

Raman and DFT simulation spectra of some prevalent herbicide metabolites

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Abstract: The use of pesticides in Europe poses significant environmental and public health challenges, leading to contamination of water sources like rivers and groundwater. Many regions exceed EU pesticide standards, highlighting the need for innovative monitoring methods that can deliver results more quickly than traditional methods, given the impact of pesticides on water quality [1]. Traditional Raman spectroscopy struggles with low sample concentrations but drop coating deposition Raman (DCDR) spectroscopy offers improved sensitivity for detecting weak signals in low-concentration samples [2]. This study investigates the Raman spectra of herbicide metabolites in Danish groundwater using the DCDR technique on gold surfaces. Key compounds examined include the pesticide metabolites Atrazine-2-hydroxy, Atrazine-desethyl, DPC, and 2,6-dichlorobenzamide (BAM). To facilitate rapid identification by this approach, we need to create a database of simulated Raman spectra for these pesticides. The spectra were acquired using a conventional Raman spectrometer (*Horiba LabRAM HR Evolution Spectrometer*), employing a 50x objective lens at maximum power (17 mW) with a 633 nm and/or 532 nm laser.

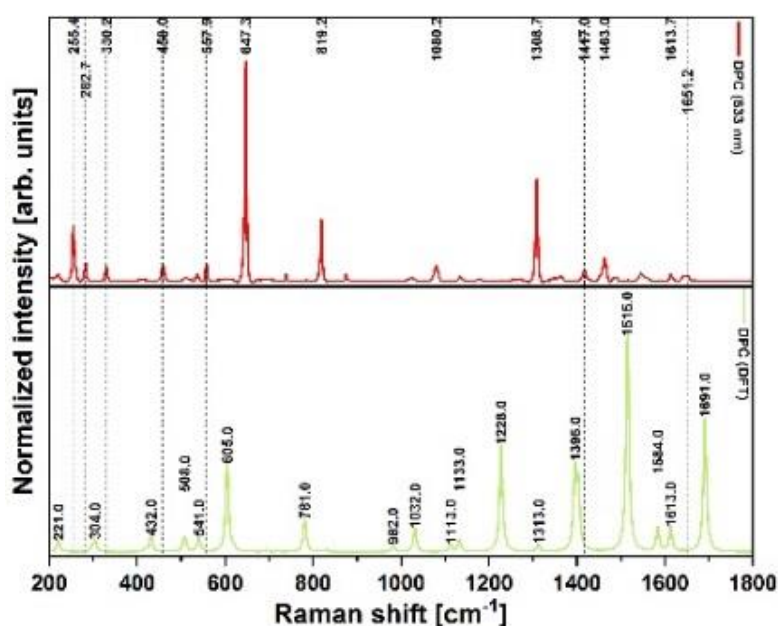


Figure 2: Desphenylchloridazon (DPC) simulated Raman spectra using DFT calculation (To enhance clarity in visual comparisons, dashed vertical lines have been drawn from the experimental maxima to the DFT spectra)

Keywords: herbicide metabolites, DCDR spectroscopy, DFT simulation

References

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