NIR Spectra Simulation in Aid of Food Analytical Framework. Understanding of Matrix Effects and Improved Detection of Adulterants

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Multi-variate analysis forms the backbone of analytical framework of NIR spectroscopy, but it lacks in providing answers on the origins of the spectral variability nor its relationships with the molecular background. In recent few years, advancement of in silico NIR spectroscopy, where spectra can be simulated *ab initio*, created an opportunity to make a decisive step beyond this barrier (Bec and Huck, 2019; Ozaki et al., 2021). This improves the comprehension of the spectral information enabling access to rich and detail molecular footprint, essential for fundamental research and providing innovative advances to analytical framework of NIR spectroscopy combined with chemometrics.

In addition to detailed NIR band assignments, accurately simulated NIR spectra enable new discoveries in physicochemical studies, e.g. the matrix effects. Intricate NIR spectral effects result from the interaction between the analyte and its chemical neighbourhood. Examples here include carbohydrates in aqueous solution, which are model system for numerous food products. On the other hand, detailed interpretation of NIR spectra of food adulterants, such as melamine, provides understanding of the differences that vibrational spectroscopic techniques (i.e. NIR vs. mid-IR) exemplify in food quality control framework.

**Keywords:** NIR interpretation, matrix effects, food adulterants, melamine, carbohydrates

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