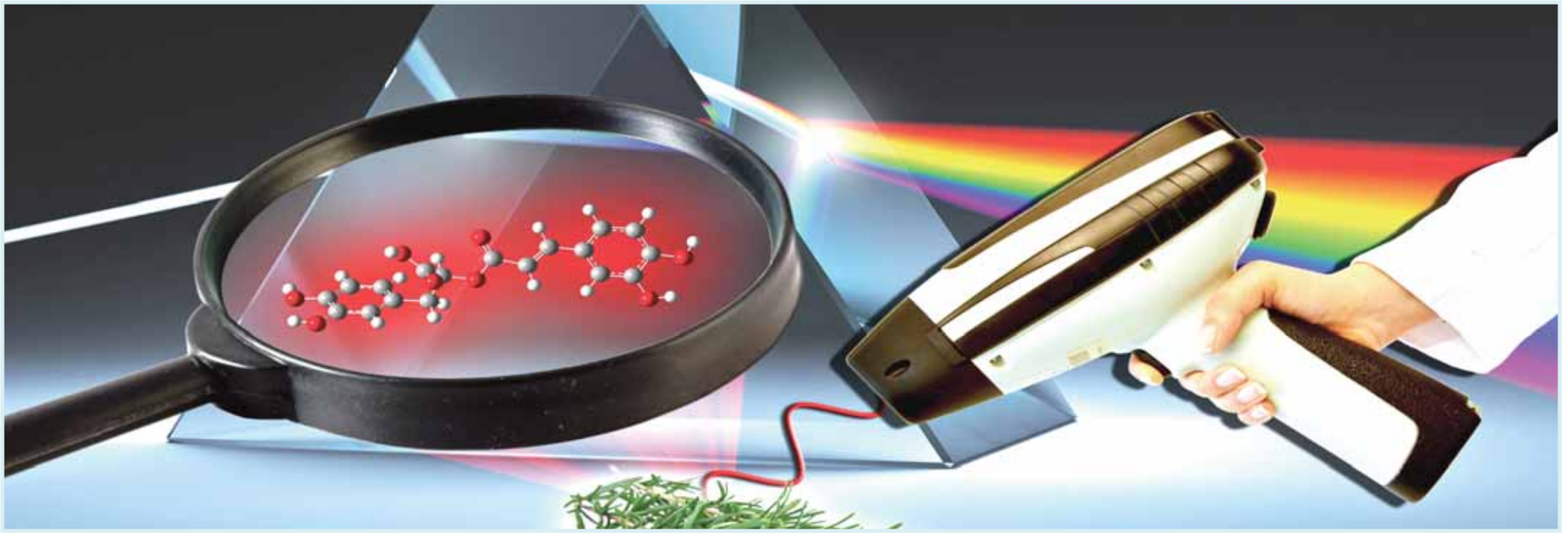
Montpellier, November 8th 2018

# Current Trends in NIR Spectroscopy Including 2D-COS and Quantum Chemistry

**Christian Huck**
**Institute of Analytical Chemistry and Radiochemistry**
**Leopold-Franzens University Innsbruck Austria**

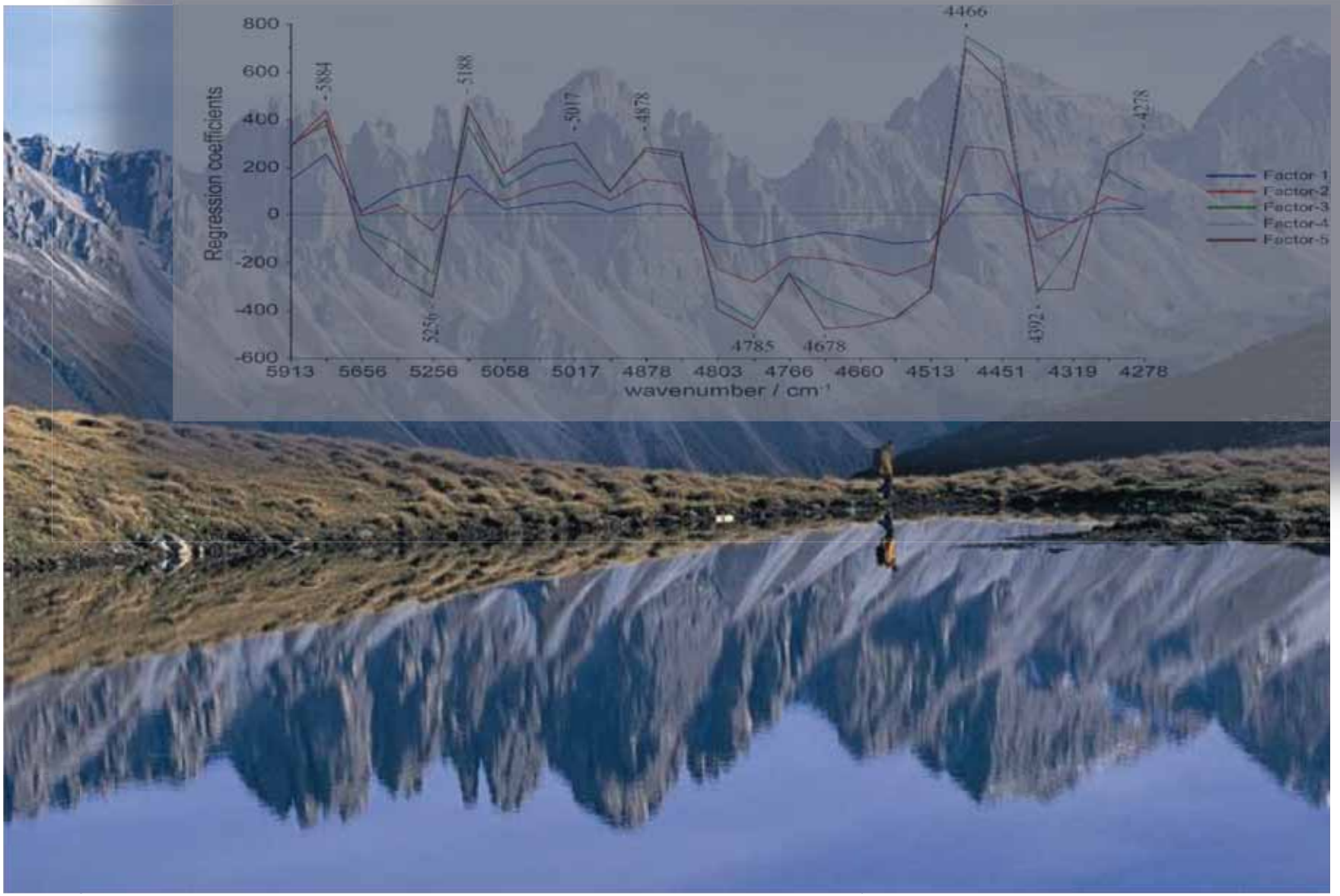



www.weltkarte.com

# Innsbruck – Heart of the Alps

# Innsbruck – Capital of the Alps

# The Alps


Regression coefficients
800
600
400
200
0
-200
-400
-600
5884
5188
5017
4878
4466
4278
5256
4785
4678
4392
5913
5656
5256
5058
5017
4878
4803
4766
4660
4513
4451
4319
4278
wavenumber / cm⁻¹
Factor-1
Factor-2
Factor-3
Factor-4
Factor-5

# Center for Chemistry and Biomedicine

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Institute of Analytical Chemistry and RadioChemistry
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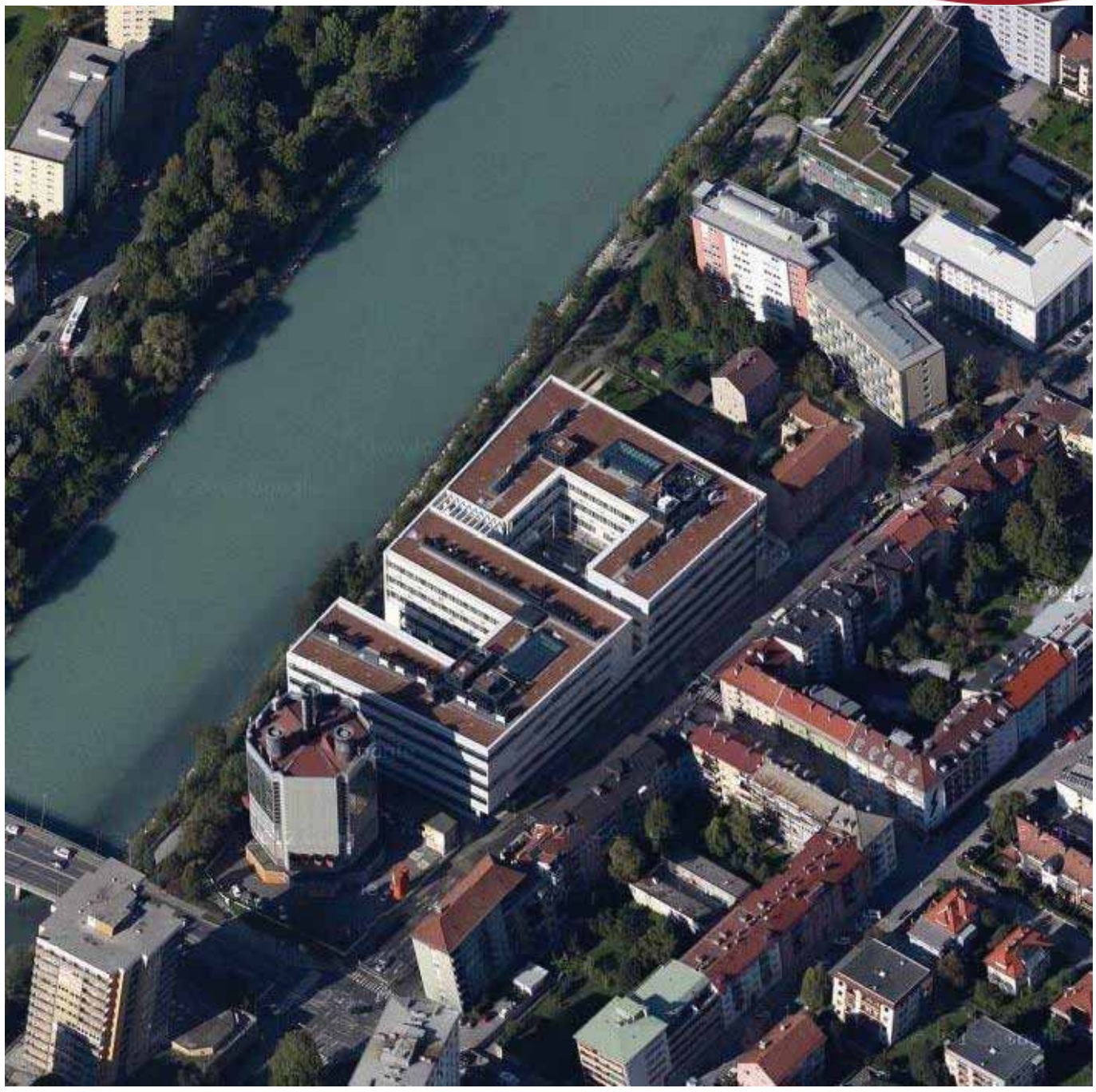

# Center for Chemistry and Biomedicine



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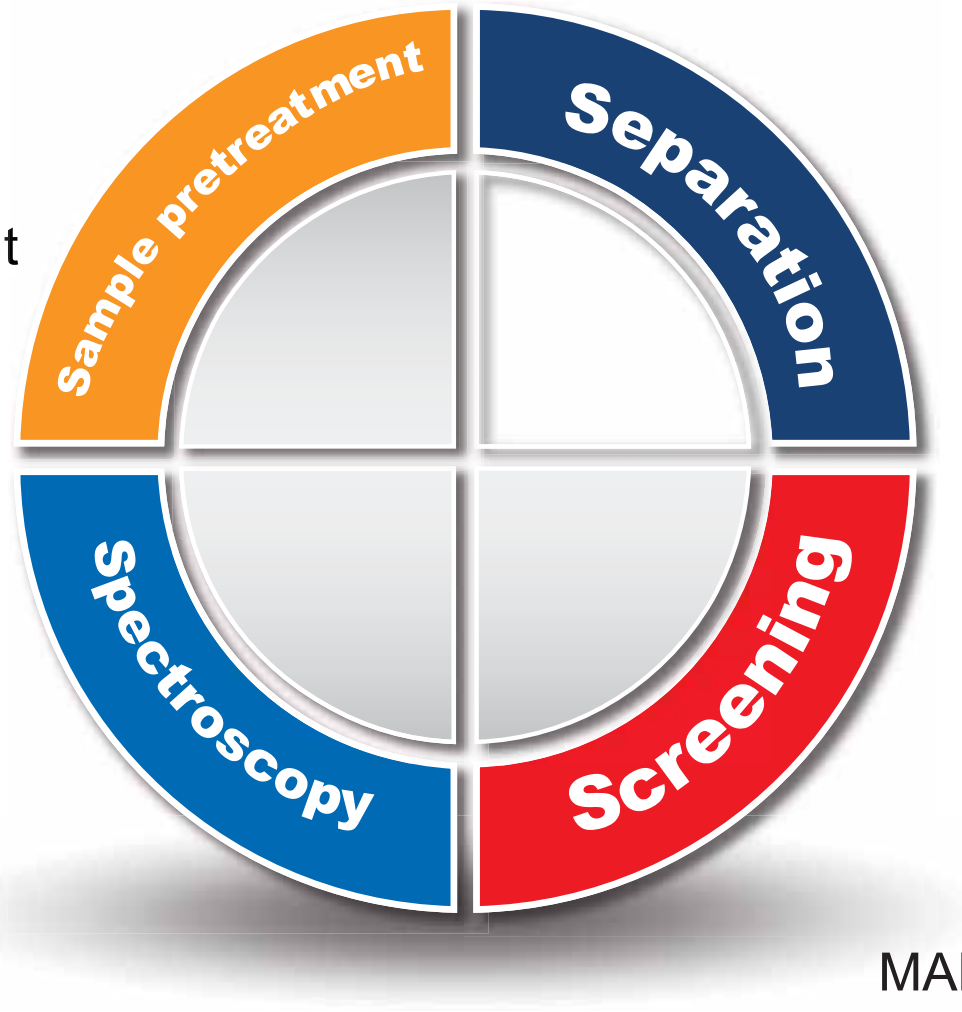
# Analytical Approaches

Innovations

Enrichment

Desalting

High-sample througput




LC, LC-MS/MS

µ-LC, µ-LC-MS/MS

CE, CE-MS

CEC

Near-infrared

Mid-Infrared

Imaging/mapping

MALDI-TOF-MS/MS

Matrixfree-MALDI

MELDI-TOF

MALDI-imaging/mapping

# Performance and Limitation of NIRS


## MILK SCANDAL IN 2008


**Melamine**

China reported an estimated 300,000 victims in total. Six infants died from kidney stones and other kidney damage with an estimated 54,000 babies being hospitalized

*Branigan, Tania (2 December 2008). "Chinese figures show fivefold rise in babies sick from contaminated milk". The Guardian. London.*

# MOTIVATION

## HORSE MEAT SCANDAL IN 2013


Of 27 beef burger products tested, 37% were positive for horse DNA, and 85% were positive for pig DNA.

*"FSAI Survey Finds Horse DNA in Some Beef Burger Products". Food Safety Authority of Ireland. 15 January 2013. Retrieved 16 January 2013.*

Charlebois S., Schwab A., Henn R., Huck C.W. An exploratory study for measuring consumer perception towards mislabeled food products and influence on self-authentication intentions. Trends Food Sci. & Technol., 50, 211-218 (2016)

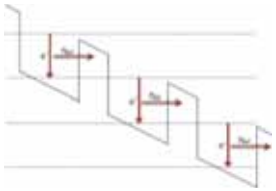
# Examples of recent severe food safety incidents

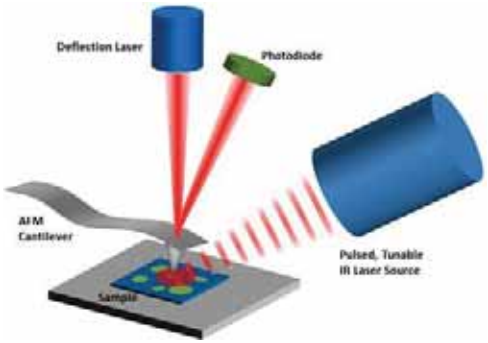
| Year | Incident | Region | Fatal casualties [persons] | Other health injuries [persons] | Estimated economy hit [EUR] |
|---|---|---|---|---|---|
| 2017 | Fipronil eggs contamination | EU | N/A | N/A | not yet estimated |
| 2016 | Plastic contamination of Mars chocolate | Worldwide (55 countries) | N/A | N/A | >10 M |
| 2016 | Punjab sweet poisoning | Pakistan | 33 | 52 | N/A |
| 2015 | *Escherichia coli* outbreak | US | N/A | 22 | >80 M |
| 2013 | Horse meat scandal | EU | N/A | N/A | N/A |
| 2008 | Milk adulteration with melamine | China | 6 | 300 000 | N/A |
| 2007 | Salmonella contamination of Cadbury sweet | UK | N/A | 42 | N/A |

# Analytical Chemistry

## Higher Performance

- Resolution
- Sensitivity
- Selectivity



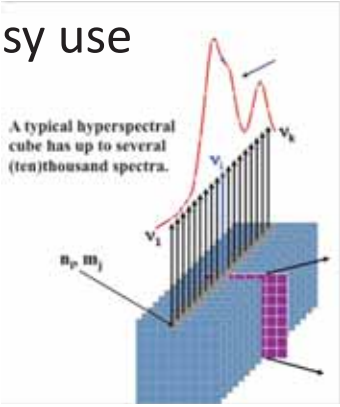



## Miniaturisation

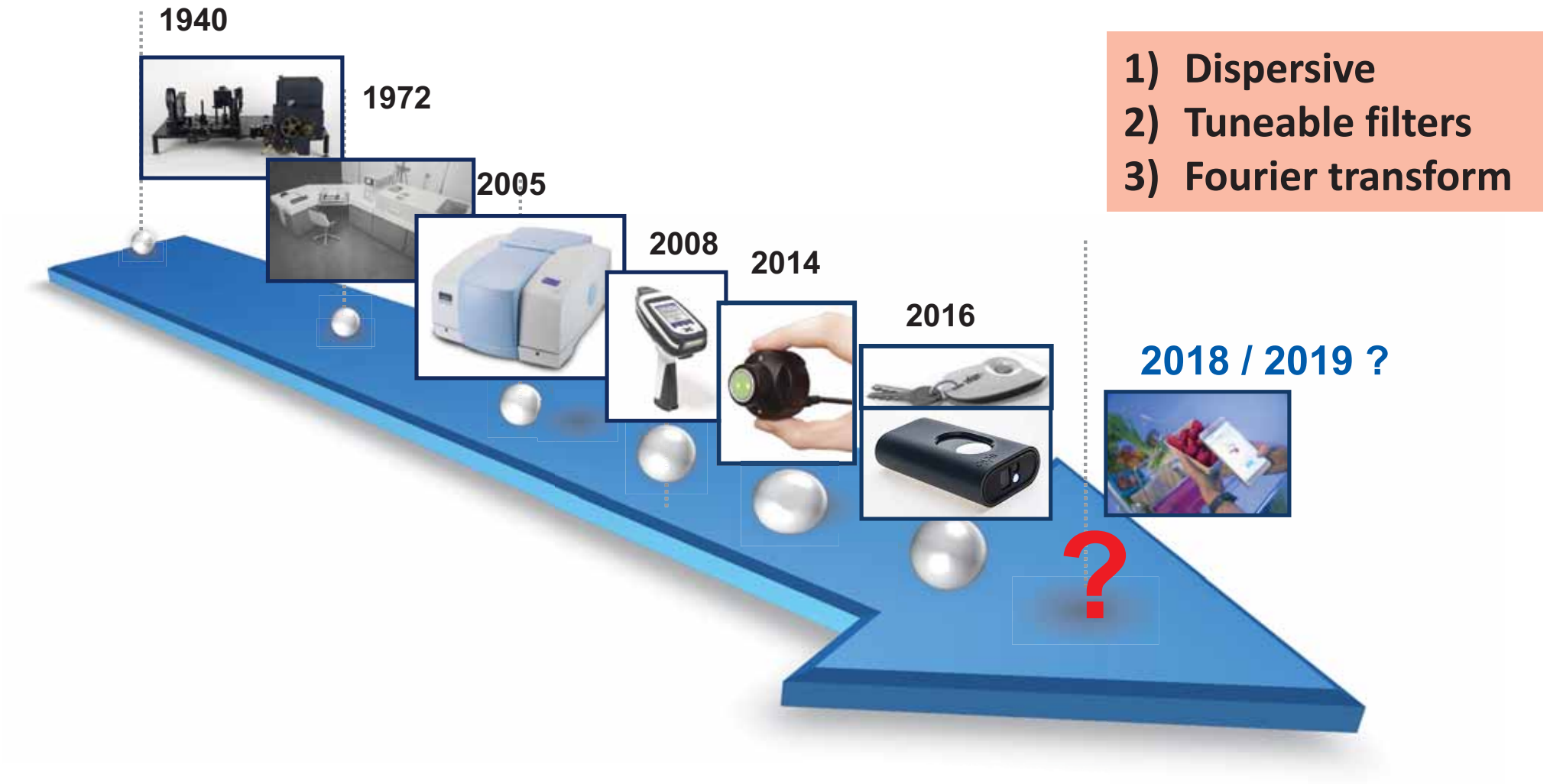
- Small, portable
- Cheap
- Easy use

## Imaging

- Fast
- Cheap
- Easy use



# TREND IN ANALYTICAL CHEMISTRY

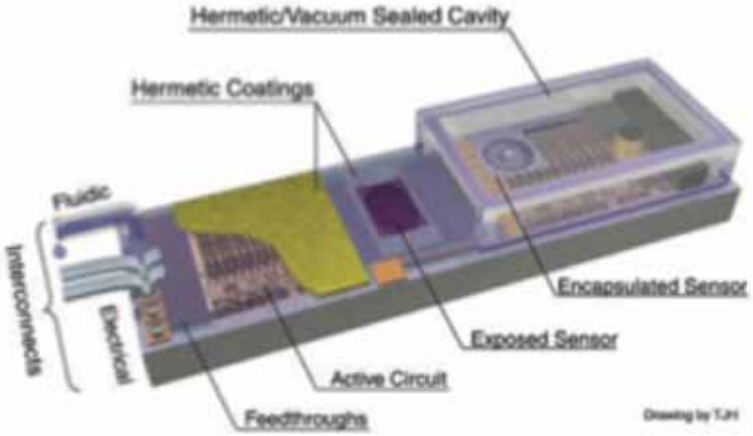


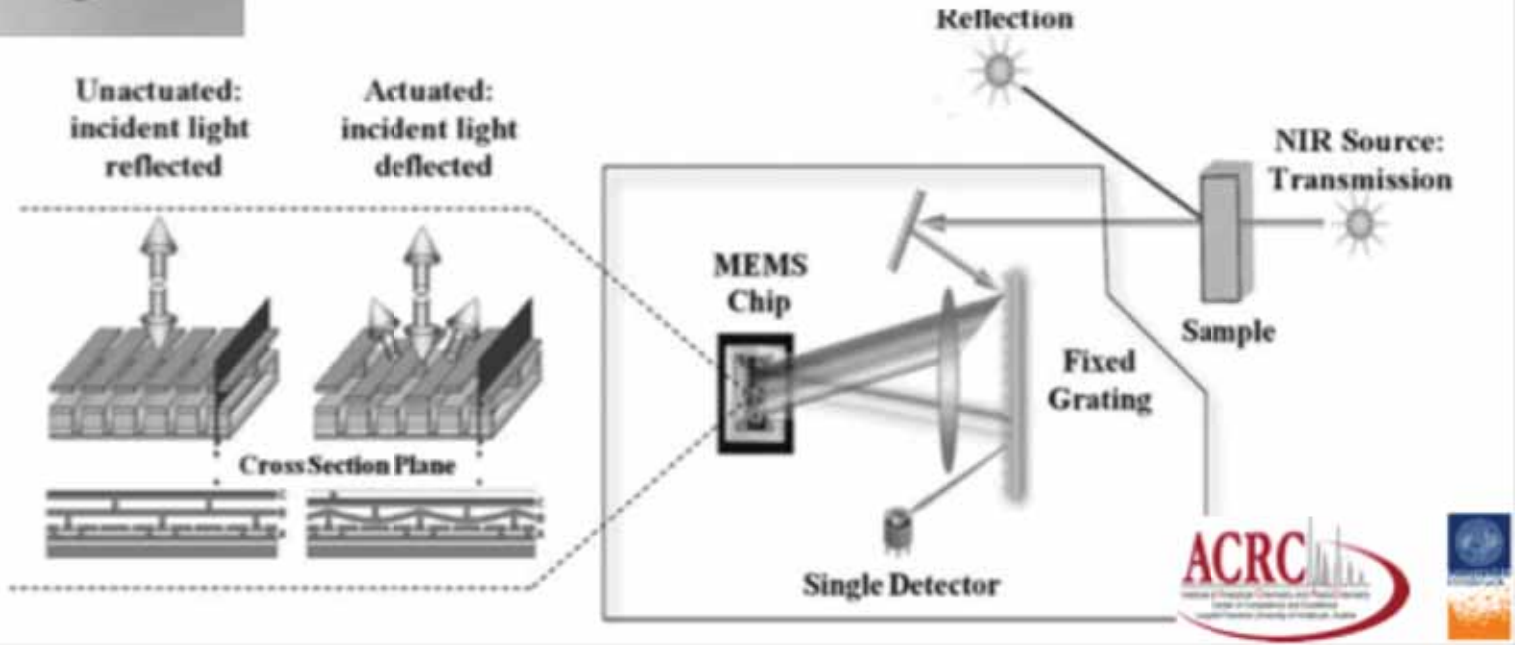

1) Dispersive
2) Tuneable filters
3) Fourier transform

Huck, C.W. Hocheffiziente neue Schwingungsspektroskopische Methoden. GIT-Laborfachzeitschrift, 5, 2-5 (2016 )

# Miniaturisation

**MEMS** is an acronym for **micro-electro-mechanical Systems**



# Miniaturisation

*…developed by JDS Uniphase Corporation*

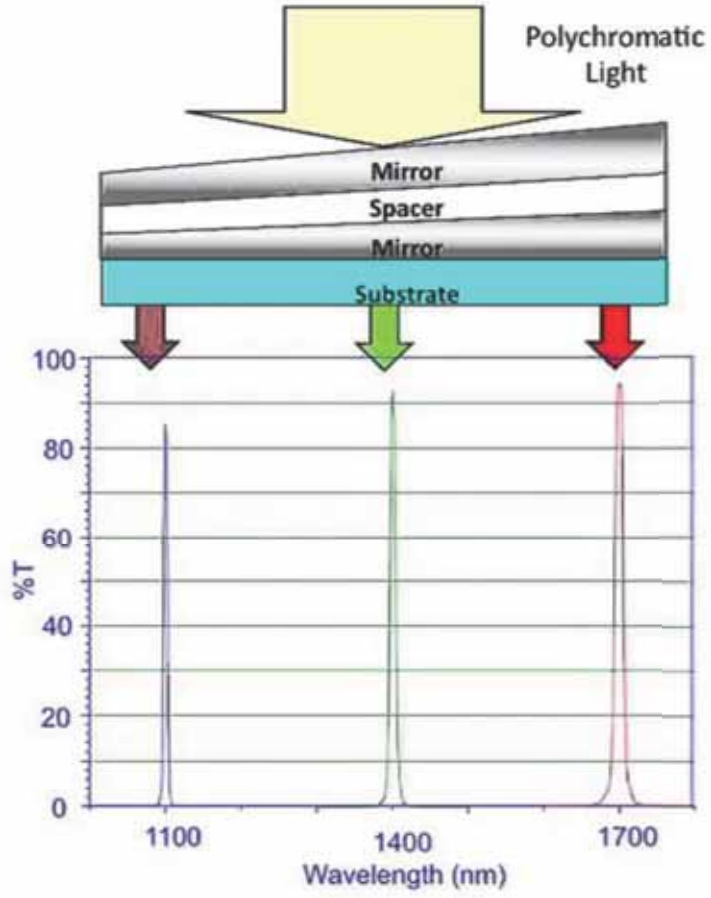
- one of worlds smallest NIR spectrometer
- extremely fast analyses
- highly cost-effective
- USB powered

# Miniaturisation

*…developed by JDS Uniphase Corporation*

## Linear Variable Filter (LVF) Technology

- LVF is a one dimensional array of continuously varying bandpass filter
  - No moving parts
  - Completely passive device
- Coating materials are deposited with wedge in one axis.



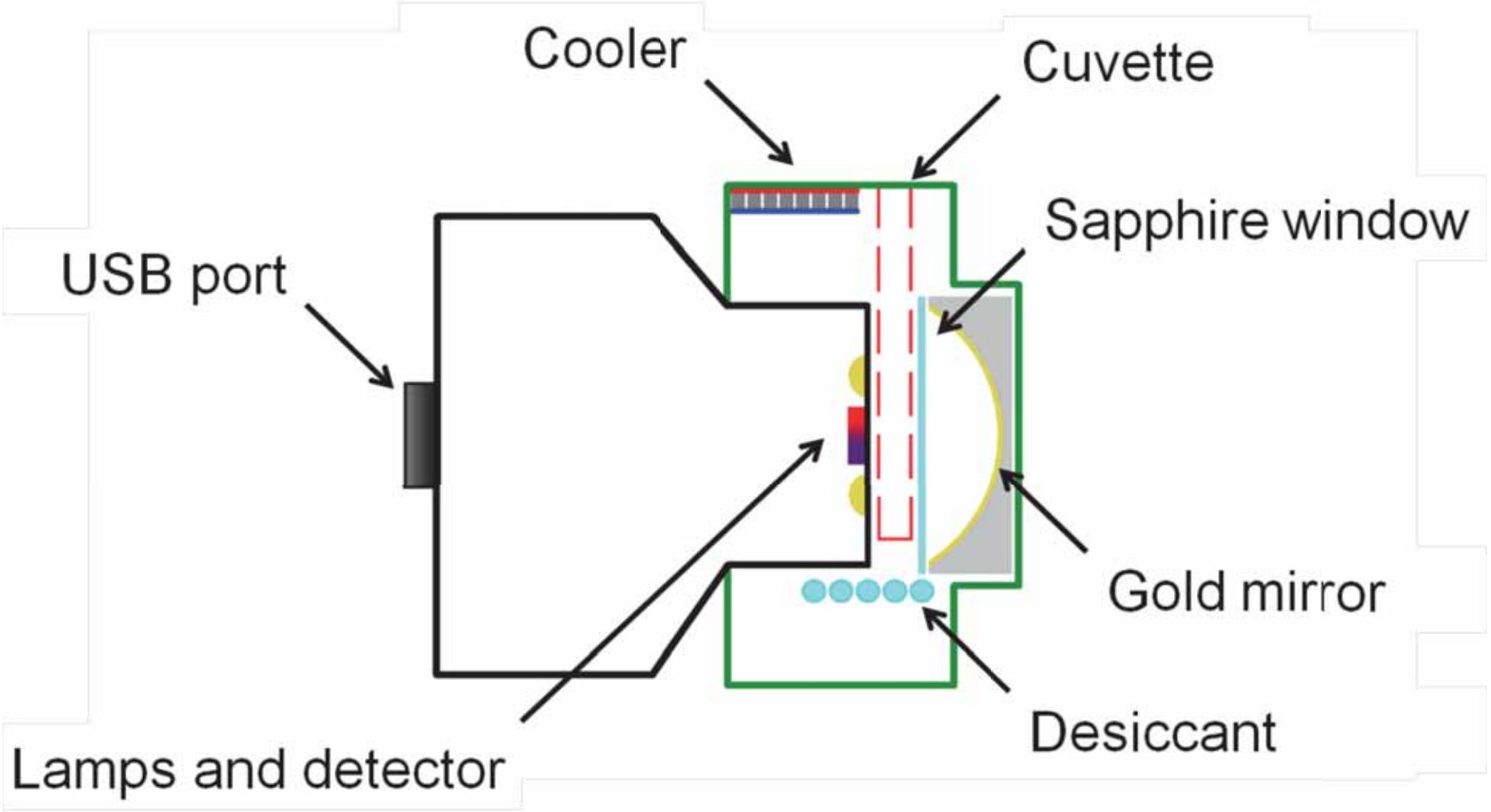
# Miniaturisation

*…a basic overview:*

- milled from solid aluminium
- 1 mm cuvette holder
- spherical gold reflector
- thermoelectric cooler

Lutz O.M.D., Bonn G.K., Rode B.M. & Huck C.W. **Analytica Chimica Acta** *2014 826 61*

# Miniaturisation




Lutz O.M.D., Bonn G.K., Rode B.M. & Huck C.W. **Analytica Chimica Acta** *2014 826 61*

# Miniaturisation

*EU directive 2009/28/EG:*

"Enforced use of ecologically derived fuel in the transport sector"

- gasoline containing ≤ 5% wt. EtOH
- gasoline containing ≤ 10% wt. EtOH

*A mobile quantification platform is desirable!*

Image: Swaroopvarma *via* Wikipedia, *2006*, Public Domain

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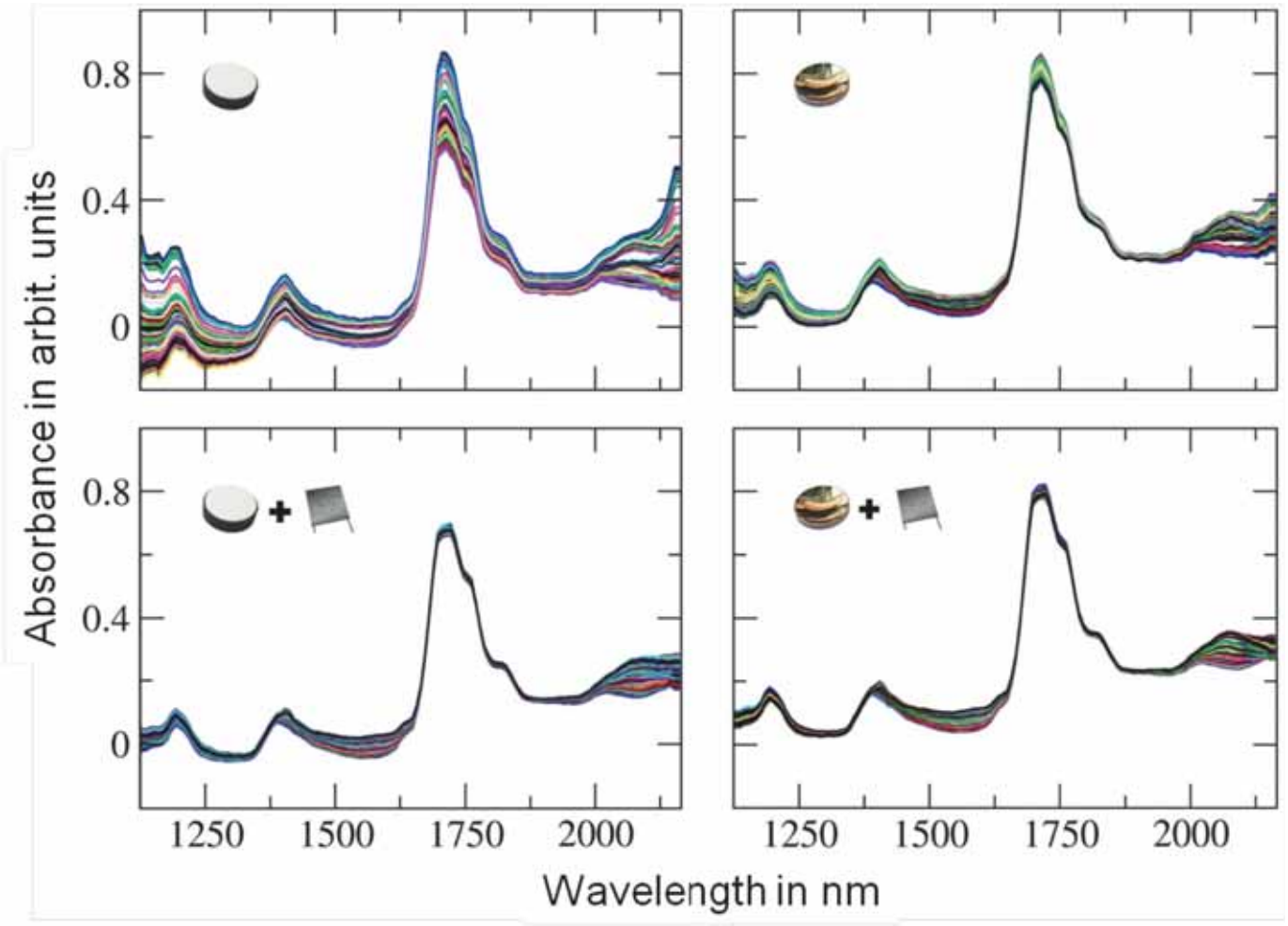
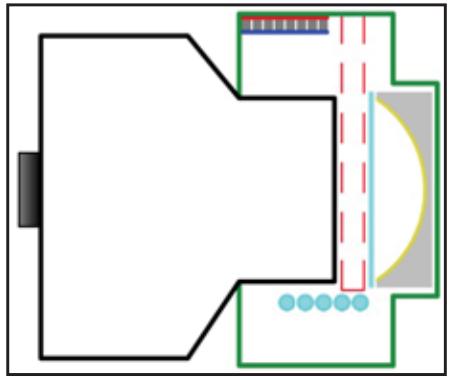
# Miniaturisation

*NIR spectra of gasoline with up to 10% w/w ethanol*



Lutz O.M.D., Bonn G.K., Rode B.M. & Huck C.W.
**Analytica Chimica Acta** *2014 826 61*

# Miniaturisation

*The PLS regression models of ethanol admixed gasoline*

| | $R^2_{val}$ | SEP (%) | LOD (%) | LOQ (%) |
|---|---|---|---|---|
|  | 0.483 | 2.45 | 8.68 | 26.04 |
|  | 0.993 | 0.35 | 0.93 | 2.79 |
|  | 0.991 | 0.33 | 1.37 | 4.11 |
|  | 0.997 | 0.21 | 0.68 | 2.04 |

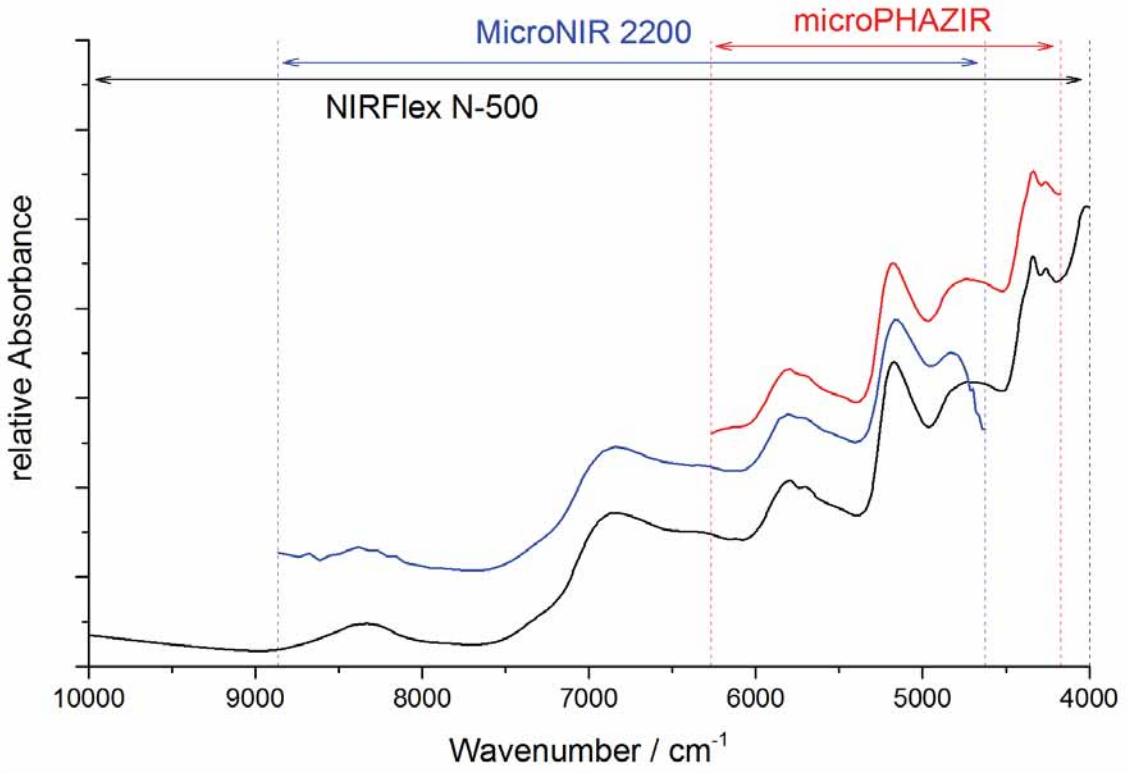
# benchtop vs. miniaturization

| device | wavenumber range / $cm^{-1}$ | resolution / $cm^{-1}$ |
|---|---|---|
| NIRFlex N-500 | 10000 - 4000 | 8 |
| microPHAZIR | 6266 - 4173 | Ø 21 |
| MicroNIR 2200 | 8865 - 4626 | Ø 33 |

NIRFlex N-500

microPHAZIR

MicroNIR 2200



**Therefore,**
**new approaches for**
**more critical evaluation is needed!**

# WORKFLOW

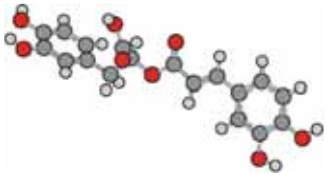
benchtop

miniaturization

NIR-spectroscopy

reference measurements

$H\Psi = E\Psi$
quantum chemical calculation



multivariate data analysis

$\mathbf{X} = \mathbf{T}\,\mathbf{P}^{T} + \mathbf{E}$

2D-COS

mLOD

critical evaluation

# APPLICATION FIELDS

## Miniaturized NIR Spectroscopy

### Medicinal Plants

- Harvest time
- Fast Quality Control
- Provenience

### Food

- Safety, fraud
- Fast Quality Control
- Provenience

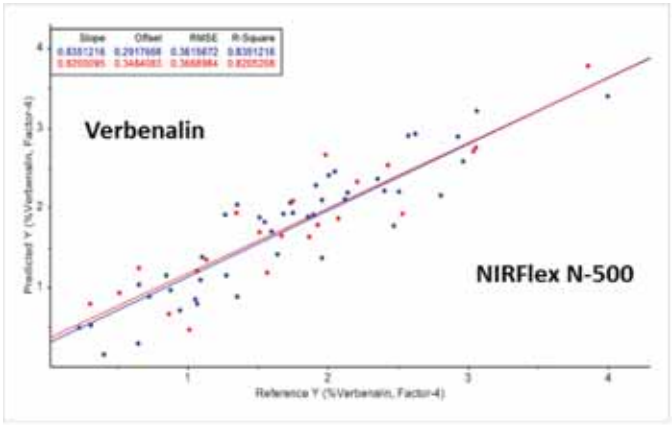
### Material analysis

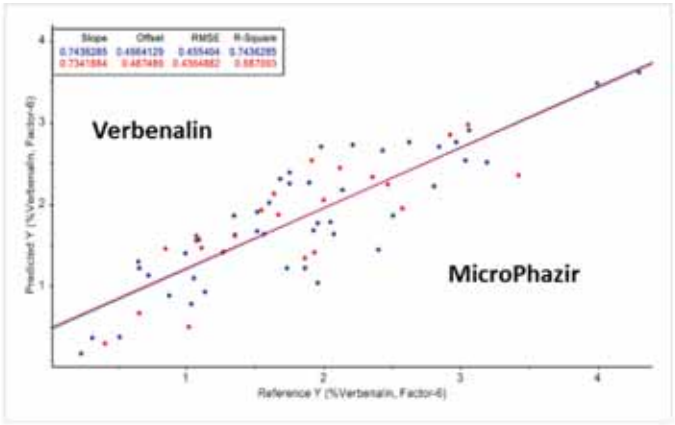
### Bioanalysis

- Cancer Research

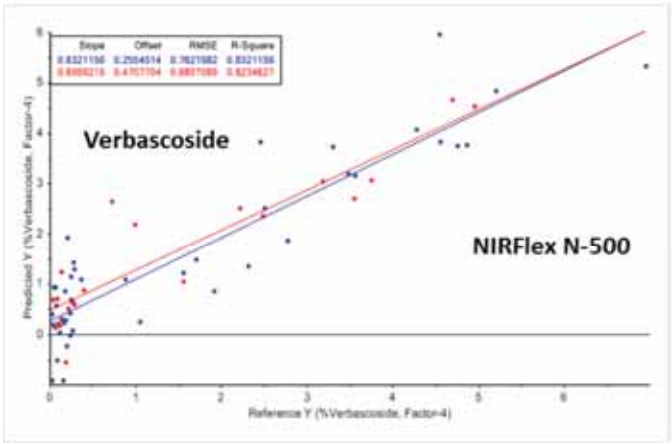

Huck C.W. Advances of Vibrational Spectroscopic Technologies in Life Sciences. Molecules, 22, 278 (2017)
Türker-Kaya S., Huck C.W. A review of mid-infrared and near-infrared imaging: principles, concepts and applications in plant tissue analysis. Molecules, 22, 168 (2017)
Huck C.W. Selected latest applications of molecular spectroscopy in natural product analysis. Phytochem. Lett., http://dx.doi.org/10.1016/j.phytol.2016.12.028 (2016)

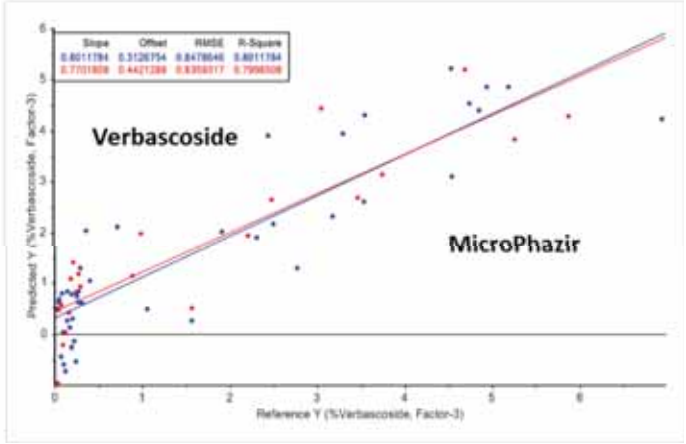
# In-field Determination of Optimum Harvest Time of MEDICINAL PLANTS: Verbena officinalis

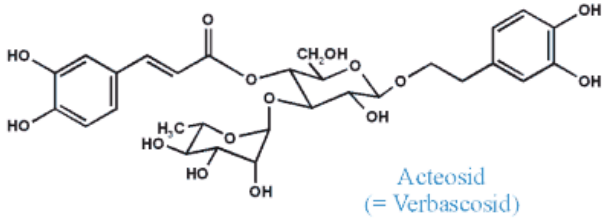




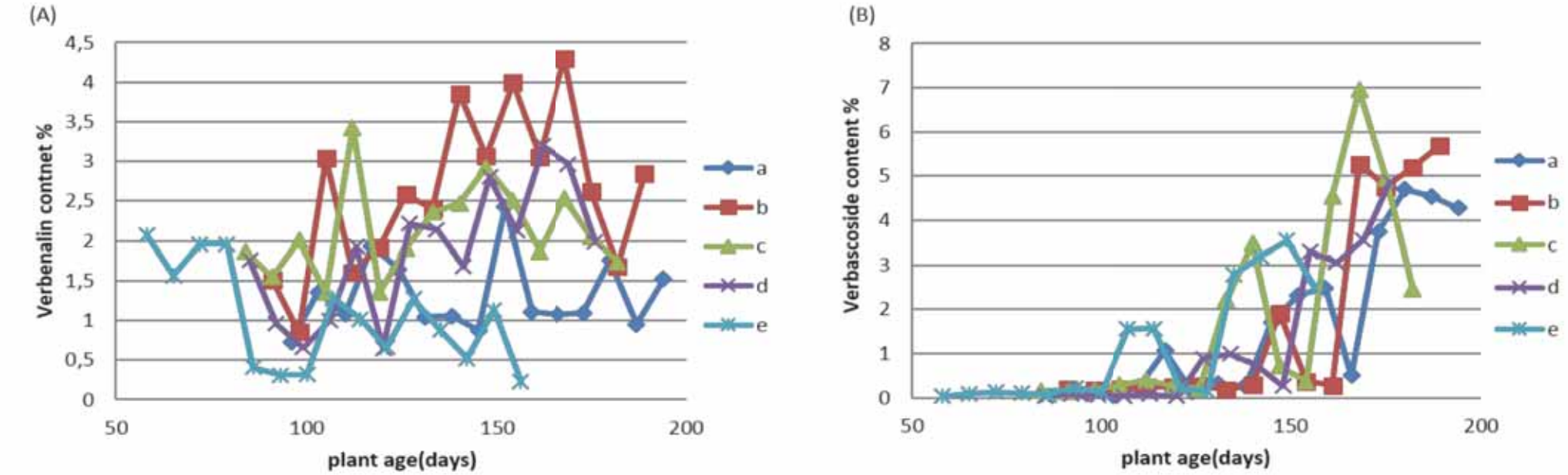


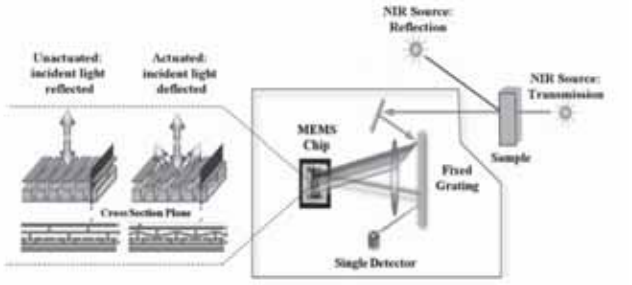



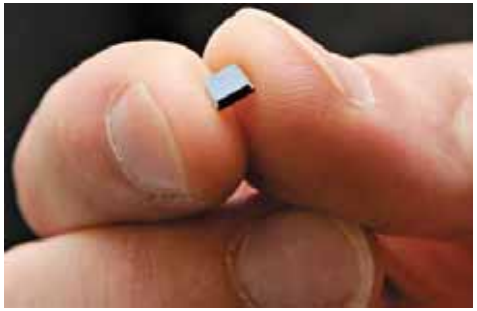

Schönbichler S.A., Bittner L.K.H., Pallua J.D., Popp M., Abel G., Bonn G.K., Huck C.W.
Simultaneous Quantification of Verbenalin and Verbascoside in Verbena officinalis by ATR-IR and NIR Spectroscopy
J. Pharm. Biomed. Anal. 84, 97 - 102 (2013)

# In-field Determination of Optimum Harvest Time of MEDICINAL PLANTS: Verbena officinalis




Graphical representation of the verbenalin (a) and verbascoside (b) content related to the dried plant material during flowering. Letter a-e stand for the five different seeding dates in March and April.



Pezzei C.K.; Schönbichler S.A.; Kirchler C.G.; Schmelzer J.; Hussain S.; Huck-Pezzei V.A.; Popp M.; Krolitzek J.; Bonn G.K.; Huck C.W. Application if benchtop and portable near-infrared spectrometers for predicting the optimum harvest time of Verbena officinalis. Talanta, 2017, http://dx.doi.org/10.1016/j.talanta.2017.03.067

# "Phytovalley®-Tirol"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Dep. of Botany
Botanical Garden

MCI
Managment
Center Innsbruck
Biotechnology

Bionorica research
Phytoneering,
GLP-Laboratories

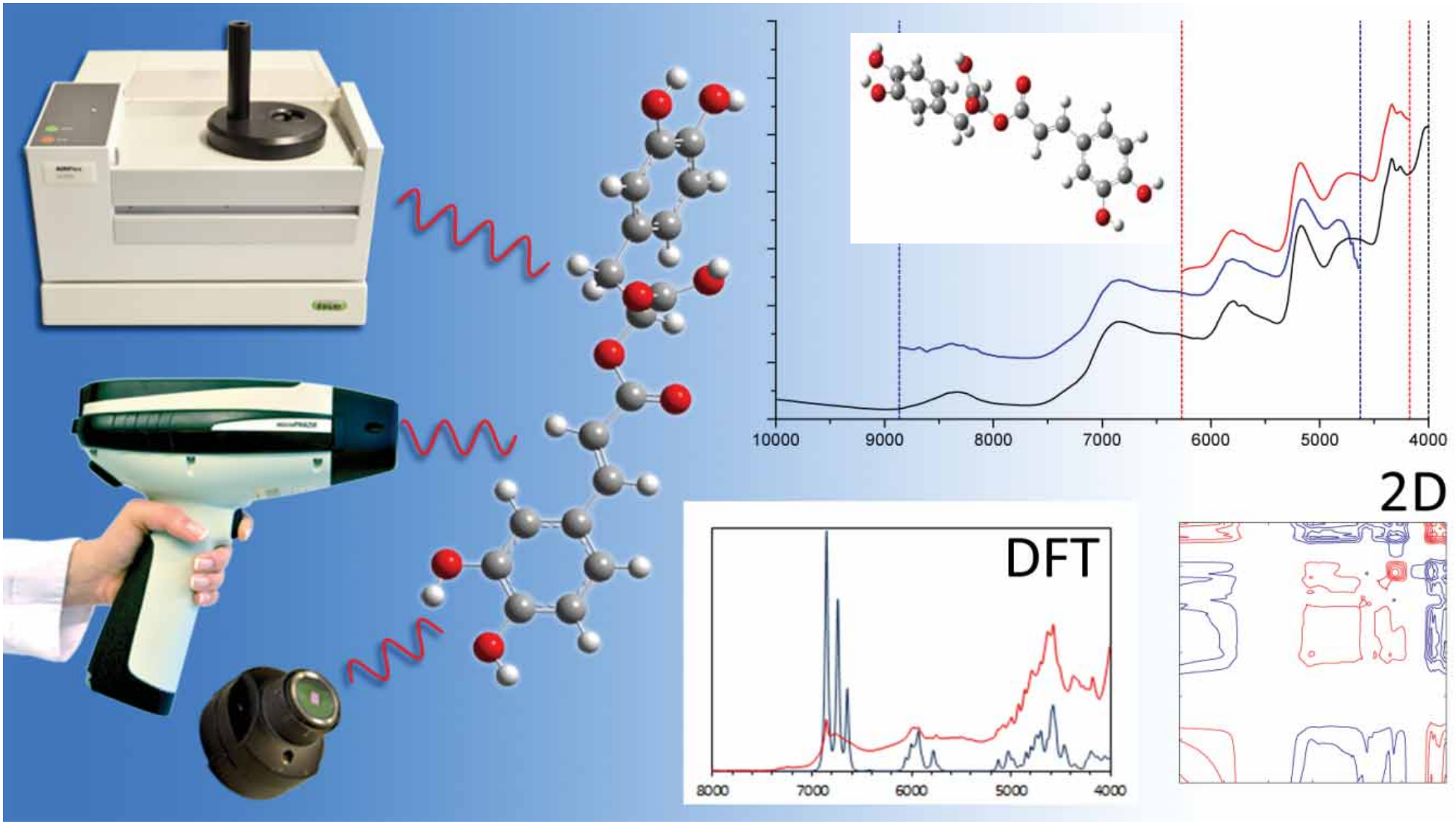
Michael Popp Research Institute
for New Phyto-Entities,
University of Innsbruck

Michael A. Popp
nature science institute

tirol kliniken
Biobank and
clinical samples

CURA
Development
Phytocosmetics
Marketing

# Fast Quality Control of MEDICINAL PLANTS: Rosmarini folium

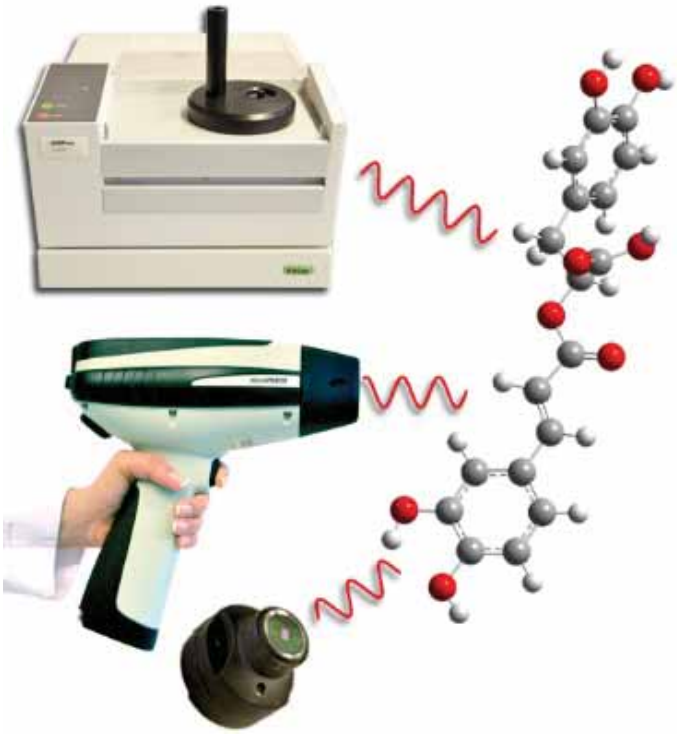



Kirchler C.G., Pezzei C.K., Bec, K.B., Mayr S., Ishigaki M., Ozaki Y., Huck C.W. Critical evaluation of spectral information of benchtop vs. portable near-infrared spectrometers: Quantum chemistry and two-dimensional correlation spectroscopy for a better understanding of PLS regression models of the rosmarinic acid content in Rosmarini folium. Analyst 142 (2017) 455

# 2D CORRELATION SPECTROSCOPY
## „the eye of the spectrometer“

2D-COS used as „the eye of the spectrometer“

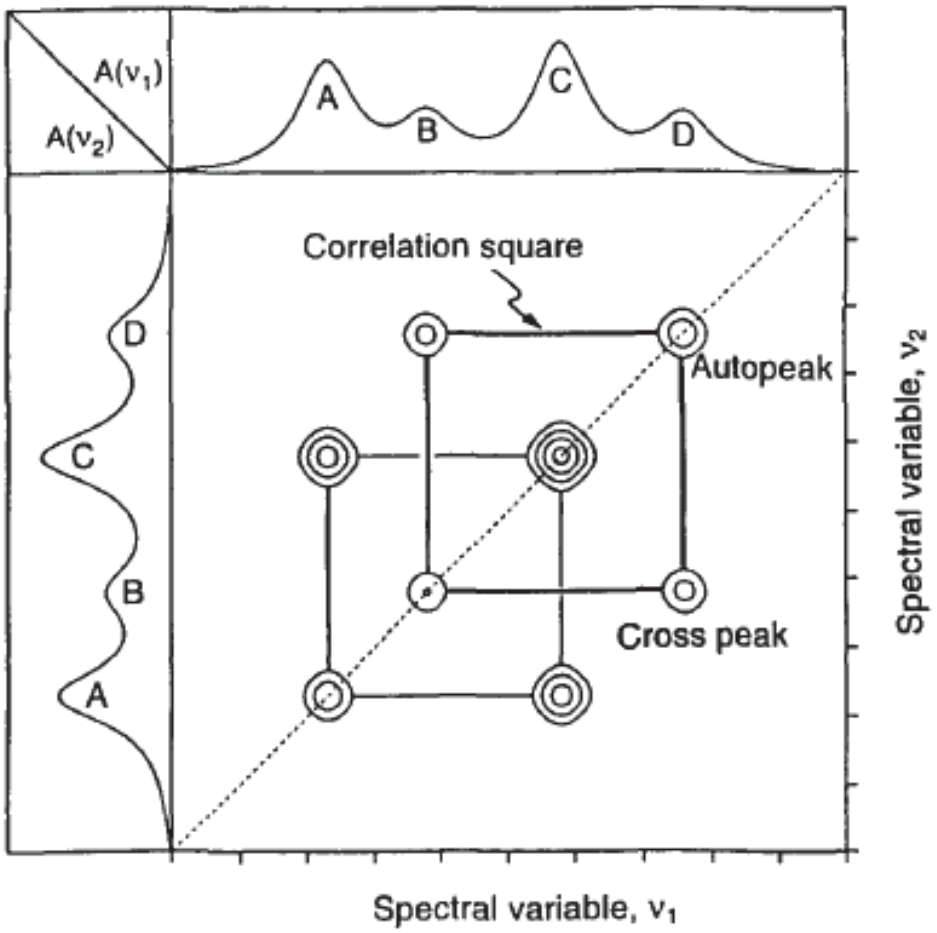
**Visual perception**



Example: rosmarinic acid content in powdered rosemary leaves (60 samples).

# 2D CORRELATION SPECTROSCOPY

What we can see is the
**dynamic variation of different spectra**
due to an external perturbation
(e.g. temperature, different
concentration, etc.)
as well as the **correlation of the variation at two different wavenumbers.**




Noda, I. Generalized Two-Dimensional Correlation Method Applicable to Infrared, Raman, and Other Types of Spectroscopy. Appl. Spectrosc. 47 (9) (1993) 1329-1336

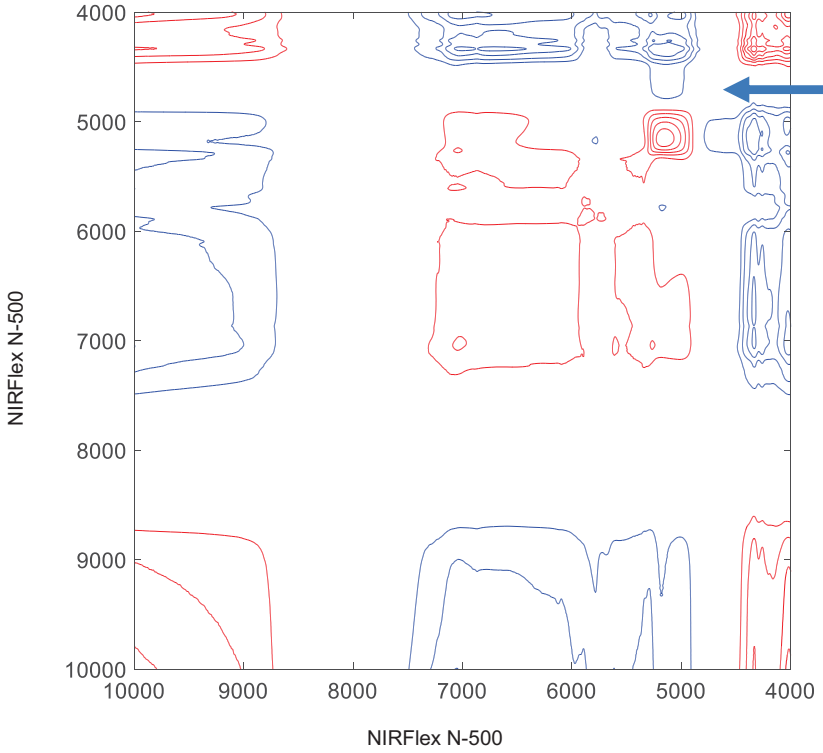
# 2D CORRELATION SPECTROSCOPY

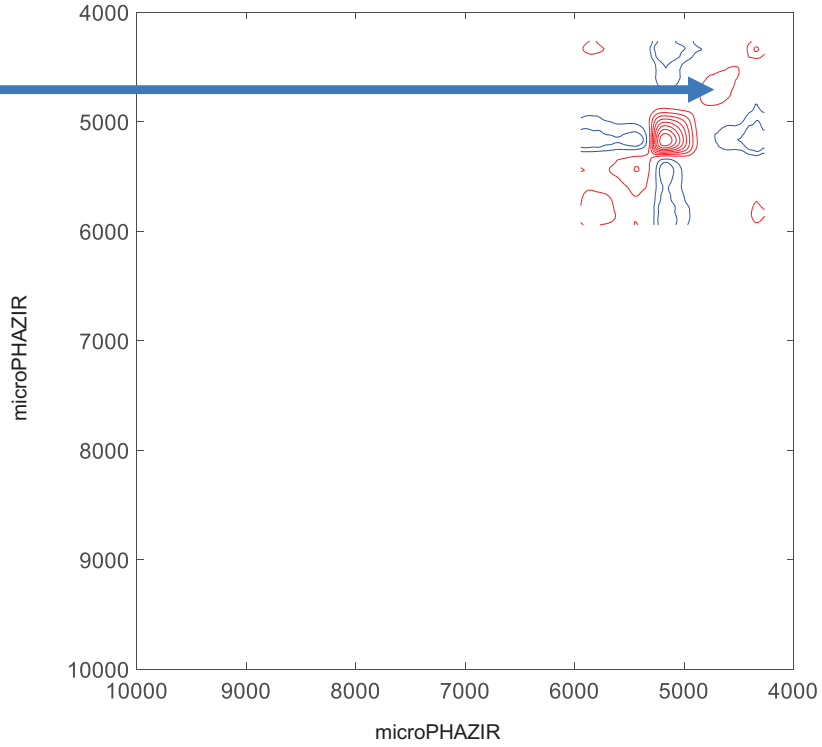
„the eye of the spectrometer“

60 rosemary samples

Benchtop
NIRFlex N-500

Miniaturized „microPhazir“



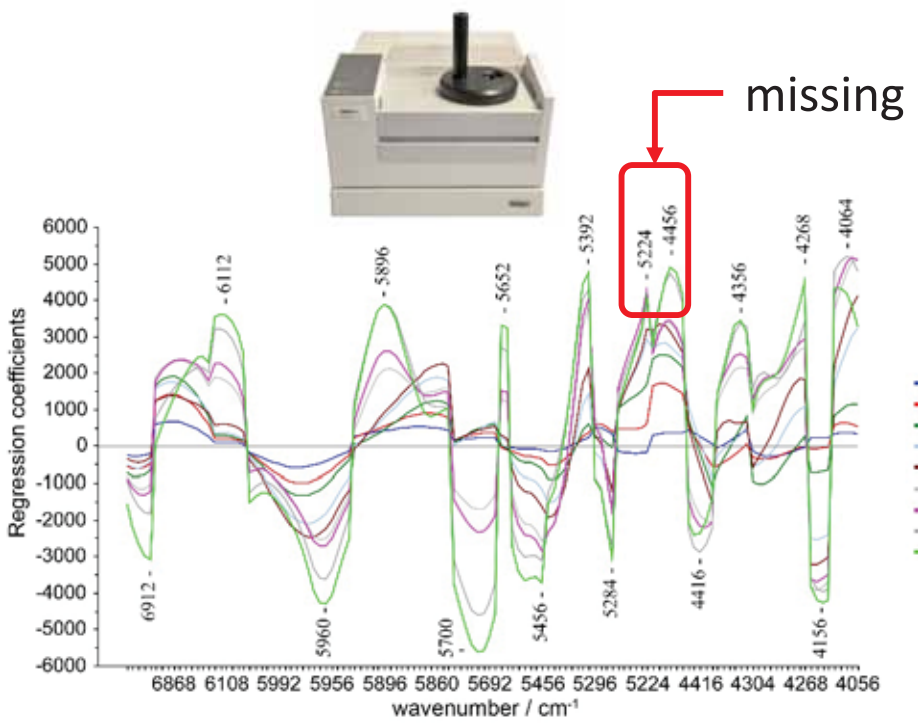

**autopeak appearance** in the visual perception of the microPHAZIR!

# 2D CORRELATION SPECTROSCOPY

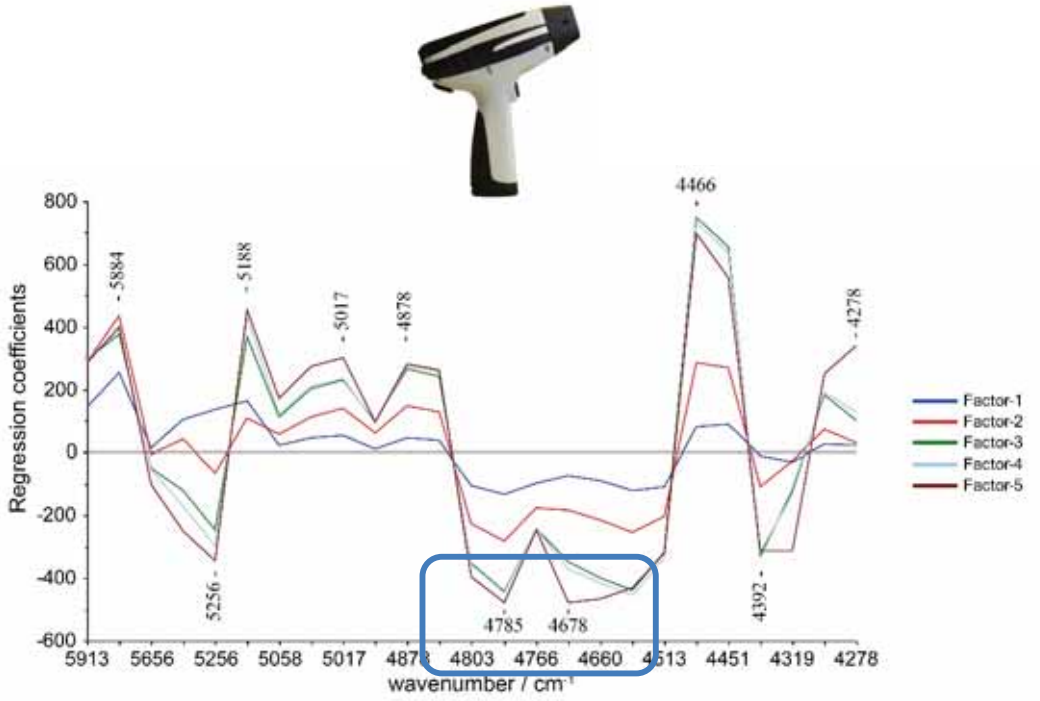
„the eye of the spectrometer“

60 rosemary samples

Benchtop „ NIRFlex N-500“




Miniaturized „microPhazir“




This region is **crucial for** the PLS-regression of **microPhazir** and **unnecessary for NIRFlex N-500!**

# 2D CORRELATION SPECTROSCOPY

„the eye of the spectrometer“

60 rosemary samples

| spectrometer | NIRFlex N-500 | | microPHAZIR | | MicroNIR 2200 | |
|---|---|---|---|---|---|---|
| samples | 60 | | 60 | | 60 | |
| outliers | 6 | | 8 | | 4 | |
| range / % | 1.138 – 2.425 | | 1.138 – 2.425 | | 1.138 – 2.425 | |
| validation method | CV | TSV | CV | TSV | CV | TSV |
| $R^2$ | 0.91 | 0.91 | 0.73 | 0.73 | 0.84 | 0.85 |
| SECV / % SEP / % | 0.072 | 0.069 | 0.12 | 0.11 | 0.091 | 0.11 |
| SECV/SEC SEP/SEC | 1.46 | 1.43 | 1.28 | 1.24 | 1.55 | 2.09 |
| factors | 8 | 8 | 5 | 5 | 11 | 12 |
| RPD | 3.27 | 3.41 | 1.88 | 2.06 | 2.46 | 2.14 |

Kirchler C.G., Pezzei C.K., Bec, K.B., Mayr S., Ishigaki M., Ozaki Y., Huck C.W. Critical evaluation of spectral information of benchtop vs. portable near-infrared spectrometers: Quantum chemistry and two-dimensional correlation spectroscopy for a better understanding of PLS regression models of the rosmarinic acid content in Rosmarini folium. Analyst 142 (2017) 455

# THYMOL – NIR ANALYTICS & QUANTUM CHEMICAL CALCULATIONS

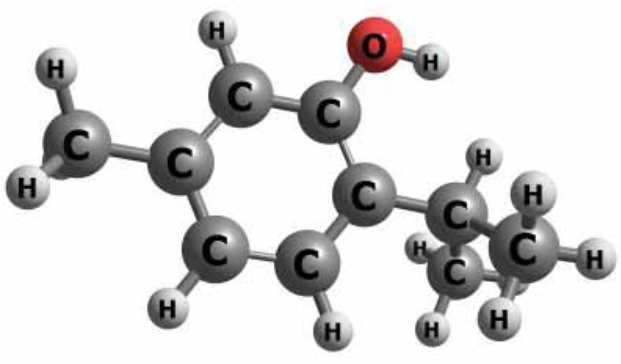


Fig. The optimized (DFT-B3LYP/SNST) molecular structure of thymol.

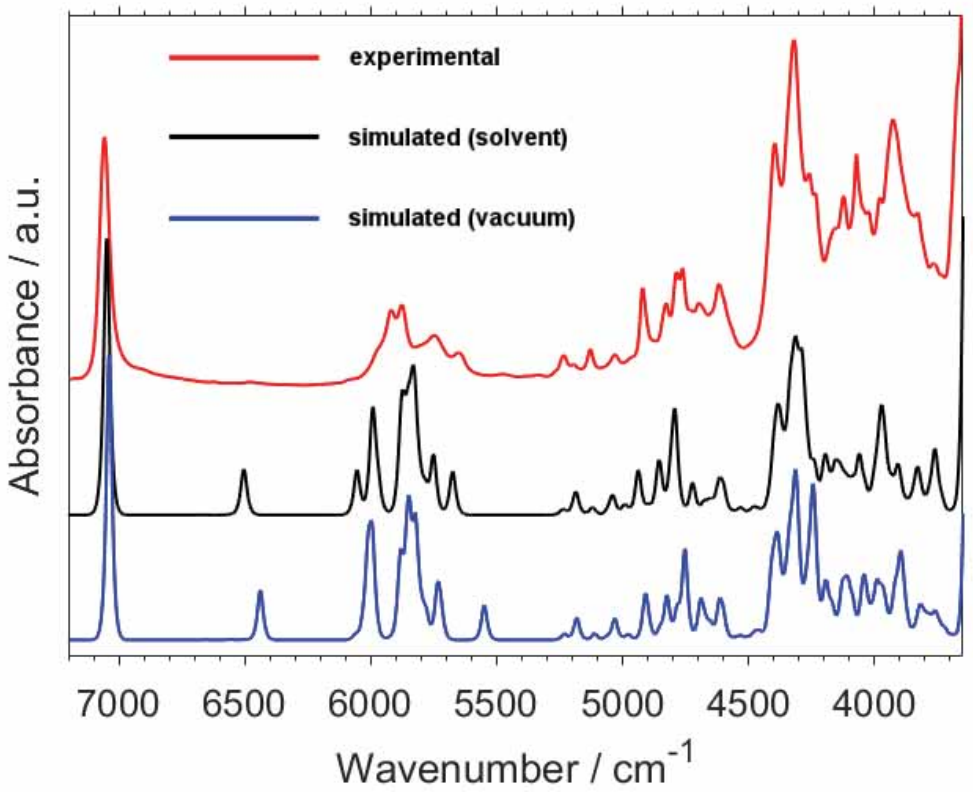



Fig. Impact of implicit solvation model (SCRF/CPCM-$CCl_4$) on the simulated (DVPT2//DFT-B3LYP/SNST+CPCM) NIR spectrum of thymol. The modeled spectral outlines compared with the experimental spectrum of thymol in solution (100 mg $mL^{-1}$ $CCl_4$).


Krzysztof B. Beć, Justyna Grabska, Christian G. Kirchler, Christian W. Huck.
NIR spectra simulation of thymol for better understanding of the spectra forming factors, phase and concentration effects and PLS regression features
Journal of Molecular Liquids, 268, 895 - 902 (2018)

# THYMOL – NIR ANALYTICS & QUANTUM CHEMICAL CALCULATIONS

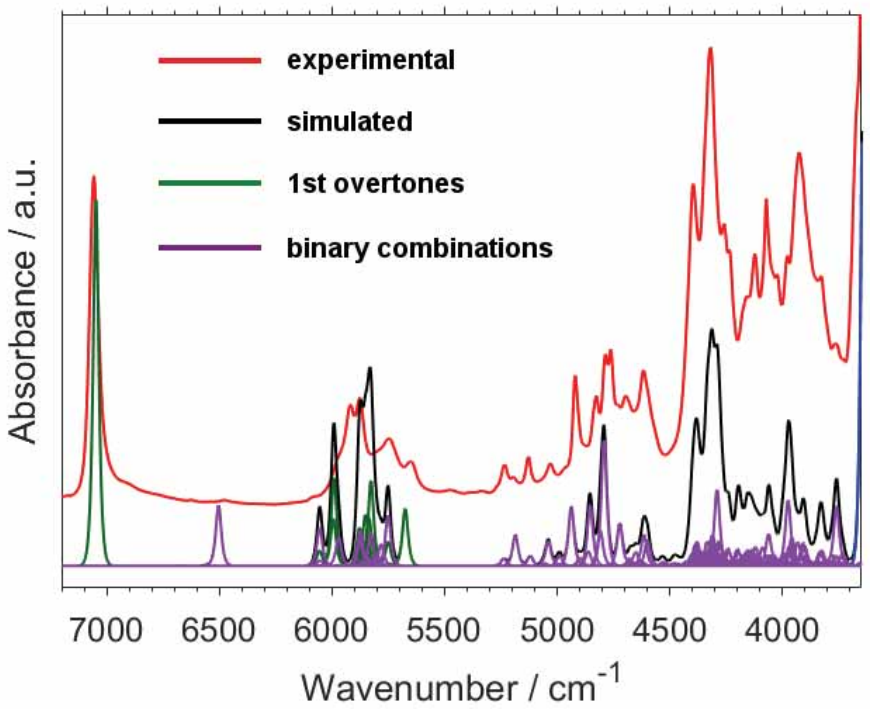



Fig. The contributions of the first overtone and binary combination bands into the NIR spectral envelope of thymol in solution phase (100 mg $mL^{-1}$ $CCl_4$) as obtained through QM spectra simulation (DVPT2//DFT-B3LYP/SNST+CPCM).

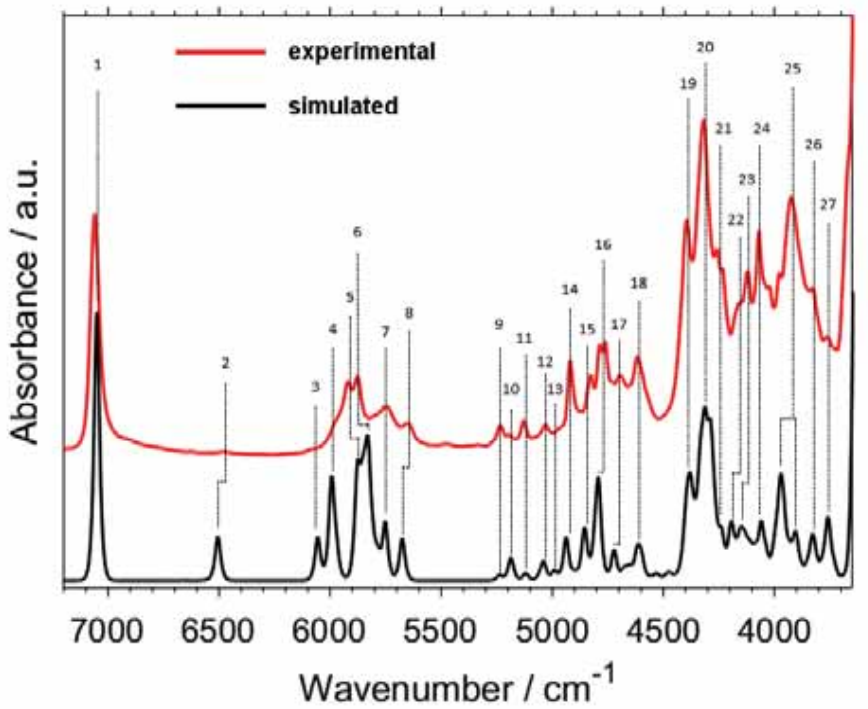


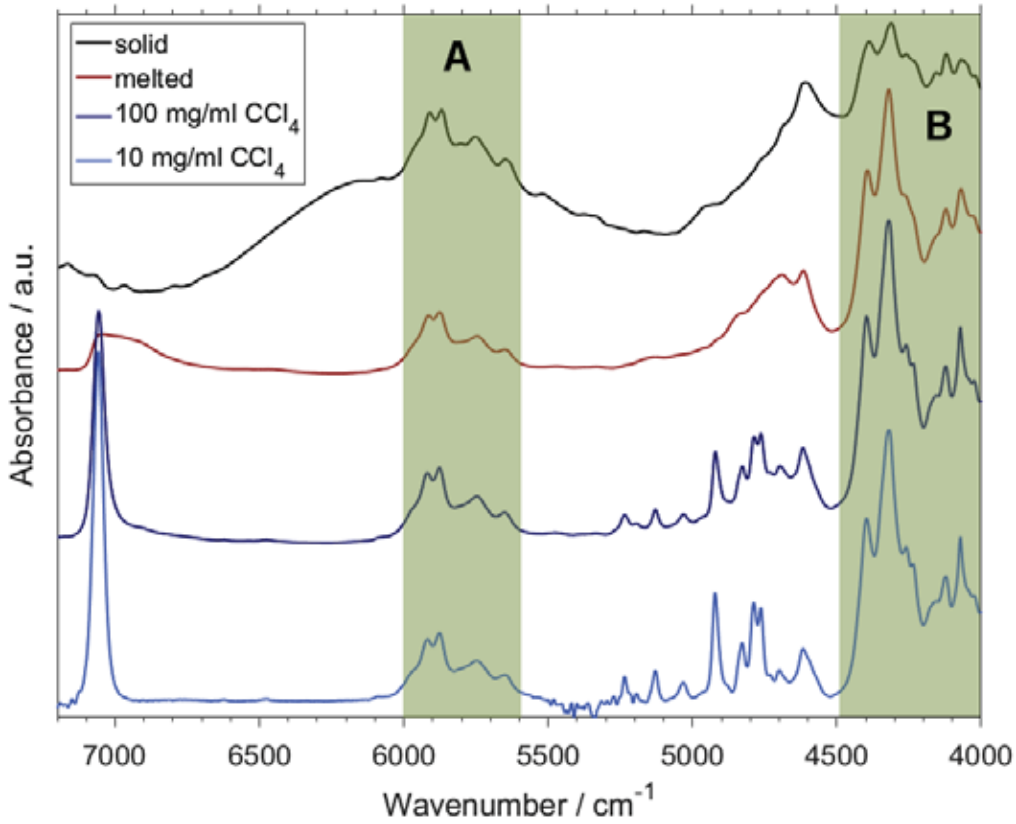

Fig. The most probable band assignments in the experimental NIR spectrum of thymol in solution phase (100 mg $mL^{-1}$ $CCl_4$) based on comparative cross-analysis with the QM simulated NIR spectrum (DVPT2//DFT-B3LYP/SNST+CPCM).

Krzysztof B. Beć, Justyna Grabska, Christian G. Kirchler, Christian W. Huck.
NIR spectra simulation of thymol for better understanding of the spectra forming factors, phase and concentration effects and PLS regression features
Journal of Molecular Liquids, 268, 895 - 902 (2018)

## Thymol – NIRS Analytics

An **in-depth analysis** of the origin of NIR spectrum of thymol and its relationship with PLSR for thymol content determination.

There are two spectral regions clearly independent of the sample state or concentration which were also crucial for the PLSR model
A: 6000-5600 $cm^{-1}$ and B: 4490-4000 $cm^{-1}$

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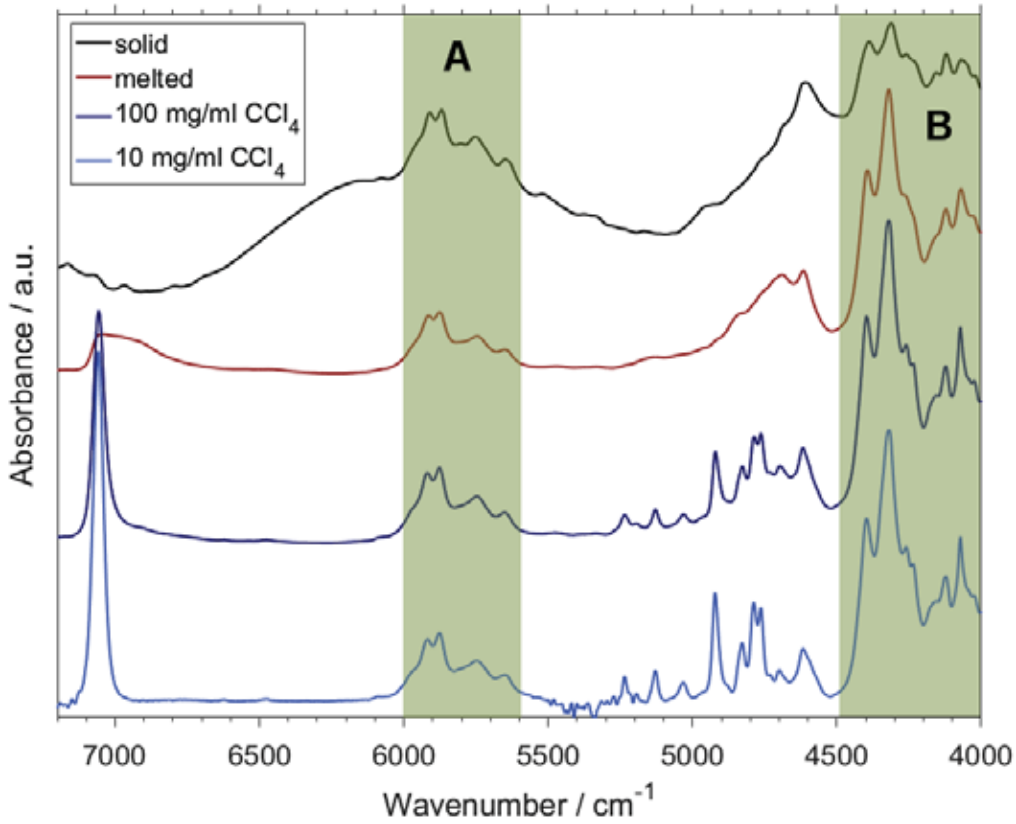


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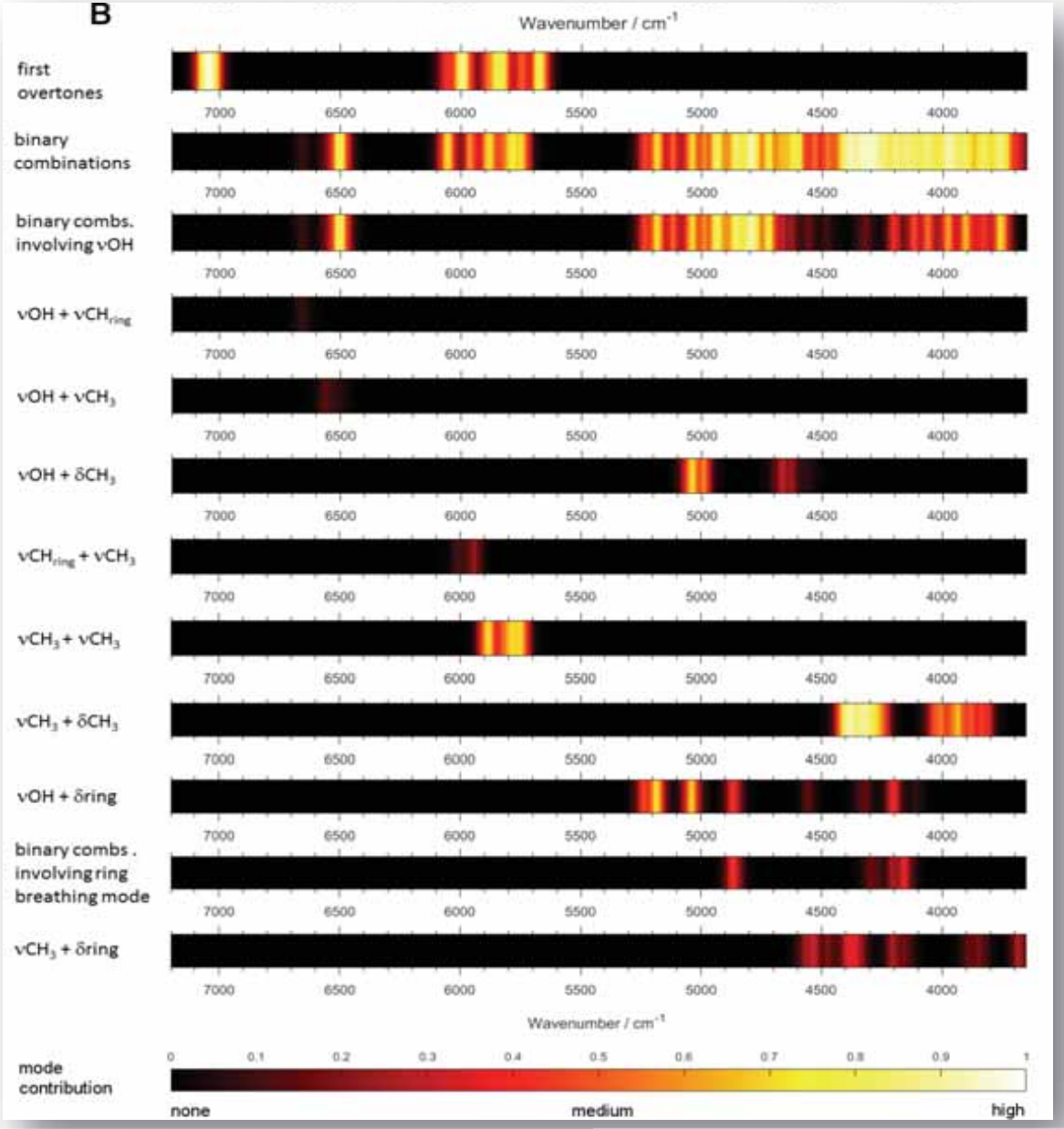
# THYMOL – NIR ANALYTICS & QUANTUM CHEMICAL CALCULATIONS

**The analysis of mode contribution into NIR spectrum of thymol (solution; 100 mg mL−1 $CCl_4$) based on the simulated data (DVPT2//DFT-B3LYP/SNST+CPCM). B: contributions of selected modes as described on the figure.**





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NIR spectra simulation of thymol for better understanding of the spectra forming factors, phase and concentration effects and PLS regression features
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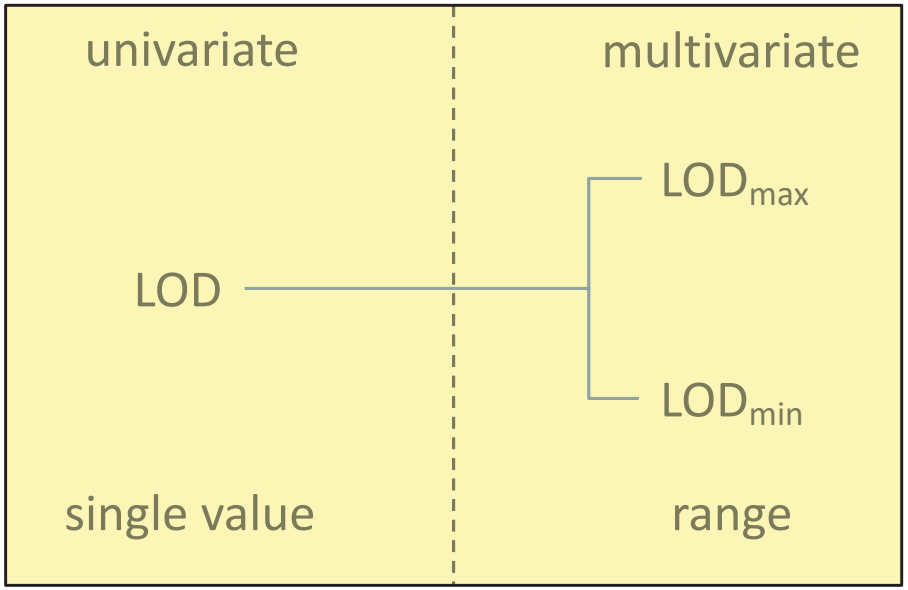
multivariate approach for calculating the LOD

Problem: instrumental signals are not specific for a particular analyte

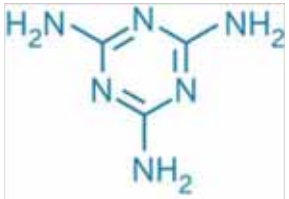
Instead of a single LOD value, an **LOD interval** is calculated which depends on the **variability of the background** composition of the calibration samples



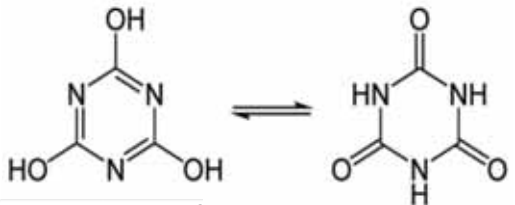



F. Allegrini, A.C. Olivieri, IUPAC-Consistent approach to the limit of detection in partial least-squares calibration. Anal. Chem. 86 (15) (2014) 7858–7866

# Comparison of sensitivity to artificial spectral errors and multivariate LOD in NIR spectroscopy: Determining the performance of miniaturizations on melamine in milk powder

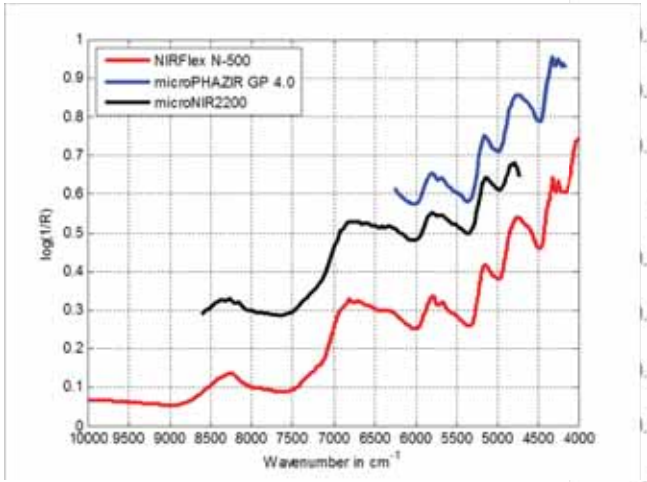



**Melamine**

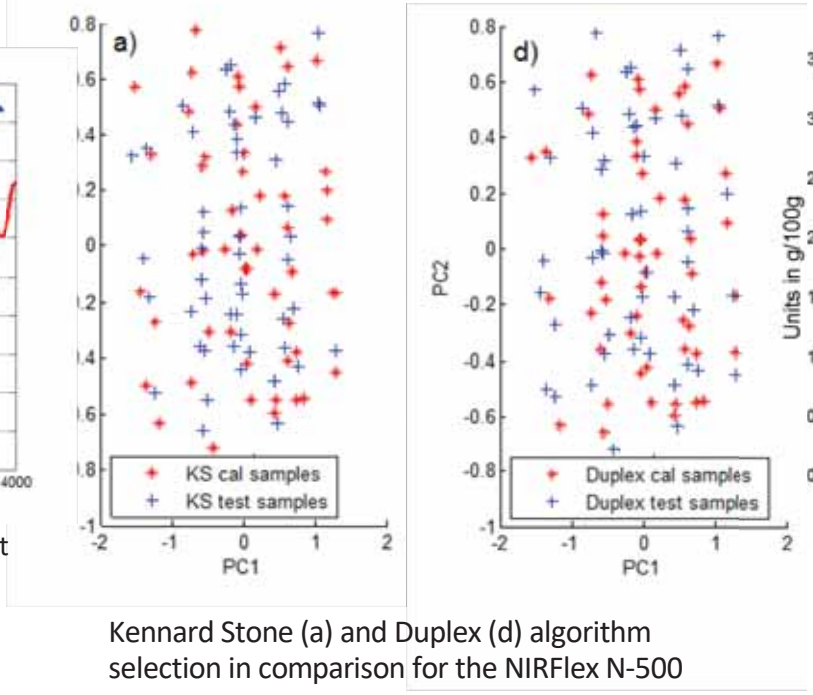



**Cynauric / isocyanuric acid**
1 2

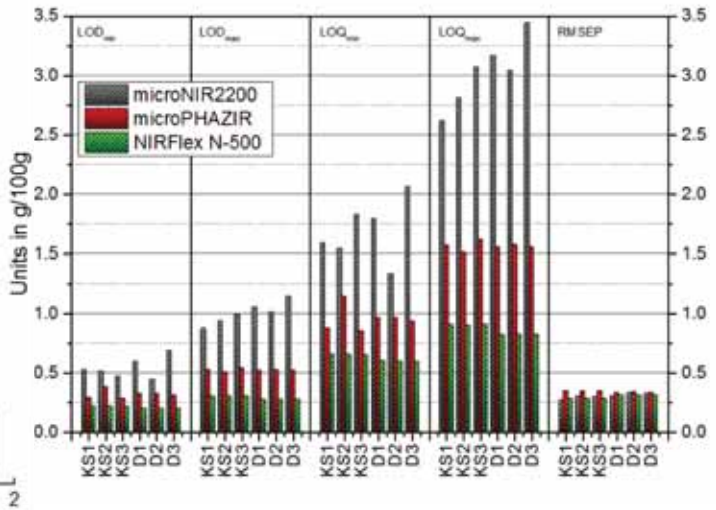
| **LOD min%** | |
|---|---|
| Benchtop | 0.20 |
| Micro Phazir | 0.28 |
| microNIR2200 | 0.44 |




Accessible spectral ranges of the different devices in comparison




Kennard Stone (a) and Duplex (d) algorithm selection in comparison for the NIRFlex N-500




LOD, LOQ and RMSEP values of the used spectrometers and constructed models in comparison. KS indicating Kennard Stone selection and D the Duplex selection

Henn R., Kirchler C.G., Grossgut M.E., Huck C.W. Comparison of sensitivity to artificial spectral errors and multivariate LOD in NIR spectroscopy – Determining the performance of miniaturizations on melamine in milk powder. Talanta, 166, 109-118 (2017)

Talanta 189 (2018) 233–240

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Talanta

journal homepage: www.elsevier.com/locate/talanta

# Evaluation of the performance of three hand-held near-infrared spectrometer through investigation of total antioxidant capacity in gluten-free grains

Verena Wiedemair, Christian W. Huck*

*Institute of Analytical Chemistry and Radiochemistry, CCB – Center for Chemistry and Biomedicine, University of Innsbruck, Innrain 80/82, 6020 Innsbruck, Austria*

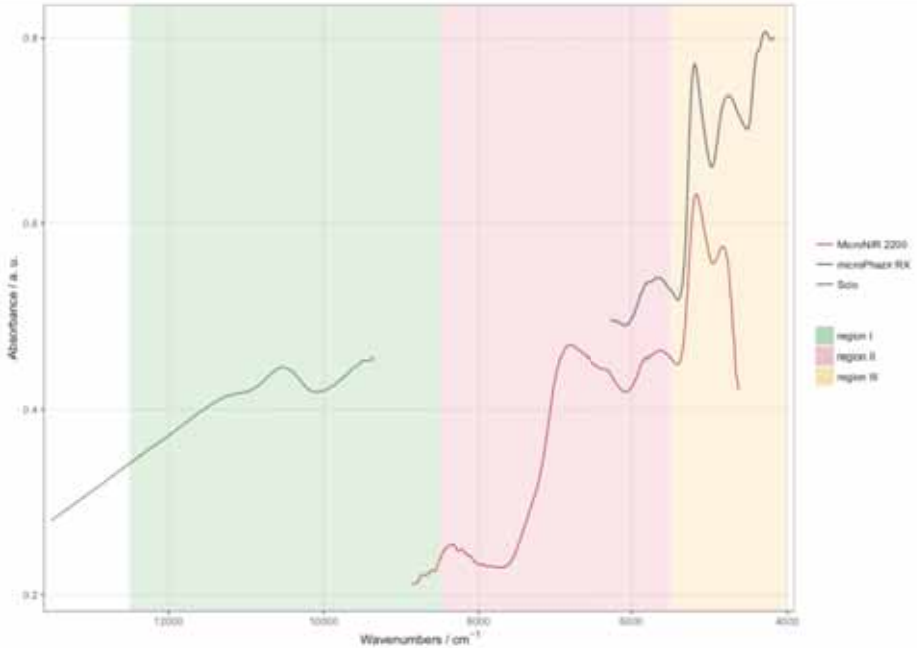



**Fig. 1.** Averaged spectrum of all samples recorded with SCiO (green), MicroNIR 2200 (red) and microPhazir RX (blue). The three regions of NIR are indicated in the background.

RPD and multivariate limit of detection (mLOD) and quantification (mLOQ) for all established models. All limits of detection and quantification are given in mgGAE/g.

| Device | State of the grains | RPD | $LOD_{min}$ | $LOD_{max}$ | $LOQ_{min}$ | $LOQ_{max}$ |
|---|---|---|---|---|---|---|
| SCiO | Non-milled | 3.93 | 1.7827 | 3.0314 | 5.3480 | 9.0943 |
| | Milled | 2.63 | 1.7029 | 2.6173 | 5.1088 | 7.8519 |
| MicroNIR 2200 | Non-milled | 4.71 | 1.2365 | 1.8338 | 3.7095 | 5.5015 |
| | Milled | 3.29 | 1.6548 | 3.2294 | 4.9643 | 9.6881 |
| microPhazir RX | Non-milled | 4.61 | 1.3958 | 2.3862 | 4.1875 | 7.1587 |
| | Milled | 2.54 | 1.4773 | 2.5487 | 4.4318 | 7.6460 |

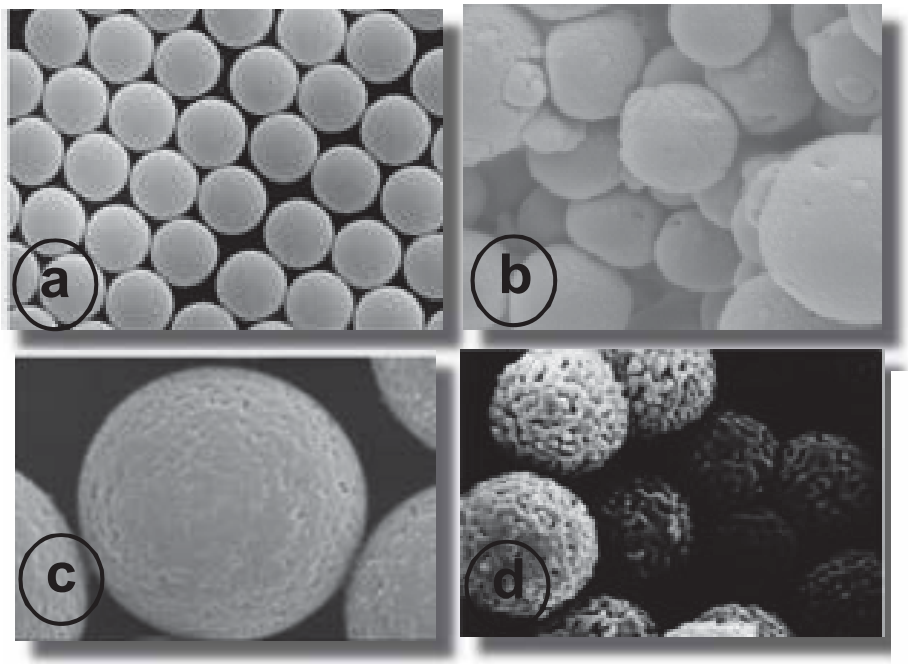
Statistical parameters of the established PLS-R models. CV denotes cross-validated models, whereas TV refers to test set validated regressions.

| Device | State of the grains | $R^2$ (CV) | RMSECV/mgGAE/g | Bias (CV) | $R^2$ (TV) | RMSEP / mgGAE/g | Bias (TV) |
|---|---|---|---|---|---|---|---|
| SCiO | Non-milled | 0.8234 | 1.9753 | 0.0116 | 0.8952 | 1.2353 | − 0.2890 |
| | Milled | 0.8240 | 2.0823 | 0.0334 | 0.8494 | 1.8572 | − 0.3235 |
| MicroNIR 2200 | Non-milled | 0.9513 | 1.1089 | − 0.0012 | 0.9519 | 1.0214 | − 0.0343 |
| | Milled | 0.9098 | 1.4647 | 0.0468 | 0.9186 | 1.4390 | − 0.2304 |
| microPhazir RX | Non-milled | 0.9213 | 1.4595 | 0.0084 | 0.8926 | 1.3716 | 0.8504 |
| | Milled | 0.9125 | 1.3501 | 0.0177 | 0.8913 | 1.7840 | − 0.4993 |

# Physicochemical Properties of Silica Materials

## Physical Properties

- Particle size distribution
- Porosity, Pore volume
- Specific surface area




**ELMI-pictures of silica particles with different porosity:**
**a**, non-porous (1000 x); **b**, 60 Å (5000 x); **c**, 300 Å (6000 x); **d**, 1000 Å (10000 x)

## Chemical Properties

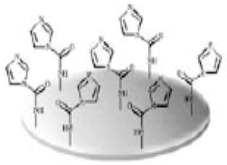
Hydrophobic

Anionic

Cationic

Metal Ion

Hydrophilic



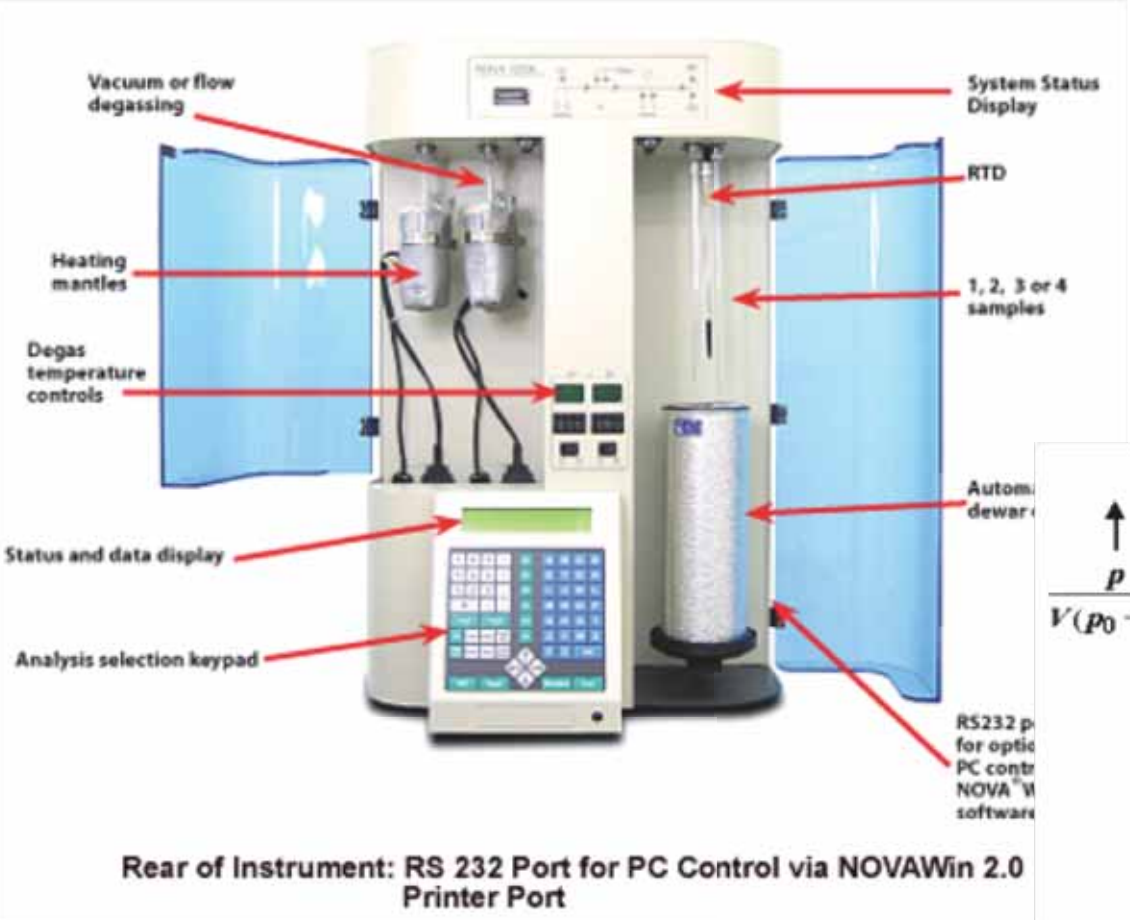
Activated Surface

Antibody – Antigen

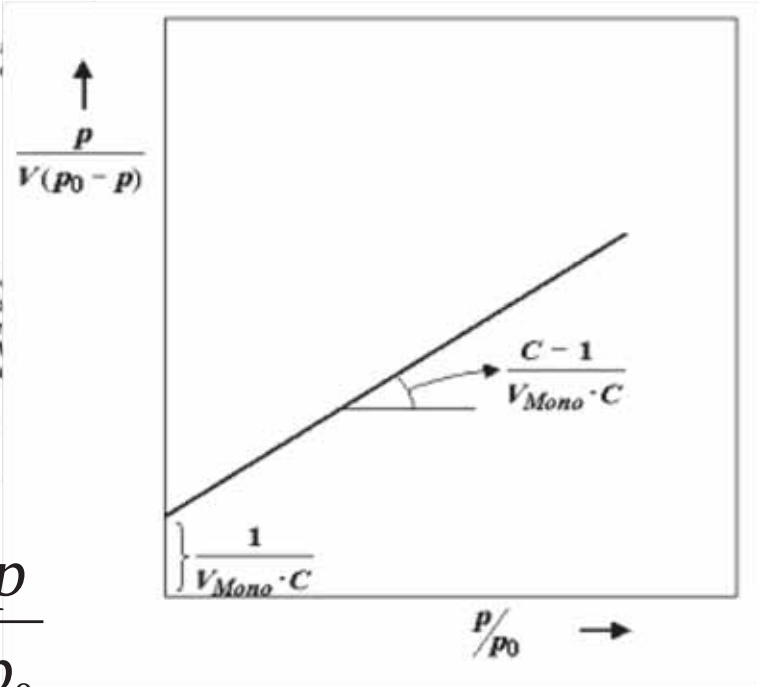
Receptor – Ligand

DNA – Protein

# Specific Surface Area – BET (Brunauer Emmett Teller)

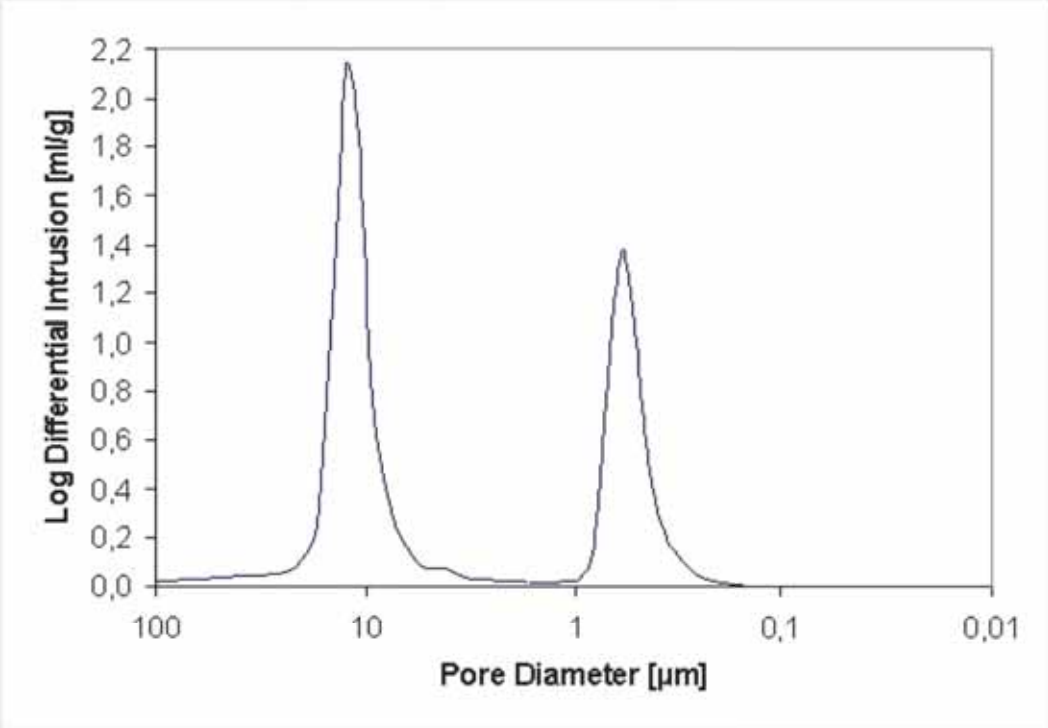



Emmett Teller




$$\frac{p}{V(p_0 - p)} = \frac{1}{V_{Mono} \cdot C} + \frac{C-1}{V_{Mono} \cdot C} \cdot \frac{p}{p_0}$$

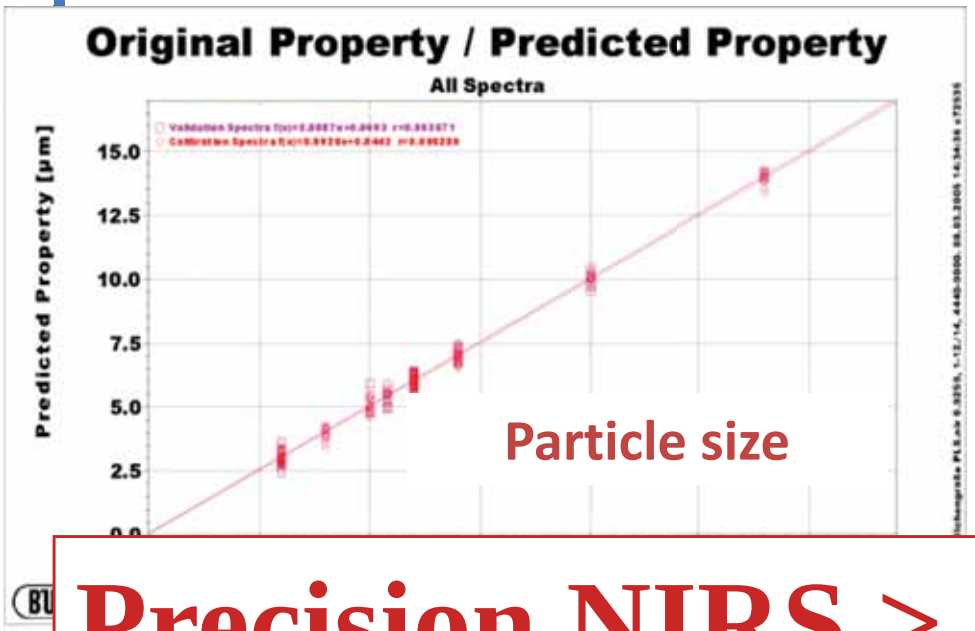
# MIP – Mercury Intrusion Porosimetry

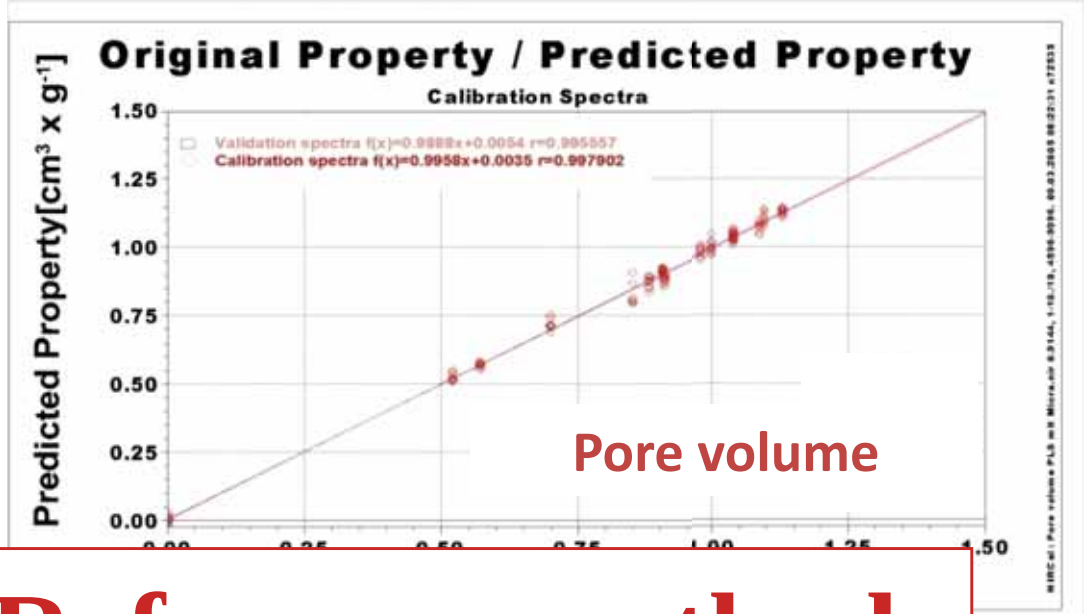




$$p = \frac{-2\gamma \cos\Theta}{r}$$

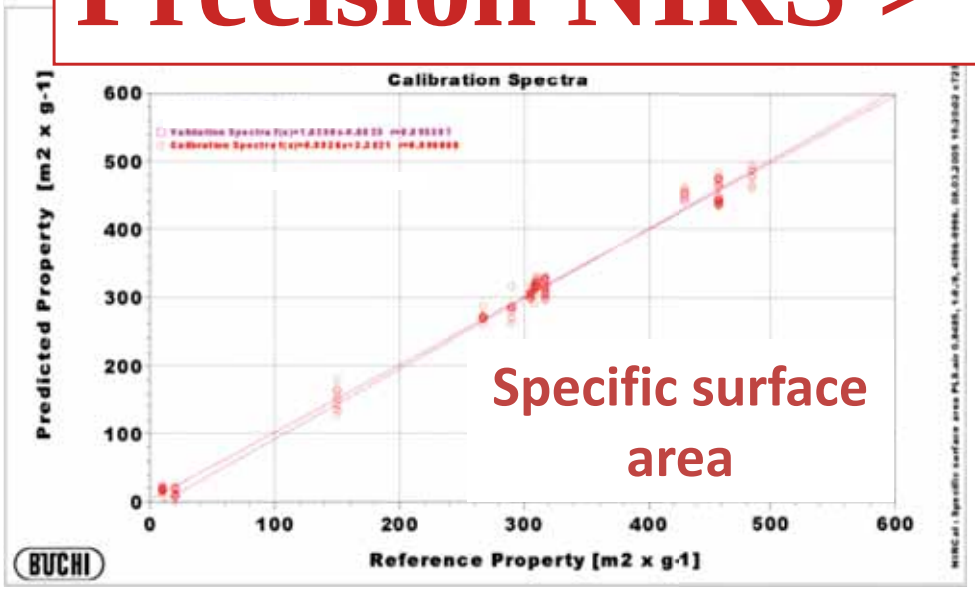
r…..pore radius
γ….surface tension of mercury
Θ…wetting angle
p….pressure

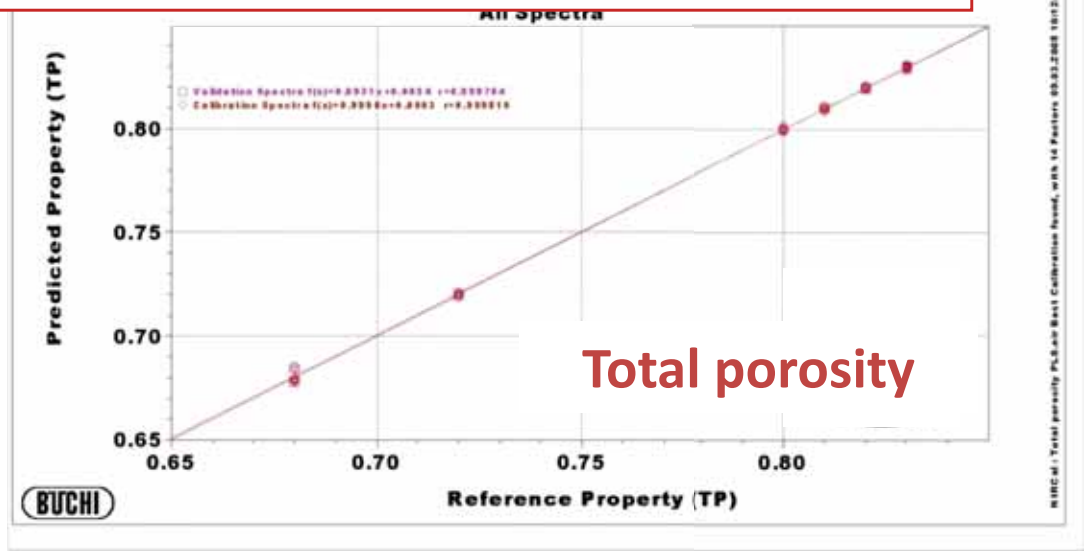
# Silica – Physical Properties



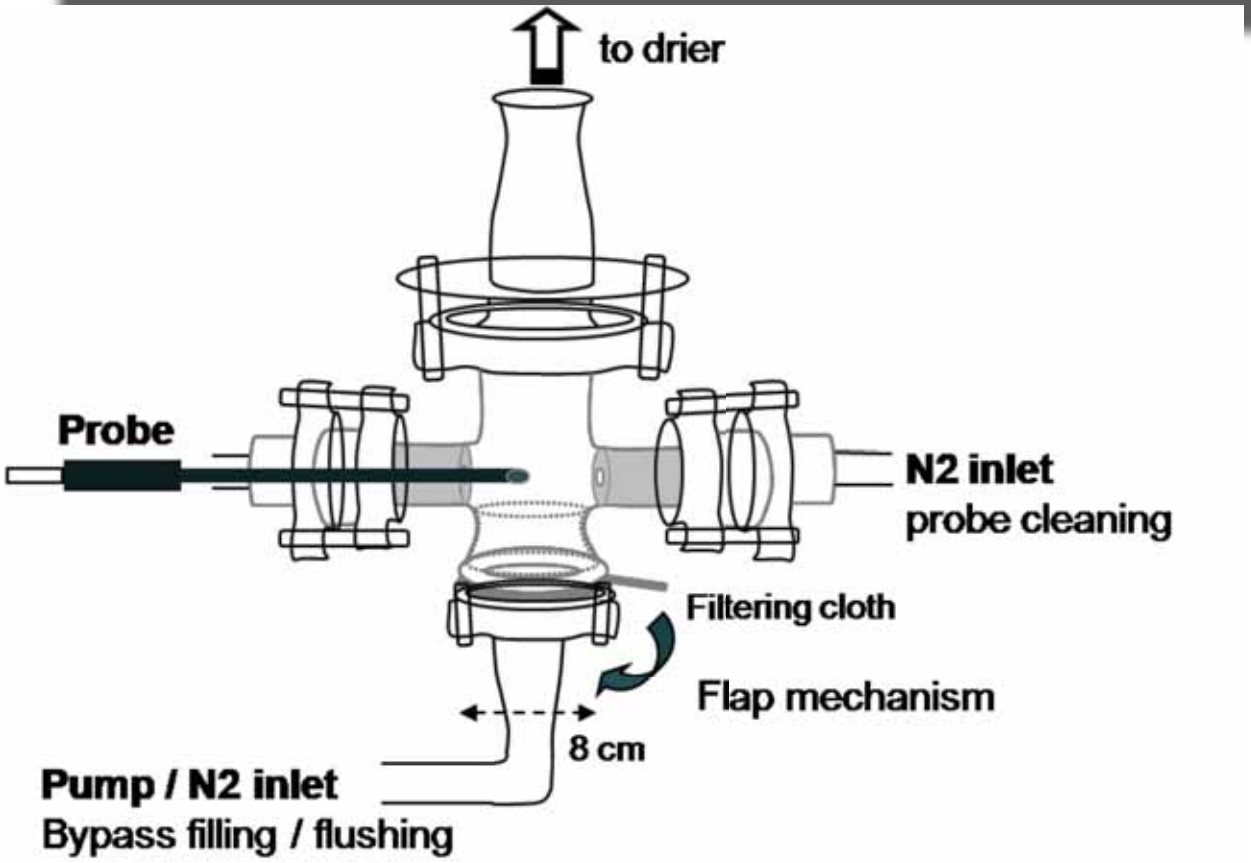




**Precision NIRS > Reference methods**



# Installation of a Bypass System



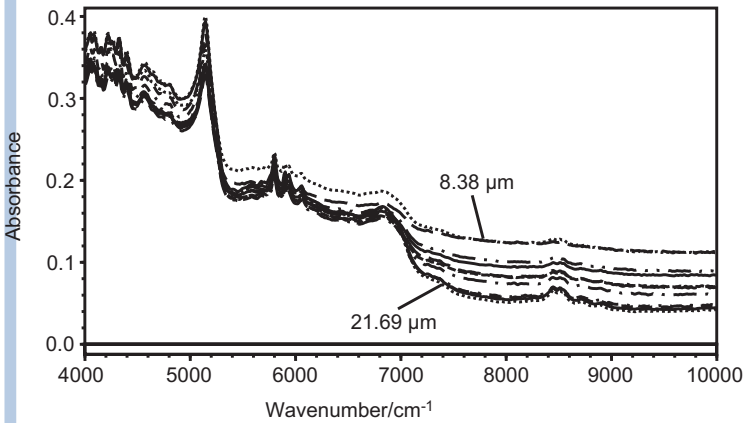

→ quick and reliable filling/purging procedure

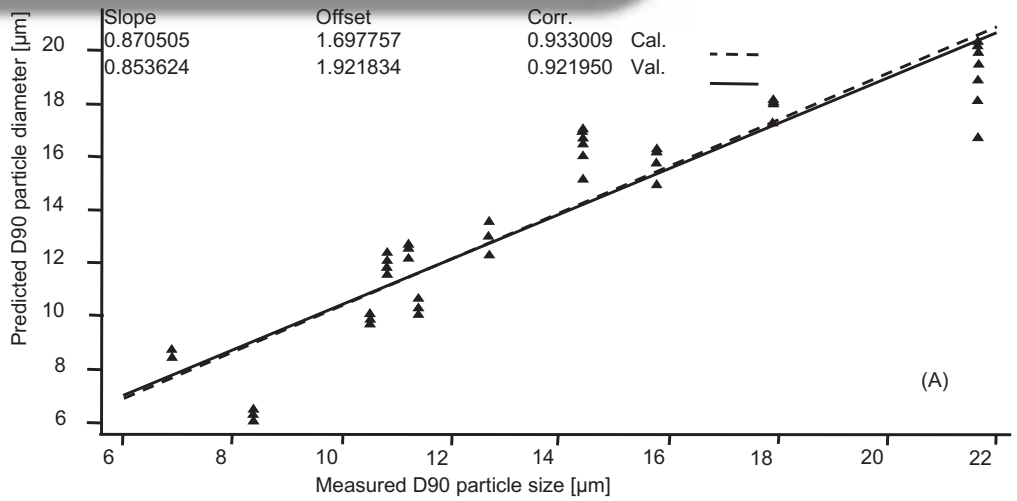
→ reproducible sample density

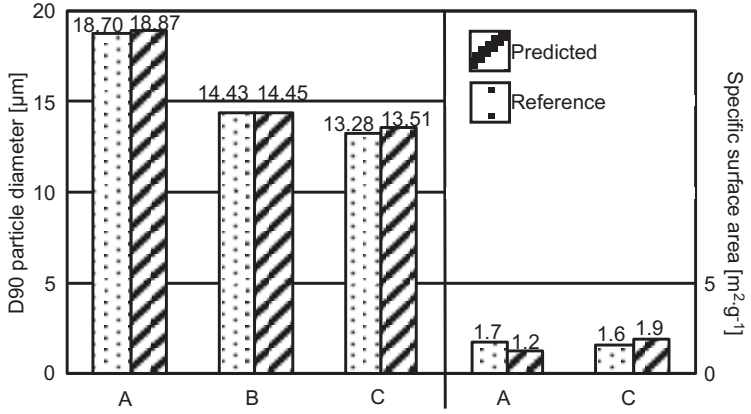
→ probe tip cleaning mechanism

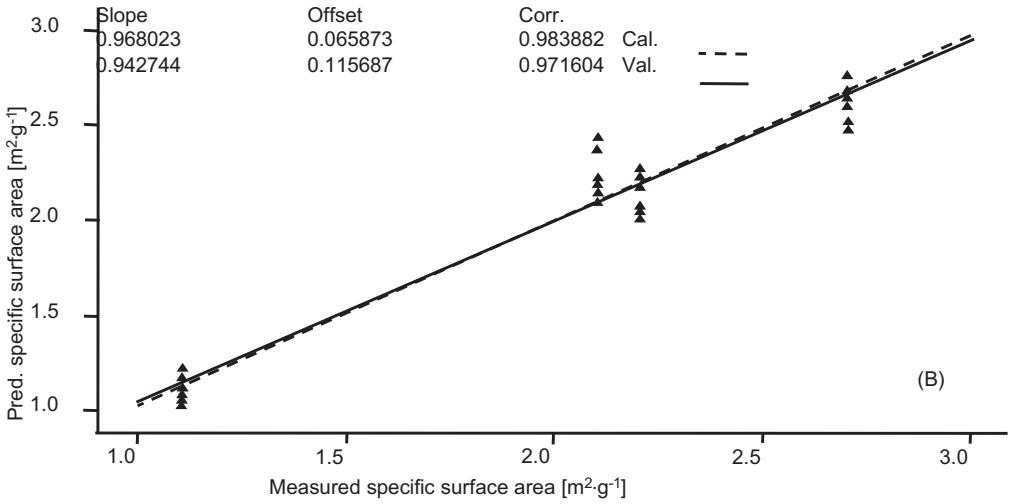
→ optical and easy mechanical access

# Particle Size and Surface Area

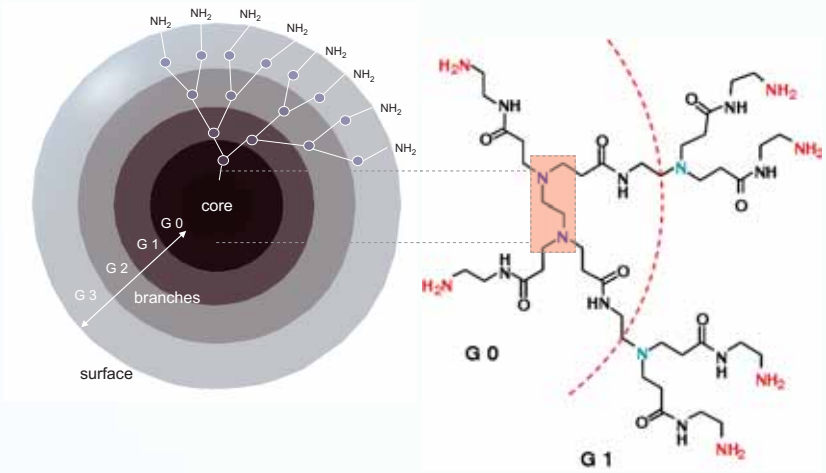


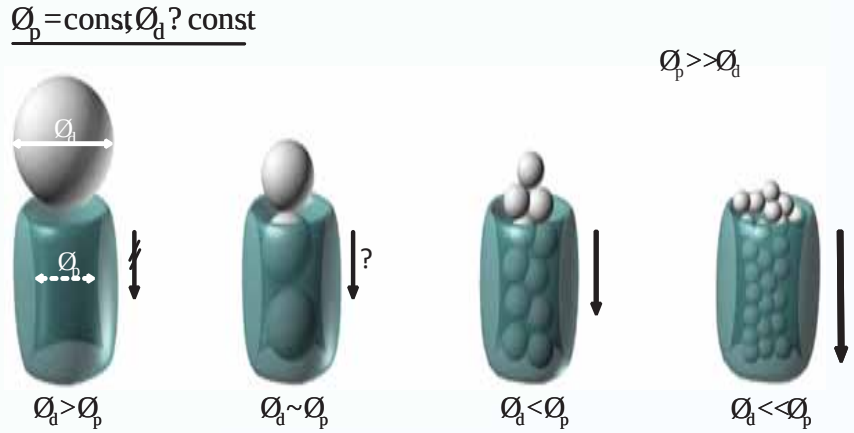



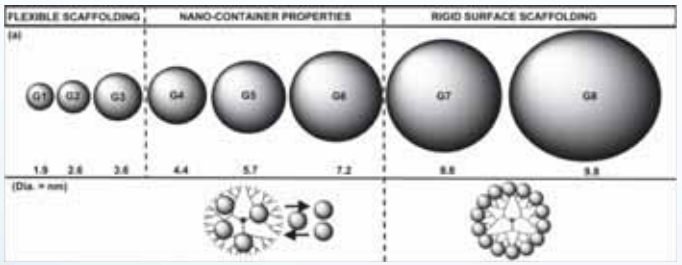



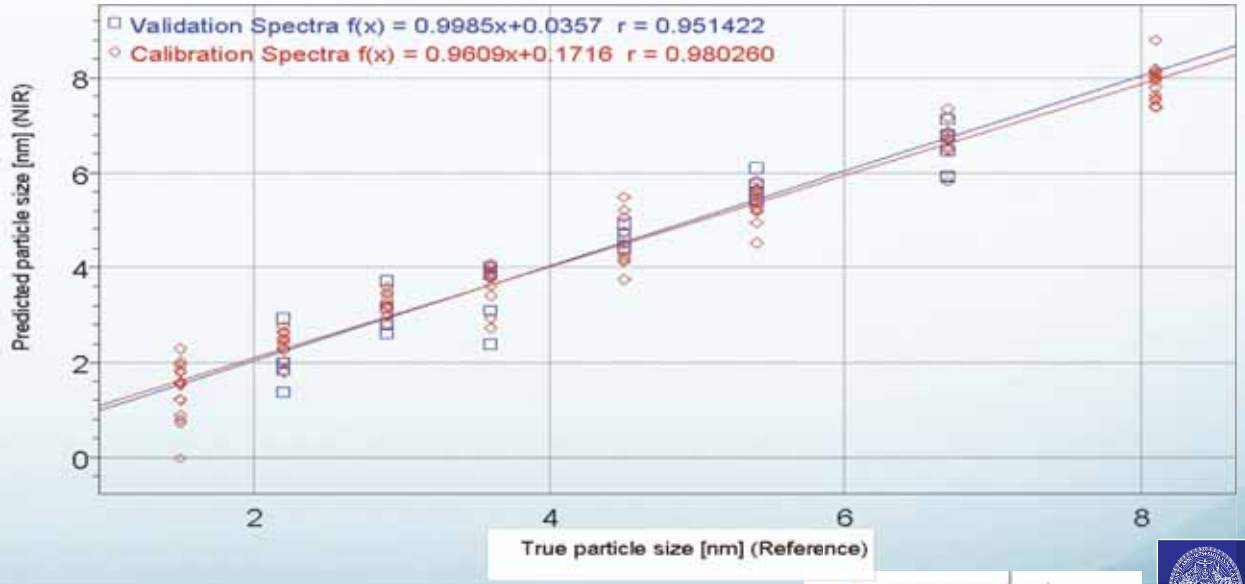



# Dendrimere




**Near-Infrared Spectroscopic Study on Guest–Host Interactions Among G0–G7 Amine-Terminated Poly(amidoamine) Dendrimers and Porous Silica Materials for Simultaneously Determining the Molecular Weight and Particle Diameter by Multivariate Calibration Techniques.** N. Heigl†, S. Bachmann†, C. H. Petter†, M. Marchetti-Deschmann‡, G. Allmaier‡, G. K. Bonn† and C. W. Huck*†· *Anal. Chem.*, **2009**, *81* (14), pp 5655–5662. **DOI:** 10.1021/ac900375z

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