

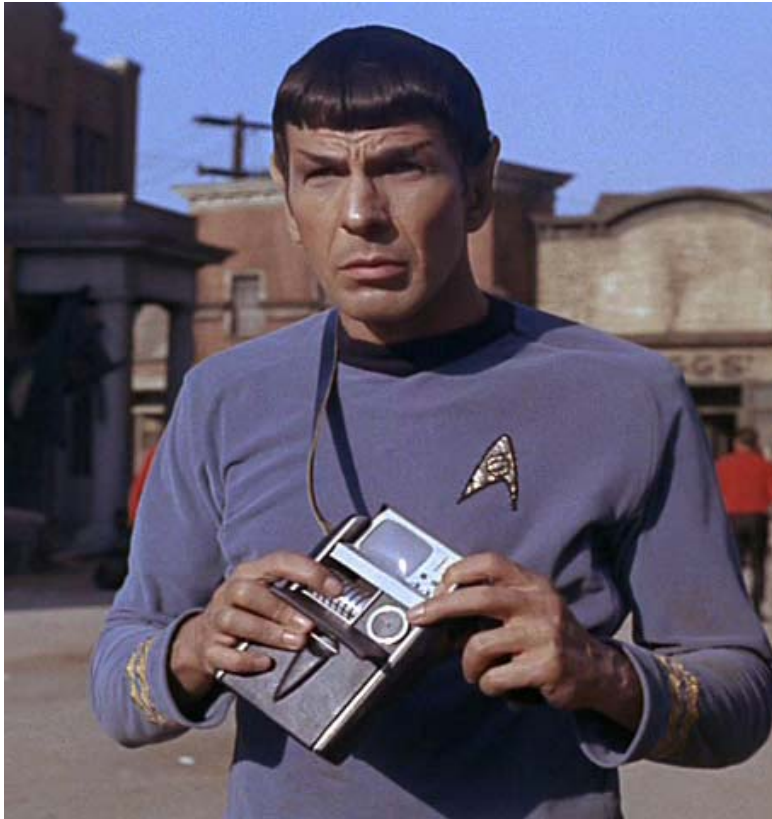
Outline

- General concepts
- Instruments
- Applications
 - reflectance, absorption, fluorescence
- Non-conventional instruments for absorption spectroscopy
- Spectroscopy by mobile devices
- Raman spectroscopy
- The kitchen of the future

Smartphone: the Swiss-knife of XXI century



Smartphone – Startrek tricorder



China and mobile phones



http://www.chinadaily.com.cn/china/2013-01/25/content_16172589.htm



Trends



- 
- Scenarios for smartphone-based sensors
 - Passive: info retrieval only
 - Plug-in sensors
 - Embedded spectroscopy

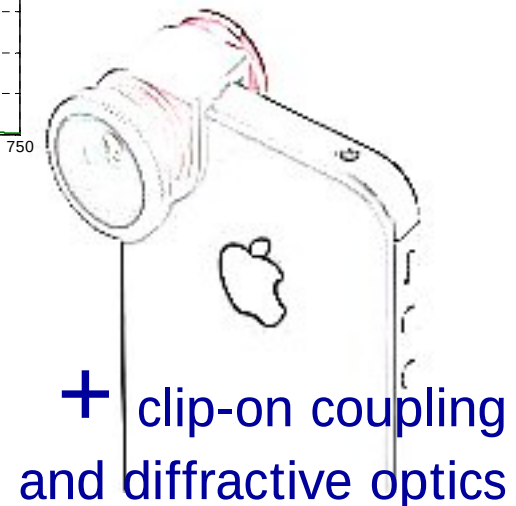
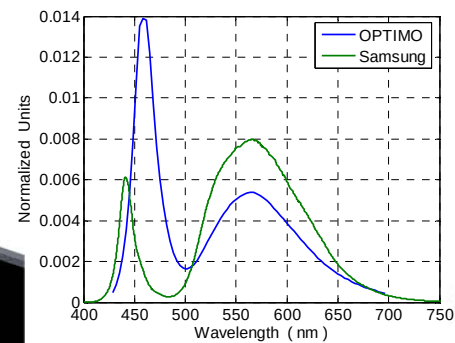
Passive: info retrieval only

- Smartphone camera used to read QR or bar-code
- QR/bar-code pic sent through internet to a data warehouse where the info is stored
- Info retrieval using internet connection
- This approach implies that the info requested by the consumer has been acquired and is available



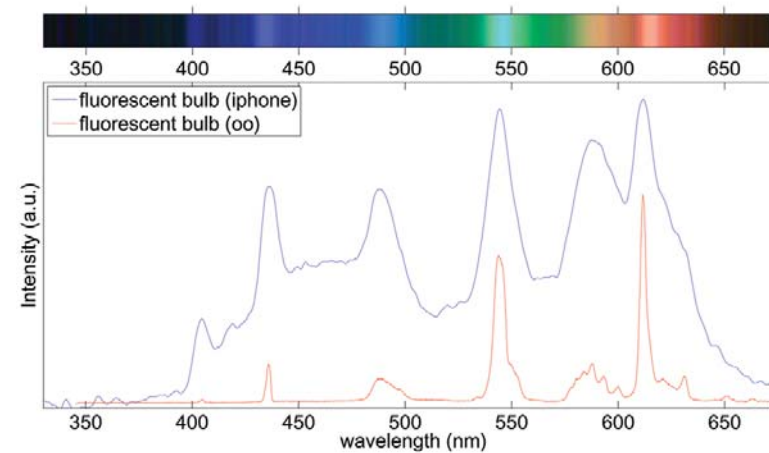
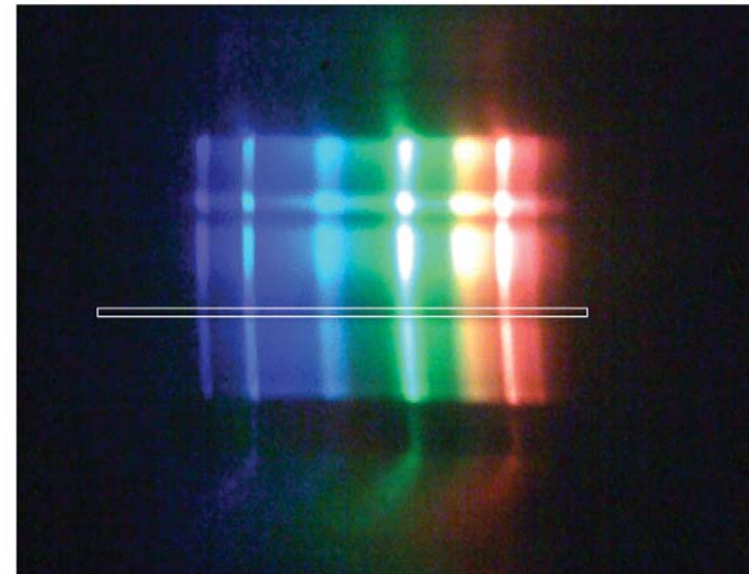
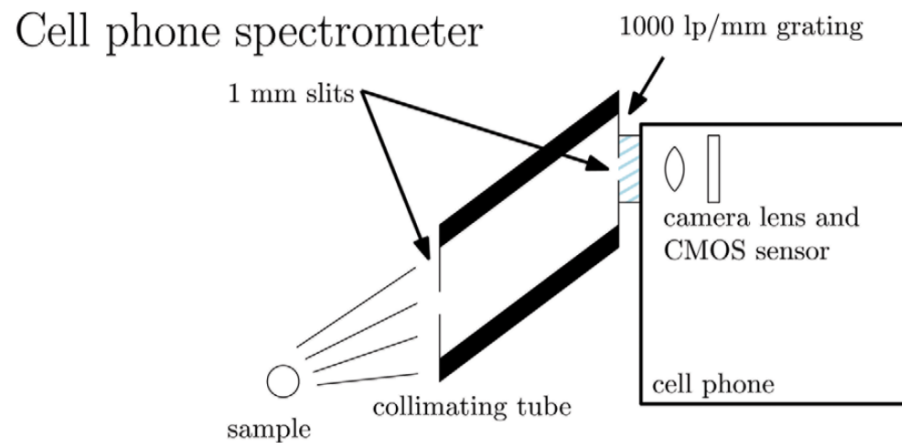
Embedded spectroscopy

- White LED = source
- Camera = spectrometer
 - 3 channels only: RGB
 - Added chemometric functionalities for a better exploitation of spectroscopic info



Embedded spectroscopy

outside source



Embedded spectroscopy

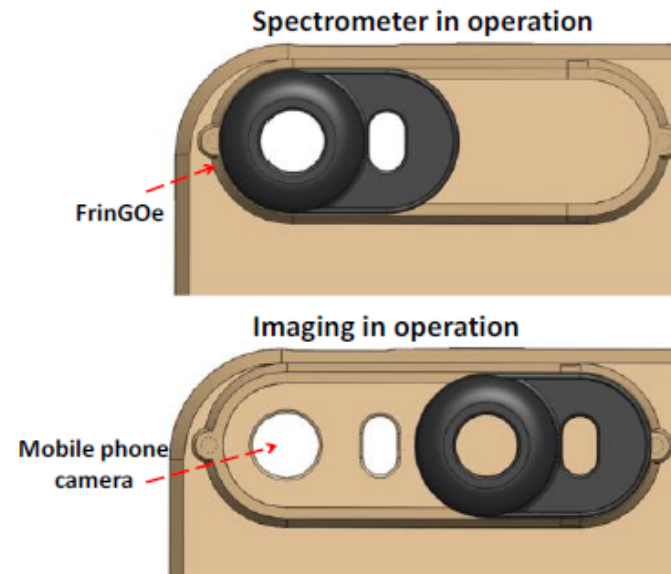
Shazam for materials..... & food

Advanced prototype - 3D printed

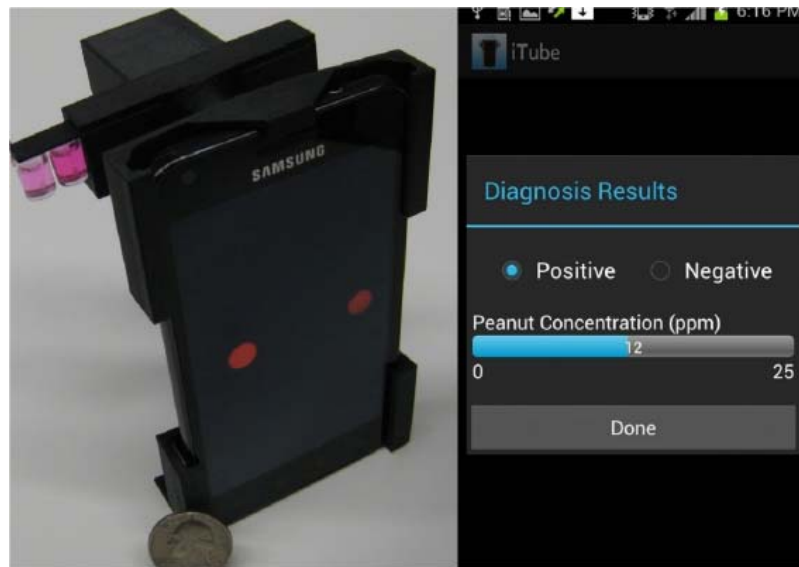




Embedded spectroscopy by means of a special cover



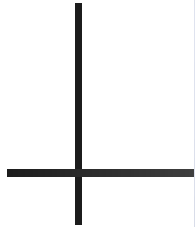
Lab in a phone



<http://innovate.ee.ucla.edu/welcome.html>



<http://www.iplaustalia.com/>



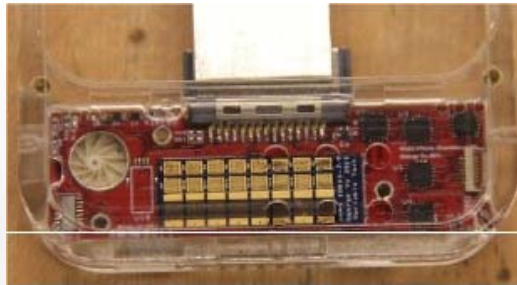
<https://phonebloks.com/plan/> - <http://www.dscout.com>



motorola
a Google company

Smartphone sensors

- External unit with sensors
 - Plug-in through socket
 - Blue-tooth connection for stand-alone units



<http://www.mydario.com/#Device>
J. Li et alii, *IEEE Sensors Conf.* 2012
<http://www.sensorcon.com/sensordrone/>

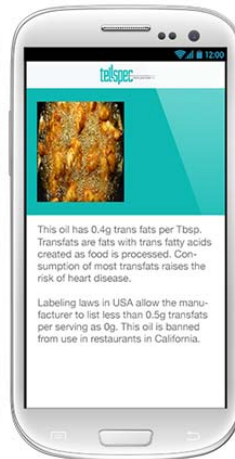
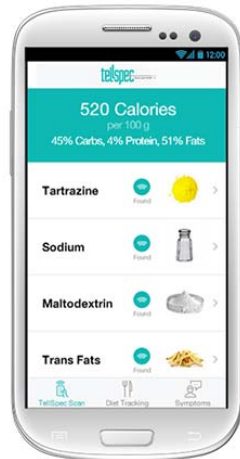
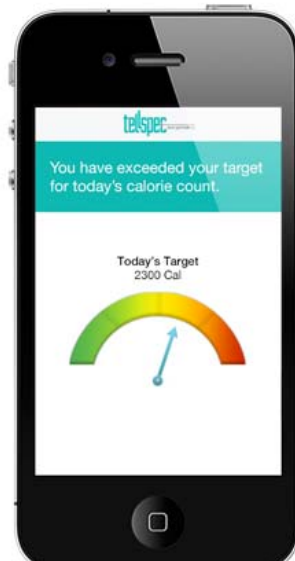
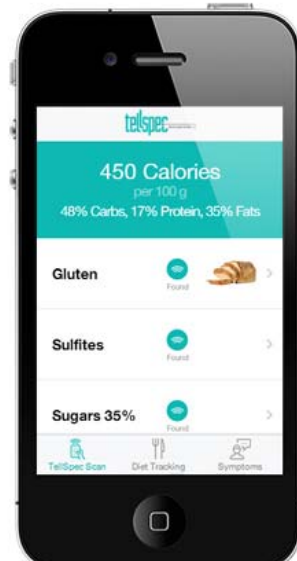


Mobile spectroscopy + cloud computing



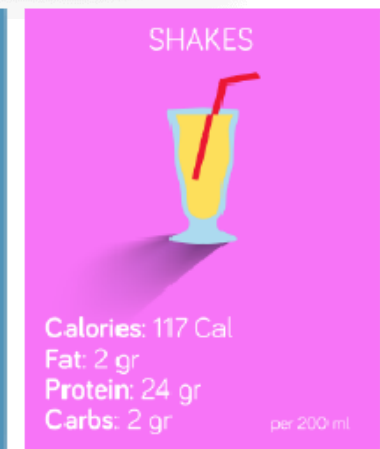
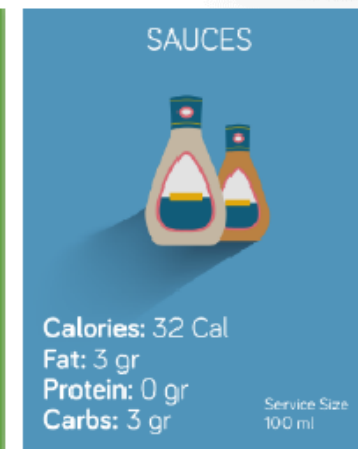
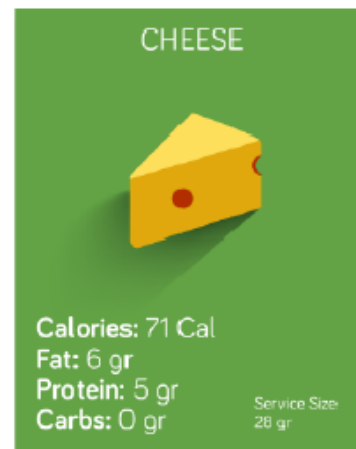
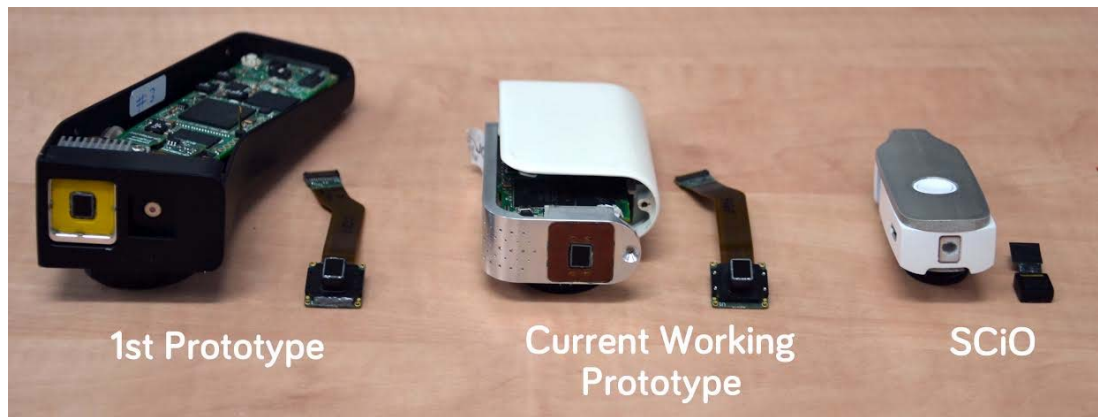
TellSpec

<http://www.tellspec.com>



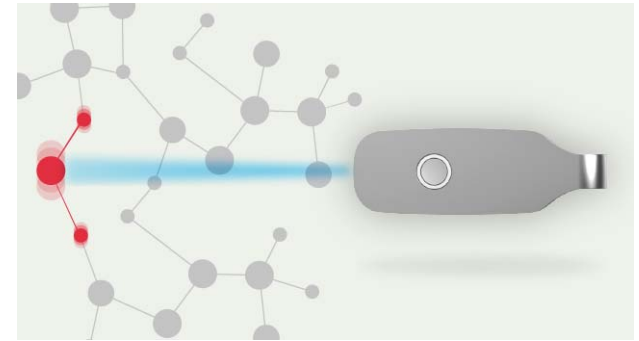
SCiO

<http://www.consumerphysics.com>



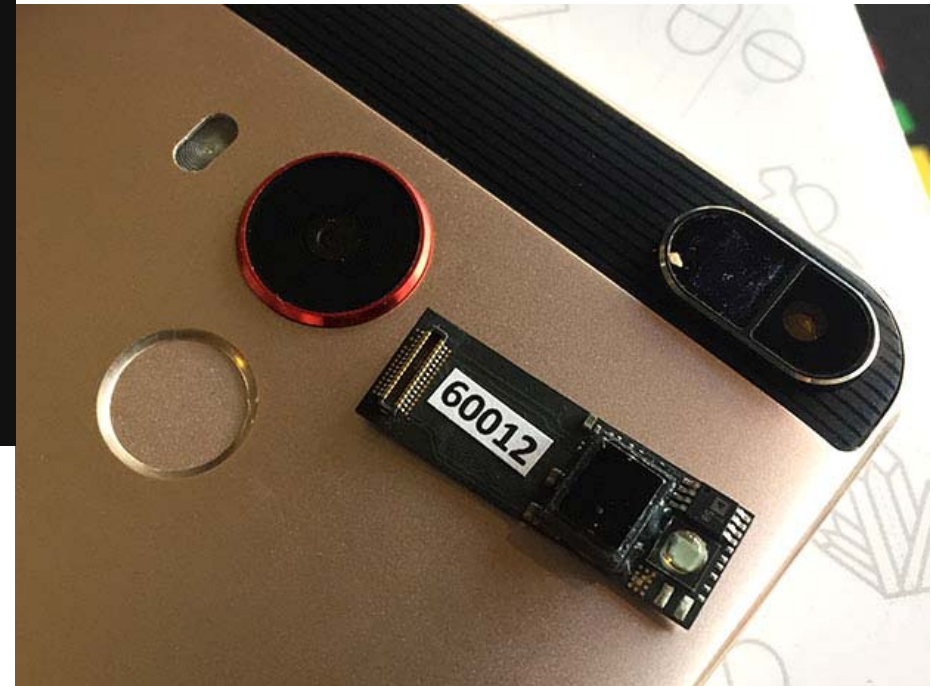
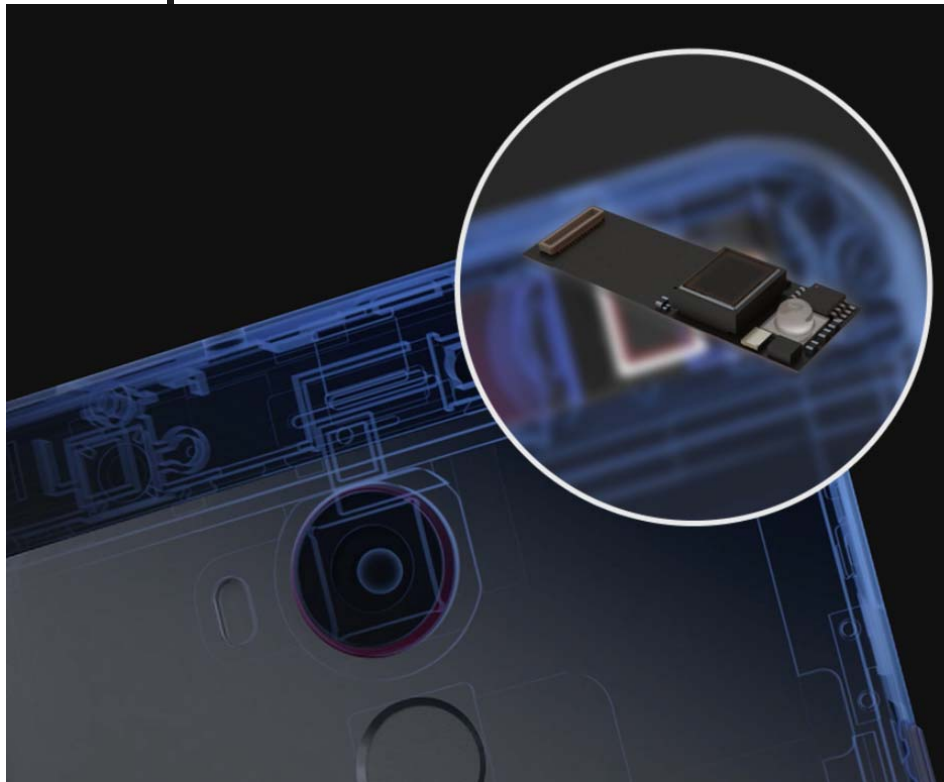
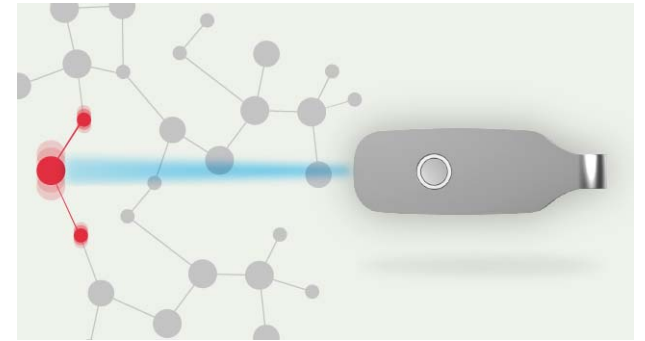
SCiO

<http://www.consumerphysics.com>



SCiO

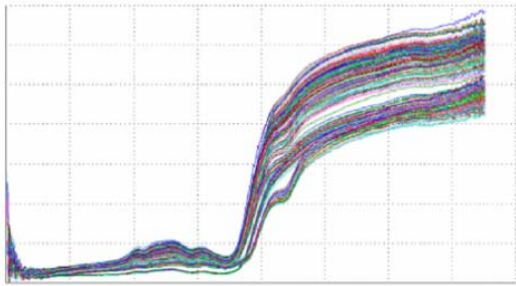
<http://www.consumerphysics.com>



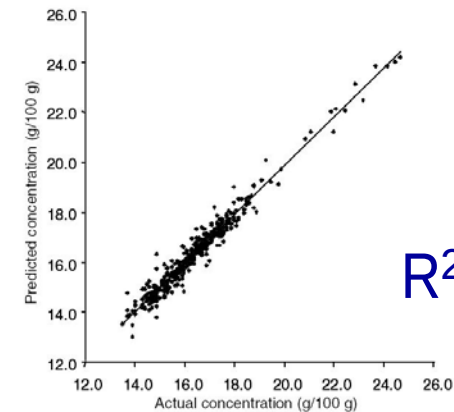
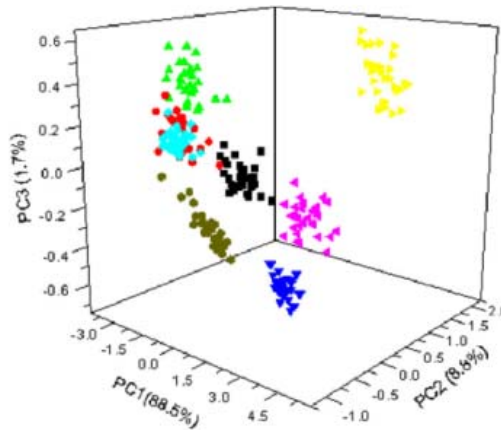
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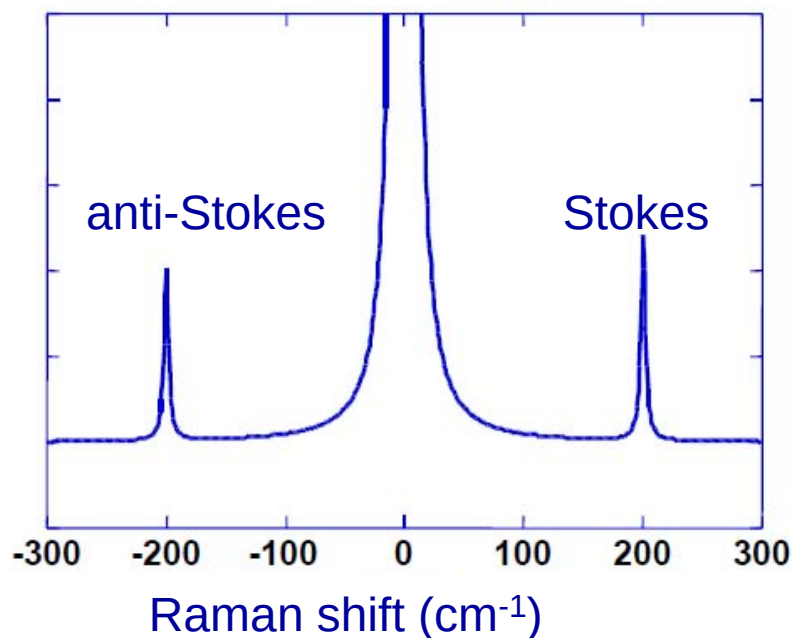
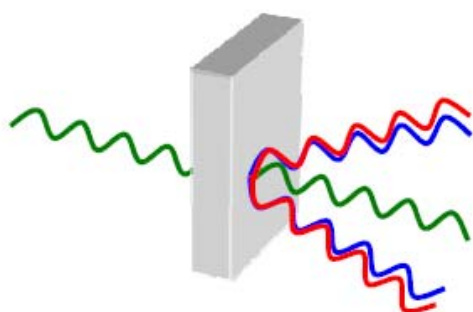
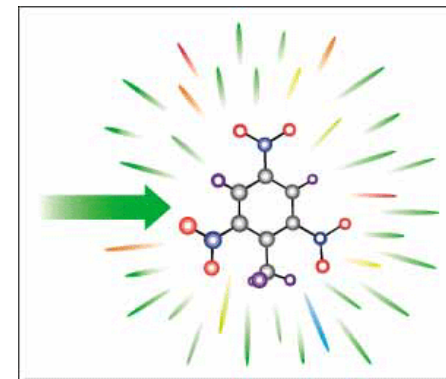
..... Steps towards multicomponent analysis



- Spectroscopy
- Chemometrics
- Classification maps
- Library of ref. spectra / analytical data
- Model for prediction of quality indicators
- Validation



Raman spectroscopy

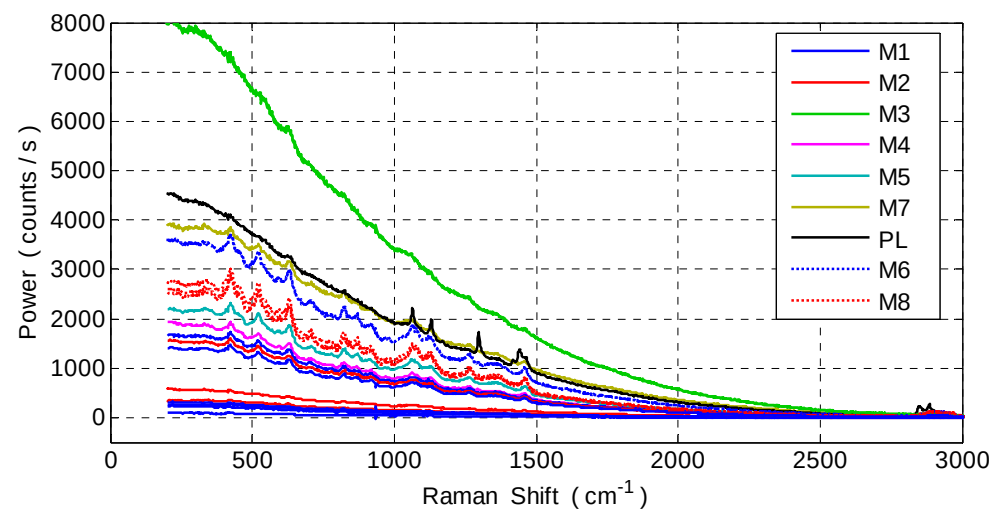


- Most of the scattered light has the same frequency/energy as that of the incident light (scattering Rayleigh)
- A slight fraction of the incident light donates or receives energy to contribute to a change in the vibrational and rotational state of molecules.
- The change in the photon energy as a result of inelastic scattering of light with molecules is the “Raman shift”

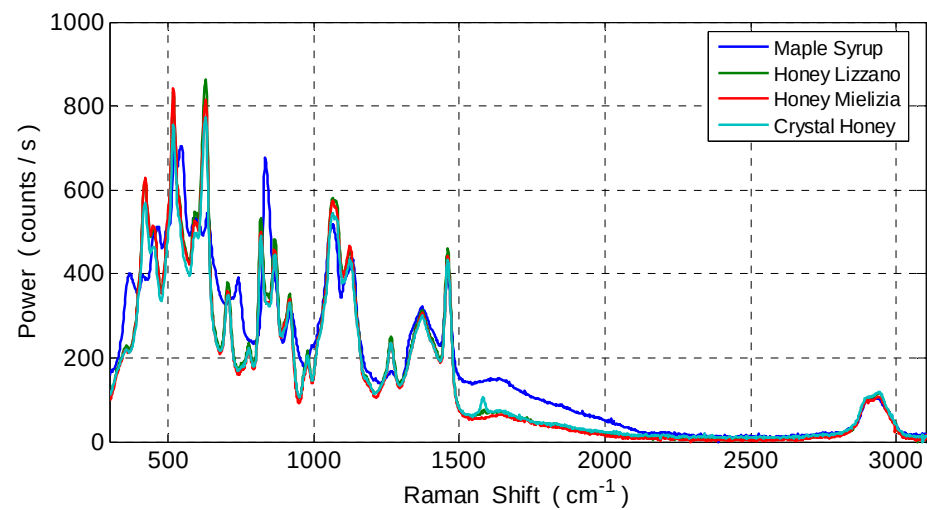
$$I_{\text{Raman}} \propto 1 / \lambda^4$$

Raman @785nm VS @1064nm

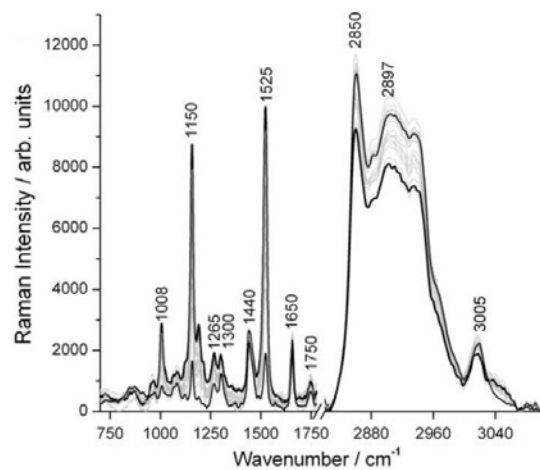
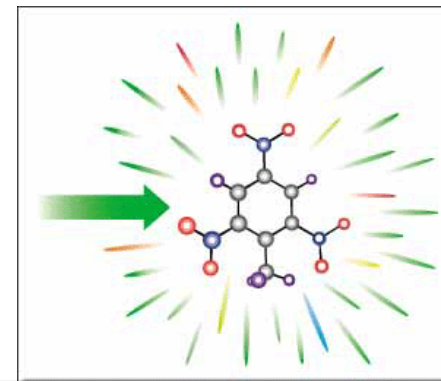
@ 785nm



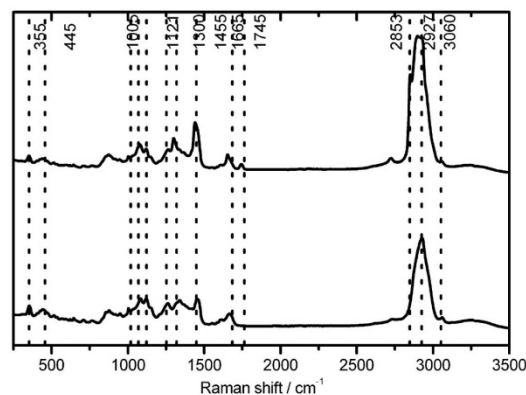
@ 1064nm



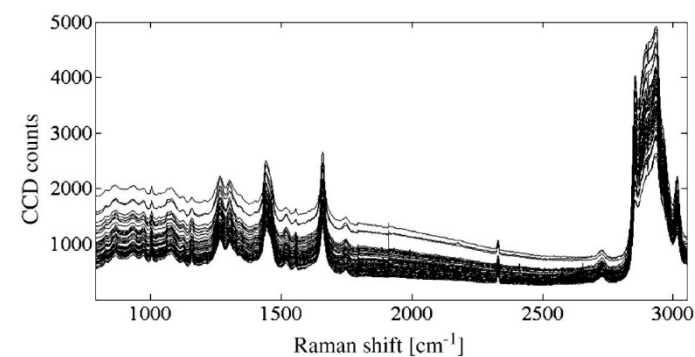
Raman – food fingerprints



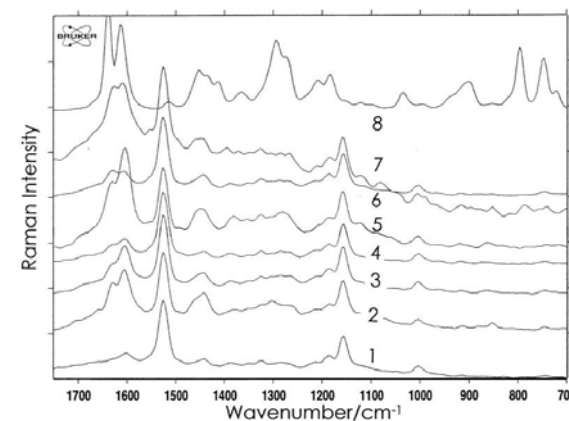
olive oil
different brands



powder milk
whole and skim



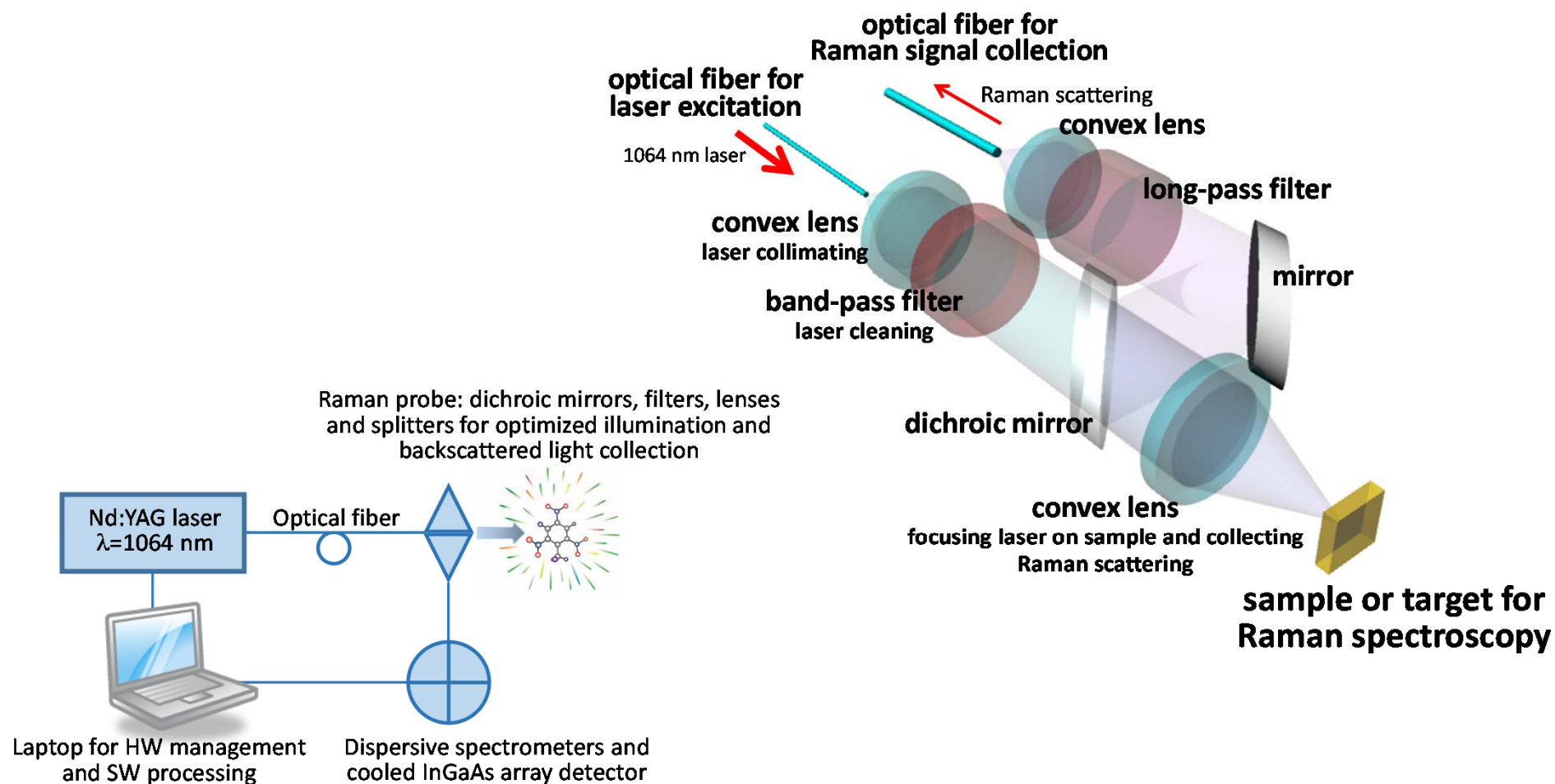
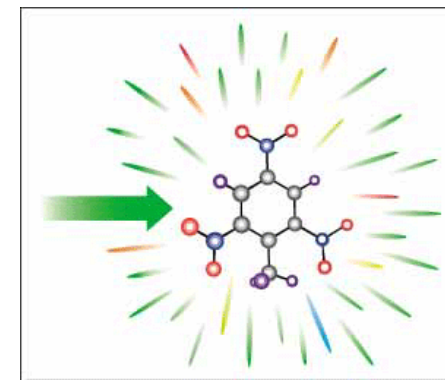
salmon



fresh herbs

R.M. El-Abassy et alii, *JAOCS*, vol. 86, 2009, pp. 507-511
C.M. McGoverin et alii, *Anal. Chim. Acta*, vol. 673, 2010, pp. 26-32
N.K. Afseth et alii, *Anal. Chim. Acta*, vol. 572, 2006, pp. 85-92
B. Schrader, *J. Mol. Str.*, vol. 480-481, 1999, pp. 21-32

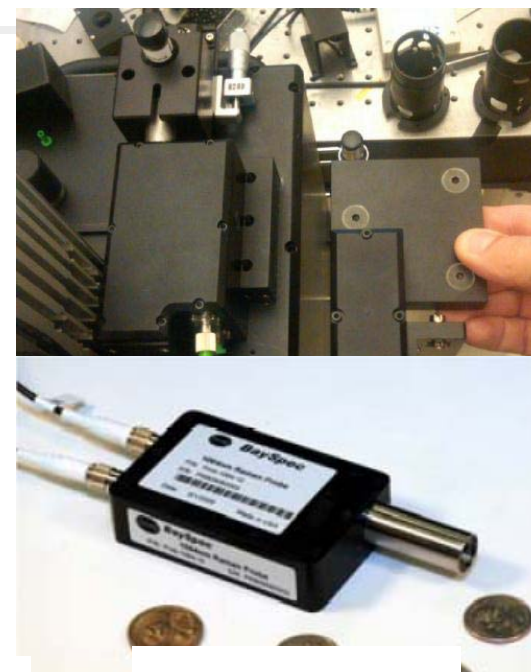
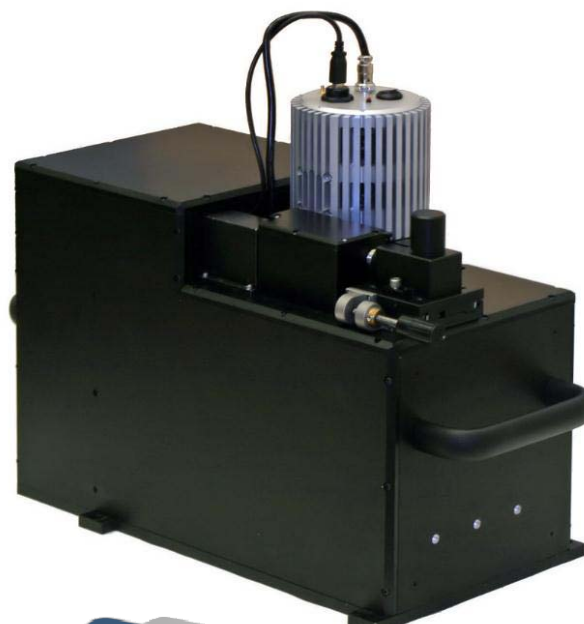
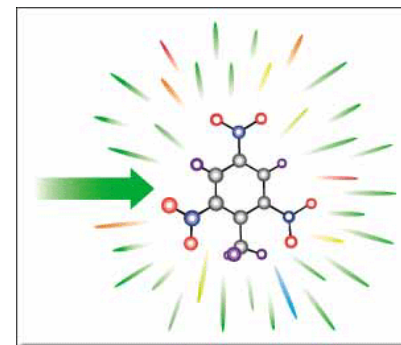
Raman spectroscopy @ 1064 nm



Raman spectroscopy @ 1064 nm

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

RamSpec-1064nm-HR
BaySpec Inc., San José CA
www.bayspec.com



www.bayspec.com



www.rigakuraman.com



www.wysri.com



www.metrohm.com

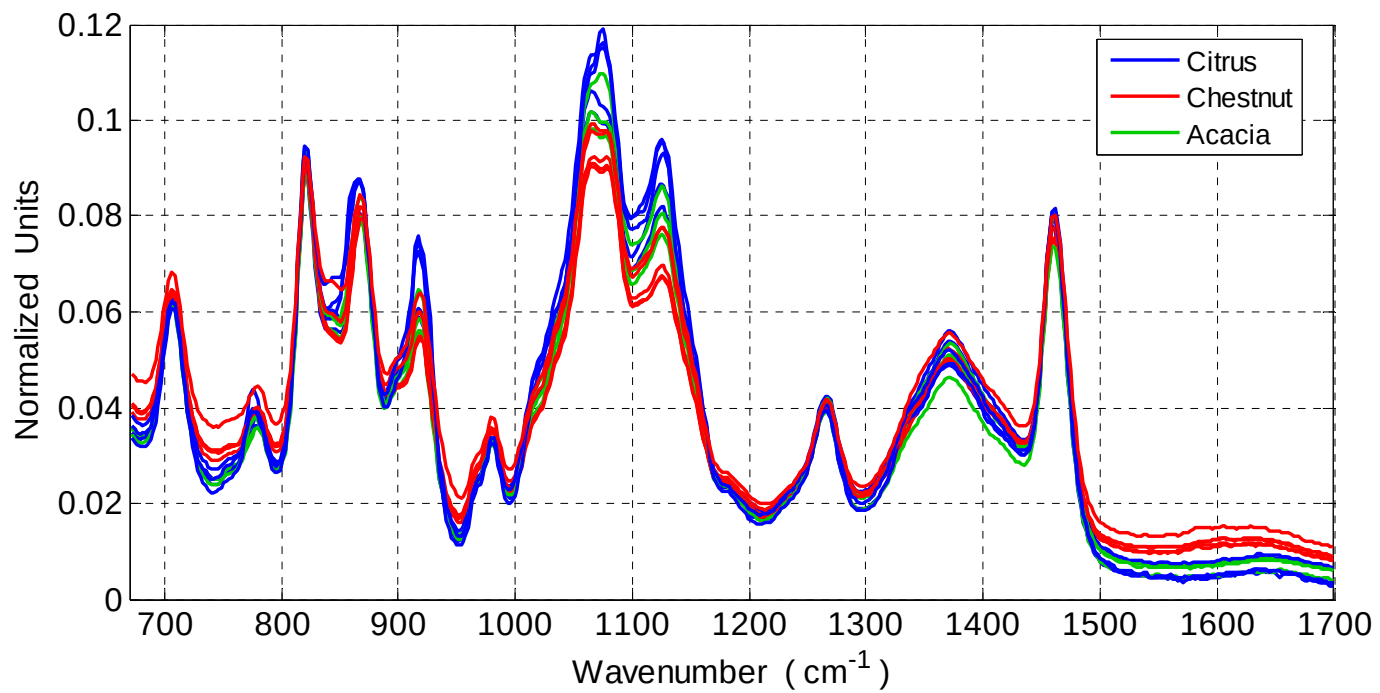
Raman spectroscopy for honey applications: the collection of honeys from Calabria

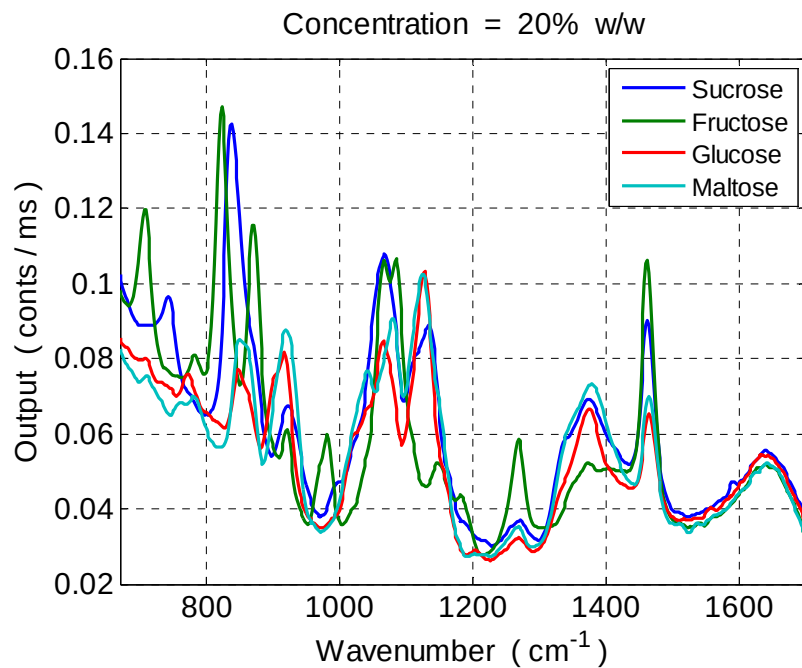
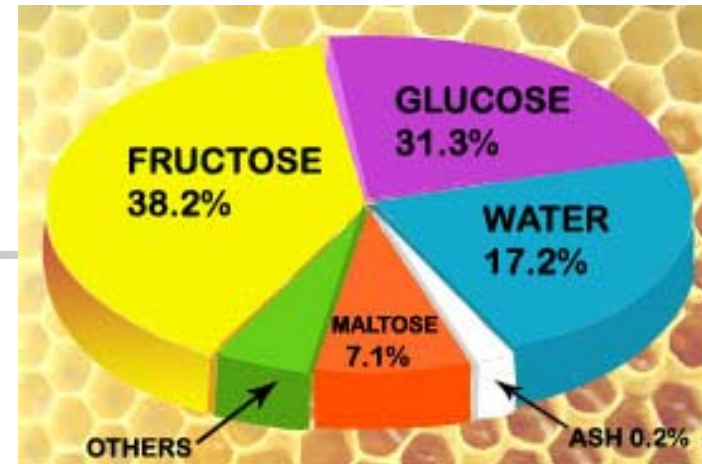
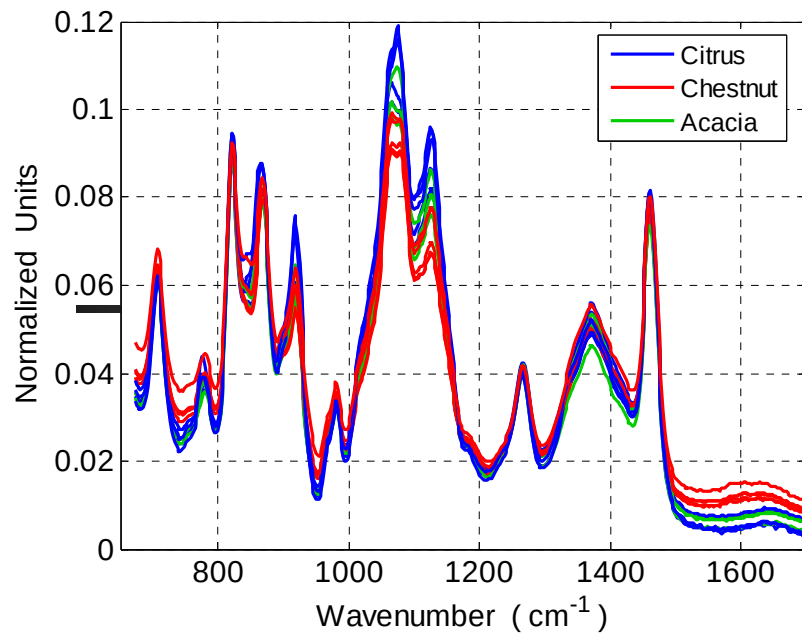


- Distinguishing the botanic origin
- Predictive models for sugar profile
- Potassium as important nutraceutic indicator



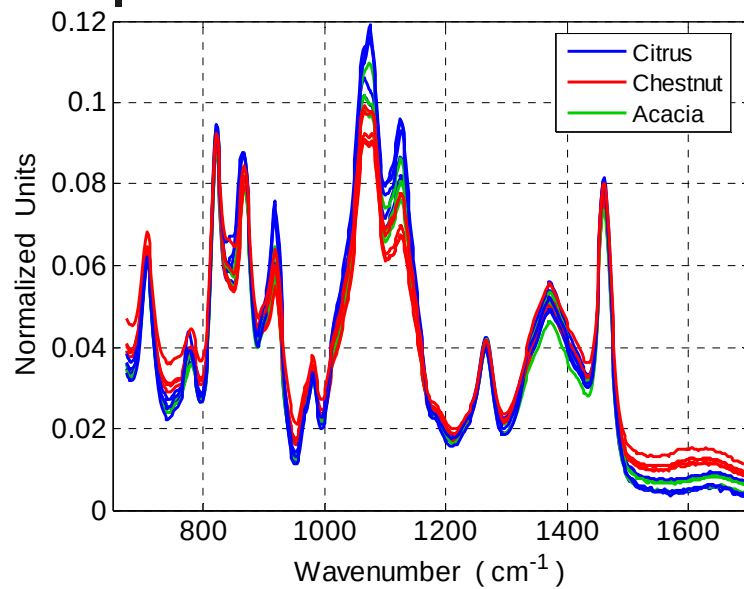
Raman spectra



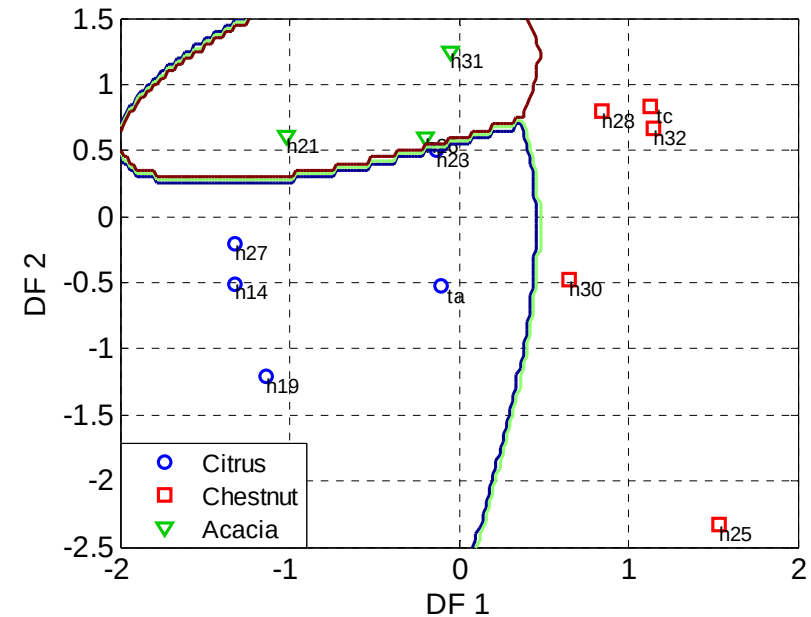


Raman band (cm^{-1})	Main contribution	Secondary contribution
707	Fructose	
821	Fructose	
867	Fructose	Glucose
917	Glucose	Maltose
1060-1080	Fructose	Glucose
1127	Glucose	Maltose
1267	Fructose	Glucose
1372	Glucose	Maltose
1460	Fructose	Glucose

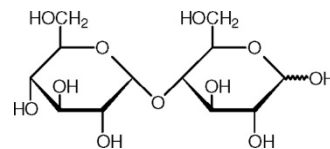
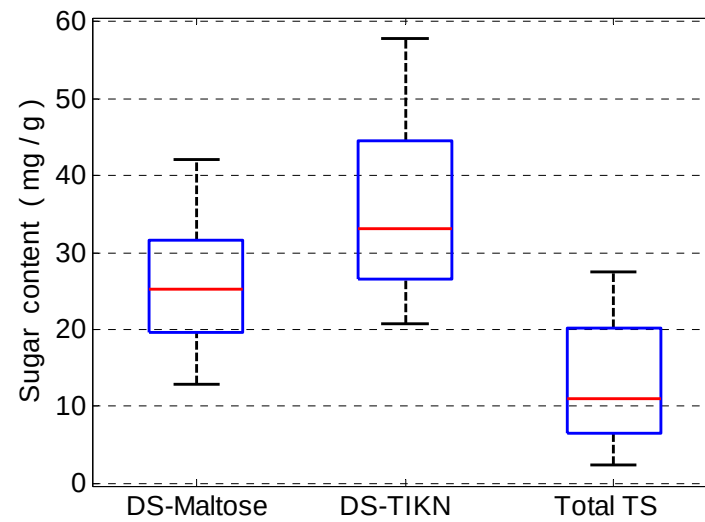
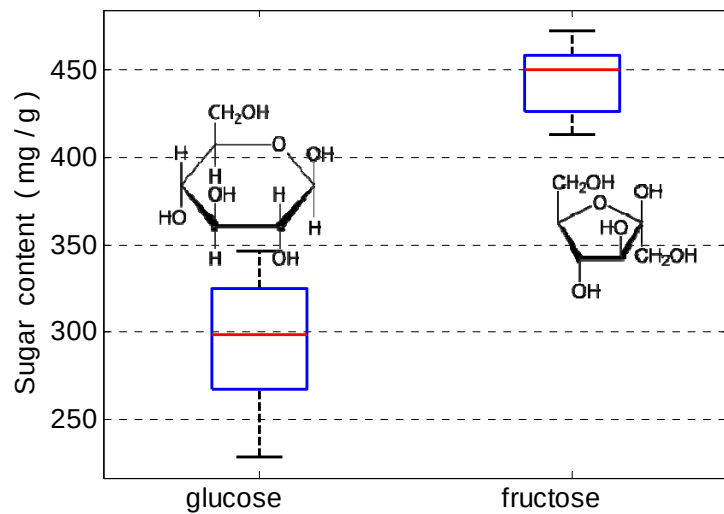
Distinguishing the botanic origin



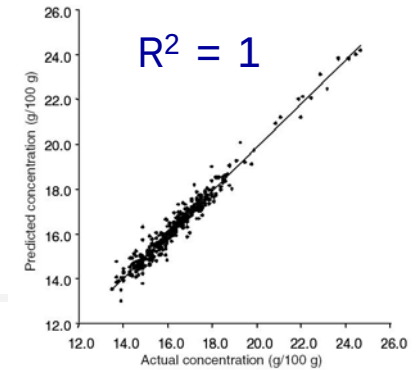
PCA + LDA + KNN



Sugar profile



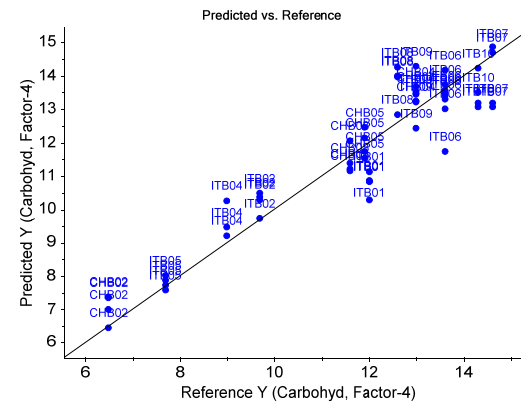
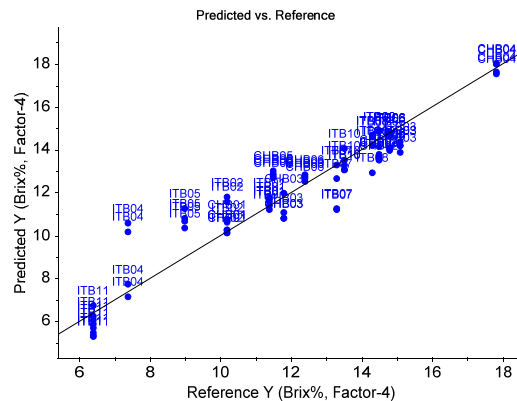
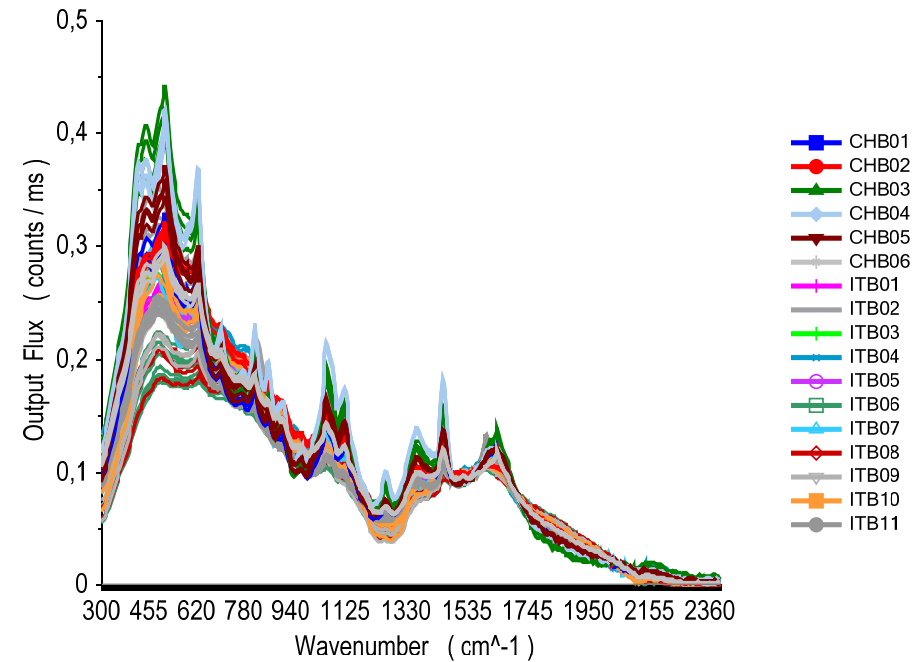
Results of PLS predictive models for sugars & potassium



Analyte			RMSEC	R^2 (cal)	RMSECV	R^2 (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 (μ g/g)			0,3	0,97	0,5	0,94

Raman fingerprints of blueberry juices

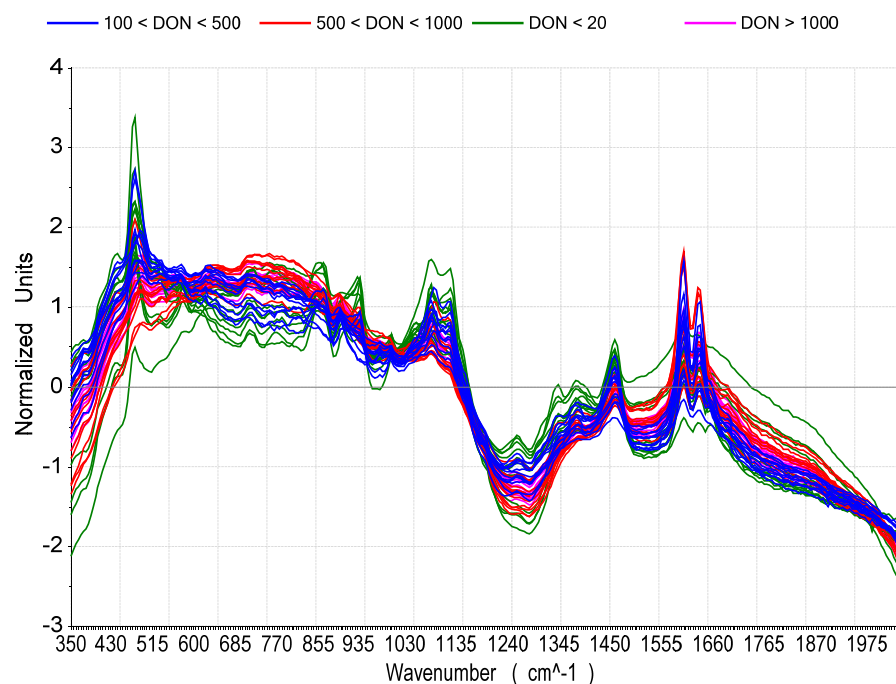
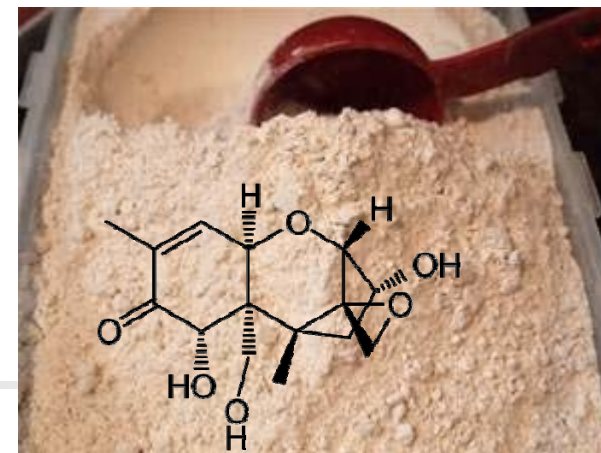
Brix and Carbohydrates



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

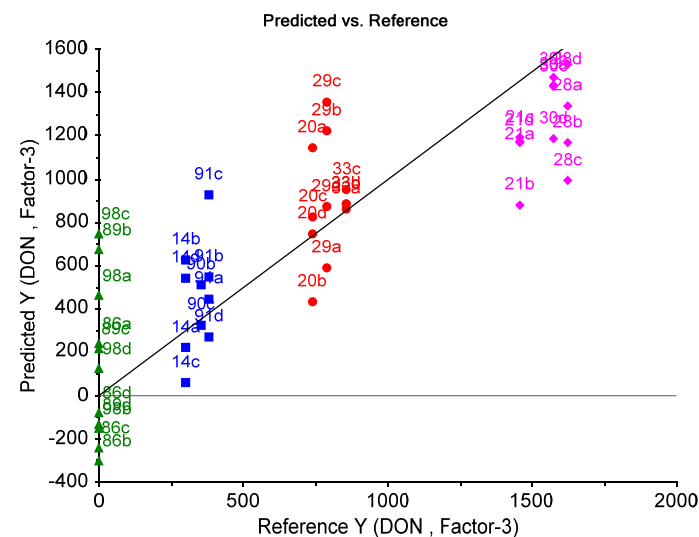
Mycotoxins in wheat flour

DON – Raman spectra and predictive model



4 levels of contamination:

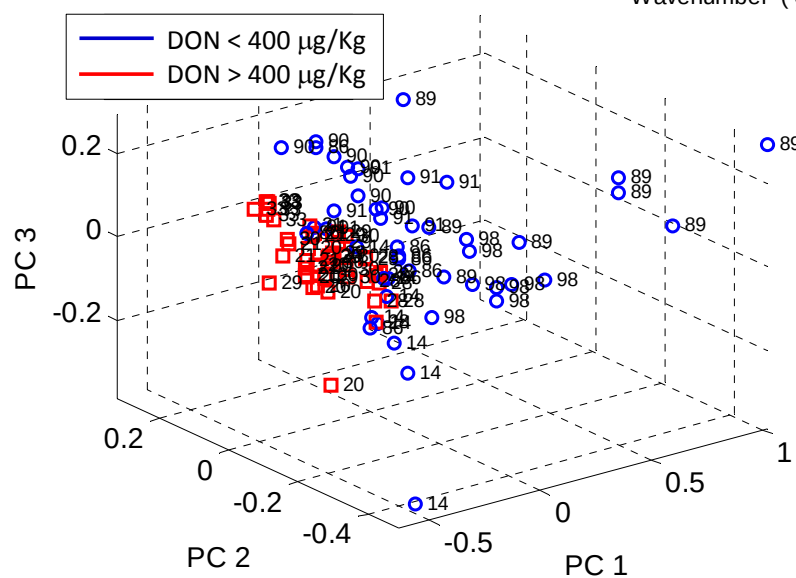
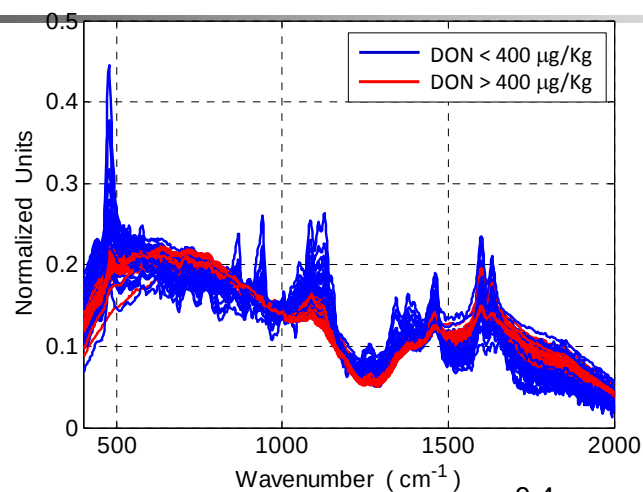
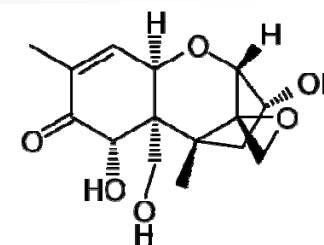
- 1) < 20 ppb
- 2) 100-500 ppb
- 3) 500-1000 ppb
- 4) > 1000 ppb



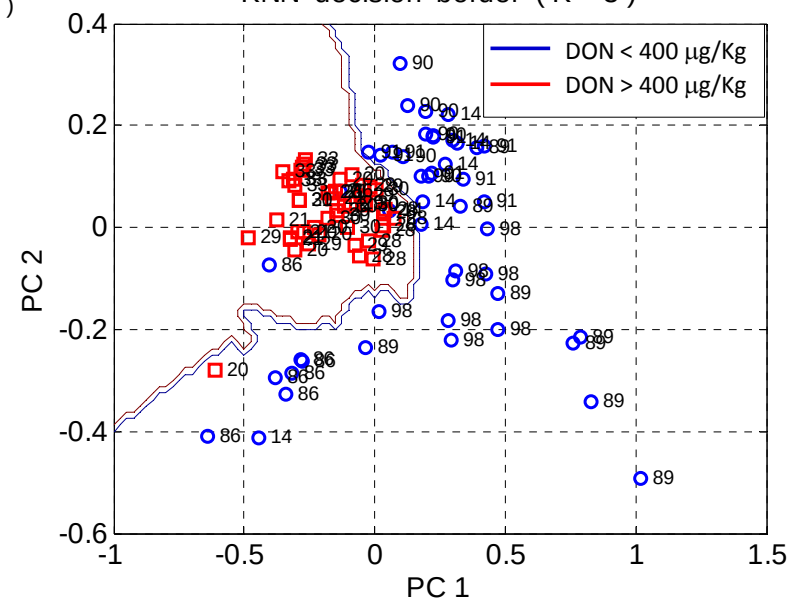
Parameter	Calibration	Cross-validation (LOO)
RMSE (ppb)	313	357
R squared	0,72	0,65

Mycotoxins in wheat flour

DON – Raman spectra and predictive model



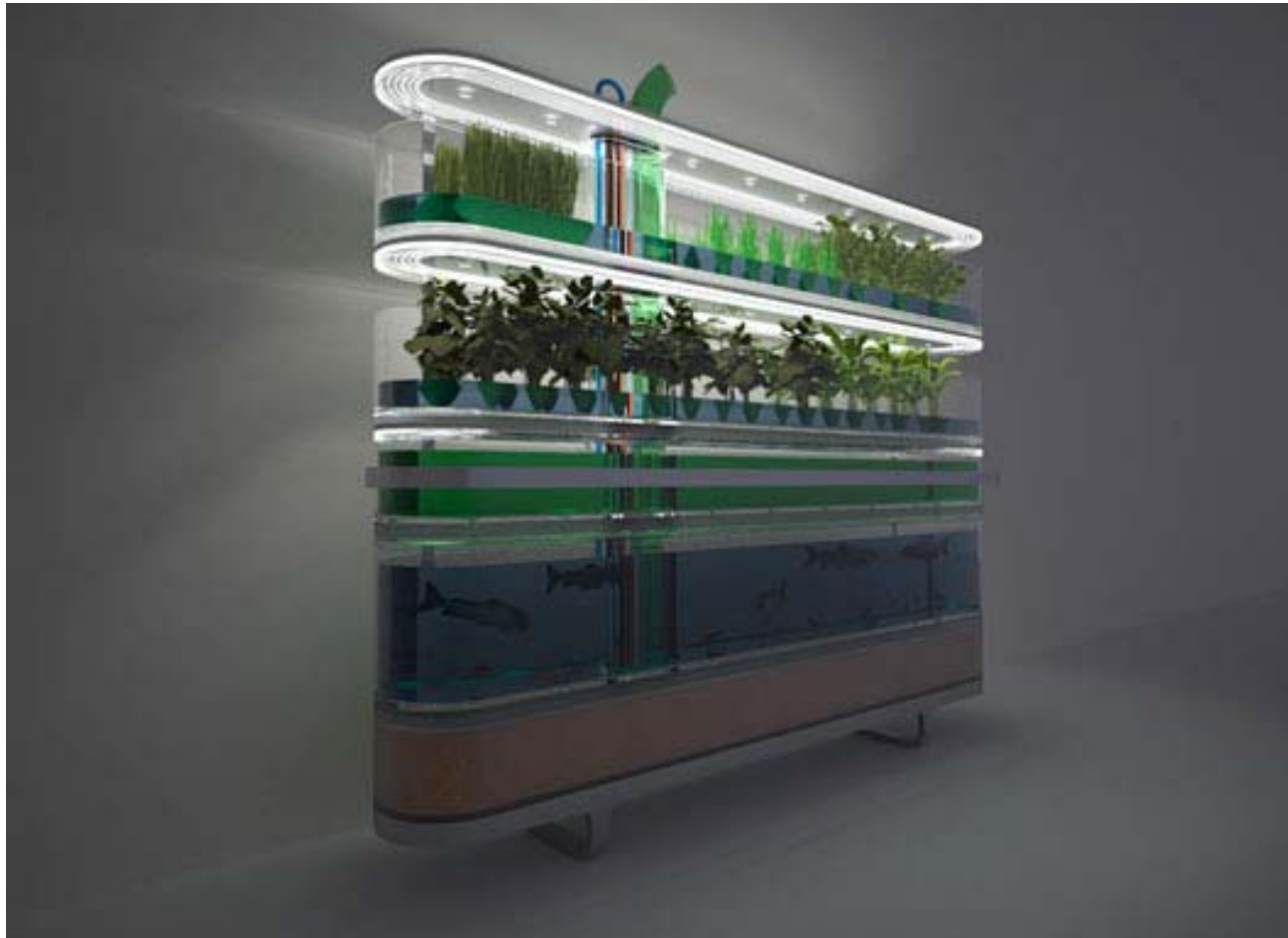
KNN decision border (K = 3)



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Home farming



<http://www.nextnature.net/2009/10/food-design-in-the-21th-century/>

<https://www.alamy.com/indoor-soil-free-gardens-with-herb-plants-and-vegetables-producing-food-on-display-at-the-consumer-electronics-show-ces-in-las-vegas-nv-usa-image221407345.html>

Home farming @ CES 2019



Digital gastronomy

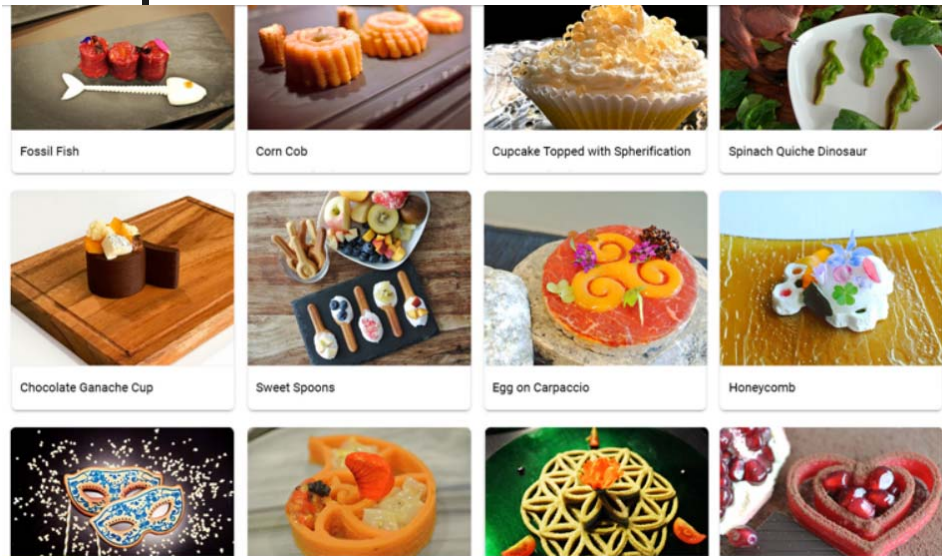


<http://www.nextnature.net/2010/01/digital-gastronomy/>

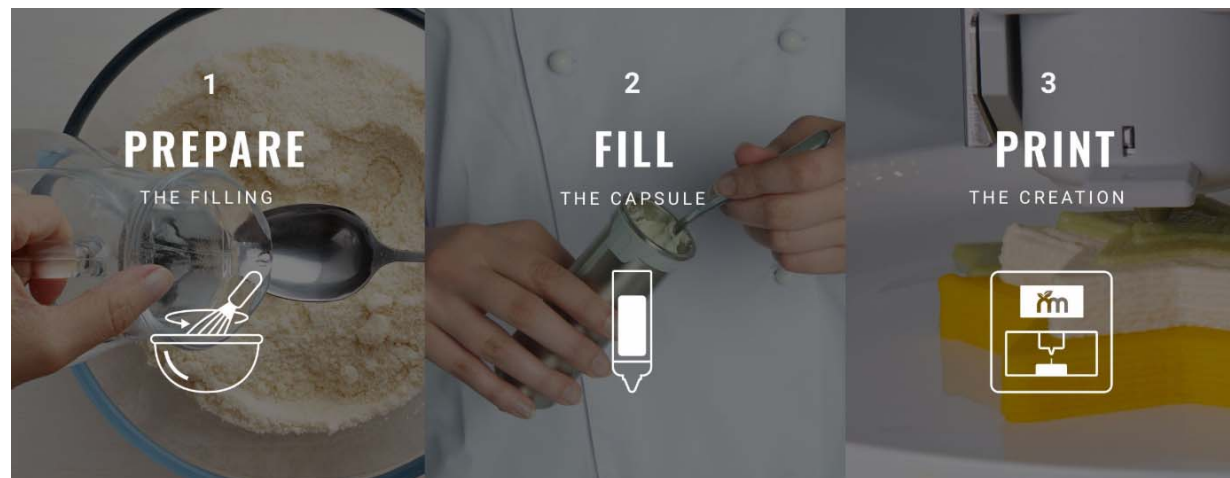


<http://www.nextnature.net/2010/05/nano-product-the-food-printer/>

Digital gastronomy



<https://www.naturalmachines.com/foodini/>



Curiosity and gadgets

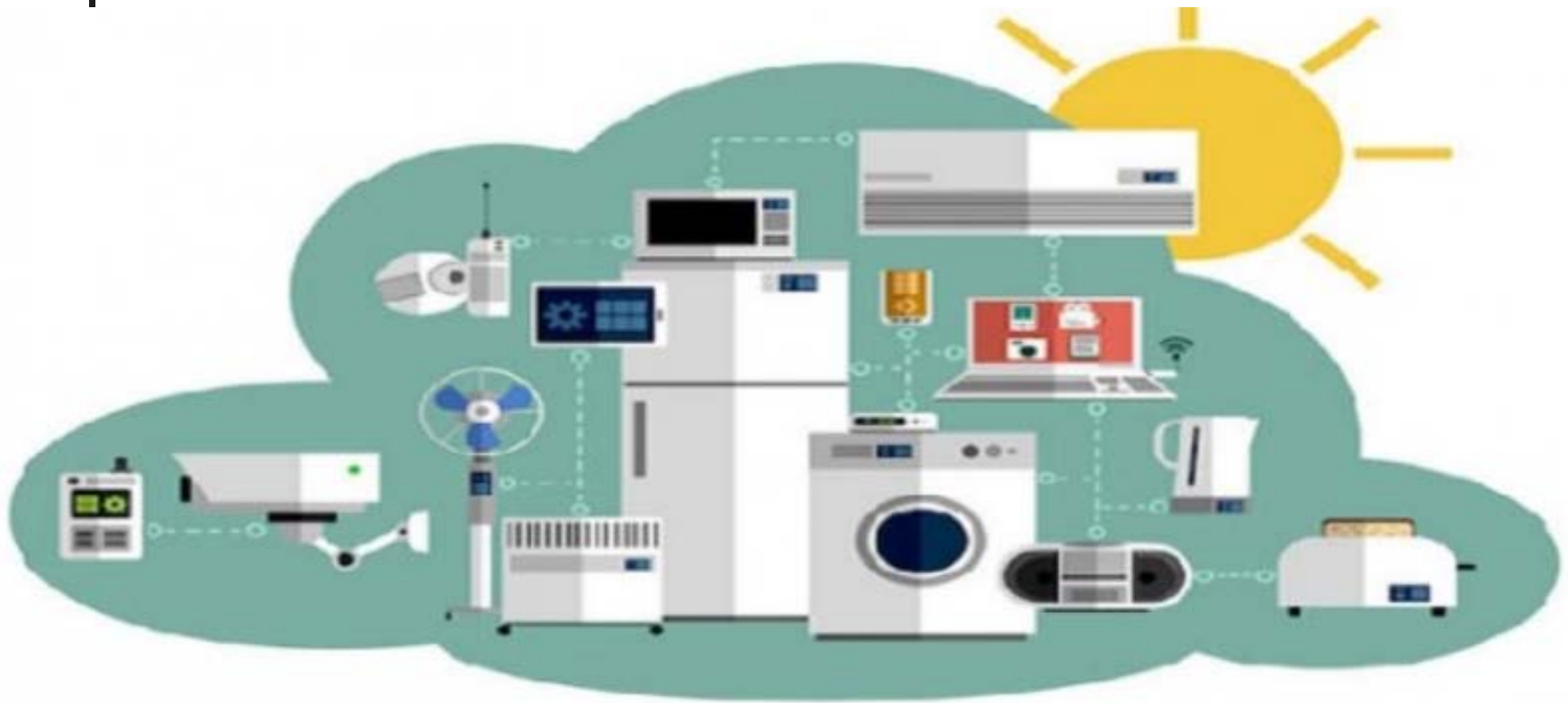


<http://situscale.com/>



<https://nimasensor.com/>

The Internet of Things - IoT



IoT Home Appliances Upgrading **Lifestyles**

The kitchen of the future



<http://www.digitaltrends.com/home/heck-internet-things-dont-yet/>

The fridge of the future – a family hub



The fridge of the future – a community hub



<https://pulsenews.co.kr/view.php?year=2017&no=565012>

What's next in food

?? Edible electronics ??

?? Edible photonics ??



<https://www.youtube.com/watch?v=oaaHLu77pQc>