Classification and Identification of Aqueous Pollen Extracts Using SERS and Artificial Neural Networks (ANN)

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The classification and identification of pollen samples is still challenging and time-consuming since it is currently based on the morphological investigation of pollen grains. In order to use specific molecular information for this analytical task, methods of vibrational spectroscopy can be combined with multivariate statistics. It has been shown that Raman[1]- and infrared-spectroscopies[2] can be applied and used for automated pollen detection. In Raman spectra of some pollen species, however, a high fluorescence background can be observed that hinders accurate pollen classification. Since SERS provides significant fluorescence quenching together with high signal enhancement, pollen detection based on SERS of aqueous pollen extracts is promising. In order to get highly reproducible SERS spectra of this extracts immobilized nanoparticles can be used.[3] Here we demonstrate that reproducible species-specific classification of pollen extract SERS data is also possible with high numbers of spectra that are obtained using nanoparticle suspensions.[4] With this simple experimental procedure several thousands of spectra can be generated in a short period of time. To make use of this high amount of data artificial neural networks (ANNs) were applied. It is shown that ANNs can be used for taxonomic classification and identification and to extract the taxonomically relevant information from the data. Since aqueous pollen extracts are used, this method enables a selective characterization of the water soluble fraction that mostly contains cellular components devoid of the spectral contributions of the insoluble sporopollenin outer layer.

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References

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