Application Note

Identification of multiple **sugars** with a solid-state FTIR sensor

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Abstract

The IRmadillo™ FTIR spectrometer was used to analyse aqueous mixtures of up to seven different sugars simultaneously. The spectrometer is capable of qualitatively and quantitatively differentiating between monosaccharides, even when the structural differences between them are minimal.

IRmadillo™ FTIR Spectrometer

Introduction

Many different processes make use of sugar molecules, for example as a feedstock for fermentation processes or as an ingredient in food and beverages.

There are many different types of sugar molecules, all with similar structures but with small differences between them. They can come in a number of different forms, some having linear, 5-membered ring and 6-membered ring varieties. A selection of sugar structures are shown in Figure 2.

Differentiating between the sugars can be extremely difficult, as conventional techniques may not detect any differences – for example, mass spectrometry cannot discriminate between compounds with the same molecular formula such as glucose and mannose. There are methods – such as refractive index measurements – that can be used to differentiate between the sugars, but they require an extract of the mixture and then separation into different components, which is time-consuming and expensive.

Here we report the use of the vibration-resistant IRmadillo spectrometer to act as a sugar sensor, designed to differentiate and quantitate a mixture of seven different sugars.

Key Words

- Sugars
- Feedstock analysis
- Food and Beverage analysis
- Bioindustry
- Biorenewables
- On-line process monitoring
- Fermentation

Features & Benefits

- Mid-infrared spectral analysis
- Solid-state sensor
- Compact design
- Real-time analysis
- Certified safe for use in hazardous and potentially explosive environment

Experimental

The IRmadillo was purged overnight with a nitrogen line at a flow rate of 0.5 L min^{-1} to ensure water vapour and carbon dioxide did not affect results. A background scan was taken for 1 hr for the best possible detection limits. The spectrometer was fitted with an AMTIR (infrared glass) ATR element. The IRmadillo probe was then inserted into a range of aqueous sugar solutions and three scans of 120 s each were taken. The spectral range of 900 – 1900 cm^{-1} was used for analysis. Two of each scan were used for model building and a third scan used for model verification. The quantification was performed using a PLS (partial least squares) model.

Results and discussion

Example spectra acquired during the experiment for the single component solutions are shown in Figure 2. The large feature at 1660 cm^{-1} present in all spectra arises from water, but the strong features between 1000 and 1200 cm^{-1} arise from the 5 and 6 membered rings (furanose and pyranose respectively) present in the sugar molecules. The exact structure of the molecule dictates the pattern and intensity of the peaks as they correspond to complicated vibrations of C-C and C-O bonds.

It should be noted that it is fairly easy using FTIR spectroscopy to differentiate between similar structures. For example, xylose and arabinose are isomers of each other, but in the MIR spectrum they show clearly different features. Other spectroscopic techniques, such as NIR, would struggle to differentiate between them.

A PLS model was made of all the mixtures and a graph showing the predicted value vs reference values is shown in Figure 1. In all cases the predictions match up very well with the reference values, showing that the model is able to predict the concentrations using the spectral features.

By calibrating the IRmadillo as a sugar sensor using the above model, it is possible to quantify and identify different mixtures of sugars. This is shown in Figure 3 where the predictions for sugar mixes have a good correlation with the reference values. Crucially, the results show that predictions are possible across a broad range of different concentrations.

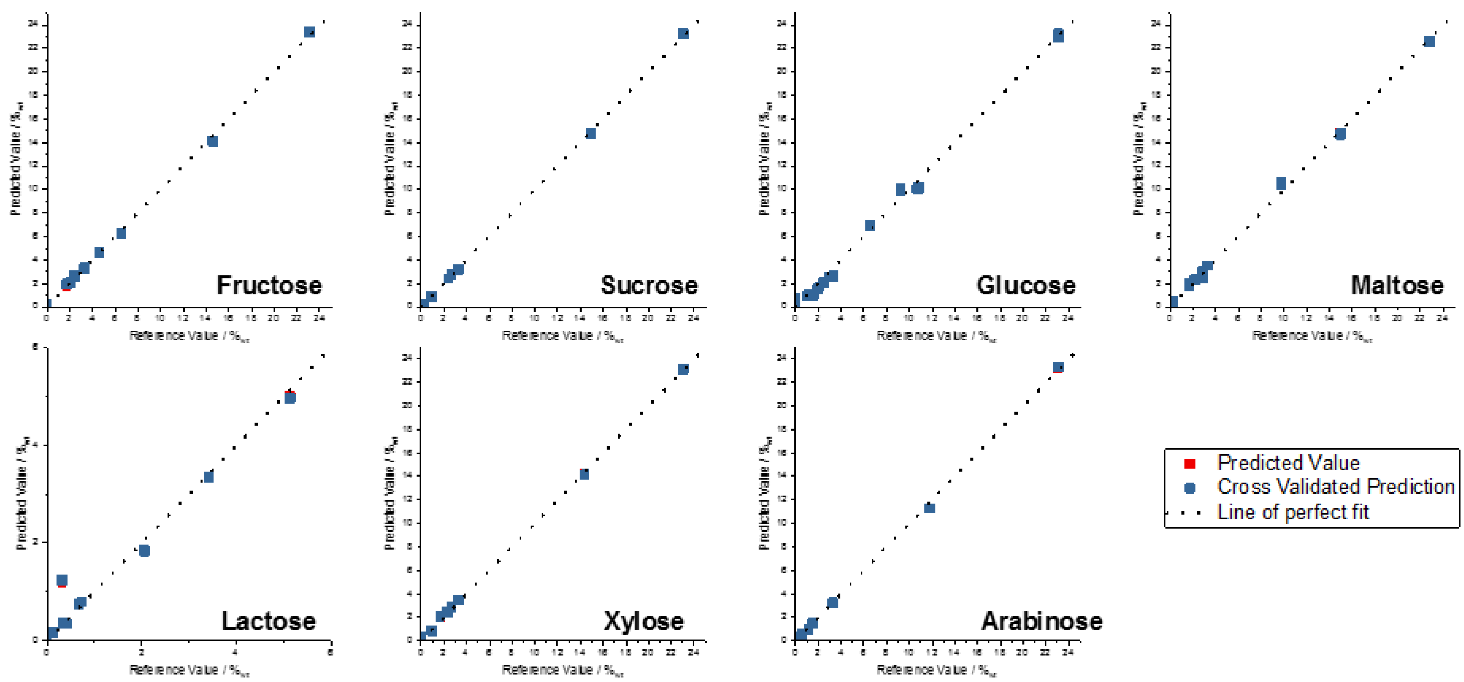

Figure 1: Collated data for predictions vs reference value for sugar quantification using a PLS model. It should be noted that the predicted values and cross validated predicted values are so close that in most cases they overlap.

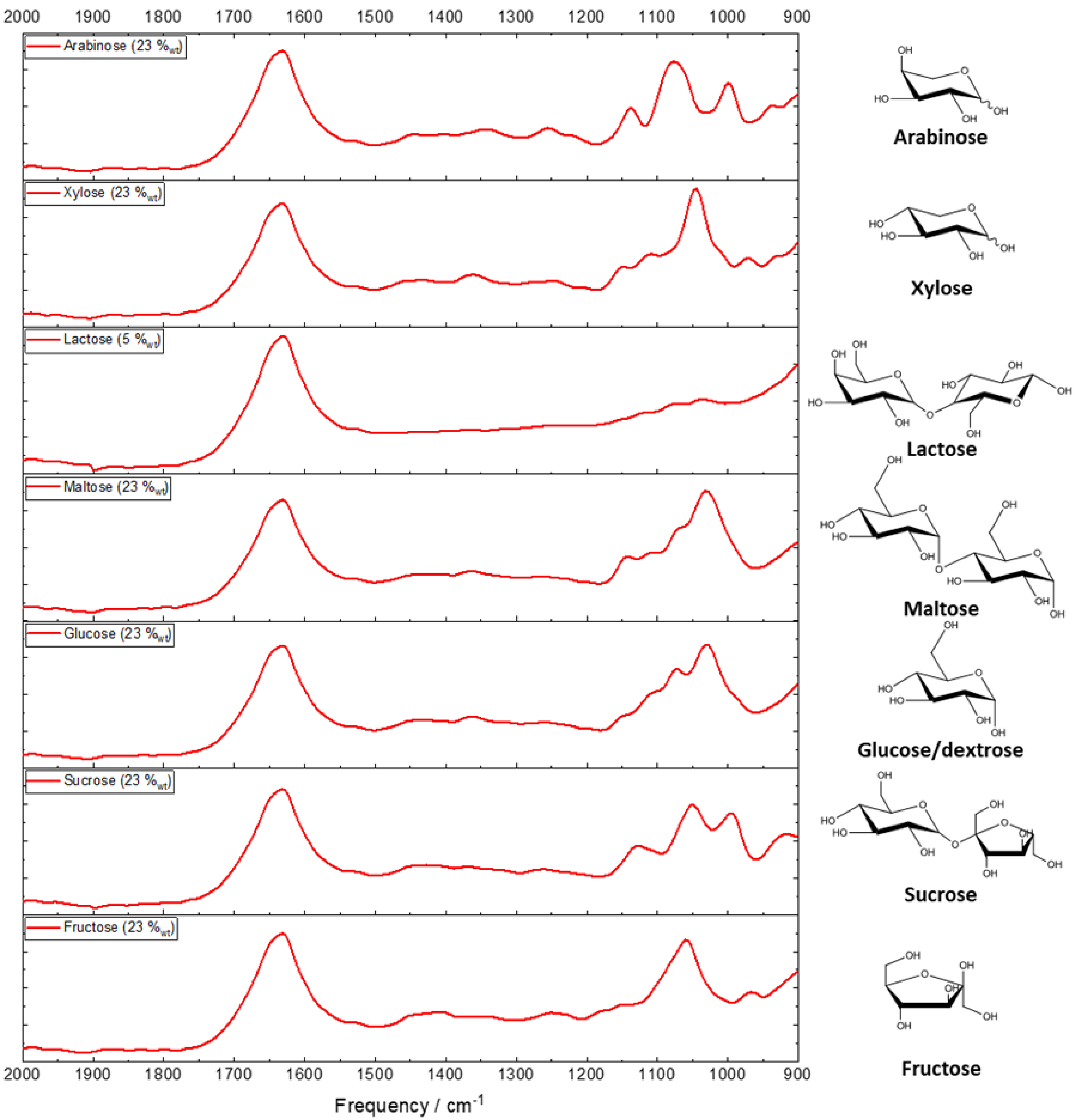

Figure 2: Spectra of seven sugar solutions acquired on an IRmadillo with a 120 s sampling time between 900 and 2000 cm^{-1}. The structures of the sugars are shown to the right.

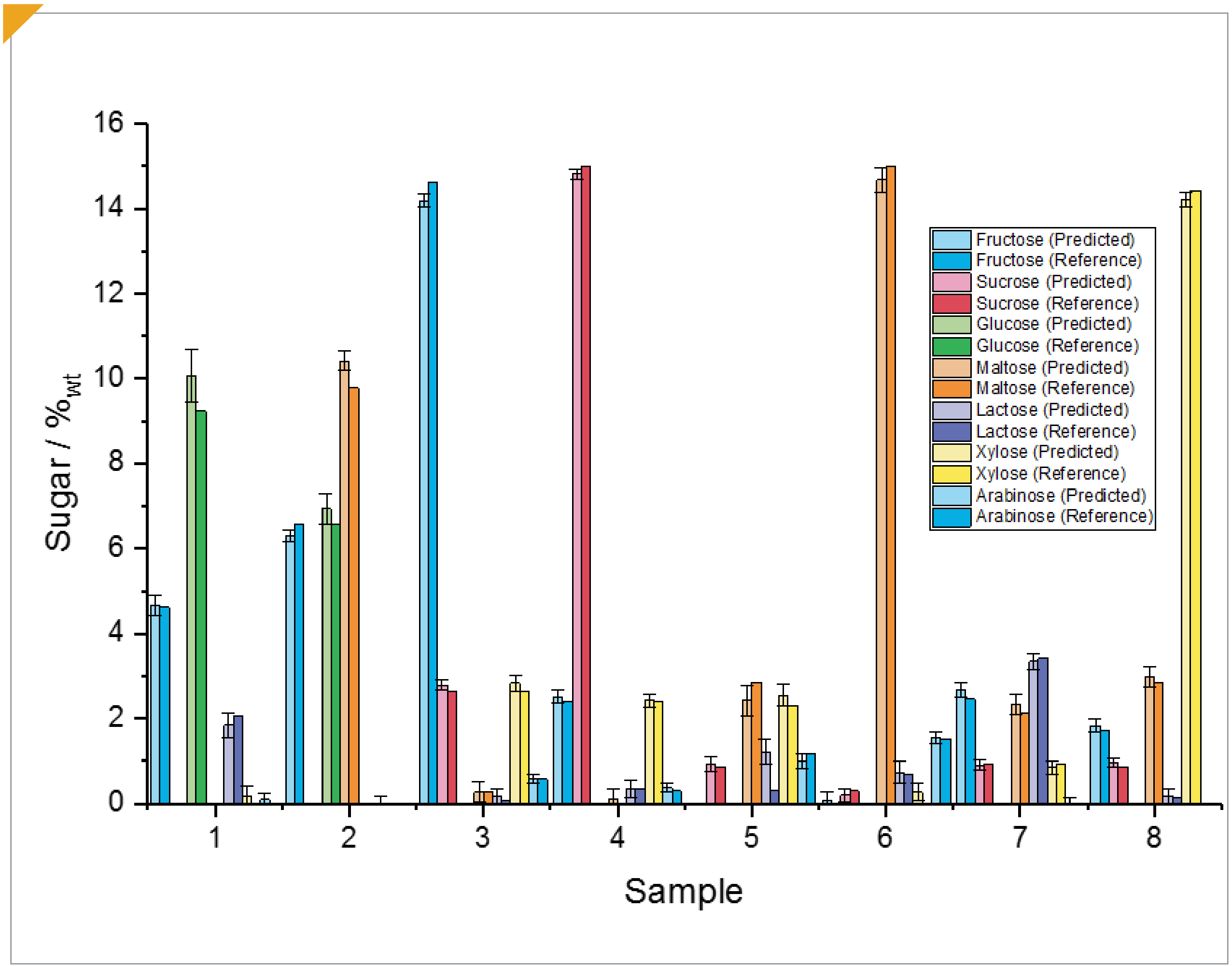

Figure 3: Predictions for mixtures of sugars using the IRmadillo and a pre-built PLS model.

Conclusions

This work shows that by building a relatively simple PLS model it is possible to calibrate the IRmadillo™ FTIR spectrometer to operate as a sugar sensor monitoring the concentrations of up to seven different sugars in an aqueous mix simultaneously. This means that real time on-line analysis of complicated mixtures is now possible, without the need for extractive sampling or HPLC. There are applications for this technology in a range of biotechnological industries (such as biorenewable energy sources), and food technology (for example in brewing).

Keep in mind

There may also be other compounds present during a process which may be of interest to you.

The IRmadillo observes all the compounds of a mixture. It can track multiple compounds simultaneously and provide a full picture of your process, with monitoring tailored to your needs.

IRmadillo™ FTIR Spectrometer

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