal Raman spectra (532 nm) were acquired from individual cells of four toxic cyanobacterial species, and the model was evaluated on a test dataset acquired in separate sessions. This configuration reached 86% accuracy with low overfitting, versus 74% for a conventional single-channel model trained on corrected spectra alone. Per-channel Shapley Additive exPlanations (SHAP) attribute classification decisions to carotenoid and chlorophyll bands and reveal distinct contributions, mainly from raw and preprocessed spectra [1]. These findings demonstrate that the proposed workflow exploits complementary information potentially suppressed by preprocessing steps, enabling more robust and interpretable results.

References

- [1] Fernández-Manteca, M. G., García García, B., Deus Álvarez, S., Gómez-Galdós, C., Pérez-Asensio, A., Algorri, J. F., Monteoliva, A. P., López-Higuera, J. M., Rodríguez-Cobo, L., Ocampo-Sosa, A. A., and Cobo, A., *Talanta*, 292 (2025) 127845.

Figures

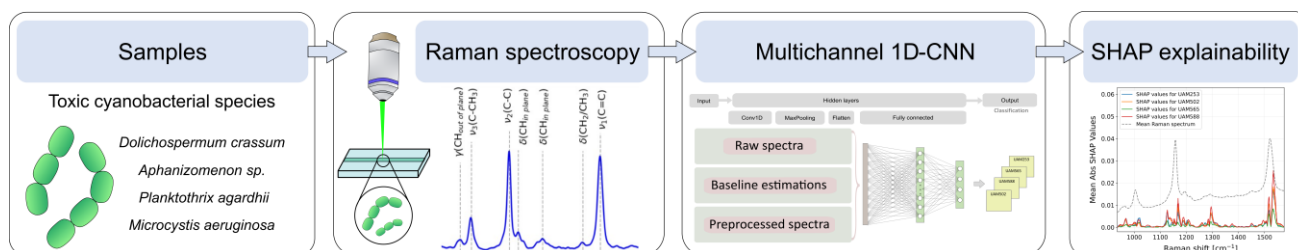


Figure 1: Schematic workflow for cyanobacterial classification using Raman, multichannel 1D-CNN and SHAP analysis.