Chemometric handling of Raman spectra for live systems monitoring and susceptibility tests

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1 The use of chemometrics for Raman spectroscopy data analysis and applications in life science

Global population forecasts dictate a rapid adoption of sustainable and user-friendly approaches to fulfil increasing food needs and improve control strategies in agro-food industry, pharmaceutical and medical field. Immunological assays, nucleic acid-based techniques (e.g. ELISA and PCR), colony forming unit test (CFU) and other classical cell vitality tests are time-consuming, destructive and expensive. Raman

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spectroscopy (RS) combined with chemometric analysis can generate a chemical fingerprinting of a sample rapidly, at low operating costs and without sample pre-processing and destruction. [1, 2]

Here, we present two examples of application of Raman spectroscopy for live systems monitoring during acute effect of an exogenous agent, attesting the possibility to build predictive models to evaluate i) susceptibility to virus infection in plants and ii) to antibiotic treatment in bacteria cells in a defined time frame. Principal Components Analysis was used for easy data visualization and exploration. Correlations between measured spectra and the effect of the virus infection of tomato plants in the first case, and the effect of drug to biomolecular profile of *E. coli* in the latter were found, separating the ageing effect that occurs in biological samples over time. Subsequently, PLS-DA classification models [3] were calculated and validated to determine the sensitivity and specificity of RS for early detection of the exogenous agent. RS captured the effect of virus infection in tomato plants when the symptoms are still not evident in plant leaves, with accuracy higher than 70% and 85% for TYLCS and TSW viruses, respectively. Moreover RS allowed the detection of different drugs action on bacterial cell in 1 hour.

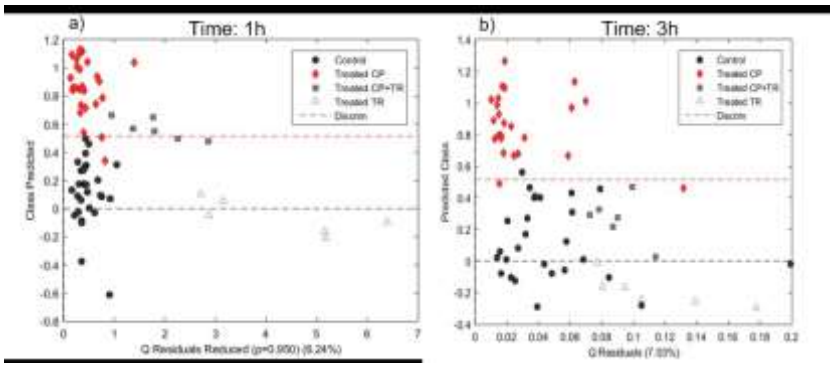

Figure 2: prediction results of induced resistance to ciprofloxacin (CP) provoked by triclosan (TR) with PLS-DA model of RS (3 LVs). Training (Red and black dots) and predicted (white and grey) set after a) 1 h and b)3 h of cell growth in presence and absence of antibiotics against Q residuals.

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