scch { software competence center hagenberg }

NIR Spectroscopy @ KremsChem

Ramin Nikzad-Langerodi

HelioSPIR 2025, Montpellier 25.06.2025

Software Competence Center Hagenberg SCCH GmbH

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Non-Profit GmbH for
Data Science & Software Science

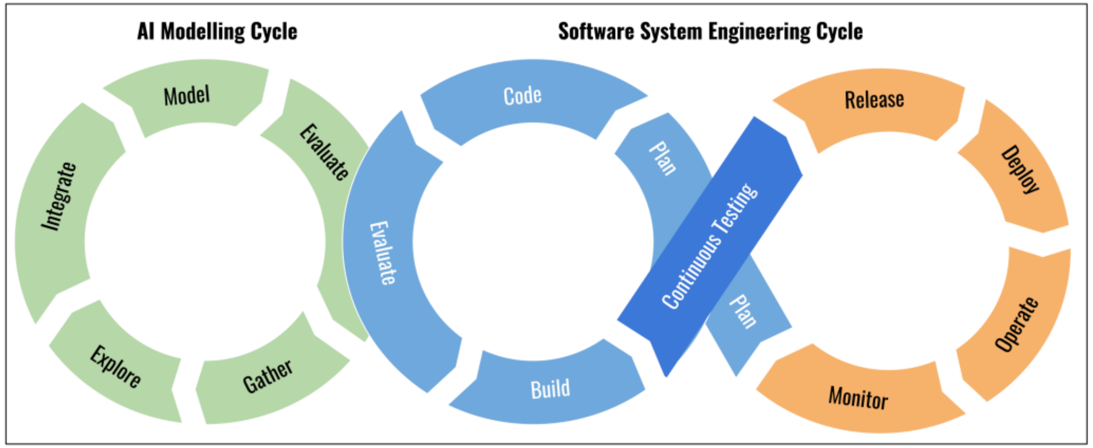
130
Employees
(over 160 with partners)

1999
founded by
the JKU Linz

Ownership
UAR Upper Austrian Research,
JKU, Association of Partner Companies

COMET K1
Competence Center for
Integrated Software-
and AI-Systems

14 million
euro total assets



Use Case

Use Case Presentation

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KremsChem Austria is the regional market and technology leader for resins, as well as a specialist in fine chemicals, surfacing materials and flame retardants.

Use Case Presentation

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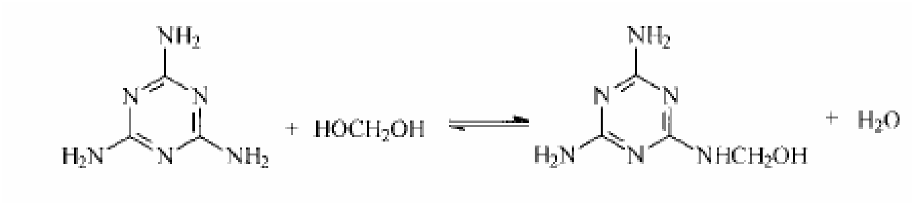
KremsChem Austria is the regional market and technology leader for resins, as well as a specialist in fine chemicals, surfacing materials and flame retardants.

BOARD & IMPRAGNATING RESINS	FLAME RETARDANTS & SURFACING MATERIALS
	FINE CHEMICALS
	FORMALDEHYDE

Source: www.tectonica-online.com

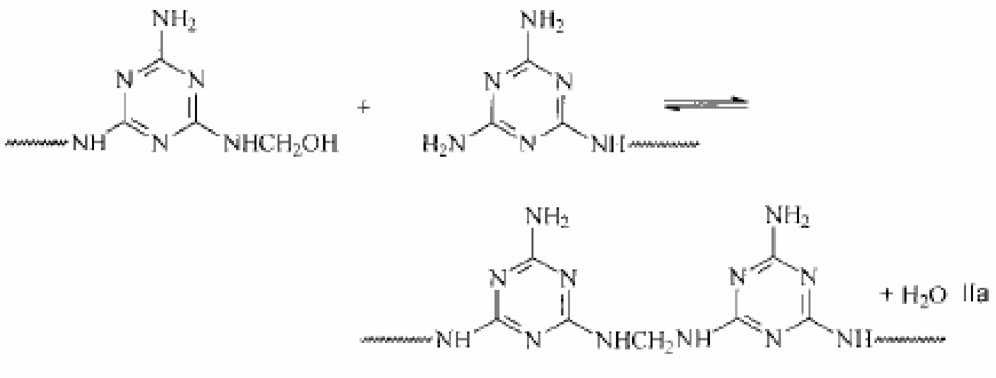
Melamin-Formaldehyde (MF) Resins

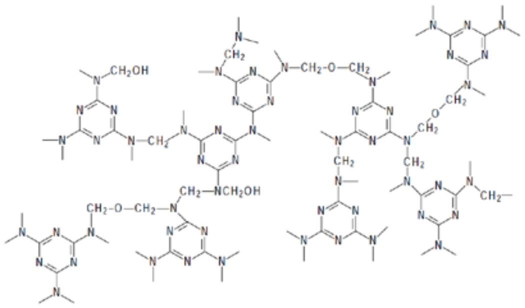
Methylolation



Jahromi *et al.* 1999

Condensation





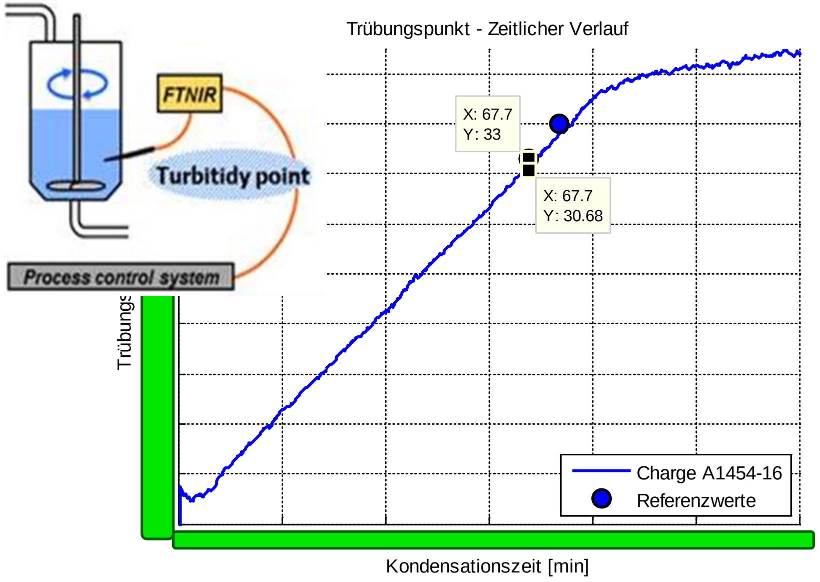
1. Melamine + Formaldehyde → Hydroxymethyl Melamine
2. (Poly) Condensation

Jahromi, S. (1999). Storage stability of melamine-formaldehyde resin solutions, 1. The mechanism of instability. *Macromolecular Chemistry and Physics*, *200*(10), 2230-2239.

Melamin-Formaldehyde (MF) Resins

scch { }

Source: www.deurowood.com



- Degree of polymerization/cross-linkage determines mechanical, thermal and electrical properties of MF resin

→ **Inline monitoring by NIR Spectroscopy**

Use Cases

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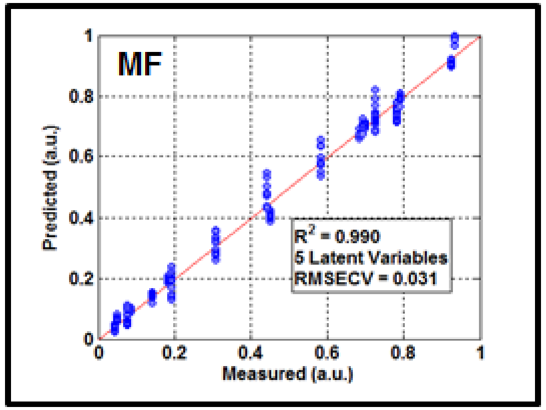
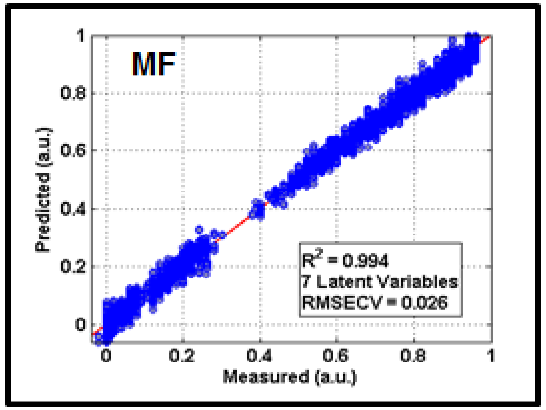
Dosage

formaldehyde
concentration



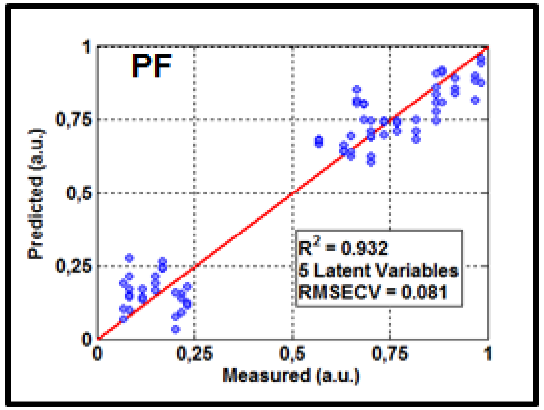
Inline process control

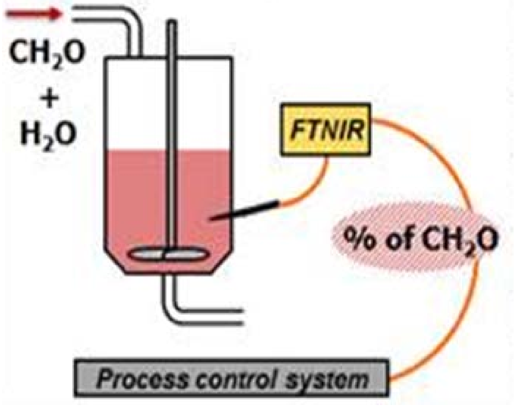
turbidity point (MF resin)
turbidity time (PF resin)

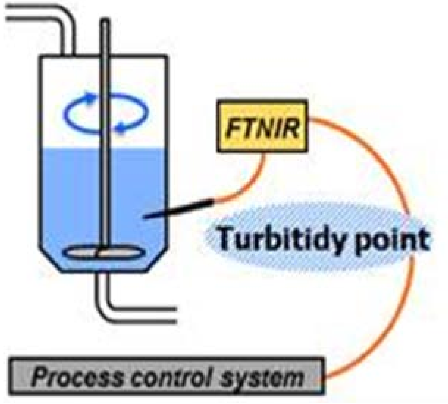


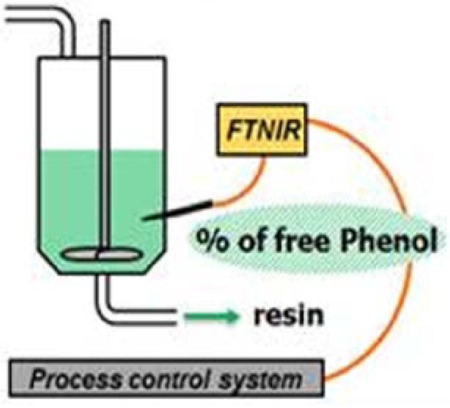
Quality control

free phenol content
in PF resin









Chemometrics as a Service (MetaLink)

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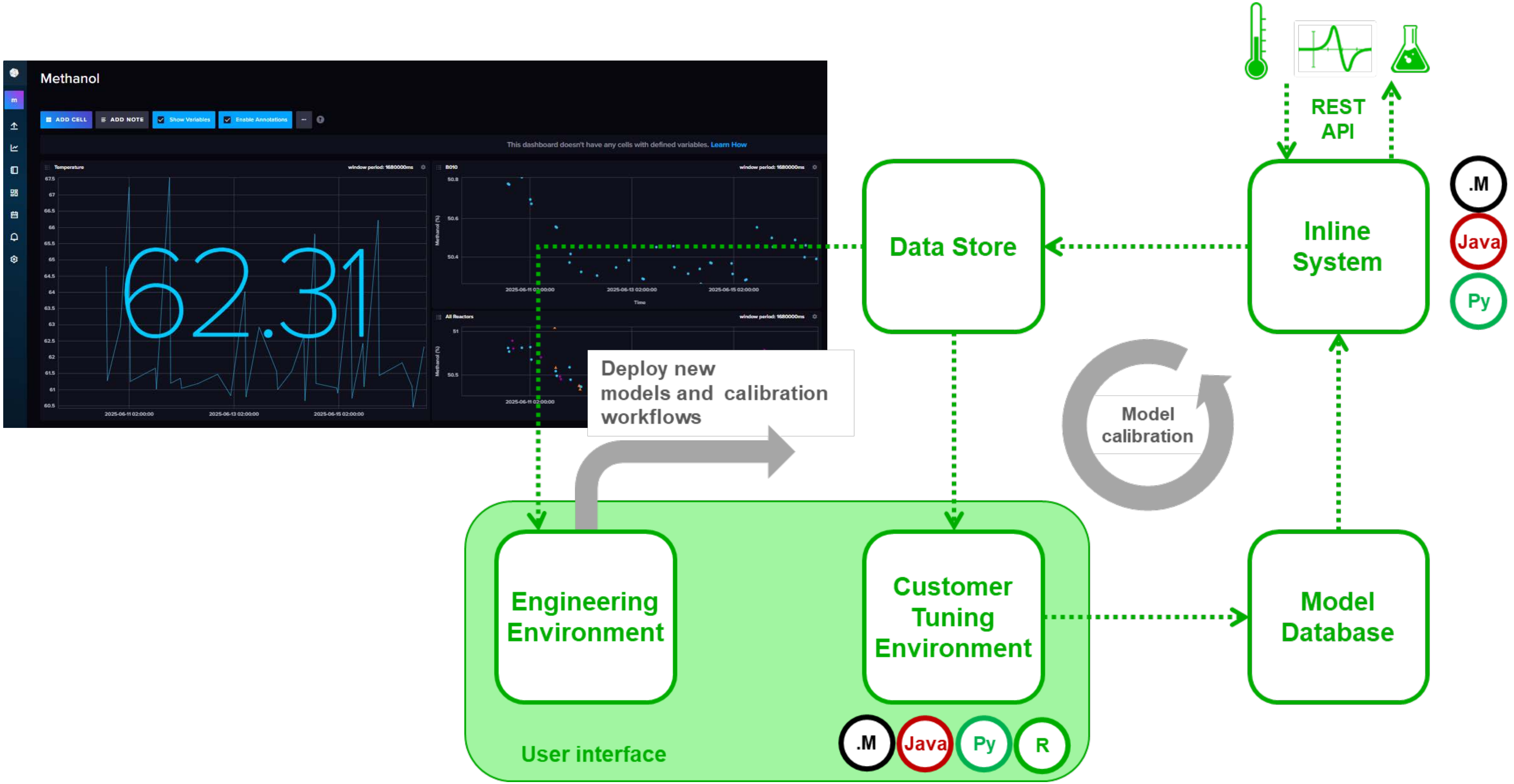

FFG Projects PAC/imPACts/PSSP

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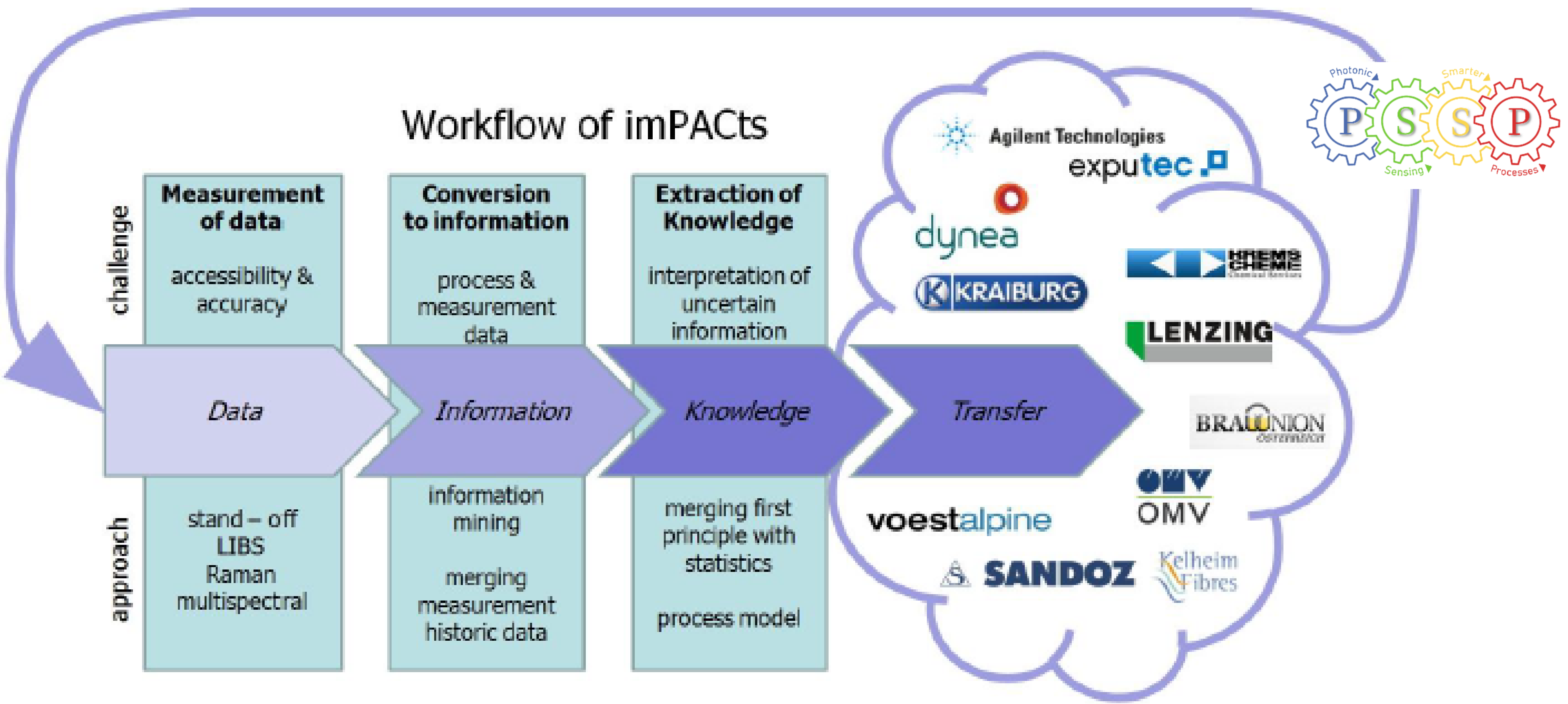

FFG Forschung wirkt.

Bundesministerium
Digitalisierung und
Wirtschaftsstandort

Bundesministerium
Klimaschutz, Umwelt,
Energie, Mobilität,
Innovation und Technologie

ober österreich

NIR Spectroscopy

NIR Spectroscopy

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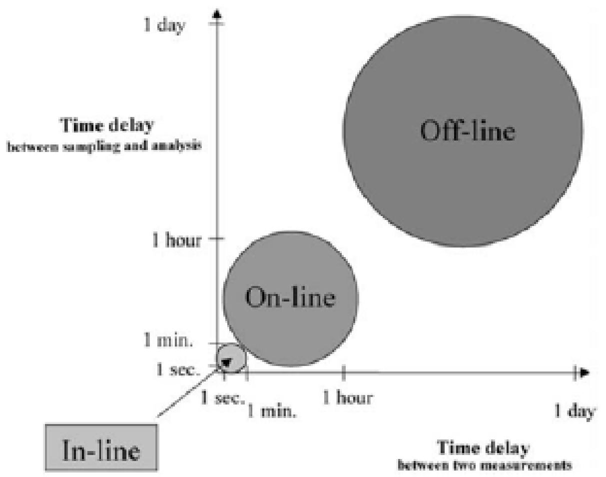
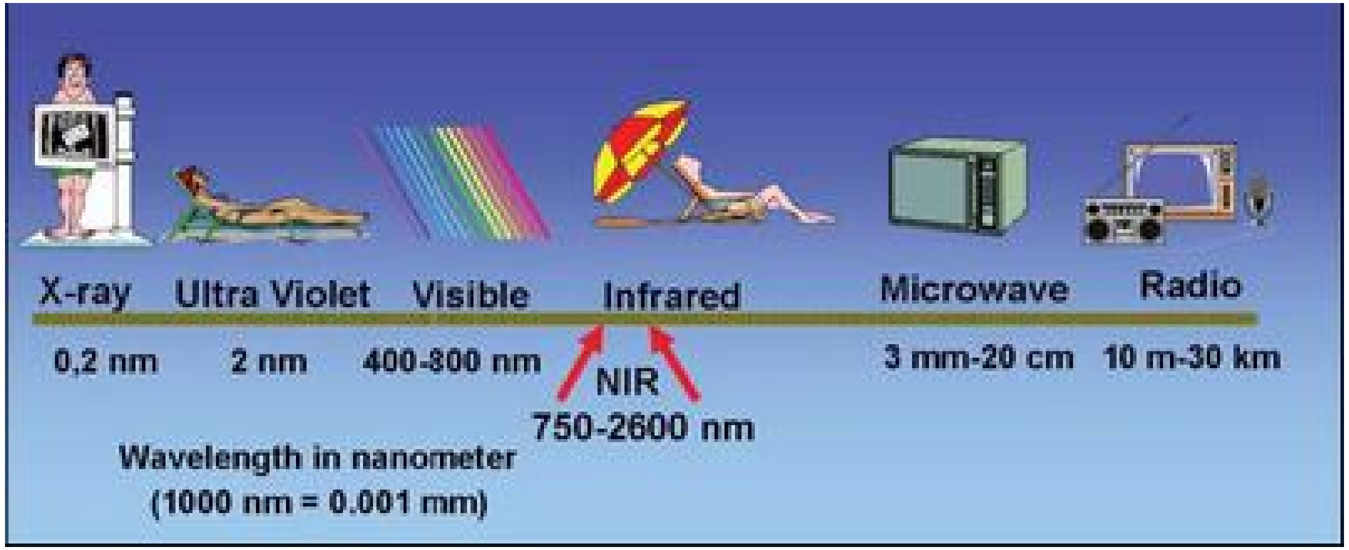
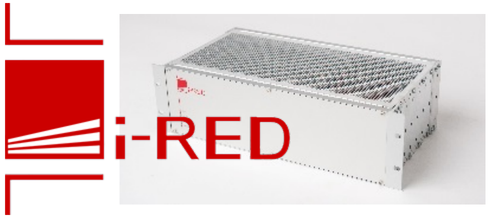
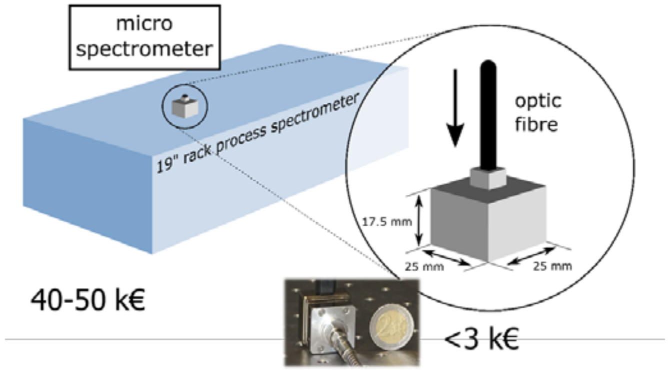


***Figure 1**: Comparison of typical time delays in off-line, at-line, on-line and in-line measurement approaches.*

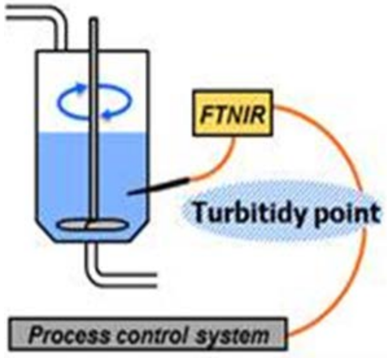


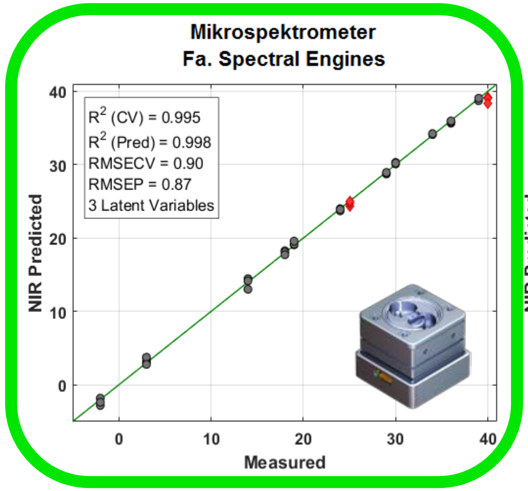


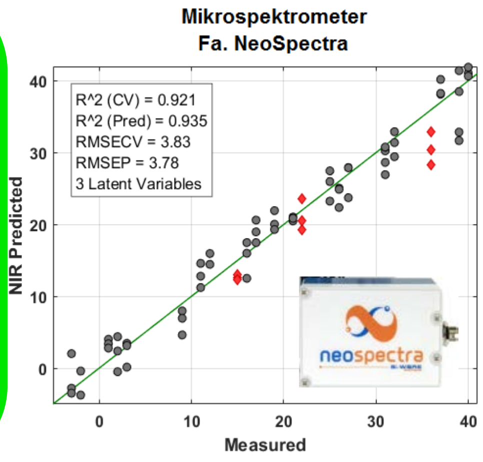


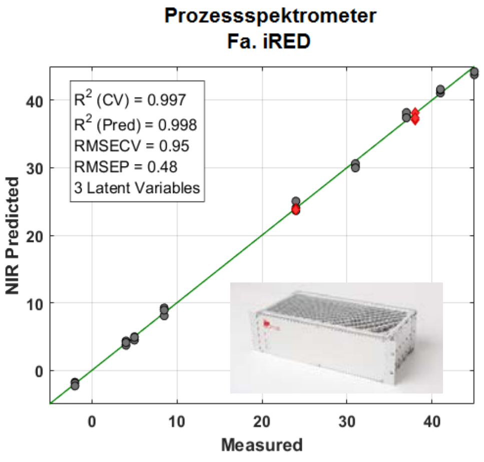
- Inline FTNIR Process Spectrometer (iRed)
- (Fabry-Pérot) Micro Spectrometer (Spectral Engines)

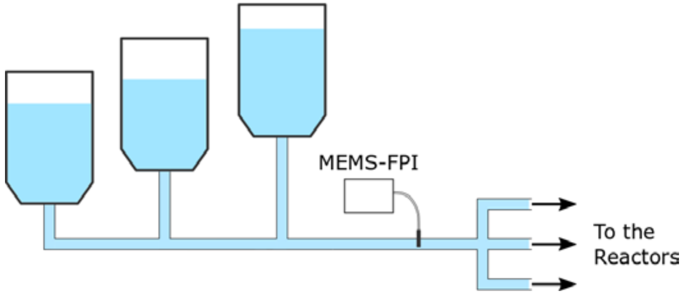
Microspectrometry





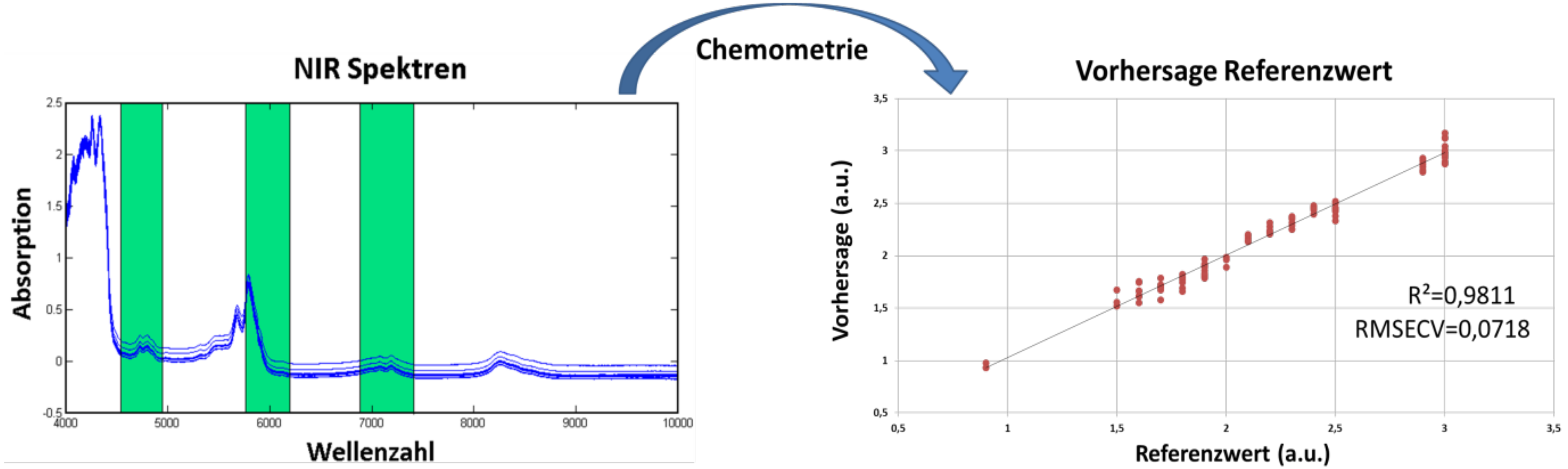






Kategorie	NIRONE 2.0 (Fa. Spectral Engines)	SWS62221-2.5 (Fa. NeoSpectra)	Prozessspektrometer Fa. iRED
SNR	>10000	>3000	>10000
Auflösung, Messzeit	2 nm, ca. 8 sek	8 nm, 8 sek	3 nm, 8 sek
Kalibrierung: R^2, RMSECV	0,995 0,90	0,921 3,83	0,997 0,95
Validierung: R^2, RMSEP	0,998 0,87	0,935 3,78	0,998 0,48
Preis (Jahr)	3290€ (2016)	2500€ (2016)	ca. 38000€ (2015)

Data Processing/Chemometrics



Spektraldaten mit den für das Modell relevanten Bereichen

Diagramm mit vorhergesagten Werten. Der große Determinations-koeffizient bestätigt die gute Eignung des zugrundeliegenden Modells

- Spectroscopy = Hardware & Experimentation & Data Processing (Chemometrics)

Experimentation - Robustness

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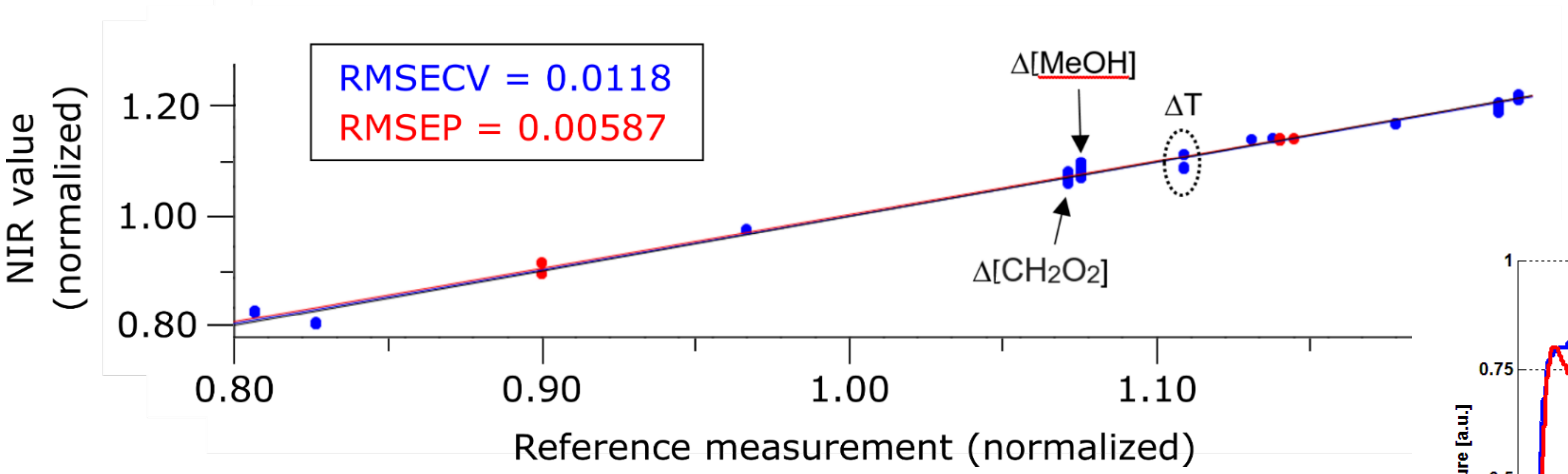

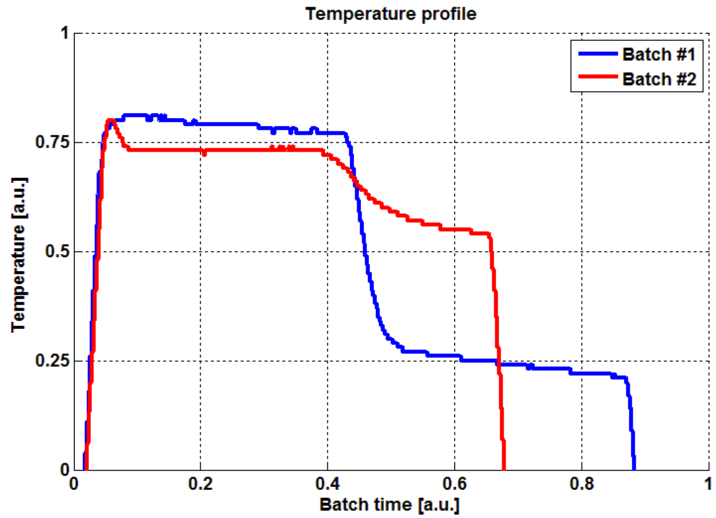

- Spiking experiments
  - → Robustify calibration against known sources of variability
  - → Validation!

Chemometrics

Data set shift & Model drift

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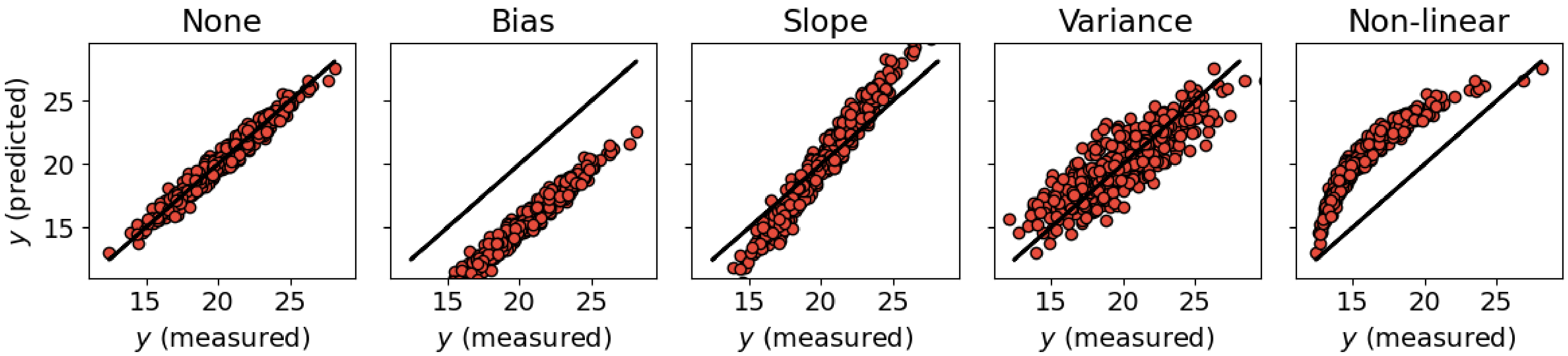
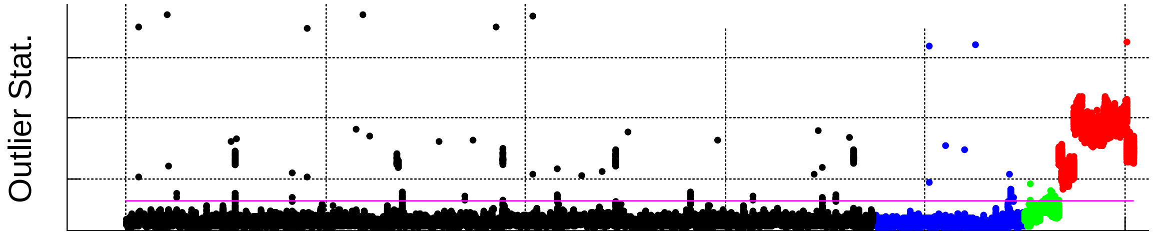


JM Roger *et al.* 2025



- Change in $P(X), P(Y), P(Y|X)$

Roger, J. M., Diaz, V. F., & Langerodi, R. N. (2025). Cloning instruments, model maintenance and calibration transfer. *TrAC Trends in Analytical Chemistry*, 118319.

Sources of Drift

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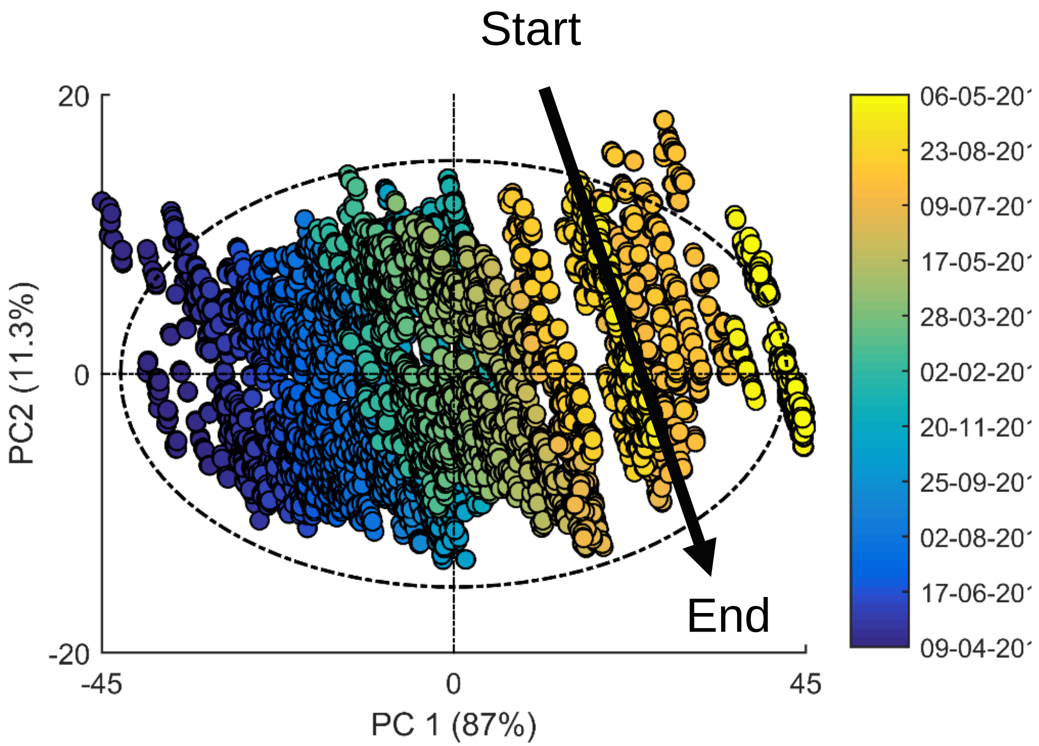

- Known (ΔT) and unknown (!) sources of variability

Robustness
Temperature

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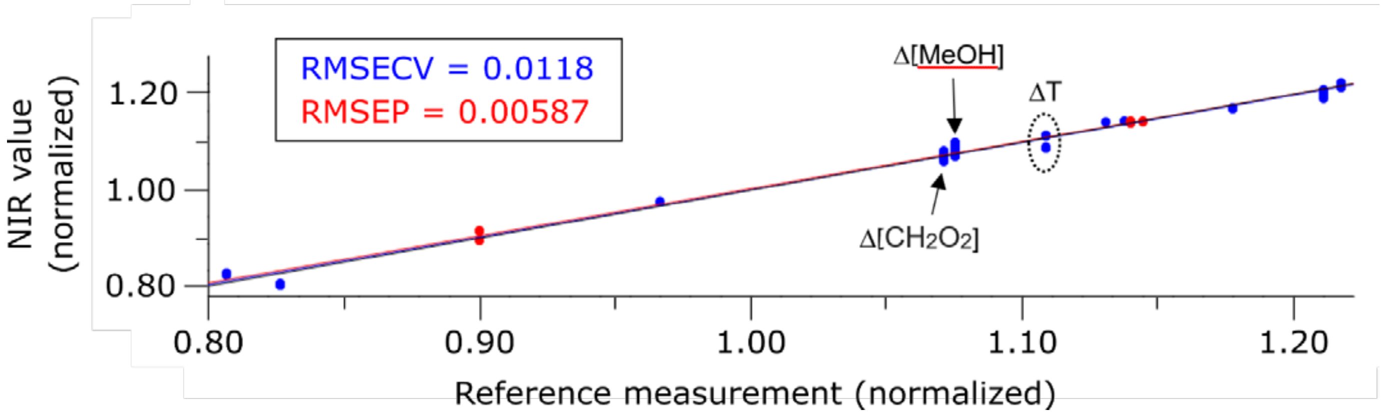
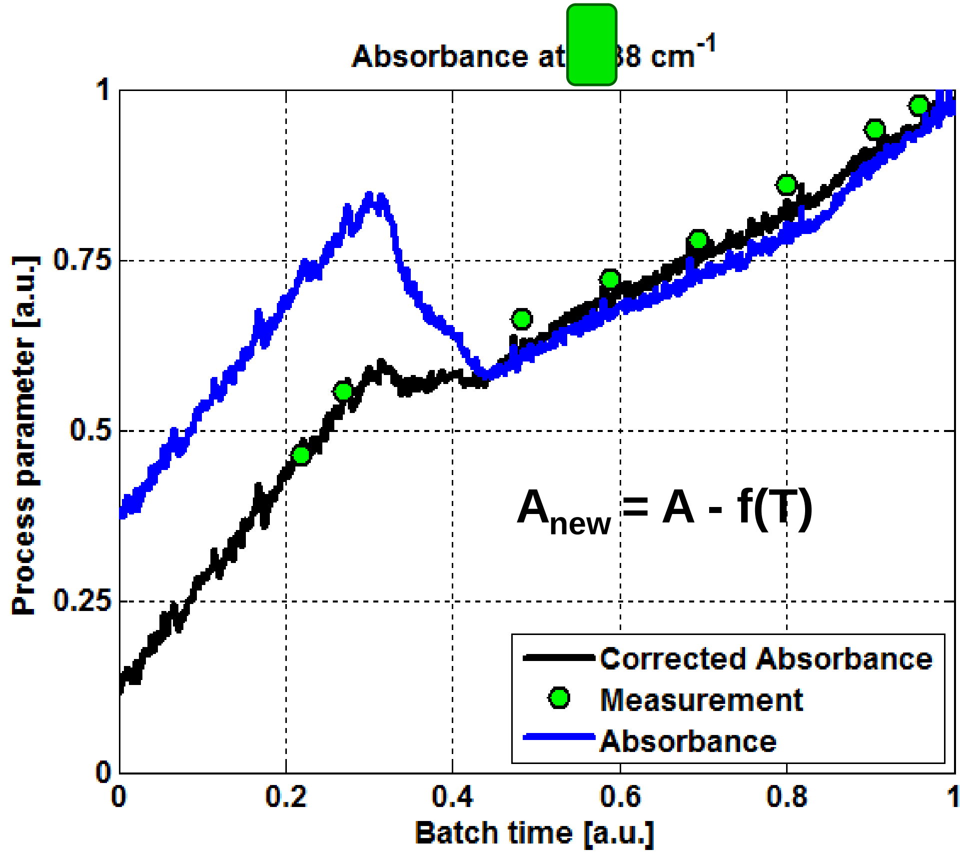


- Temperature correction
  - **„Spiking“ experiments**
  - Modeling out the temperature dependence
  - Variable selection

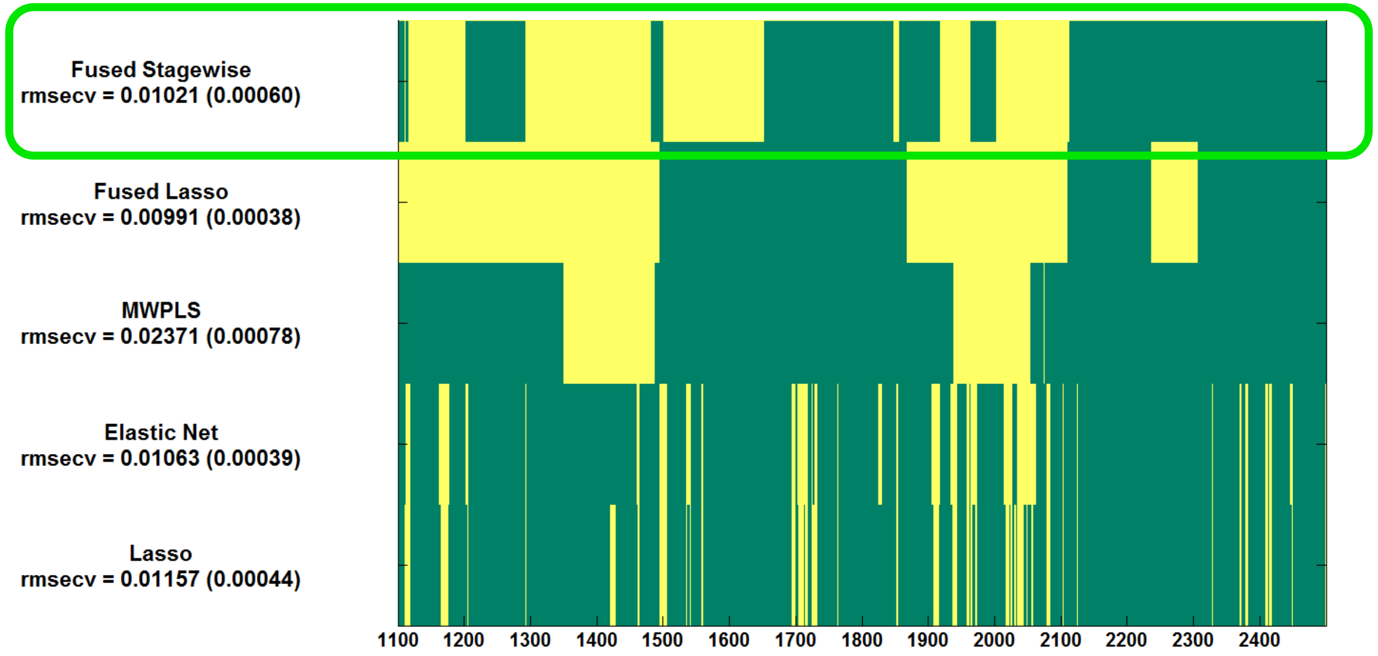
Robustness
Temperature



- Temperature correction
  - „Spiking“ experiments
  - **Modeling out the temperature dependence**
  - Variable selection

Variable Selection

$$\min_{\beta}\left\{\|y - X\beta\|_2^2 + \underbrace{\lambda_1\|\beta\|_1}_{\text{Variables}} + \underbrace{\lambda_2\sum_{j=1}^{p-1}|\beta_{j+1} - \beta_j|}_{\text{Regions}}\right\}$$



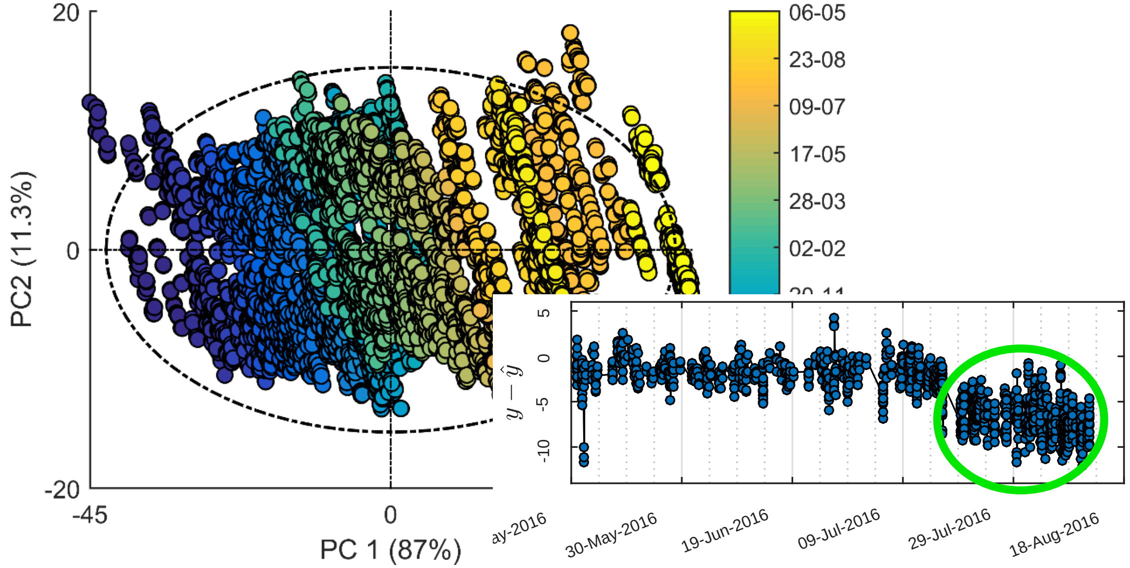
Malli et al. 2015

- Temperature correction
  - Spiking experiments
  - Modeling out the temperature dependence
  - **Variable selection**

Malli, B., & Natschläger, T. (2015). Fused stagewise regression—A waveband selection algorithm for spectroscopy. *Chemometrics and Intelligent Laboratory Systems*, *149*, 53-65.

Robustness
Unknown Drift

Calibration Data



„Drift Component“

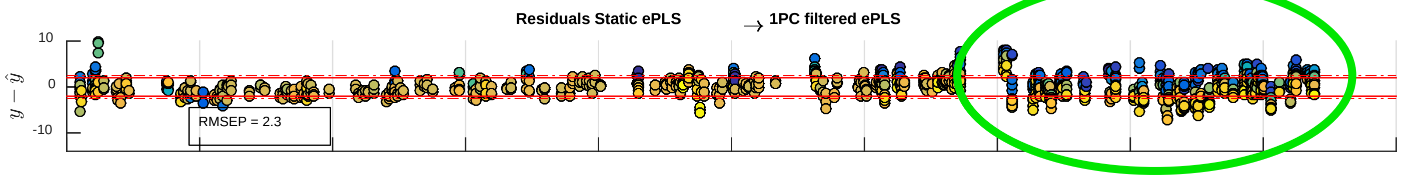
Removal of Drift Component

1) $X^t_{res} = X^t - t_1 p_1'$ (PCA)

2) $\beta_0, \beta_{PLS} \leftarrow X^t_{res}, Y^t$ (PLS on Residuals)

3) $x^{new}_{filtered} = x^{new} - (x^{new} p_1) p_1'$ (Filter)

4) $y^{new} = \beta_0 + \beta' x^{new}_{filtered}$ (Prediction)



- Removing unknown sources of variability
  - → Preprocessing

Drift Detection

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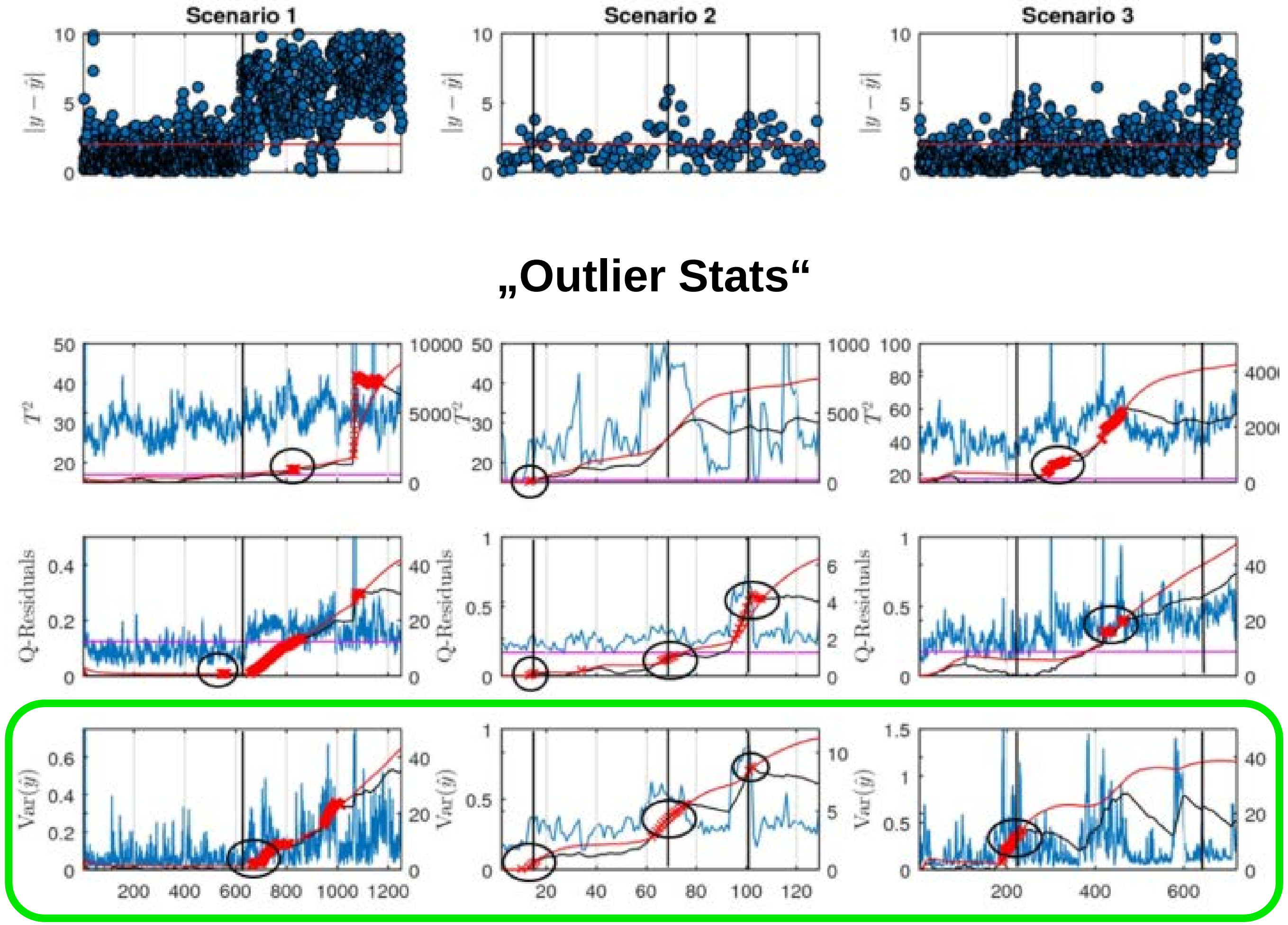
Nikzad-Langerodi *et al.* 2018

Prediction Error

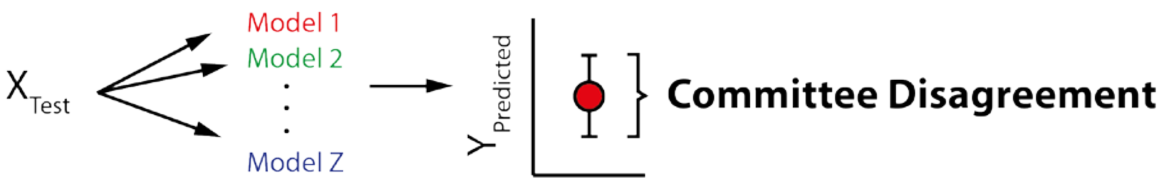
„Outlier Stats“



- Traditional outlier stats (T^2, Q_{Res})
  - False Alarms
  - Violation of crit. limits not always useful

Nikzad-Langerodi, R., Lughofer, E., Cernuda, C., Reischer, T., Kantner, W., Pawliczek, M., & Brandstett model adaptation. *Analytica Chimica Acta*, *1013*, 1-12.

Drift Detection

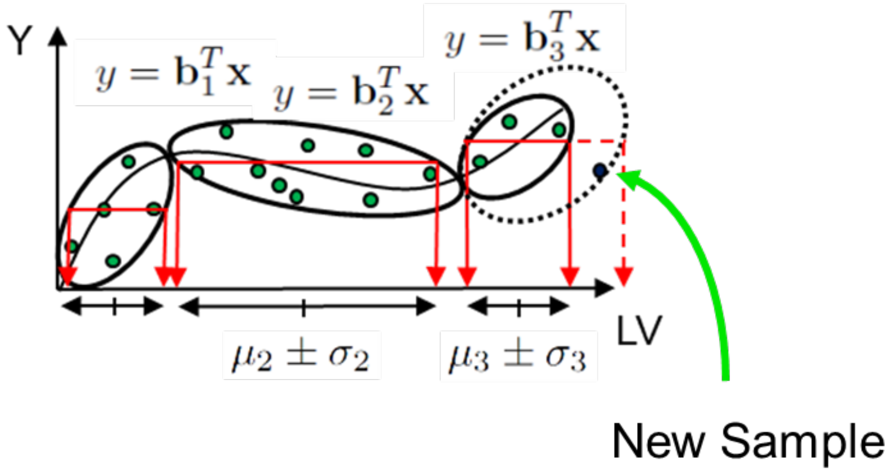


Nikzad-Langerodi *et al.* 2018

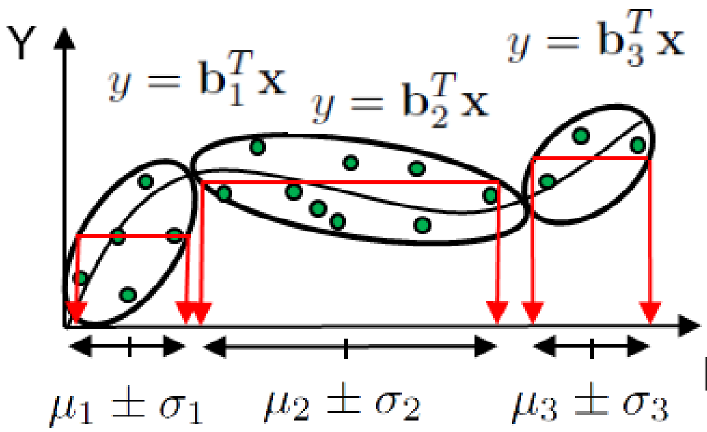
- „Committee Disagreement“
  - Prediction variance of a PLS ensemble

Nikzad-Langerodi, R., Lughofer, E., Cernuda, C., Reischer, T., Kantner, W., Pawliczek, M., & Brandstetter, M. (2018). Calibration model maintenance in melamine resin production: Integrating drift detection, smart sample selection and model adaptation. *Analytica Chimica Acta*, *1013*, 1-12.

Model Maintenance (Dynamic)

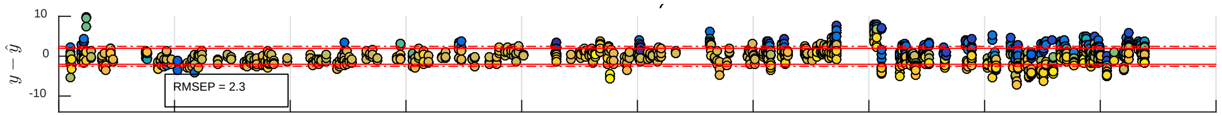


Fuzzy - PLS



$$\hat{y} = \sum_{i=1}^{C} f_i(\mathbf{t}) \underbrace{\frac{\exp(-1/2(\mathbf{t}-\mathbf{c}_i)\Sigma_i^{-1}(\mathbf{t}-\mathbf{c}_i))}{\sum_{i=1}^{C}\exp(-1/2(\mathbf{t}-\mathbf{c}_i)\Sigma_i^{-1}(\mathbf{t}-\mathbf{c}_i))}}_{\text{Normalized Membership Degree}}$$

- Fuzzy Systems & Latent Variable Models
  - „Locally Weighted Regression“
  - (Unsupervised) updating of fuzzy rule bases



Nikzad-Langerodi, R., Lughofer, E., Cernuda, C., Reischer, T., Kantner, W., Pawliczek, M., & Brandstetter, M. (2018). Calibration model maintenance in melamine resin production: Integrating drift detection, smart sample selection and model adaptation. *Analytica Chimica Acta*, *1013*, 1-12.

Model Maintenance
Transfer Learning/Domain Adaptation

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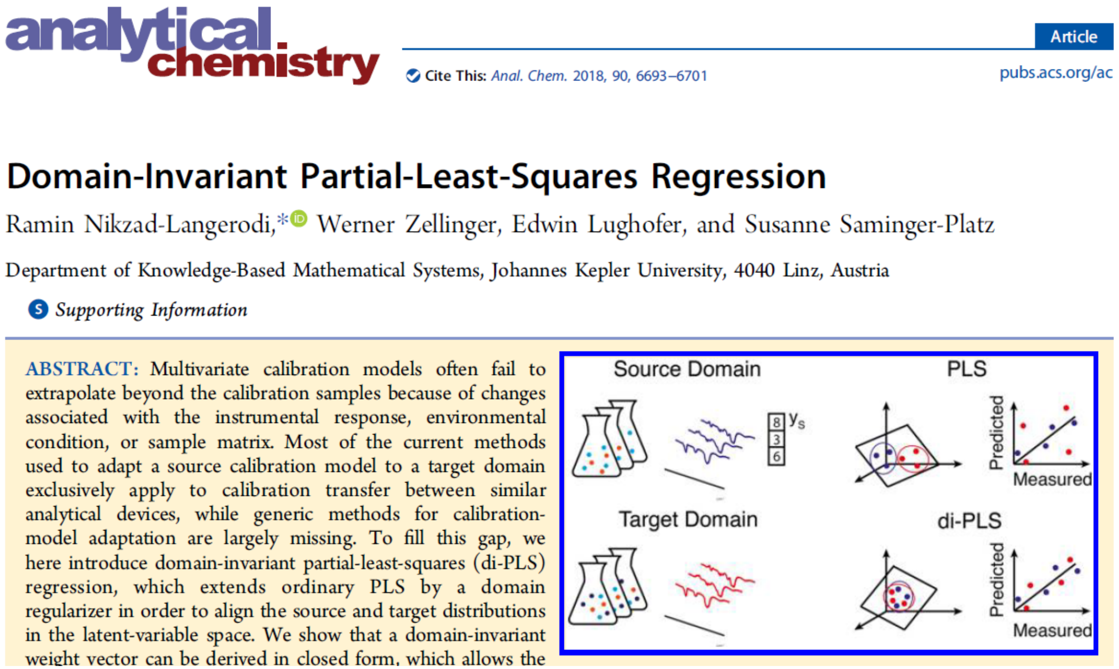


analytical chemistry

Article

Cite This: *Anal. Chem.* 2018, 90, 6693–6701

pubs.acs.org/ac

Domain-Invariant Partial-Least-Squares Regression

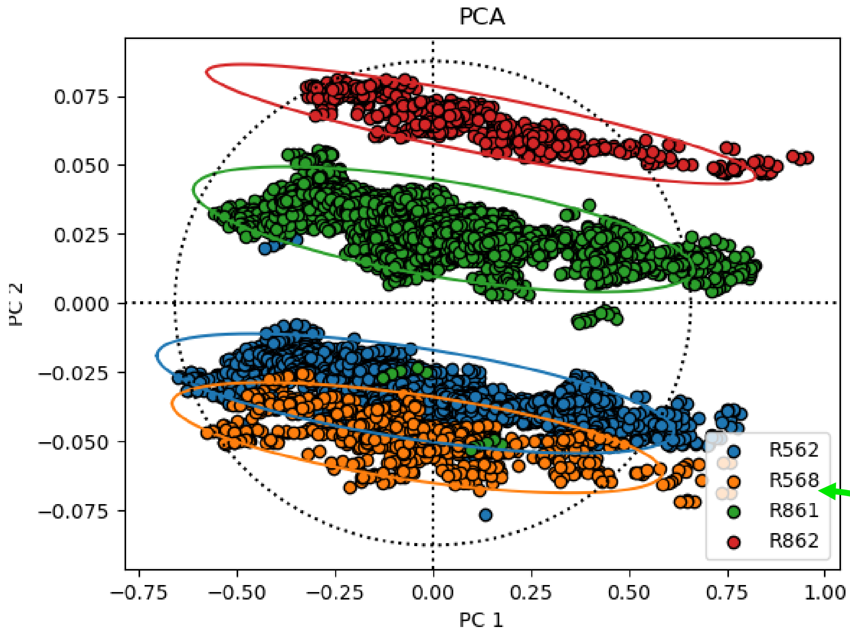
Ramin Nikzad-Langerodi,* Werner Zellinger, Edwin Lughofer, and Susanne Saminger-Platz

Department of Knowledge-Based Mathematical Systems, Johannes Kepler University, 4040 Linz, Austria

Supporting Information

ABSTRACT: Multivariate calibration models often fail to extrapolate beyond the calibration samples because of changes associated with the instrumental response, environmental condition, or sample matrix. Most of the current methods used to adapt a source calibration model to a target domain exclusively apply to calibration transfer between similar analytical devices, while generic methods for calibration-model adaptation are largely missing. To fill this gap, we here introduce domain-invariant partial-least-squares (di-PLS) regression, which extends ordinary PLS by a domain regularizer in order to align the source and target distributions in the latent-variable space. We show that a domain-invariant weight vector can be derived in closed form, which allows the

Nikzad-Langerodi *et al.* 2018



https://github.com/RNL1/Melamine-Dataset

Melamine Recipes

- Transfer Learning
  - Re-use Data/Model from related domain to help learning in new domain (e.g., recipe/device etc.)

Nikzad-Langerodi, R., Zellinger, W., Lughofer, E., & Saminger-Platz, S. (2018). Domain-invariant partial-least-squares regression. *Analytical chemistry*, *90*(11), 6693-6701.

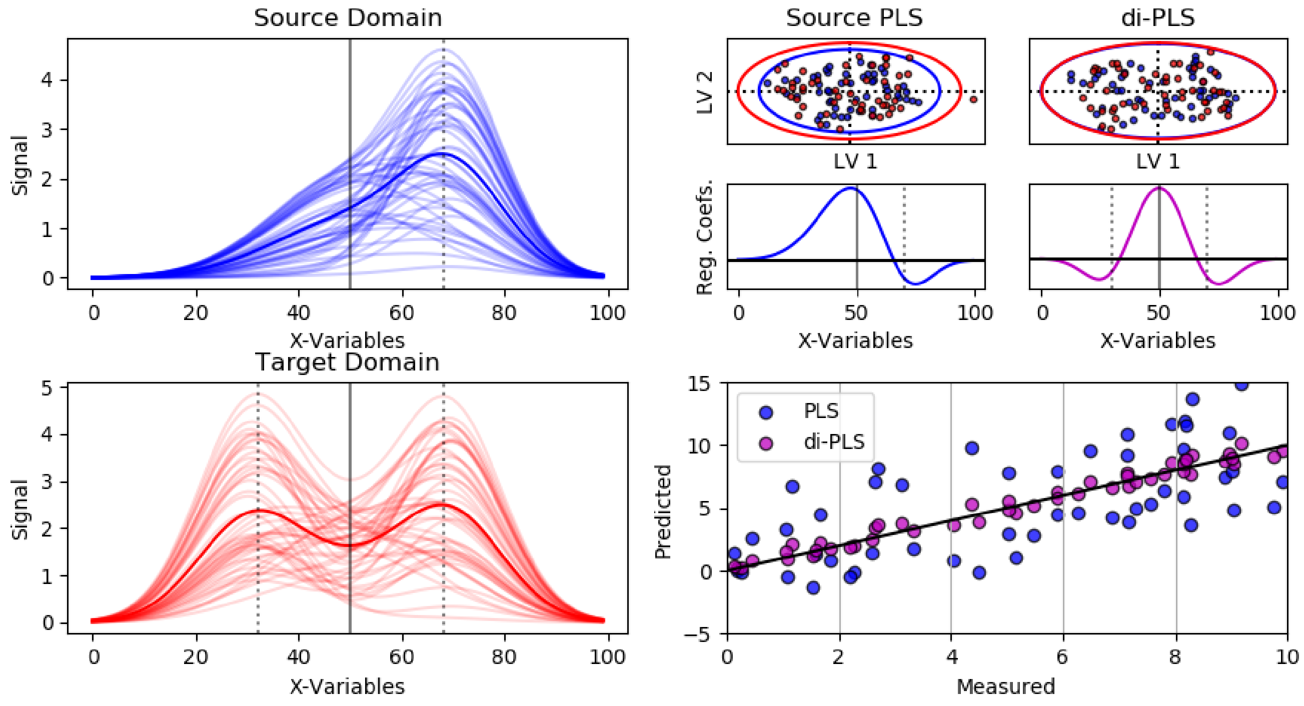
Model Maintenance
Transfer Learning/Domain Adaptation

scch { }

$$\min_{\mathbf{w}^{\mathrm{T}}\mathbf{w}=1} \|\mathbf{X}_S - \mathbf{y}\mathbf{w}^{\mathrm{T}}\|_{\mathrm{F}}^2 + \underbrace{\gamma \mathbf{w}^{\mathrm{T}}\mathbf{\Lambda}\mathbf{w}}_{\text{Domain Regularization}}$$

$$\Lambda \sim \frac{1}{n_S - 1}\mathbf{X}_S^T\mathbf{X}_S - \frac{1}{n_T - 1}\mathbf{X}_T^T\mathbf{X}_T$$

Nikzad-Langerodi *et al.* 2018

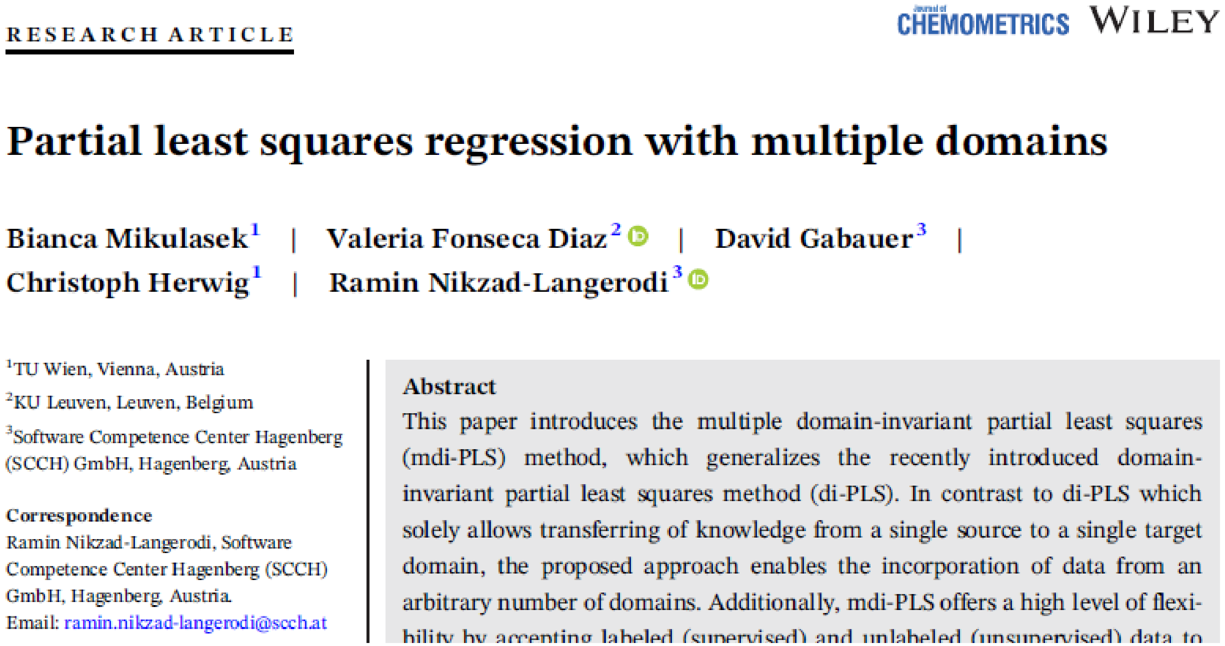


- di-PLS
  - Partial Least Squares with Domain Regularization
  - Aligns Distributions in Latent Space

https://github.com/B-Analytics/diPLSlib

Nikzad-Langerodi, R., Zellinger, W., Lughofer, E., & Saminger-Platz, S. (2018). Domain-invariant partial-least-squares regression. *Analytical chemistry*, *90*(11), 6693-6701.

Model Maintenance
Transfer Learning/Domain Adaptation



RESEARCH ARTICLE

CHEMOMETRICS WILEY

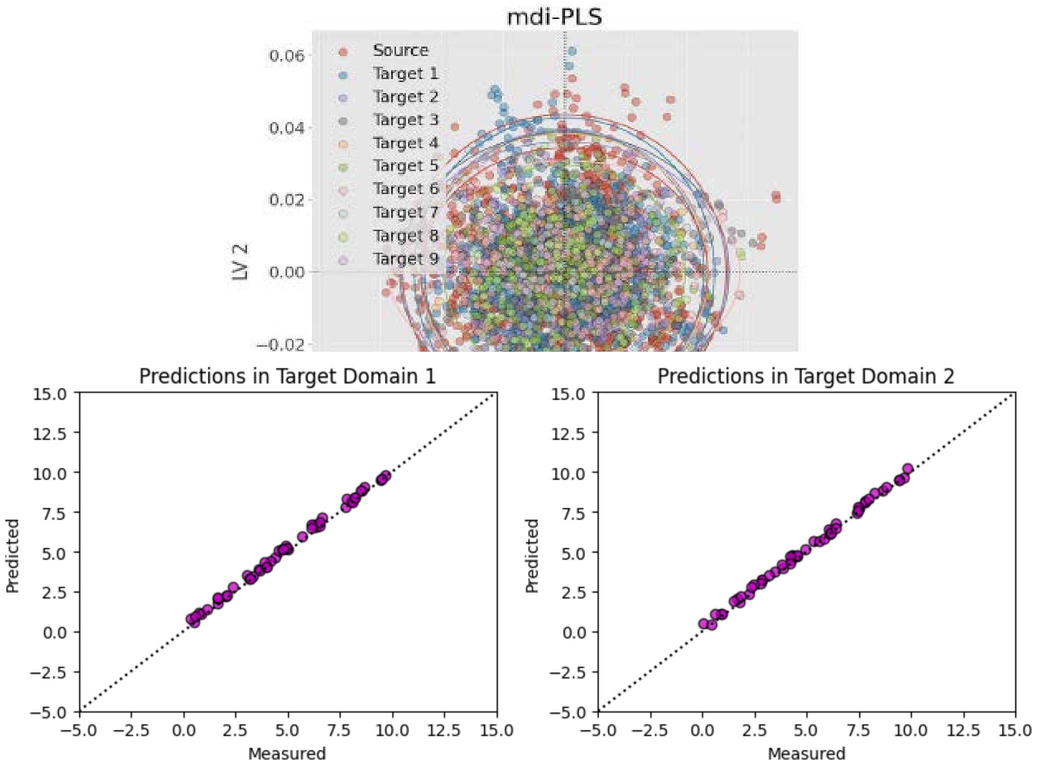
Partial least squares regression with multiple domains

Bianca Mikulasek[1] | Valeria Fonseca Diaz[2] | David Gabauer[3] | Christoph Herwig[1] | Ramin Nikzad-Langerodi[3]

[1]TU Wien, Vienna, Austria
[2]KU Leuven, Leuven, Belgium
[3]Software Competence Center Hagenberg (SCCH) GmbH, Hagenberg, Austria

Correspondence
Ramin Nikzad-Langerodi, Software Competence Center Hagenberg (SCCH) GmbH, Hagenberg, Austria.
Email: ramin.nikzad-langerodi@scch.at

Abstract
This paper introduces the multiple domain-invariant partial least squares (mdi-PLS) method, which generalizes the recently introduced domain-invariant partial least squares method (di-PLS). In contrast to di-PLS which solely allows transferring of knowledge from a single source to a single target domain, the proposed approach enables the incorporation of data from an arbitrary number of domains. Additionally, mdi-PLS offers a high level of flexi-



Mikulasek *et al.* 2023

- mdi-PLS
    - Global models over multiple domains

Mikulasek, B., Fonseca Diaz, V., Gabauer, D., Herwig, C., & Nikzad-Langerodi, R. (2023). Partial least squares regression with multiple domains. *Journal of Chemometrics*, *37*(5), e3477.

Model Maintenance
Transfer Learning/Domain Adaptation

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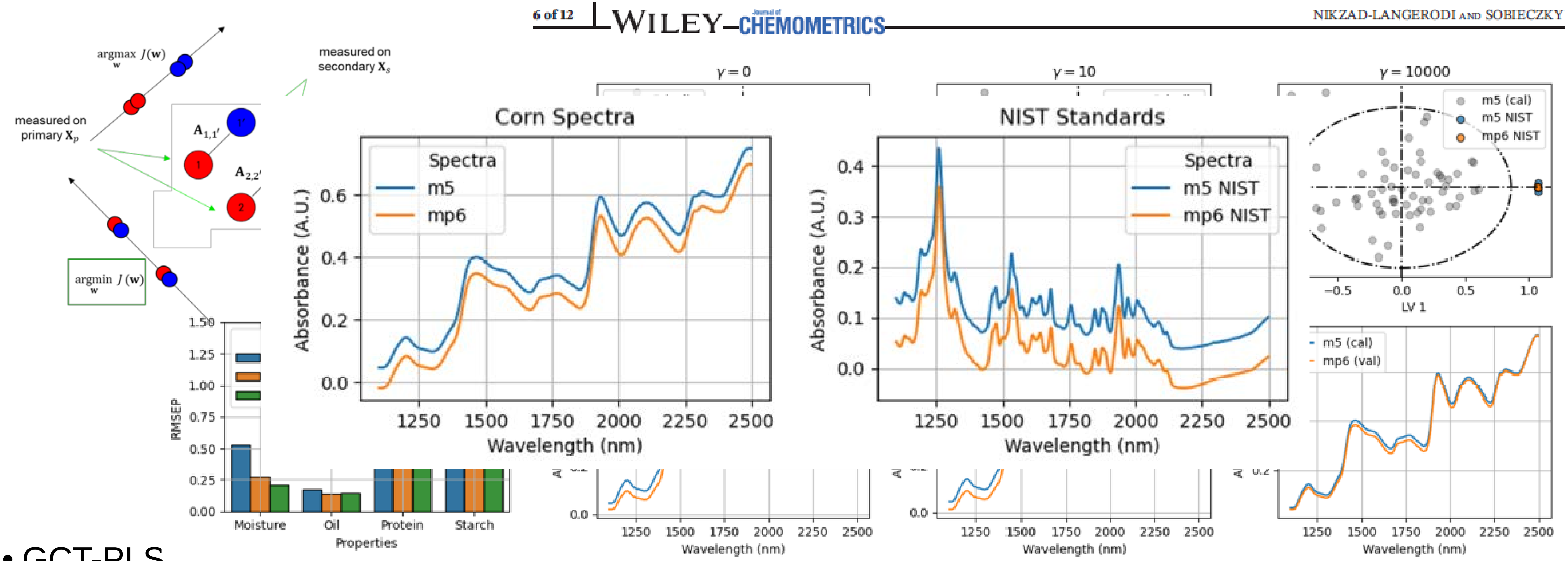
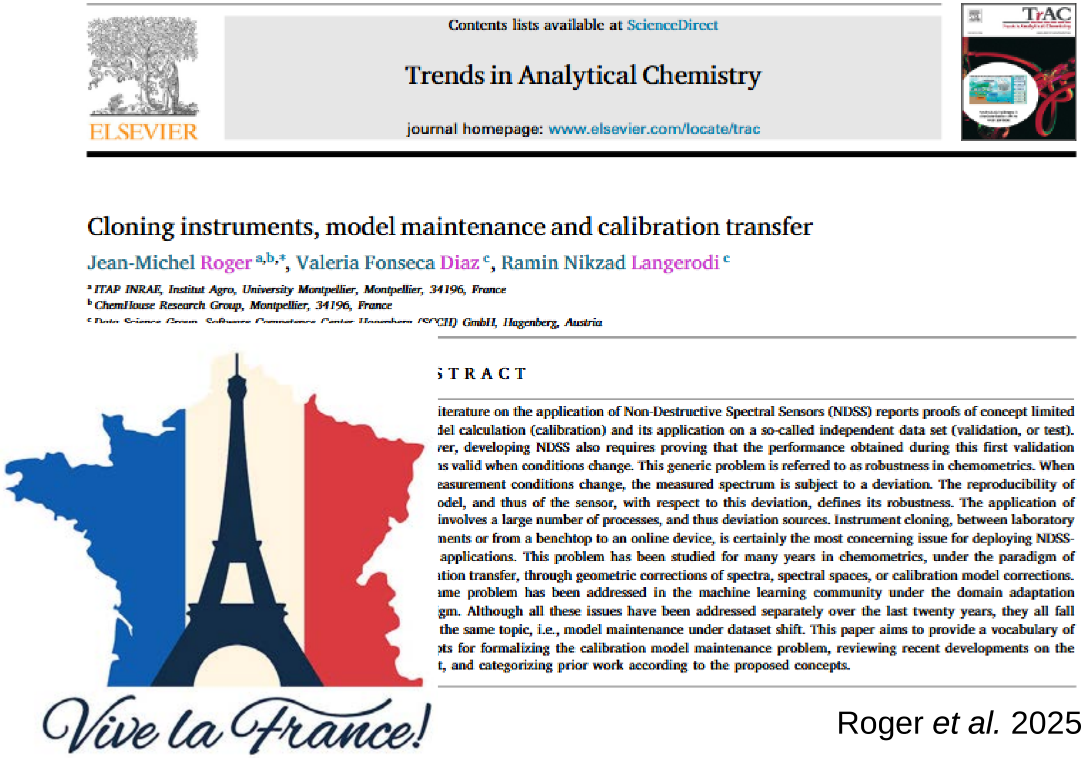


- GCT-PLS
  - Domain regularization for calibration transfer

Nikzad-Langerodi & Sobieczky 2021

Nikzad-Langerodi, R., & Sobieczky, F. (2021). Graph-based calibration transfer. *Journal of Chemometrics*, *35*(4), e3319.

Model Maintenance
Transfer Learning/Domain Adaptation



Contents lists available at ScienceDirect

Trends in Analytical Chemistry

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

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TrAC

Cloning instruments, model maintenance and calibration transfer

Jean-Michel Roger[a,b,*], Valeria Fonseca Diaz[c], Ramin Nikzad Langerodi[c]

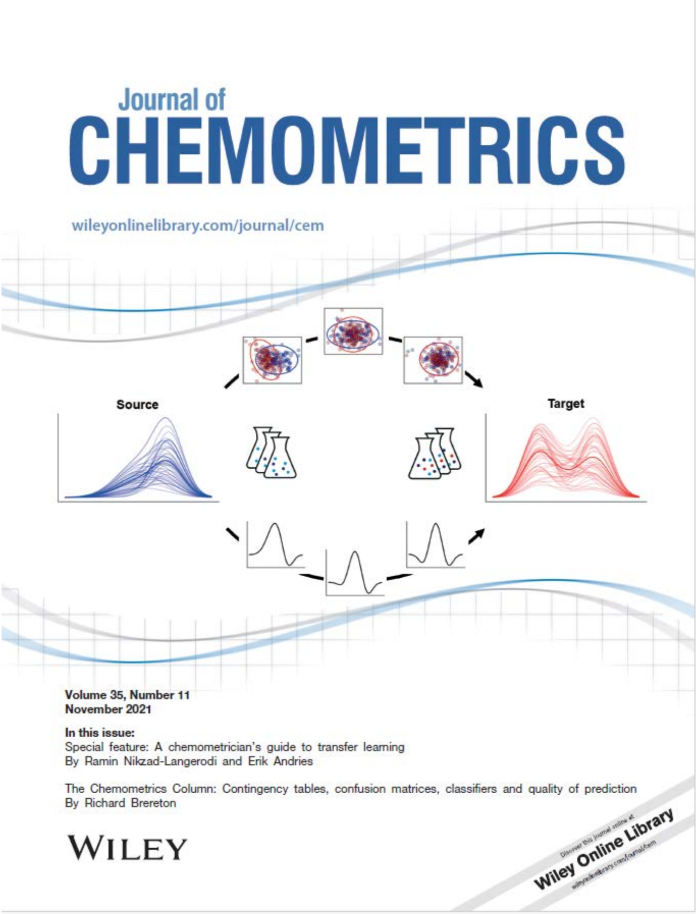
[a] ITAP INRAE, Institut Agro, University Montpellier, Montpellier, 34196, France
[b] ChemHouse Research Group, Montpellier, 34196, France
[c] Data Science Group, Software Competence Center Hagenberg (SCCH) GmbH, Hagenberg, Austria

STRACT

iterature on the application of Non-Destructive Spectral Sensors (NDSS) reports proofs of concept limited del calculation (calibration) and its application on a so-called independent data set (validation, or test). ver, developing NDSS also requires proving that the performance obtained during this first validation as valid when conditions change. This generic problem is referred to as robustness in chemometrics. When easurement conditions change, the measured spectrum is subject to a deviation. The reproducibility of odel, and thus of the sensor, with respect to this deviation, defines its robustness. The application of involves a large number of processes, and thus deviation sources. Instrument cloning, between laboratory nents or from a benchtop to an online device, is certainly the most concerning issue for deploying NDSS- applications. This problem has been studied for many years in chemometrics, under the paradigm of ation transfer, through geometric corrections of spectra, spectral spaces, or calibration model corrections. ame problem has been addressed in the machine learning community under the domain adaptation gm. Although all these issues have been addressed separately over the last twenty years, they all fall the same topic, i.e., model maintenance under dataset shift. This paper aims to provide a vocabulary of pts for formalizing the calibration model maintenance problem, reviewing recent developments on the t, and categorizing prior work according to the proposed concepts.

Vive la France!

Roger *et al.* 2025



Nikzad-Langerodi & Andries 2021

- Further Reading

Nikzad-Langerodi, R., & Andries, E. (2021). A chemometrician's guide to transfer learning. *Journal of Chemometrics*, *35*(11), e3373.

Conclusion

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- Bringing NIR to industry requires an **<u>interdisciplinary effort</u>**
- Spectroscopy = Sensor + Experiment + Chemometrics
- Industrial projects are important drivers of scientific advancements (in chemometrics)

Acknowledgements

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Thomas Reischer
(KremsChem)

IR & Raman Group
(RECENDT GmbH)

Data Science Group
(SCCH GmbH)

Edwin Lughofer
(JKU Linz)

Thank You!

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Innovation und Technologie

ober österreich

The research reported in this presentation has been funded by the Federal Ministry for Innovation, Mobility and Infrastructure (BMIMI), the Federal Ministry for Economy, Energy and Tourism (BMWET), and the State of Upper Austria in the frame of the SCCH competence center INTEGRATE [(FFG grant no. 892418)] in the COMET - Competence Centers for Excellent Technologies Programme managed by Austrian Research Promotion Agency FFG.