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


BEIJING - The number of Chinese mobile phone users reached 1.11 billion as of the end of 2012, according to official data unveiled Thursday.

The Ministry of Industry and Information Technology (MIIT) said in a statement that mobile phone users represent 80 percent of all phones users in the country.
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

![Diagram of a camera and spectroscopic graph]

+ clip-on coupling and diffractive optics
Embedded spectroscopy outside source

Cell phone spectrometer

1 mm slits

1000 lp/mm grating

sample
collimating tube

camera lens and CMOS sensor
cell phone

Smith et alii, *PLOS ONE*, vol. 6, 2011, e17150
Embedded spectroscopy
Shazam for materials........ & food
Advanced prototype - 3D printed

http://store.publiclab.org/products/smartphone-spectrometer
Embedded spectroscopy by means of a special cover

https://fringoe.com/
Lab in a phone

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

http://www.iplaustralia.com/
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
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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”.

\[ I_{\text{Raman}} \propto \frac{1}{\lambda^4} \]
Raman @785nm VS @1064nm

@ 785nm

@ 1064nm
Raman – food fingerprints

- salmon
- olive oil, different brands
- powder milk, whole and skim
- fresh herbs

R.M. El-Abassy et alii, JAOCs, vol. 86, 2009, pp. 507-511
Raman spectroscopy @ 1064 nm

Nd:YAG laser $\lambda=1064$ nm

Optical fiber

Laptop for HW management and SW processing

Dispersive spectrometers and cooled InGaAs array detector

Raman probe: dichroic mirrors, filters, lenses and splitters for optimized illumination and backscattered light collection

Nd:YAG laser 1064 nm laser

optical fiber for laser excitation

optical fiber for Raman signal collection

convex lens
laser collimating

band-pass filter
laser cleaning

dichroic mirror

cmpex lens
focusing laser on sample and collecting Raman scattering

sample or target for Raman spectroscopy

long-pass filter

mirror

Raman scattering
**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 nutraceutical indicator
Raman spectra

![Raman spectra graph]

- Citrus
- Chestnut
- Acacia
## Raman Band (cm⁻¹)

### Main Contribution
- 707 Fructose
- 821 Fructose
- 867 Fructose
- 917 Glucose
- 1060-1080 Fructose
- 1127 Glucose
- 1267 Fructose
- 1372 Glucose
- 1460 Fructose

### Secondary Contribution
- Sugar Concentration = 20% w/w

### Concentration = 20% w/w
- Sucrose
- Fructose
- Glucose
- Maltose

### Chart
- **Normalized Units**
- **Wavenumber (cm⁻¹)**
- **Output (counts/ ms)**

### Pie Chart
- **Citrus**
- **Chestnut**
- **Acacia**
- **Fructose 31.3%**
- **Glucose 17.2%**
- **Maltose 7.1%**
- **WATER 17.2%**
- **OTHERS**

### Table
<table>
<thead>
<tr>
<th>Raman band (cm⁻¹)</th>
<th>Main contribution</th>
<th>Secondary contribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>707</td>
<td>Fructose</td>
<td></td>
</tr>
<tr>
<td>821</td>
<td>Fructose</td>
<td></td>
</tr>
<tr>
<td>867</td>
<td>Fructose</td>
<td>Glucose</td>
</tr>
<tr>
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<td>Glucose</td>
<td>Maltose</td>
</tr>
<tr>
<td>1060-1080</td>
<td>Fructose</td>
<td>Glucose</td>
</tr>
<tr>
<td>1127</td>
<td>Glucose</td>
<td>Maltose</td>
</tr>
<tr>
<td>1267</td>
<td>Fructose</td>
<td>Glucose</td>
</tr>
<tr>
<td>1372</td>
<td>Glucose</td>
<td>Maltose</td>
</tr>
<tr>
<td>1460</td>
<td>Fructose</td>
<td>Glucose</td>
</tr>
</tbody>
</table>
Distinguishing the botanic origin

PCA + LDA + KNN
Sugar profile

<table>
<thead>
<tr>
<th>Sugar content (mg/g)</th>
<th>glucose</th>
<th>fructose</th>
<th>DS-Maltose</th>
<th>DS-TIKN</th>
<th>Total TS</th>
</tr>
</thead>
<tbody>
<tr>
<td>250</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>300</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>350</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>400</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>450</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Sugar content (mg/g)
## Results of PLS predictive models for sugars & potassium

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

A.G. Mignani et alii, IEEE-JLT, 2016
Raman fingerprints of blueberry juices
Brix and Carbohydrates

Parameter and model results

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Carbohydrates</th>
<th>BRIX degrees</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMSEC</td>
<td>0,80 g/hg</td>
<td>0,97%</td>
</tr>
<tr>
<td>RMSCV</td>
<td>0,97 g/hg</td>
<td>1,1%</td>
</tr>
<tr>
<td>(R^2) (cal)</td>
<td>0,887</td>
<td>0,9</td>
</tr>
<tr>
<td>(R^2) (val)</td>
<td>0,840</td>
<td>0,88</td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Calibration</th>
<th>Cross-validation (LOO)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMSE (ppb)</td>
<td>313</td>
<td>357</td>
</tr>
<tr>
<td>R squared</td>
<td>0.72</td>
<td>0.65</td>
</tr>
</tbody>
</table>
Mycotoxins in wheat flour
DON – Raman spectra and predictive model
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Home farming

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
The kitchen of the future

The fridge of the future – a family hub
The fridge of the future – a community hub

What’s next in food
?? Edible electronics ??
?? Edible photonics ??

https://www.youtube.com/watch?v=oaHLu77pQc