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Infrared spectroscopy combined with machine learning techniques to monitor starch in vitro digestibility

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In vitro digestion techniques are a popular way to study the digestion of different foods. However, these methods can be time-consuming, and only measure one analyte at a time (e.g. glucose, maltose, protein).[(1)] Infrared (IR) spectroscopy is a non-invasive technology that can be used to identify many chemical compounds in a sample simultaneously and can be used to collect information about the whole sample and a process (e.g. digestion).[(2)] The aim of this research is to evaluate the ability of IR spectroscopy combined with machine learning (ML) methods to determine the overall changes and trends during the in vitro digestion of different starches (potato, rice, pregelatinized starch). Samples ($n = 280$) (200 µl aliquots) were collected at different time points (5, 10, 15, 20, 25, 30, 40, 50, 60, 75, 90, 105, and 120 minutes) during *in vitro* digestion (INFOGEST method). Maltose concentration was measured using the reducing end (PAHBAH) assay. Near (NIR) and mid-infrared (MIR) spectra of the aliquots were also collected and were used to predict the concentration of maltose at each time point using partial least squares (PLS) regression. Principal component analysis (PCA) was used to visualise trends and changes in the spectra associated with starch digestion. The PCA score plot showed differences in the data set associated with the type of starch analysed and the time of sampling. The coefficient of determination (R^2) and the standard error in cross-validation (SECV) for the prediction of maltose at each time point in the set of samples analysed using MIR spectroscopy were 0.94 and 914 $\mu g mL^{-1}$. The results of this study indicated that ML methods applied to the IR spectra can be used to evaluate changes and trends in the spectra associated with *in vitro* starch digestion. The future studies shall explore and validate the results with digestion of complex foods.

References

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