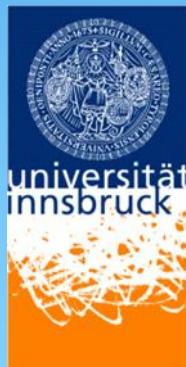


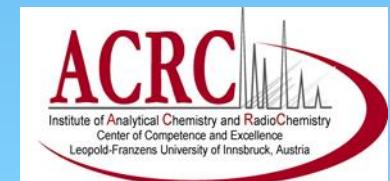
# Future Applications of Aquaphotomics in Natural Product Analysis

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Christian Huck

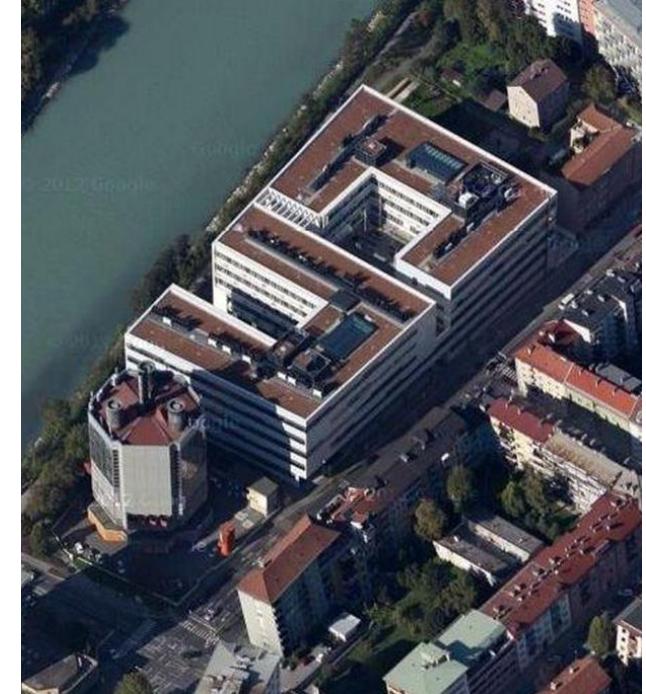
Institute of Analytical Chemistry and Radiochemistry  
CCB – Center for Chemistry and Biomedicine  
Leopold-Franzens University  
Innsbruck, Austria  
Mail: Christian.W.Huck@uibk.ac.at



# Innsbruck



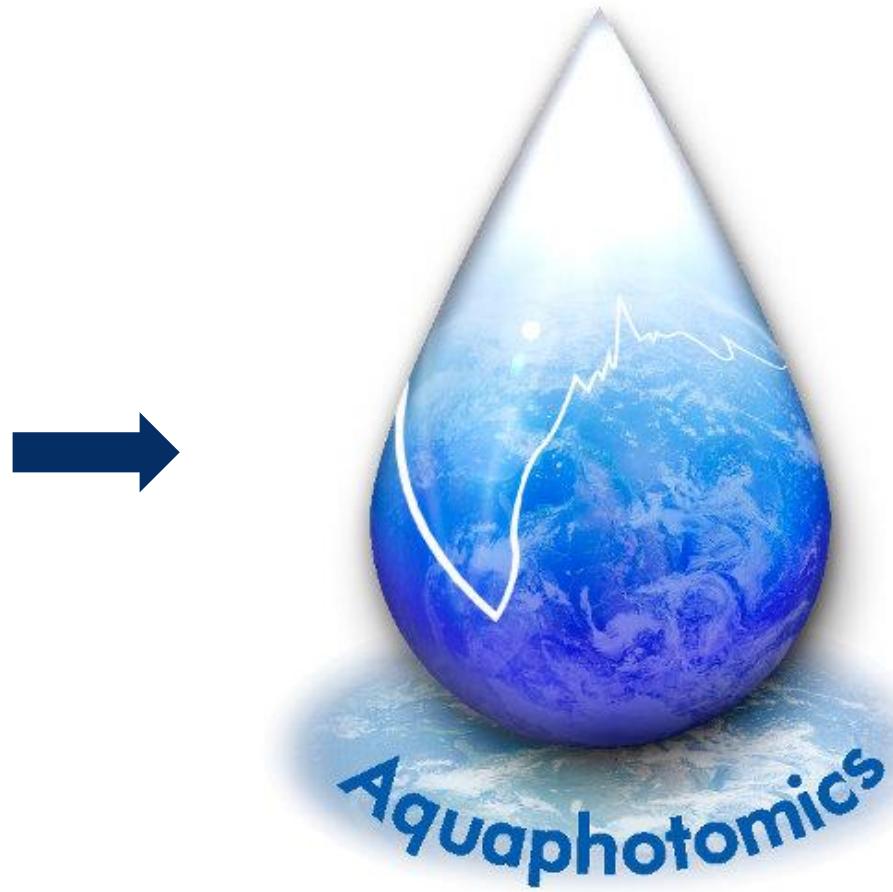
# CCB – Center for Chemistry and Biomedicine



# Tirol – Country in the Alps



# Tirol – Country of Waterfalls + Lakes



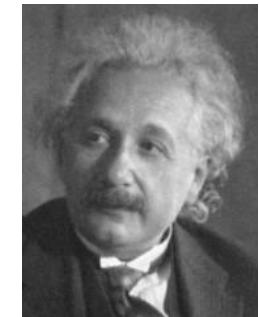
# Future...

# ... Applications

- \* I do not concern myself with what has been done.  
I'm interested in what needs to be done. *Marie Curie*



- \* More than in the past I am interested in the future,  
because in it I intend to live. *Albert Einstein*



# Future...

# ... Applications

- \* Food products



- \* Medicinal plants



- \* Medical applications



Future applications...

# Food Products

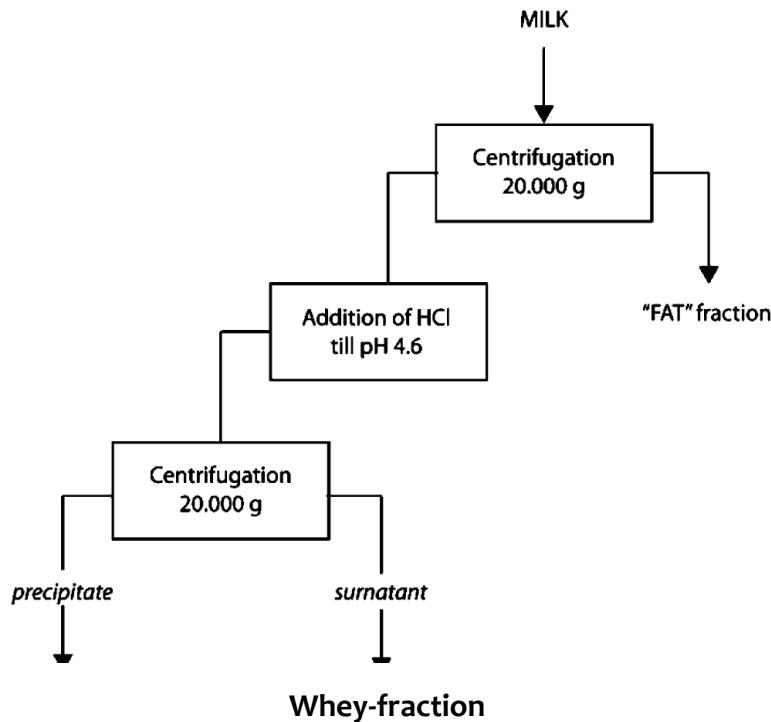
## Origin

- \* Farming gets more and more pressurized by its high production costs, opening of the markets and globalization.
- \* To compete against cheaper sustainably producing competitors, the added value of these products must be made credible for the consumer in order to achieve reasonable prices.

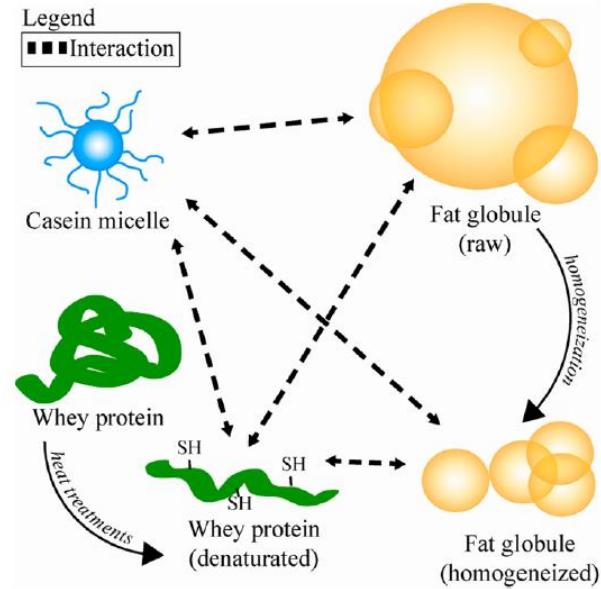
Future applications...

# Food Products: Milk

Steps for the fractionation



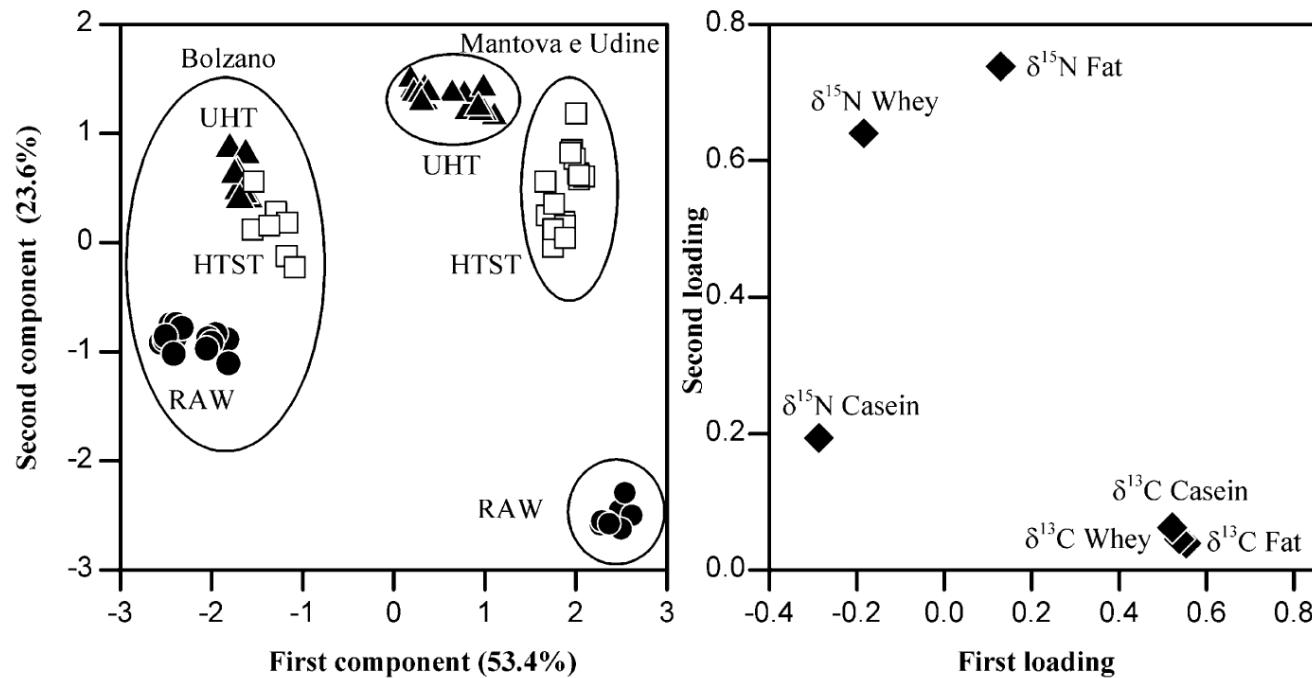
Scheme 2. Sketch of the Main Effects and Interactions between Whey, Casein, and Fat during Heat and Homogenization Processing<sup>a</sup>



Future applications...

# Food Products: Milk

isotope ratio of  $\delta^{13}\text{C}$  and  $\delta^{15}\text{N}$  for the milk samples and their fractions :  
fat, casein, and whey



Score (left) and loading (right) plots for the principal component analysis based on a data set containing 72 samples from different regions of Italy

Scampicchio M., Mimmo T., Capici C., Huck C., Innocente N., Drusch S., Cesò S. **Identification of Milk Origin and Process-Induced Changes in Milk by Stable Isotope Ratio Mass Spectrometry.**  
J. Agric. Food Chem. 60, 11268 – 11273 (2012)

Future applications...

# Food Products: Milk

## ORIGIN

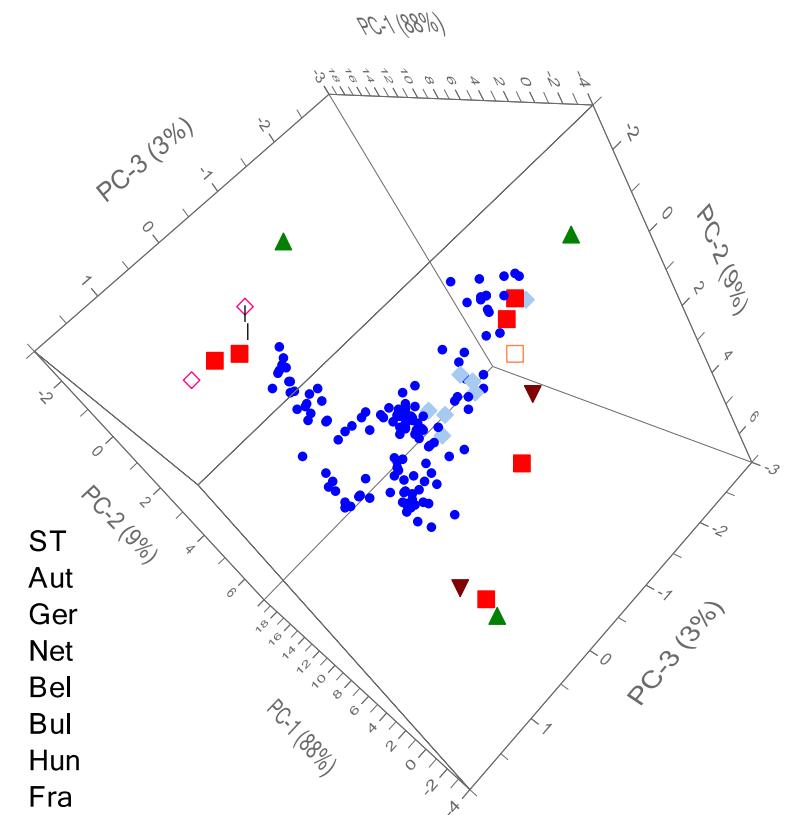
PCA Clustering – 3D Scores Plot

- mean spectra (three measurements per sample)
- n = 158 samples
- pre-treatment: SNV
- Wavelength region: 1000–2326 nm
- PCA-Clustering to separate according to the origin
- Samples from Belgium, Bulgaria, France, Germany and Hungary from those of South Tyrol
- Austrian milk samples largely separated from South Tyrolean samples

Huck-Pezzei V.A., Seitz I., Karer R., Schmutzler M., De Benedictis L., Wild B., Huck C.W.

**Alps Food Authentication, Typicality, and Intrinsic Quality by Near Infrared Spectroscopy.**

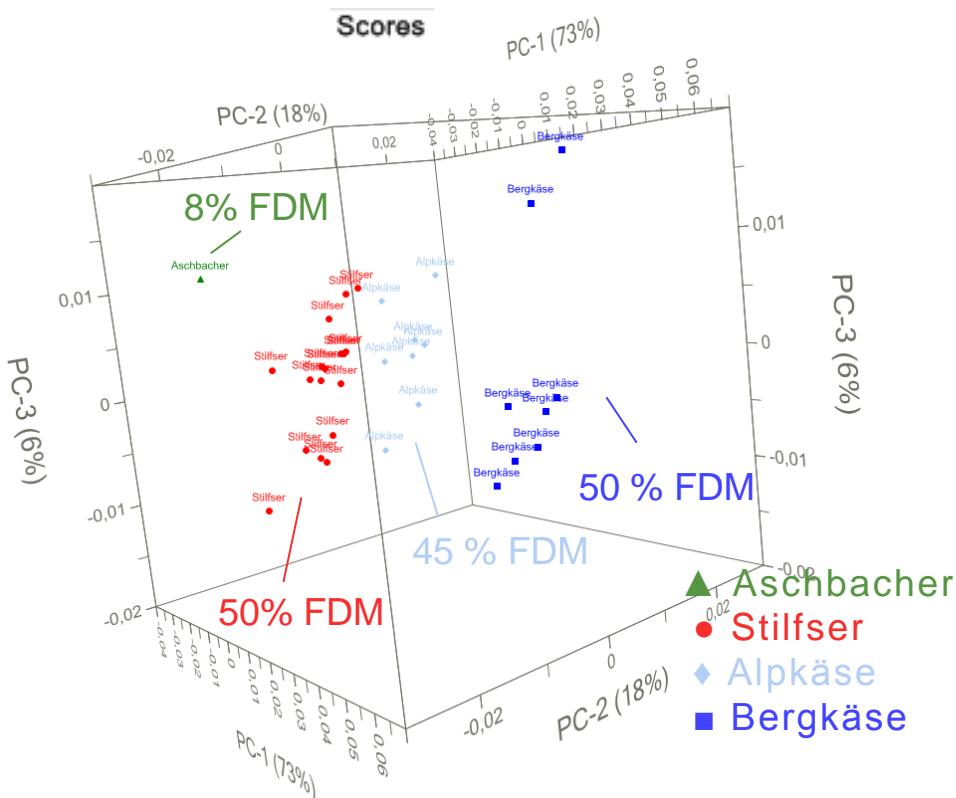
Food Res. Internat., 2014, 62, 984-990



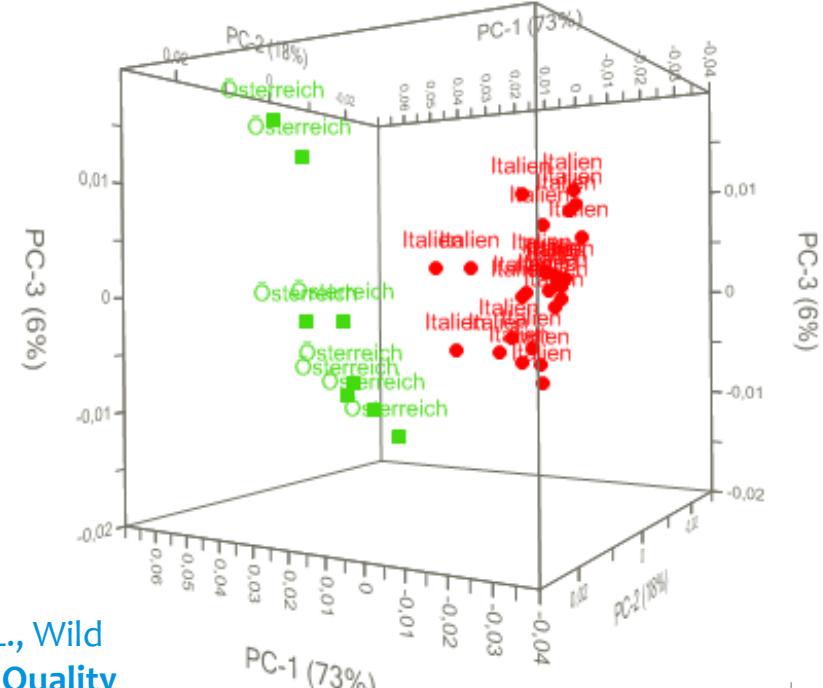
Future applications...

# Food Products: Cheese

Different species



Different origin  
Hard cheese

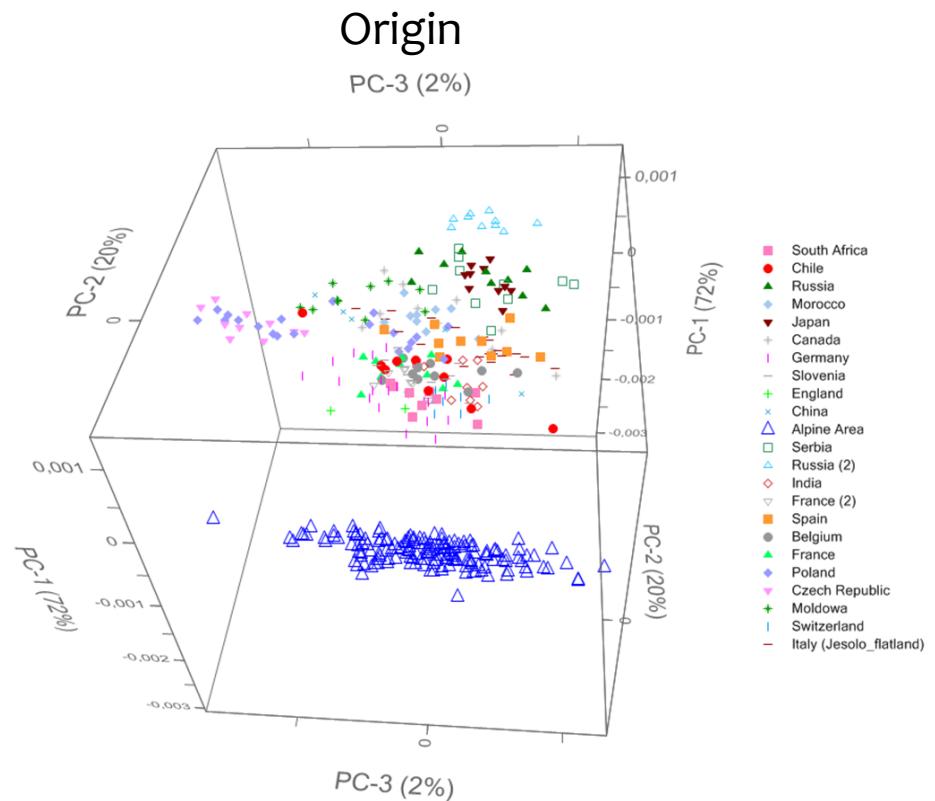
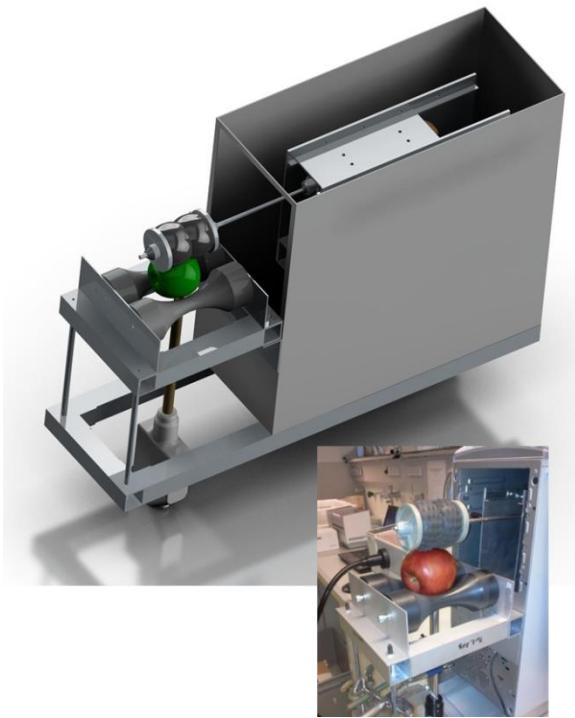


Huck-Pezzei V.A., Seitz I., Karer R., Schmutzler M., De Benedictis L., Wild B., Huck C.W. **Alps Food Authentication, Typicality, and Intrinsic Quality by Near Infrared Spectroscopy.** Food Res. Internat., 2014, 62, 984-990

Future applications...

# Food Products: Apple

Surface scanning

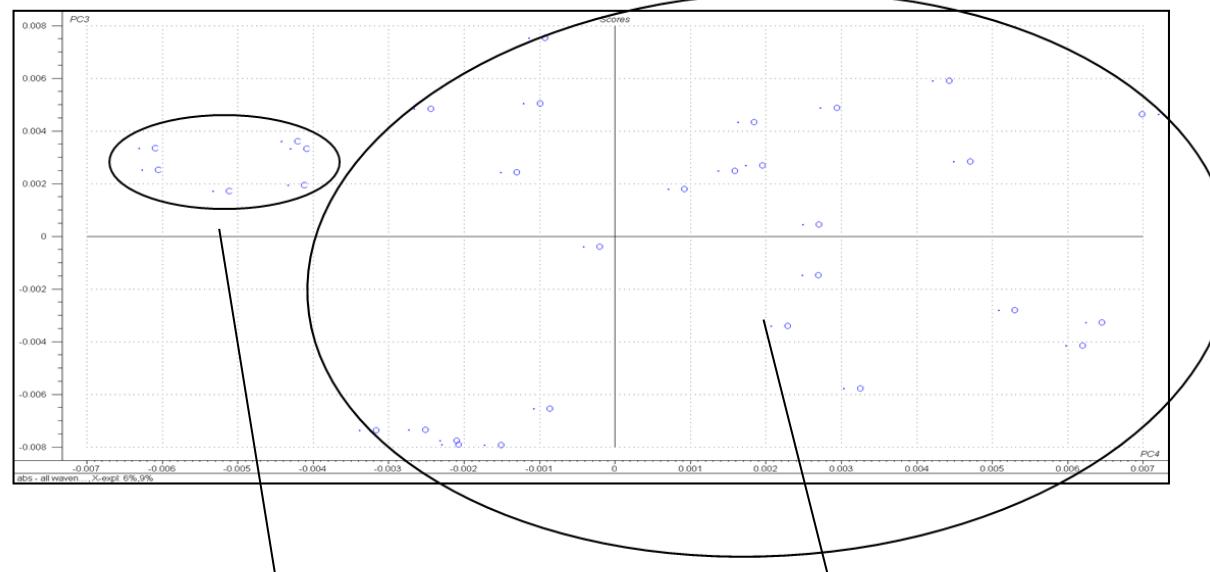
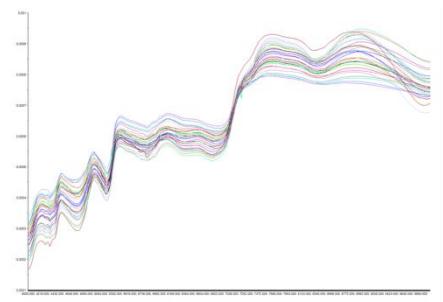


Schmutzler M., Huck C.W. Automatic Sample Rotation for Simultaneous Determination of Geographical Origin and Quality Characteristics of Apples based on Near Infrared Spectroscopy (NIRS).  
Vibr. Spectrosc., 72, 97-104 (2014)

Future applications...

# Medicinal Plants

St. John's wort is used against moderate depression



Hypericum perforatum

Hypericum hirsutum

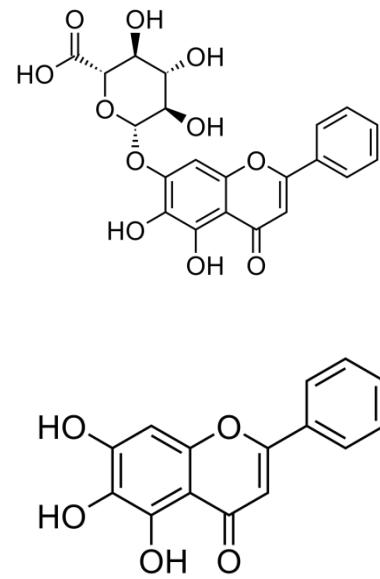
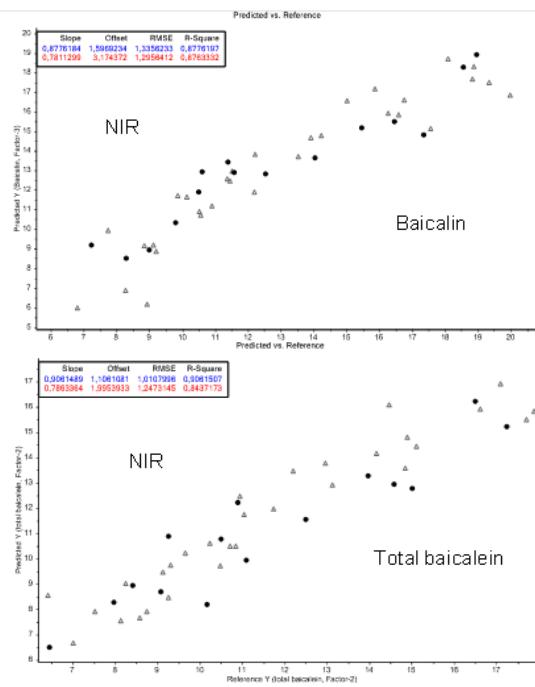
Huck-Pezzei V.A., Bittner L.K., Pallua J.D., Sonderegger H., Abel G., Popp M., Bonn G.K., Huck C.W. A Chromatographic and Spectroscopic Analytical Platform for the Characterization of St. John's wort Extract Adulterations. *Anal. Methods* 5, 616 – 628 (2013)

# Future applications...

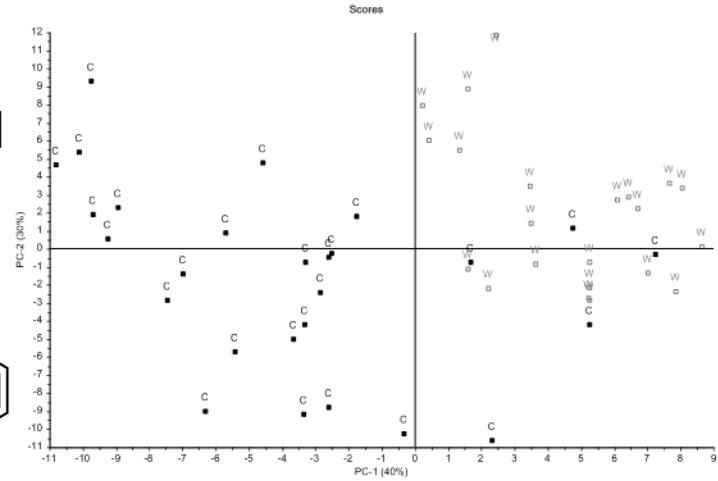
# Medicinal Plants

## Radix scutellariae against inflammation

### Quality control



### Wild vs. Cultivated species



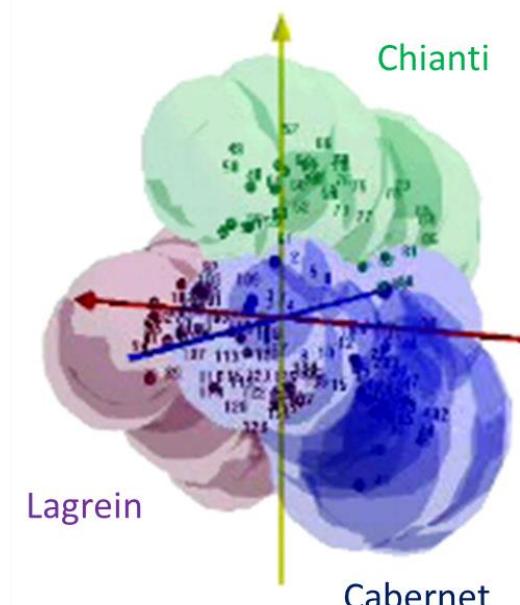
Principal components score image of the wild and cultivated *radix scutellariae* samples.

Navarro Escamilla M., Rodenas Sanz F, Li H., Schönbichler S.A., Yang B., Bonn G.K., Huck C.W.

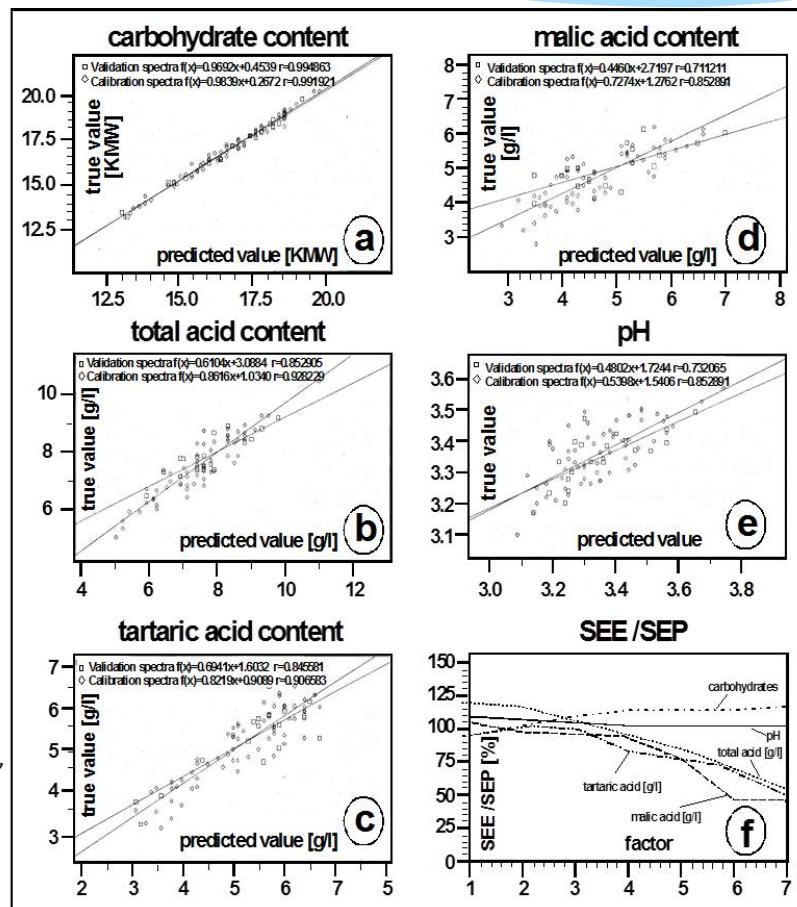
Rapid determination of baicalin and total baicalein content in *Scutellariae radix* by ATR-IR and NIR spectroscopy

Talanta 114, 304 – 310 (2013)

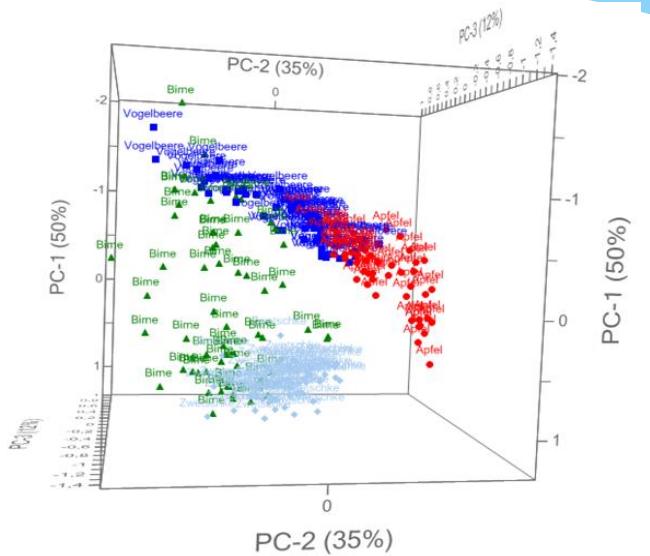
# Wine Analysis



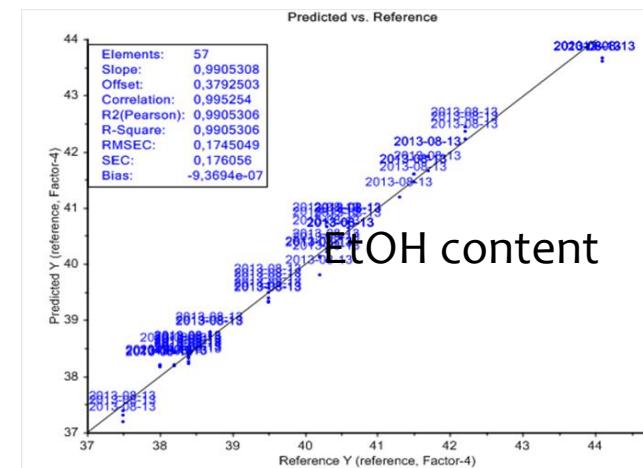
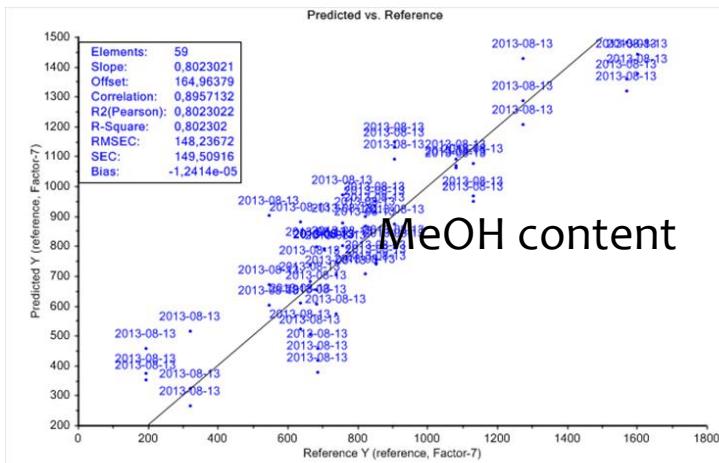
Factor plot of 141 spectra of different wines (Lagrein, Chianti, Cabernet Sauvignon). Conditions: Normalisation, 1st derivative; wavenumber range, 4500 - 10000 cm<sup>-1</sup>; thickness, 3 mm; scans, 10; temperature, 23° C.



# Schnaps Analysis

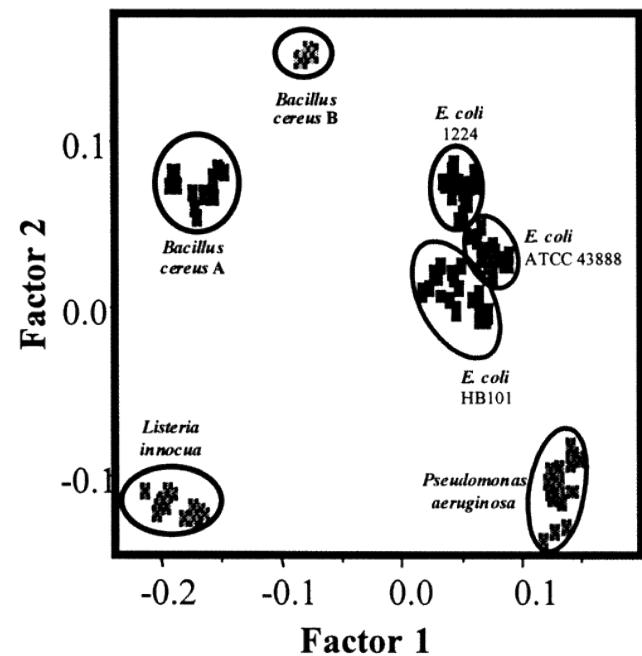
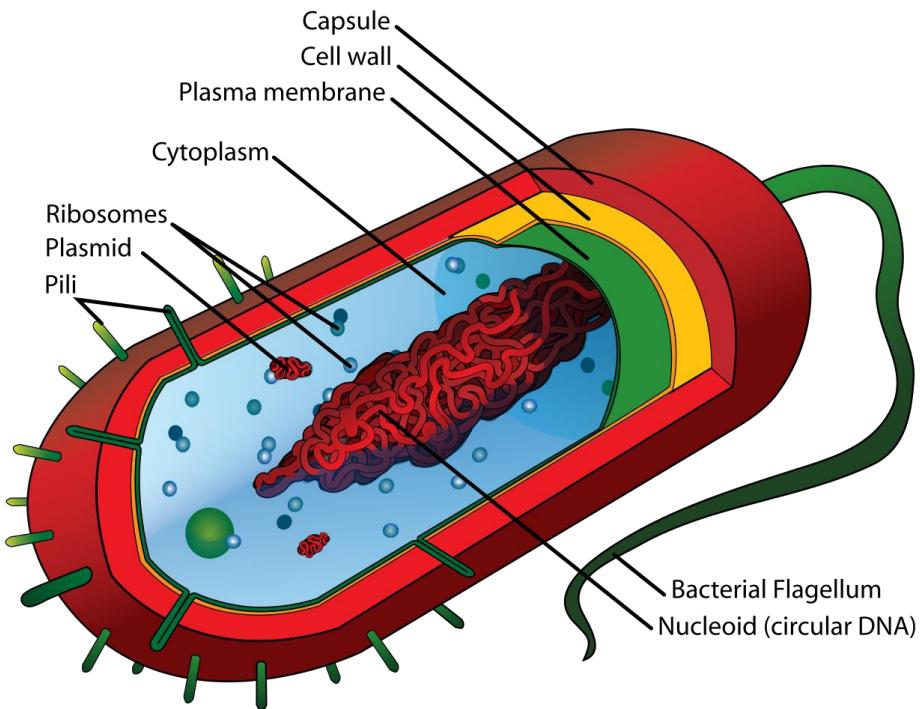


Apple  
Pear  
Plum  
Rowan berry



Future applications...

# Medicinal Plants



[J Agric Food Chem. 2001 Feb;49\(2\):574-9.](#)

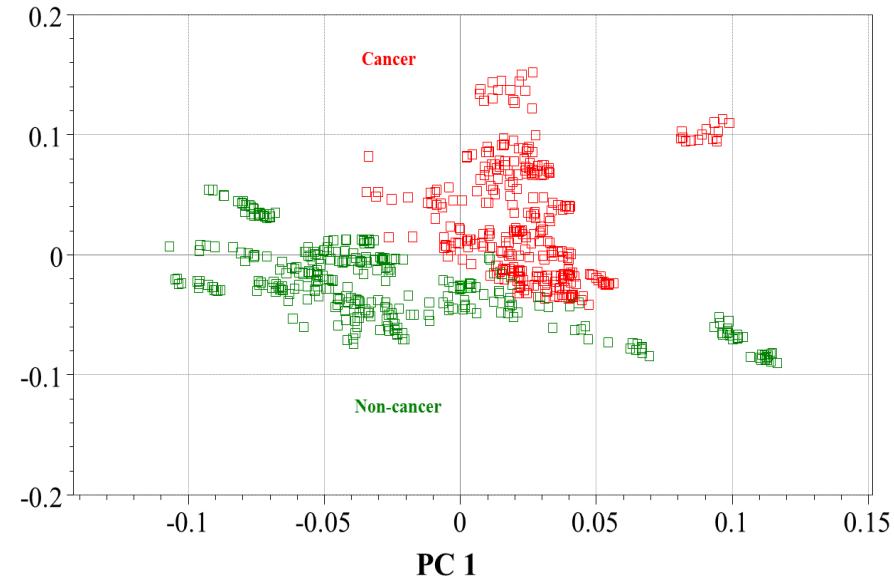
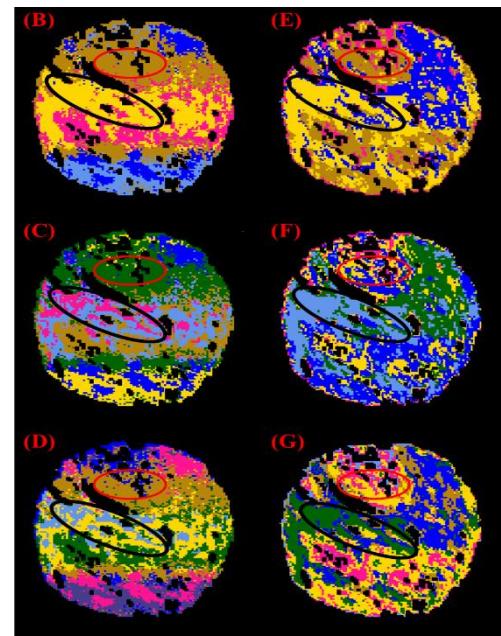
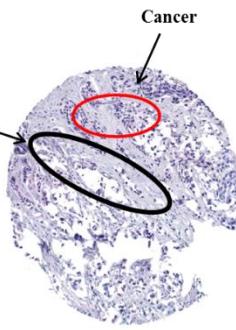
Rapid detection and identification of bacterial strains by Fourier transform near-infrared spectroscopy.

Rodriguez-Saona LE<sup>1</sup>, Khambaty FM, Fry FS, Calvey EM.

Future applications...

# Medical Applications

(A)



(A) HE stained section with marked regions of cancer and non-cancer areas from a FFPE tissue. (B) – (D) HCA images with 5, 6 and 7 clusters. (E) – (G) KMC images with 5, 6 and 7 clusters.

Pezzei C., Brunner A., Bonn G.K., Huck C.W.

**Fourier Transform Infrared Imaging Analysis in Discrimination Studies of Bladder Cancer**

Analyst 138, 5719-5725 (2013)

# Acknowledgments

- European Efre Project "Originalp"
- Agrarmarketing Tirol and Austria
- Ministry for Science, Research and Economy





# Questions?

I will be happy to answer !