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PCA ANALYSIS OF SURFACE ENHANCED RAMAN SPECTRA OF NATURAL DYES ADSORBED ON NOBLE METAL SURFACES

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Raman spectroscopy is a valuable technique for detecting and characterizing dyes used in the past, but the Raman spectra of most of such dyes, especially the organic ones, present a strong fluorescence background. Surface-enhanced Raman scattering (SERS) can be used to overcome these inconveniences providing useful information in terms of chemical composition by using very small sample quantities. In this paper, alizarin and purpurin have been studied in low concentrations using SERS by noble metal substrates deposited using pulsed laser deposition (PLD) technique. Principal Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA) are the two statistical tools employed for this study, they can provide quick access to relevant information otherwise buried in big datasets of spectra which are particularly unfriendly for direct human inspection (due to data size). We have shown that both PCA and HCA are chemical-composition sensitive and can discriminate alizarin and purpurin in a joint dataset composed by SERS maps recorded on the two samples despite the similarity in their chemical structure and the intricacies due to the interplay of chemisorption and tautomerism. The possible impact of the latter has been explored with Density Functional Theory calculations showing that simulated spectra of different tautomers of alizarin and purpurin are markedly different.