Identification of -glucosidase inhibitors in apple peel - a chemometric approach

Schmidt, Jeppe Secher; Daykin, Clare A.; Stærk, Dan

Publication date:
2012

Document version
Early version, also known as pre-print

Citation for published version (APA):
Identification of $\alpha$-glucosidase inhibitors in apple peel - A chemometric approach

Jeppe S. Schmidt, Clare A. Daykin, Dan Stærk

Scope
To identify $\alpha$-glucosidase inhibitors in apple peel by multivariate data analysis of the combined $^1$H NMR spectra and IC$_{50}$ values from $\alpha$-glucosidase assay of raw apple peel extract.

Hypothesis
Compounds that are correlated with the $\alpha$-glucosidase inhibitory activity can be identified by applying partial least squares (PLS) regression on $^1$H NMR spectra and IC$_{50}$ 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.

Results
The PLS regression of $^1$H NMR spectra and IC$_{50}$ values of raw apple peel extract identified chlorogenic acid, (-)-epicatechin and phlorizin to correlate with the $\alpha$-glucosidase inhibitory activity. These three compounds are correlated with the $\alpha$-glucosidase inhibitory activity, but correlation does however not imply causation. Therefore, it still needs to be determined whether these three compounds are responsible for the observed activity or not.