



# Fingerprinting food by means of Raman spectroscopy – a photonic tasting

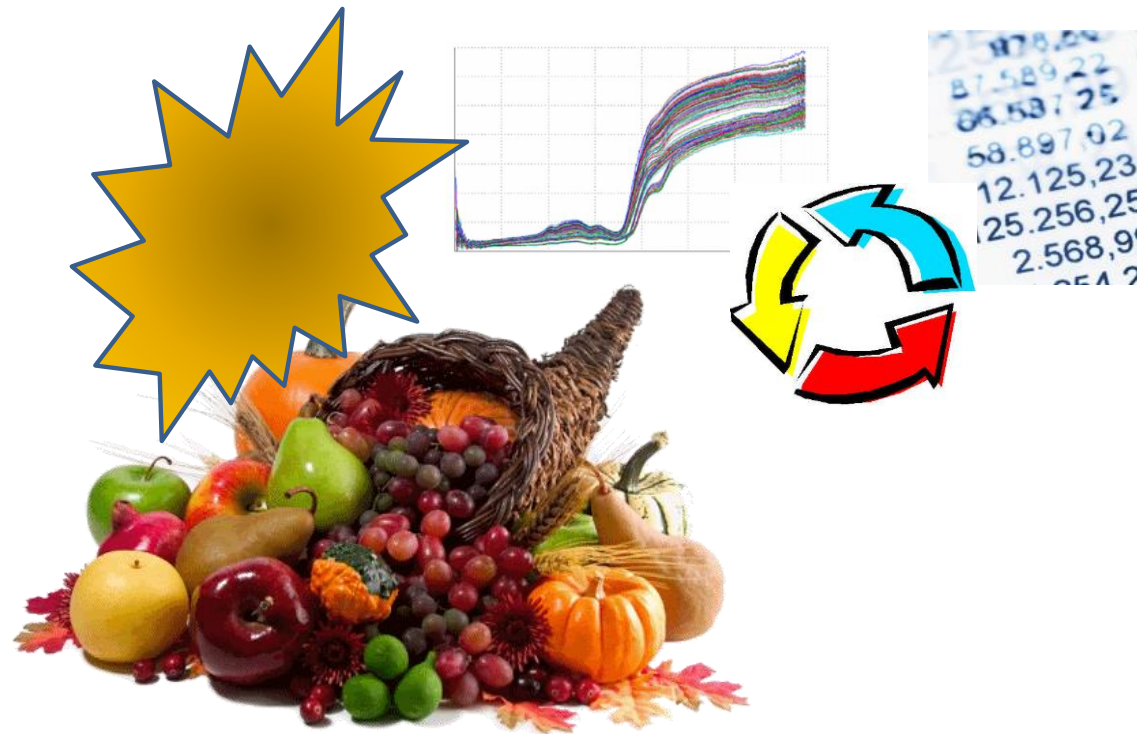
A.G. Mignani , L. Ciaccheri, A.A. Mencaglia  
CNR-Istituto di Fisica Applicata “Nello Carrara”,  
Sesto Fiorentino (FI), Italy  
[a.g.mignani@ifac.cnr.it](mailto:a.g.mignani@ifac.cnr.it)



# Ambition – Photonics for food tasting

One shot of light  
for multi-component analysis

- 'green' analytics
- non-destructive
- rapid

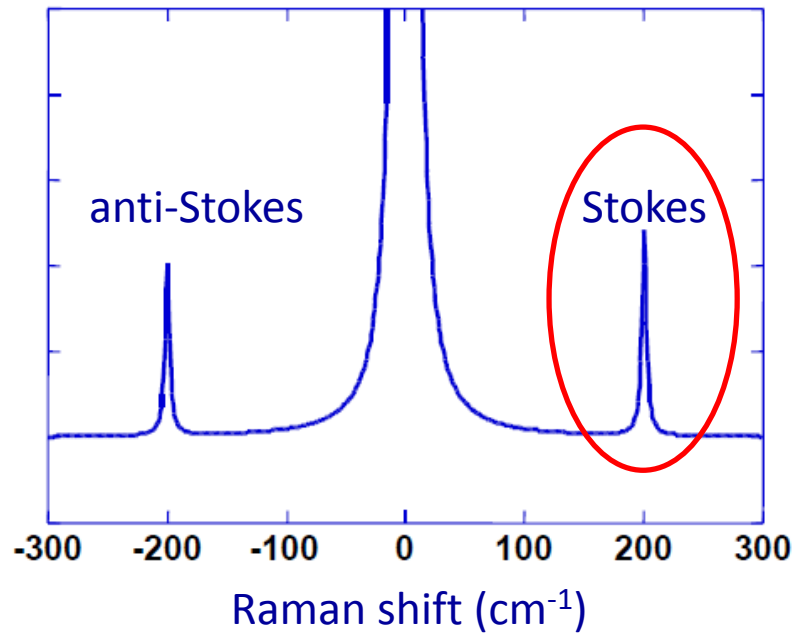
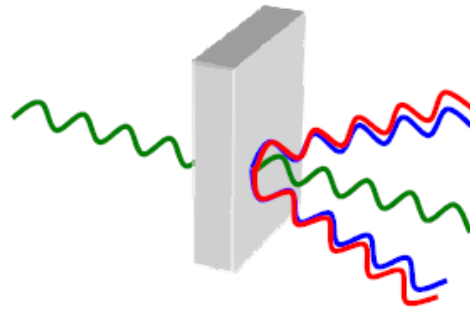
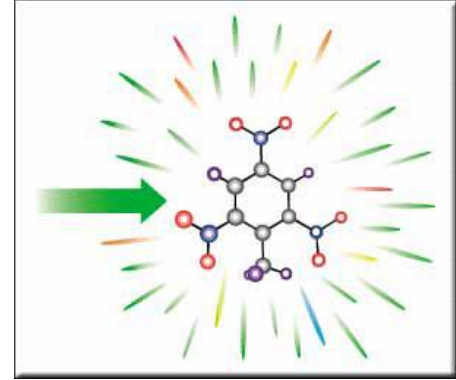


# Motivation

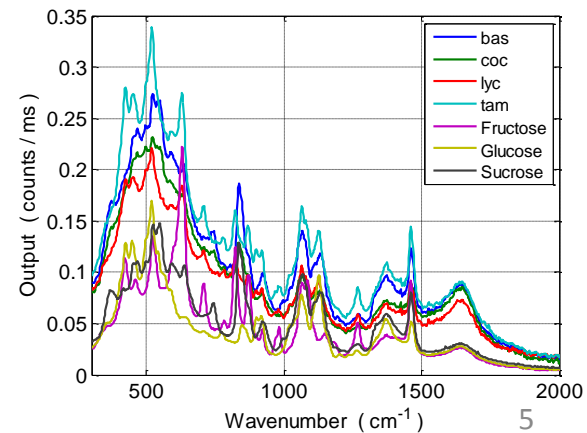
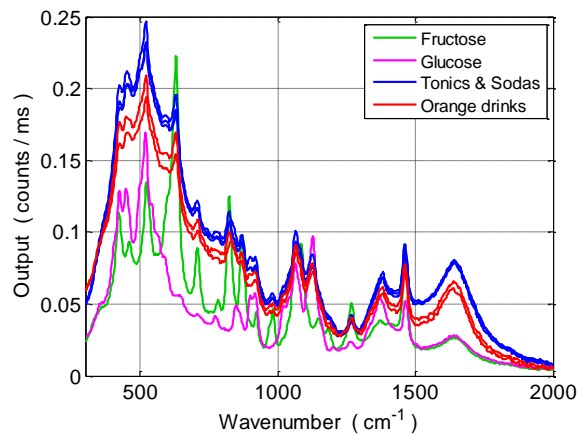
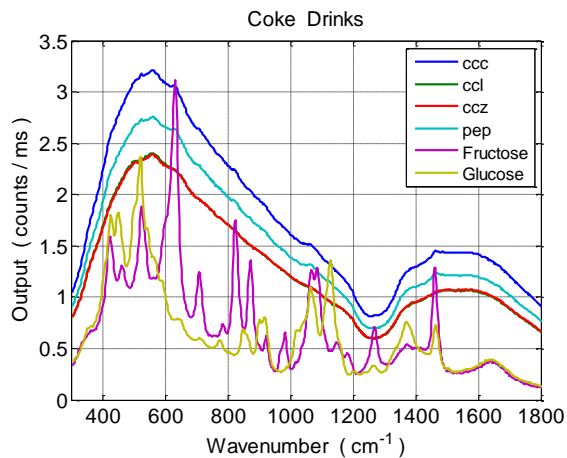
- Online monitoring of nutraceutical and quality indicators
- Towards a modern nutraceutical labelling of natural products for QR codes



# Raman spectroscopy



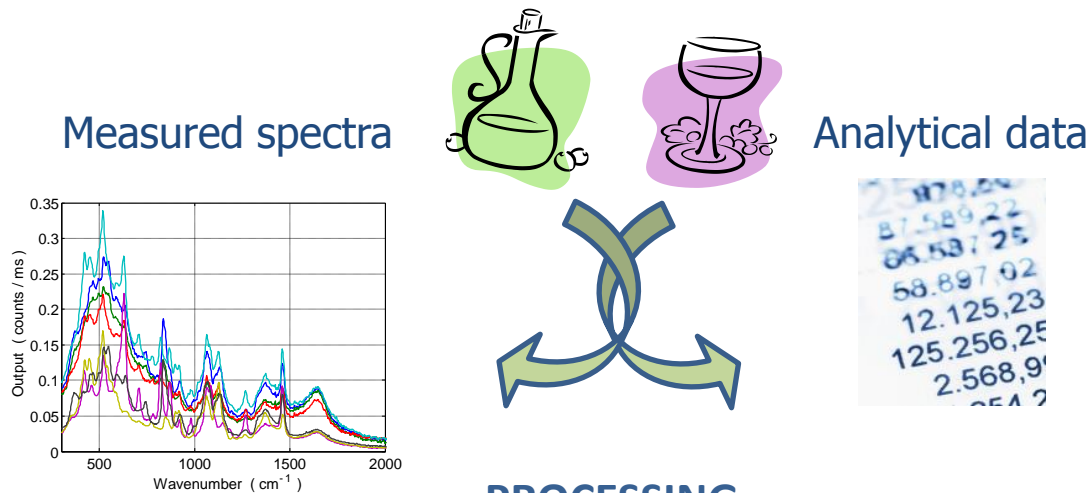
# Raman fingerprints of beverages & sodas



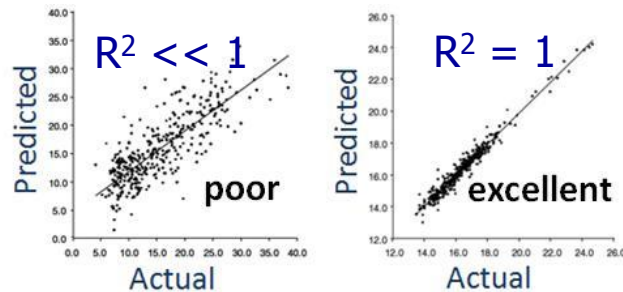
# Data processing issues

extraction of information from spectra

Selected reference samples



PROCESSING



Validation

# PLS predictive models

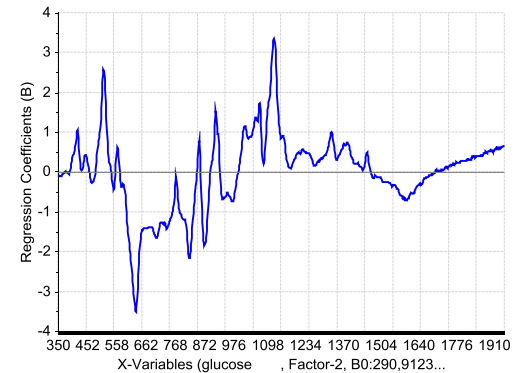
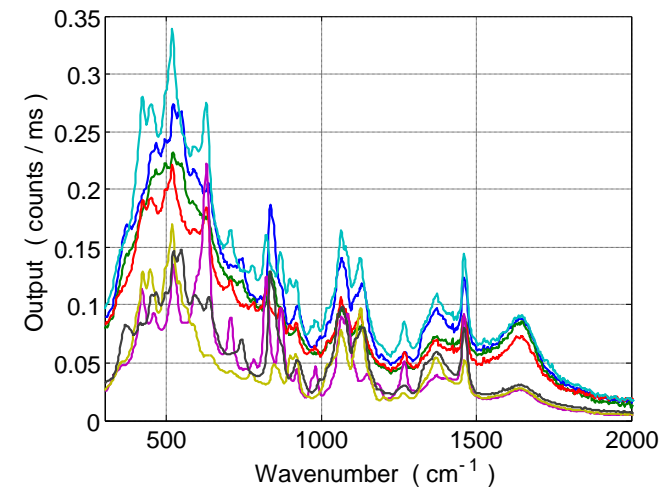
$$\hat{y}_n = \sum_{m=1}^M r_m (x_{n m} - \langle x \rangle_m)$$

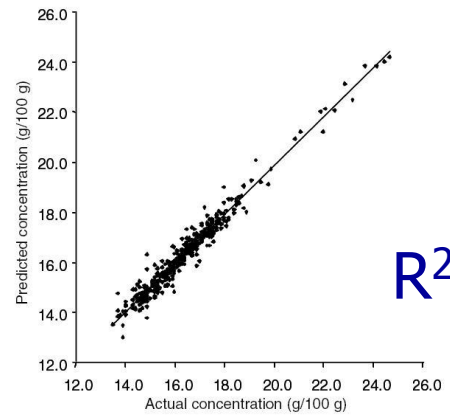
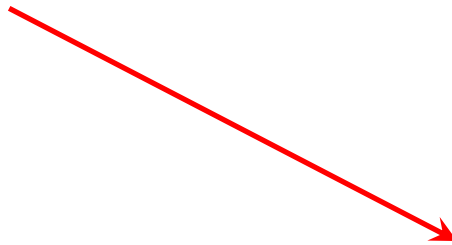
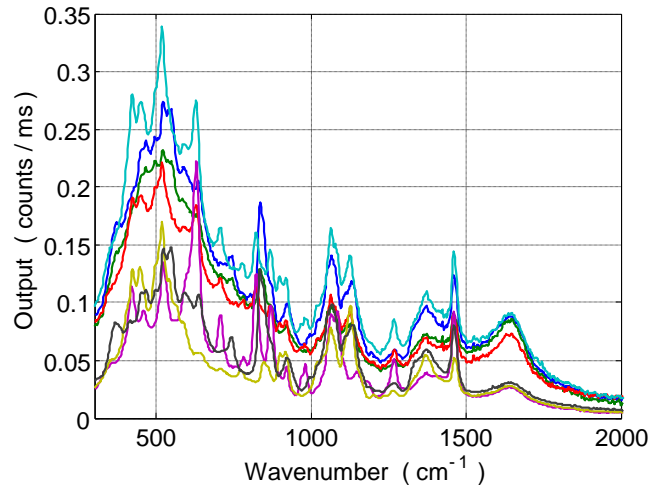
M = number of spectral channels (discrete wavenumbers)

$r_m$  = regression coefficient corresponding to m-th wavenumber

$x_{n m}$  = value of the Raman spectrum of n-th sample at m-th wavenumber

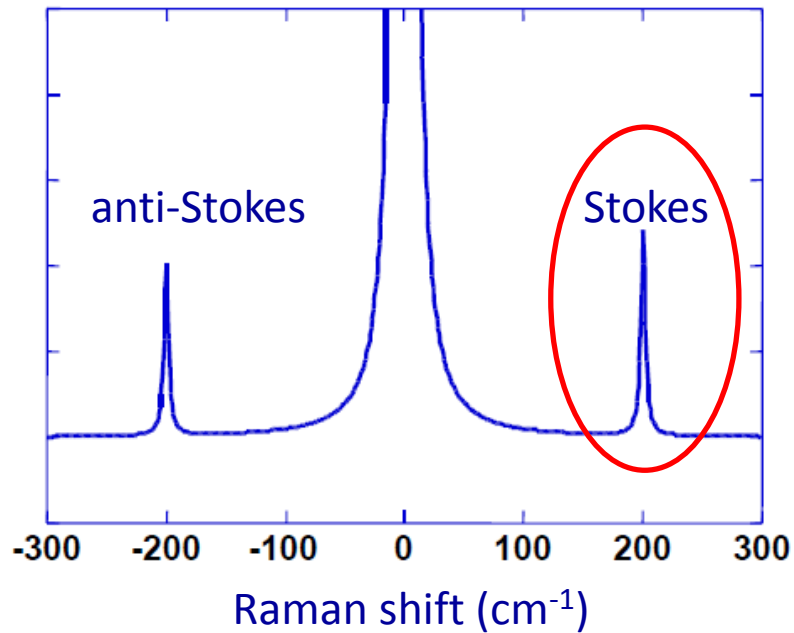
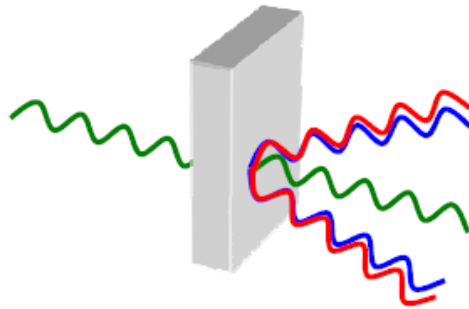
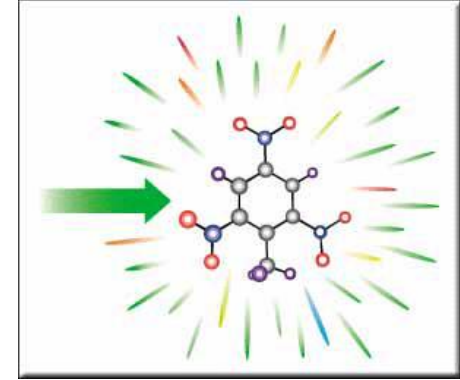
$\langle x \rangle_m$  = mean value of Raman spectrum at m-th wavenumber, for the calibration set







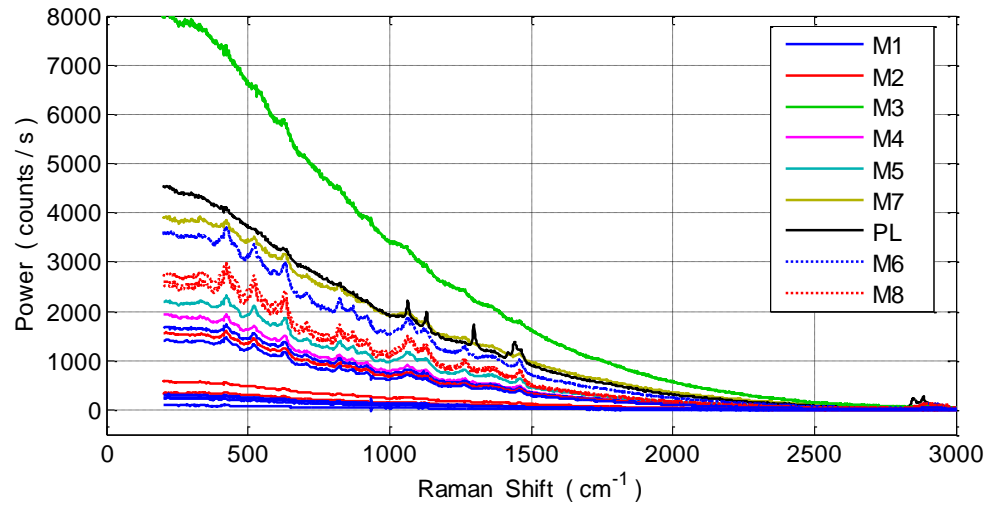
# Raman spectroscopy



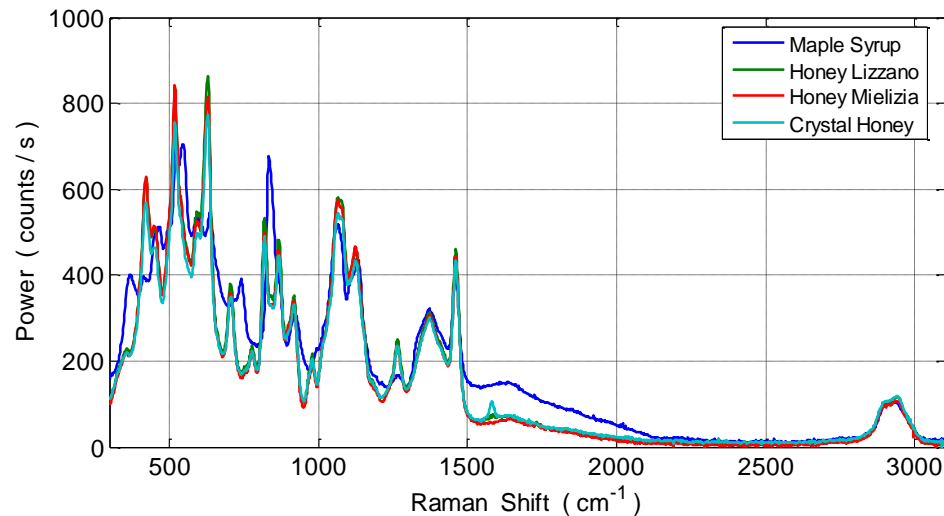
$$I_{\text{Raman}} \propto 1 / \lambda^4$$

# Raman spectra – 785 nm versus 1064 nm

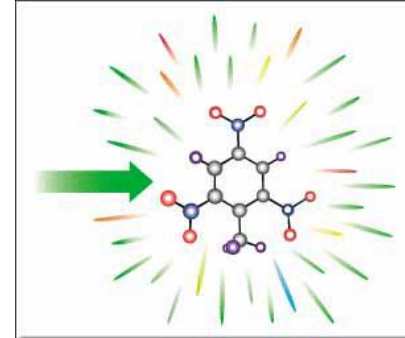
@ 785nm



@ 1064nm

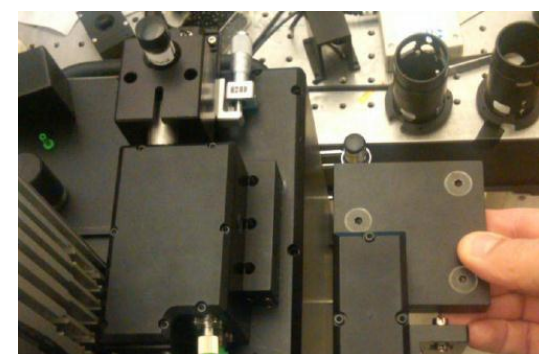
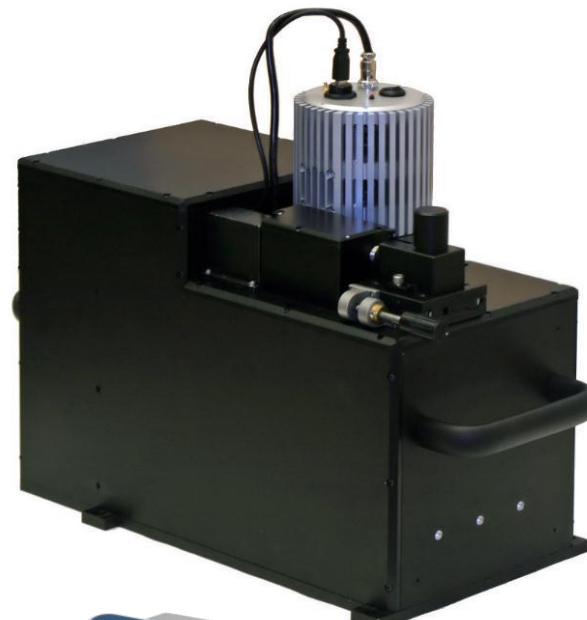


# Raman spectroscopy @ 1064 nm



Laser power: 400 mW  
Detector cooling: - 55°C

RamSpec-1064nm-HR  
BaySpec Inc., San José CA  
[www.bayspec.com](http://www.bayspec.com)



[www.bayspec.com](http://www.bayspec.com)



[www.rigakuraman.com](http://www.rigakuraman.com)

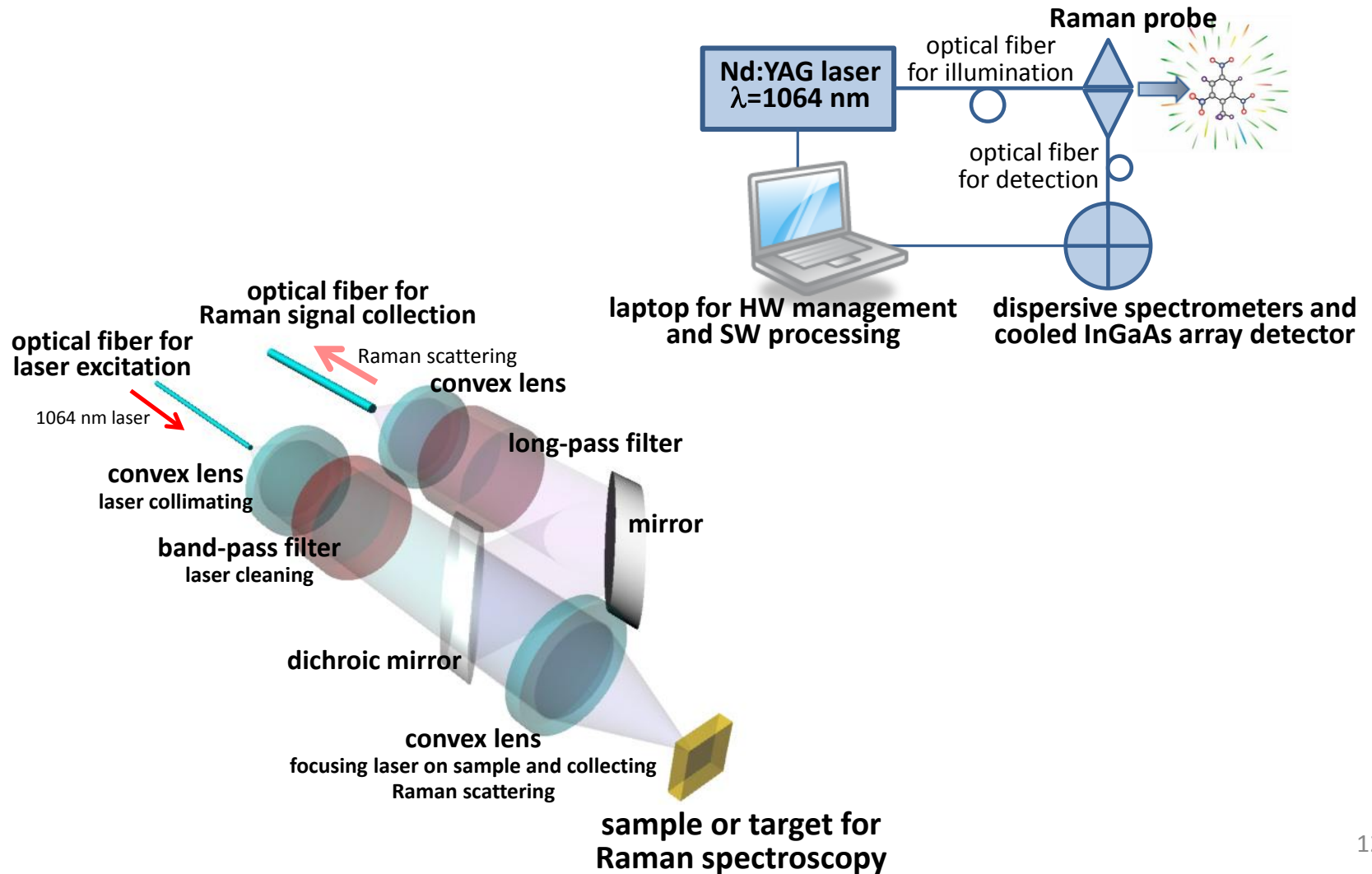


[www.wysri.com](http://www.wysri.com)



[www.metrohm.com](http://www.metrohm.com)

# Raman spectroscopy @ 1064 nm



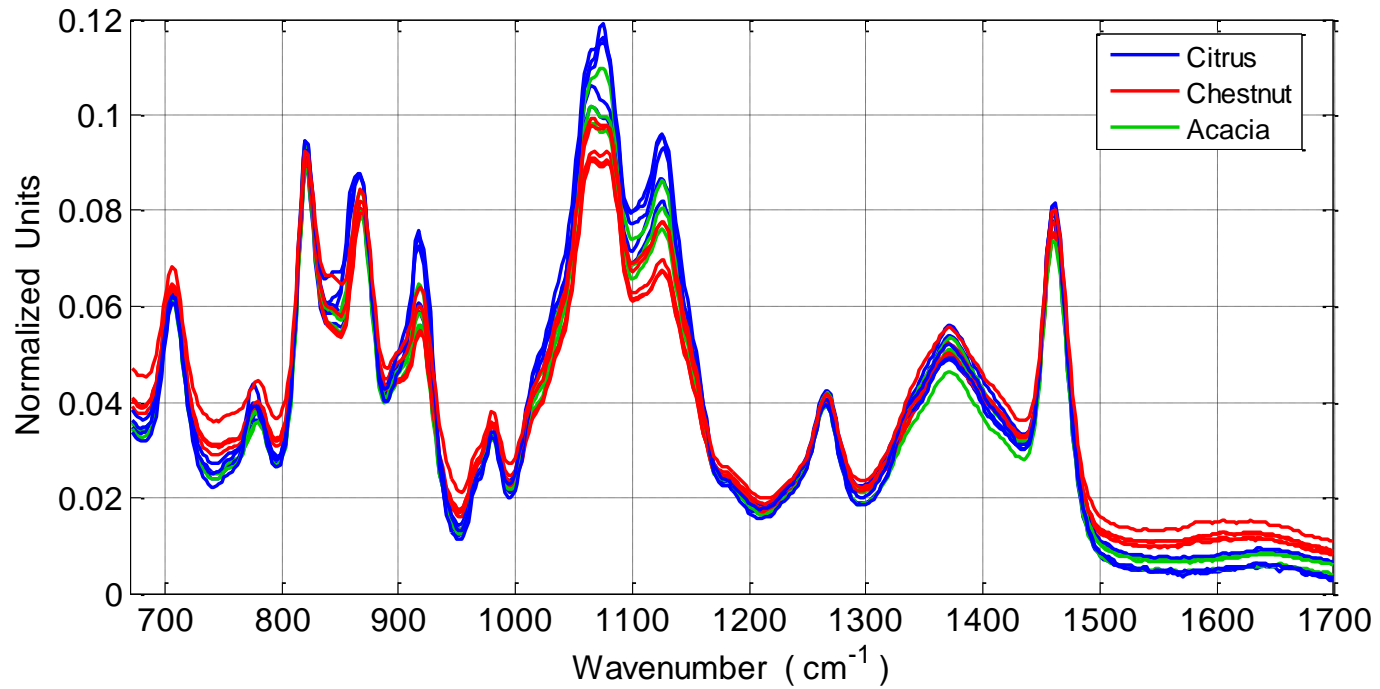
# Honeys from Calabria

Raman spectra + some maths = QR codes

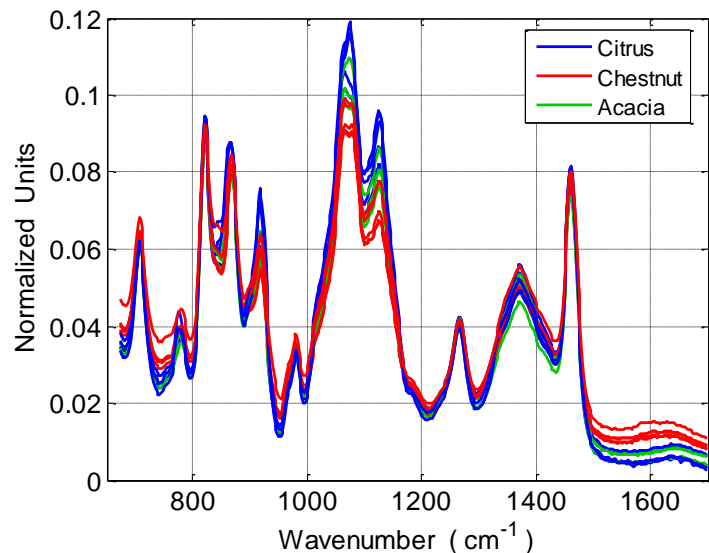
- Distinguishing the botanic origin
- Predictive models for sugar profile
- Potassium as important nutraceutical indicator



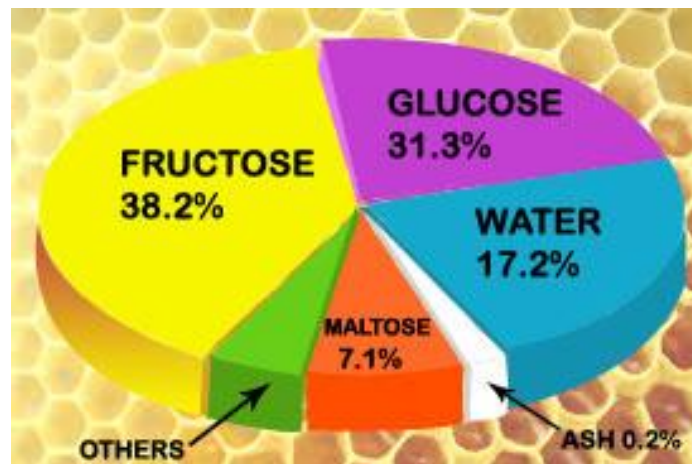
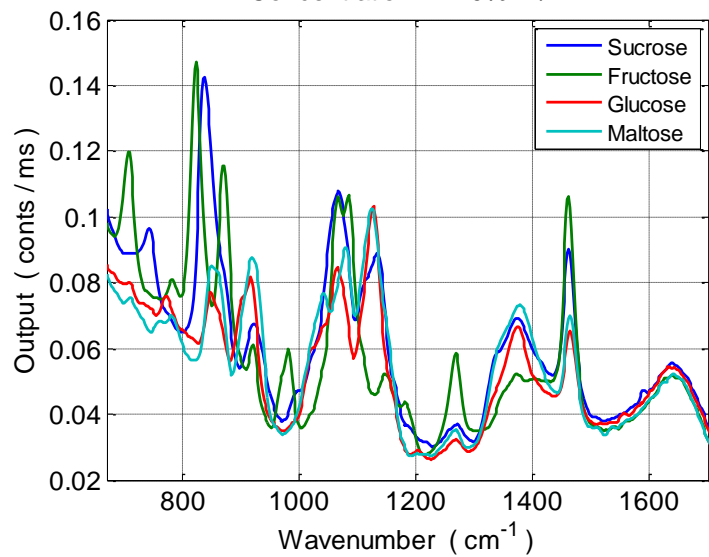
# Raman spectra of honeys



# Honeys and sugars

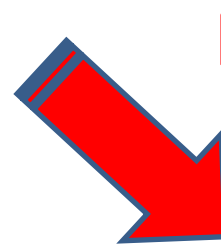
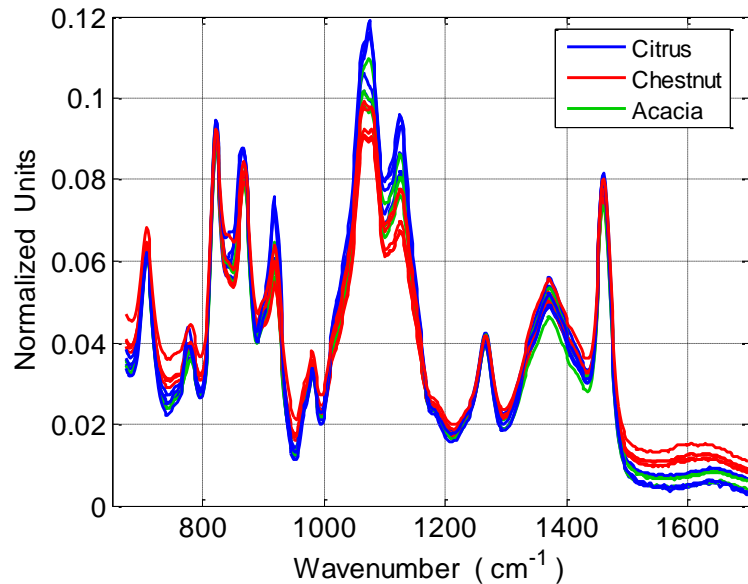


Concentration = 20% w/w

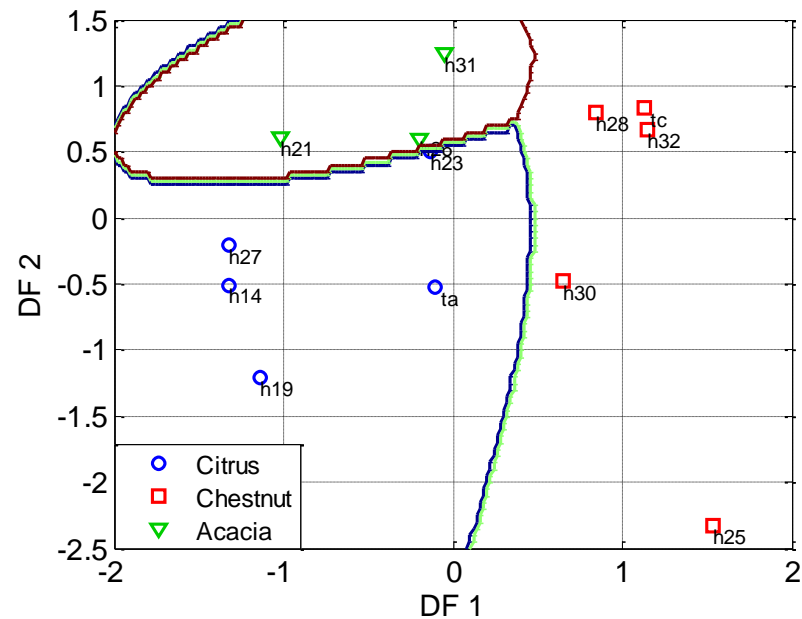


Raman band (cm <sup>-1</sup> )	Main contribution	Secondary contribution
707	Fructose	
821	Fructose	
867	Fructose	Glucose
917	Glucose	Maltose
1060-1080	Fructose	Glucose
1127	Glucose	Maltose
1267	Fructose	Glucose
1372	Glucose	Maltose
1460	Fructose	Glucose

# Distinguishing the botanic origin

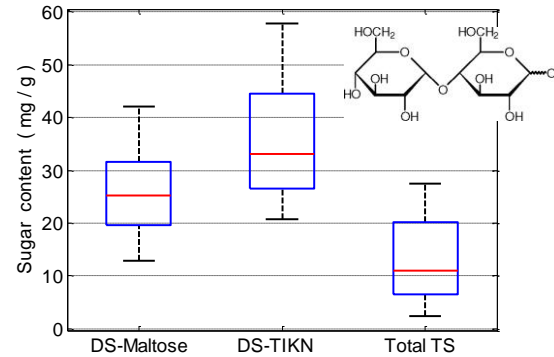
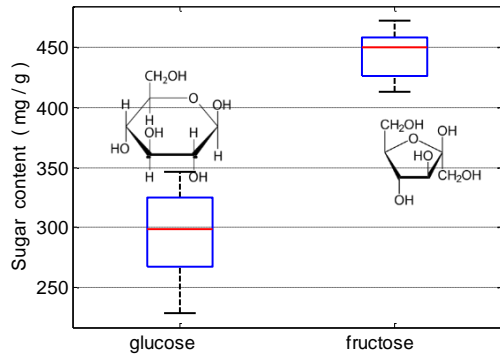


**PCA + LDA + KNN**



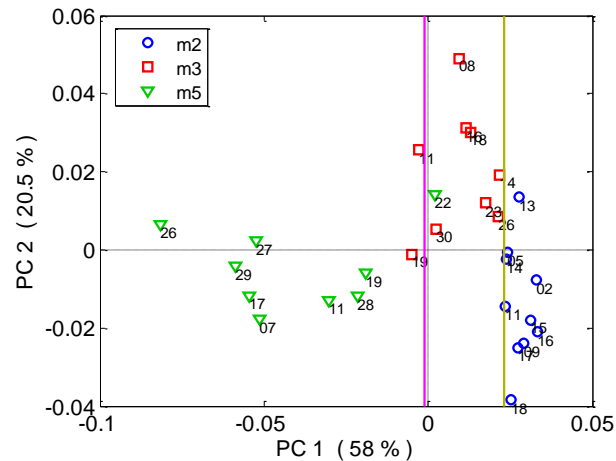
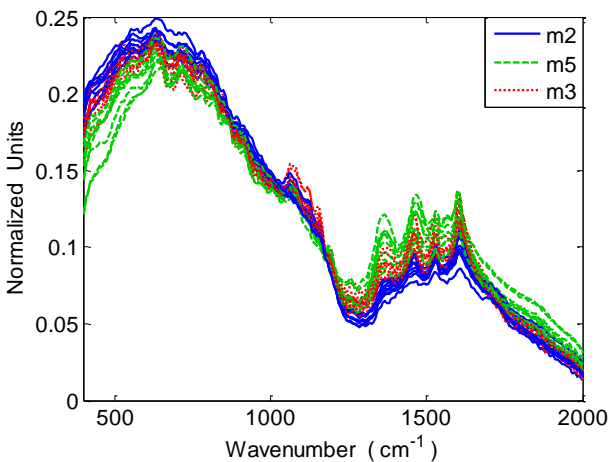


# Honey: PLS predictive models for sugars & potassium



Analyte		RMSEC	R <sup>2</sup> (cal)	RMSECV	R <sup>2</sup> (val)	
SUGARS	Monosaccharides (mg/g)	Glucose	7,3	0,96	11	0,92
		Fructose	5,5	0,89	7,6	0,82
	Disaccharides (mg/g)	Maltose	3,5	0,83	5,3	0,66
		Trehalose+Isomaltose +Kojibiose+Nigerose	2,3	0,91	3,6	0,83
	Trisaccharides (mg/g)	Erlose+Isomaltotriose +Panose	2,6	0,89	3,9	0,80
POTASSIUM (μg/g)		0,3	0,97	0,5	0,94	

# Blueberry powder anthocyanins as quality indicators



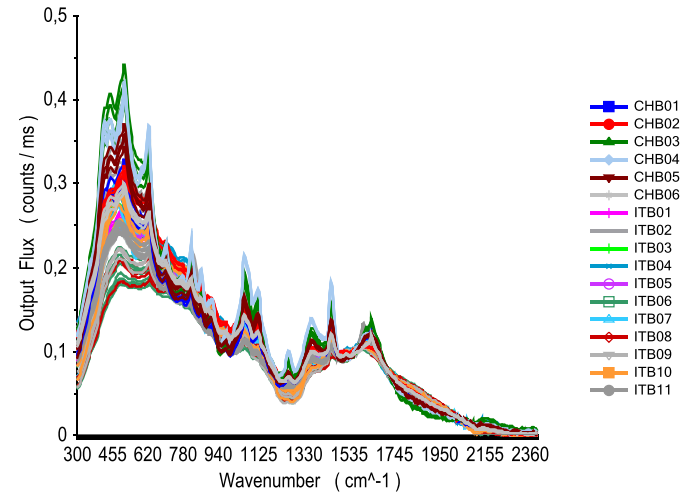
## Total Anthocyanins parameters of predictive model

$R^2$ – calibration	0,78
RMSEC (mg/hg)	43
$R^2$ – validation	0,75
RMSECV (mg/hg)	48

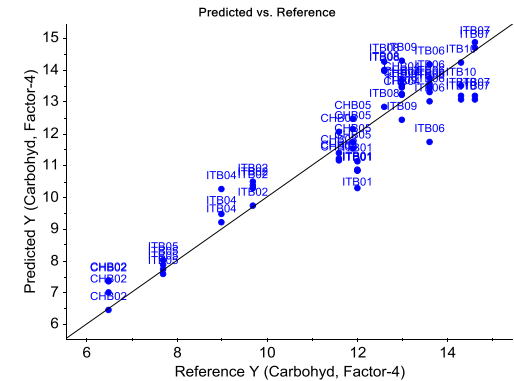
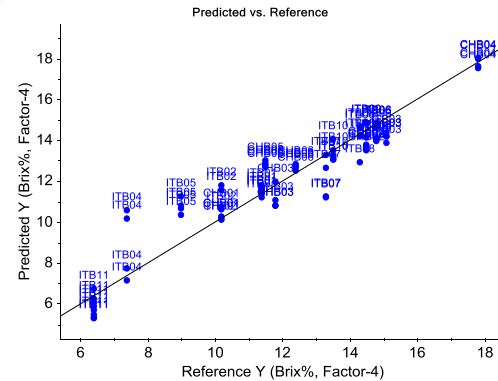


# Blueberry juices

## °Bx and carbohydrates as quality indicators

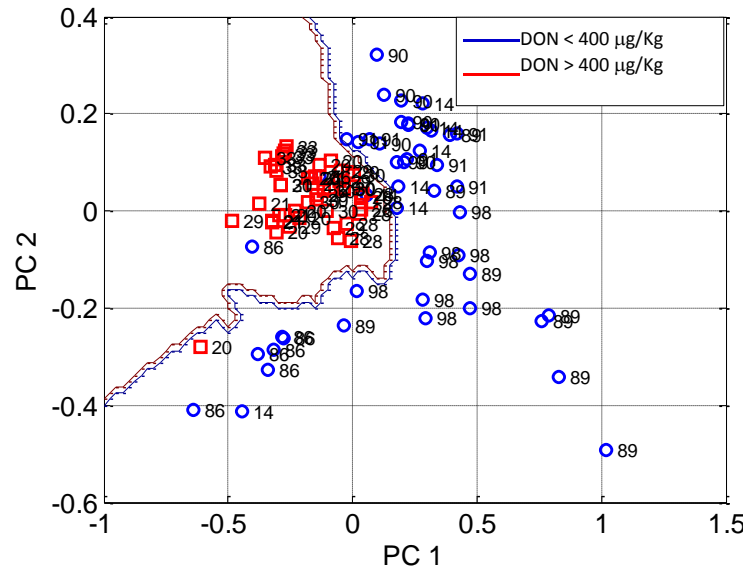
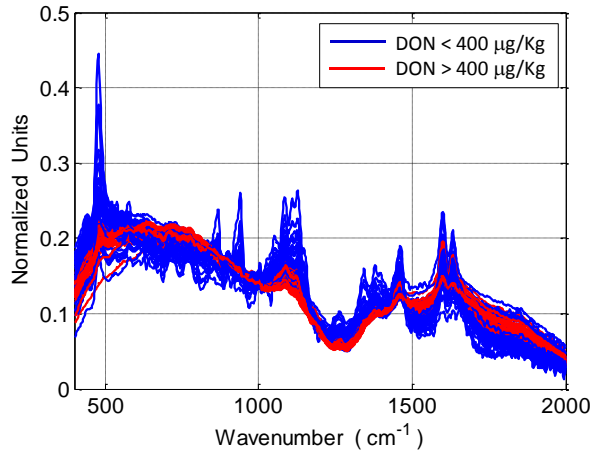
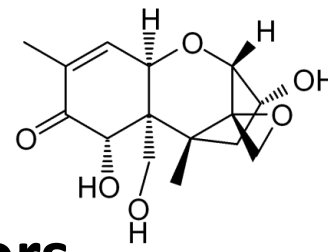


Parameter and model results	Carbohydrates	BRIX degrees
RMSEC	0,80 g/hg	0,97%
RMSCV	0,97 g/hg	1,1%
R <sup>2</sup> (cal)	0,887	0,9
R <sup>2</sup> (val)	0,840	0,88



# Wheat bran

## DON aflatoxin as safety indicators



Sample ID code	DON (µg/kg)	Classes
86	< LOD	Class A DON < 400 µg/kg
89	< LOD	
98	< LOD	
14	301	
90	355	
91	379	
20	738	Class B DON > 400 µg/kg
33	790	
29	857	
21	1459	
30	1567	
28	1623	

KNN confusion matrix (K = 3)		
	Predicted negative	Predicted positive
True negative	42	6
True positive	1	47



# Acknowledgements

- For honeys:
  - Project MIUR PON #00636 “FingerImball” , and Mariateresa Russo, Rosa Di Sanzo, Sonia Carabetta, Università di Reggio Calabria, Italy
- For blueberries:
  - Powders: Spanish Project “P11-AGR-7843”, and B. Gordillo Arrobas, F.J. Rodríguez-Pulido, C. Stinco, M.L. González-Miret, F.J. Heredia – Food Colour and Quality Lab., Dept. Nutrition and Food Science, Facultad de Farmacia, Universidad de Sevilla, Spain
  - Juices: Libo Yuan, Tingting Yuan, Shaoxian Zhang – Harbin Engineering University, College of Science, PR China
- For aflatoxins:
  - Project MIUR CL.A.N. #CTN01\_00230\_248064 “Safe&Smart”, and A. De Girolamo, V. Lippolis, M. Pascale – CNR Institute of Sciences of Food Production CNR , Bari, Italy

..... **Thank you** 😊