

Supplementary

Table S1. Theoretical (provided by the manufacturer) and experimental (measured by densimeter) average sugar values of fruit juices.

Juice	Theoretical sugar concentration (g/100mL)	Experimental sugar concentration (g/100mL)
ORANGE	9.6	10.31
APPLE	10.67	10.77
PINEAPPLE	11.43	11.31
GRAPE	15.77	15.85

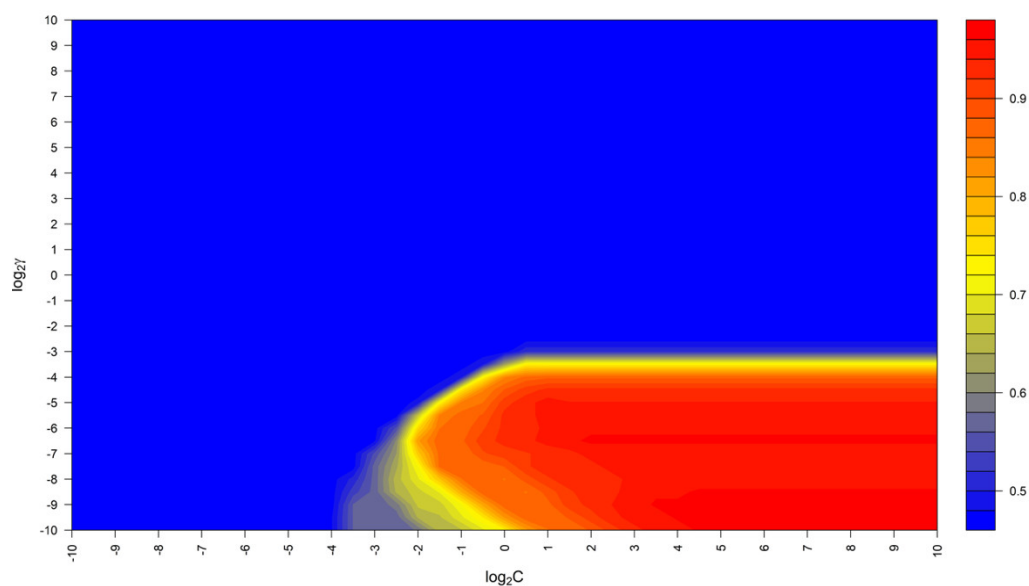


Figure S1. Search for the best combination of hyperparameters (C and γ) for the Gaussian SVM model obtained by CV of 5 folds using the FT-IR spectrum of all training set samples ($D_{540 \times 138}$).

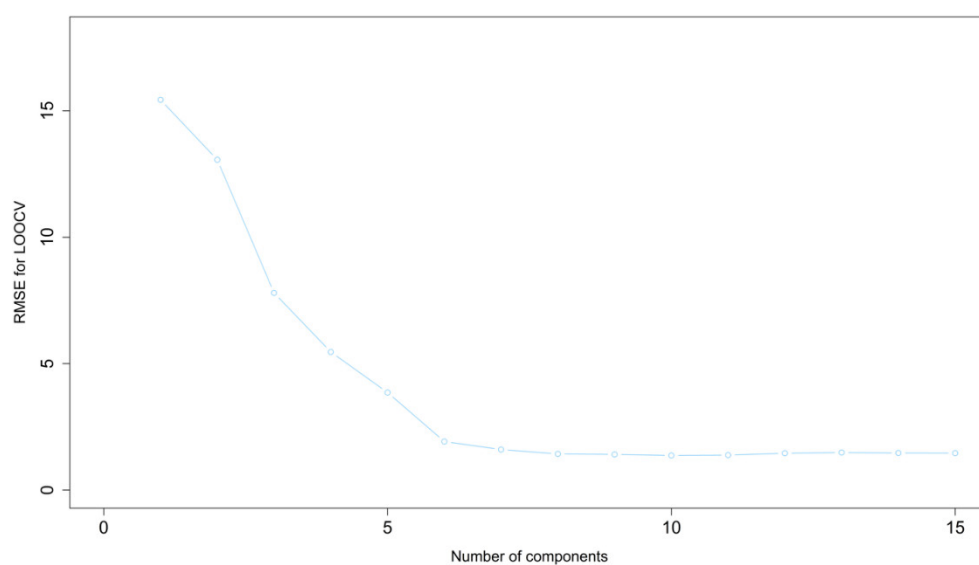


Figure S2. Evolution of the root mean square error (RMSE), as a function of the number of components used in PLS analysis. The LOOCV error has been used for the FT-IR spectrum of the adulterated and unadulterated juice samples from the training set.

Link to the web application:

<https://joseluispcalle.shinyapps.io/Application/>

This application is a prototype and includes Gaussian SVR and SVM models in combination with FT-IR spectra. The user only needs to enter the Excel file generated directly from the analysis by FT-IR and press the "Submit" button. Additionally, the option of using the CSV format and choosing the corresponding field separators has been introduced to facilitate its use. A "Download" button has been implemented to download a sample file. This file can be uploaded to the application, select the ".xlsx" option and click on "Submit" to display the predictions obtained. It should be noted that the model will learn as more samples are analyzed and, consequently, will cover more variability. Thus, adulterating a fruit juice without being detected will be increasingly difficult.