AN INSIGHT INTO THE PROBLEMS OF DETERMINING THE ADULTERATION OF ALMOND FLOUR WITH LOW-COST MINIATURISED NIR INSTRUMENTS

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Introduction

Miniaturized NIR instruments have gained more interest in recent years to solve relevant analytical problems[1], also in the agri-food sector. In this work, we will apply four different miniaturized low-cost NIR devices[2] to the measurement of almond flour[3-4] adulterated with bitter almond. The instruments cover together the spectroscopic range between 740 and 2558 nm, being complementary in the spectroscopic information. Three different granulometries of almond flour will be analysed with all the instruments in different days to assess the performance of the different instruments in the construction of the calibration models for the prediction of the percentage of bitter almond in almond flour.

Instrumentation and experimental work

SCiO (Consumer Physics)

- 740-1070 nm (331 λ)
- Dispersive element
- Osram broadband IR led
- Photodiode array
- Contact to 1 cm-distance measurements

NeoSpectra MDK (Si-Ware)
2 different instruments

- 1350-2558 nm (134 λ)
- MEMS Michelson interferometer
- Three tungsten halogen lamps
- Single InGaAs photodetector
- Contact measurements

NeoSpectra Scanner (Si-Ware)

- 1350-2550 nm (134 λ)
- MEMS Michelson interferometer
- Tungsten halogen lamps
- Single InGaAs photodetector
- Contact measurements

Samples
Almond flour was obtained from whole sweet and whole bitter almonds. 3 different granulometries (small, medium, large) were obtained using a coffee-grinder and different sieves (5, 12 and 22 openings per inch: openings about 500 μm, 200 μm and 100 μm).

Pre-processing methods evaluated
Different spectral pre-processing methods were tested in the preliminary results: standard normal variate (SNV) and second Savitzky–Golay derivative with a different number of smoothing points. Data were always mean-centered before calculation.

Validation of the methods
Leave-one-out was used for cross-validation of the preliminary models here presented. The PLS Toolbox running on Matlab was used for calculations.

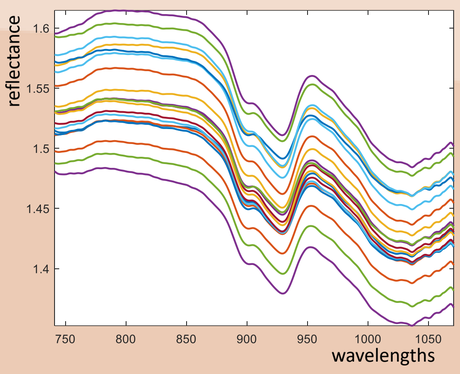
Experimental design
20 different percentages from 0% bitter almonds to 100% bitter almonds were used. 5 analytical replicates for the NeoSpectra MDK and 15 for SCiO were done for each percentage. 2 different calibration models in different days were built for each instrument and type of granulometry.

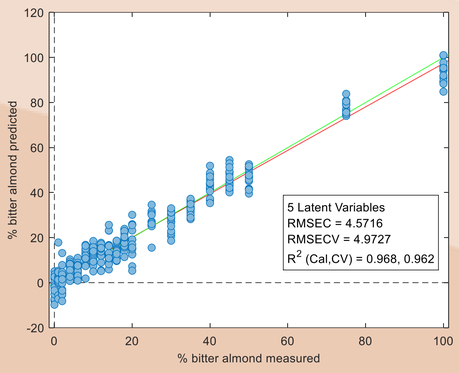
Preliminary results

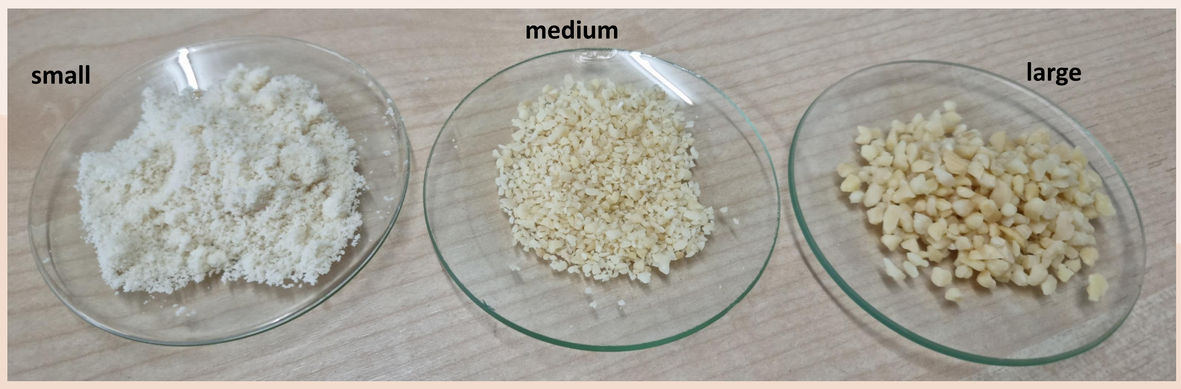
A study about the variability of the spectra when doing instrumental replicates and analytical replicates showed the possibility of only using analytical replicates, skipping the need for including instrumental replicates and therefore shortening the time of analysis. This is especially valid for the NeoSpectra MDK, which have the highest variability of all the instruments included in this study doing analytical replicates.

As examples, reported results include SCiO and a NeoSpectra MDK. Other models are currently under construction. Pictures show the average spectra at each percentage of bitter almond and the best regression line for each type of instrument obtained so far.

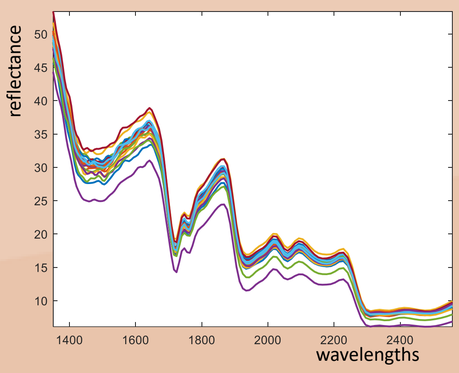
SCiO – large almond flour

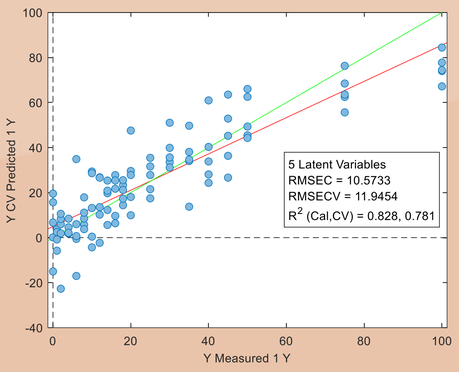






NeoSpectra MDK – small almond flour





	Pre-processing	Granulometry	LVs	RMSEC	RMSECV	R^2CV
SCiO	mean centering	small	6	8.817	9.175	0.870
SCiO	smooth+2nd der+centering	medium	6	5.186	5.629	0.951
SCiO	smooth+2nd der+centering	large	5	4.571	4.973	0.962
NeoSpectra MDK	mean centering	small	7	9.343	11.928	0.783
NeoSpectra MDK	smooth+2nd der+centering	medium	5	10.573	11.945	0.781
NeoSpectra MDK	smooth+2nd der+centering	large	6	12.357	14.419	0.681

Conclusions

- 4 different miniaturized NIR instruments are being applied to the analysis of % of bitter almond in almond flour of 3 different granulometries
- SCiO obtains so far the best results in all 3 types of granulometries, specially for small almond flour
- The obtained results show that the ability of prediction not only depends on the range of wavelengths but also on the specific technical configuration of the instruments and on the physicochemical characteristics of almond flour
- Analysis with the NeoSpectra Scanner are ongoing and future results will include a comparison of the calibration models made in different days

References

[1] B Giussani, G. Gorla, J. Riu, Crit. Rev. Anal. Chem 2022, DOI: 10.1080/10408347.2022.2047607

[2] K.B. Beć, J. Grabska, C.W. Huck, Chem. Eur. J. 2021, 27, 1514-1532

[3] M.A. Faqeerzada, S. Lohumi, R. Joshi, M.S. Kim, I. Baek, B.K. Cho, Foods 2020, 9, 876

[4] J.M. Netto, F.A. Honorato, P.G. Celso, M.F. Pimentel, J. Food Compost. Anal. 2023, 115, 104981

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