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Identification of α-glucosidase inhibitors in apple peel - A chemometric approach

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Scope
To identify α-glucosidase inhibitors in apple peel by multivariate data analysis of the combined ¹H NMR spectra and IC₅₀ values from α-glucosidase assay of raw apple peel extract.

Hypothesis
Compounds that are correlated with the α-glucosidase inhibitory activity can be identified by applying partial least squares (PLS) regression on ¹H NMR spectra and IC₅₀ values of raw extract.

Introduction
There is an increasing interest in bioactive compounds responsible for the health-promoting properties of fruits and vegetables. However, plant extracts are very complex matrices containing hundreds of compounds, and identification of the individual constituents responsible for the bioactivity is a time-consuming task. The use of conventional (bio)analytical tools like in vitro bioassay and NMR spectroscopy in combination with multivariate data analysis might be an efficient way to speed up this process.

The enzyme α-glucosidase is involved in the hydrolysis of di-, tri- and oligo-saccharides to mono-saccharides in the small intestine. This makes α-glucosidase inhibitors potential leads for the management of blood glucose level in patients with type 2 diabetes.

Conclusion
PLS regression of ¹H NMR spectra and IC₅₀ values of apple peel extract identified chlorogenic acid, (-)-epicatechin and phlorizin to correlate with the α-glucosidase inhibitory activity.