

# Chemometrics Workshop - Wien 2010

Monday, 28 June 2010, 9:30 - 13:00

## Schedule

- 9:30 - 9:40 A. Friedl:  
Short presentation of the *Institute of Chemical Engineering*  
and the Research Division *Thermal Process Engineering and Process Simulation*
- 9:40 - 10:05 O. Rodionova\*, A.L. Pomerantsev, L. Houmøller, A.V. Shpak, O. Shpigun:  
Application of NIR for counterfeit drug detection. Another proof that chemometrics is usable: NIR confirmed by HPLC-DAD-MS and CE-UV
- 10:05 - 10:30 A.L. Pomerantsev\*, O. Rodionova:  
PAT solution to the drug release prediction
- 10:30 - 10:40 A. Friedl:  
Chemical engineering and chemometrics
- 10:40 - 10:50 Discussion
- 10:50 - 11:10 *Break*
- 11:10 - 11:25 B. Liebmann\*, A. Friedl, K. Varmuza:  
Applicability of near-infrared spectroscopy for process monitoring in bioethanol production
- 11:25 - 11:40 K. Varmuza:  
A curious method for data from curious experiments:  
Random projection with TOF-SIMS data from comet-relevant samples
- 11:40 - 12:00 O. Rodionova, A.L. Pomerantsev:  
Chemometrics in Excel
- 12:00 - 12:20 R. Dutter, A. Zainzinger\*, A. Alfons\*:  
*DAS+R*: A graphical user interface for multivariate data analysis in *R*
- 12:20 - 12:40 P. Filzmoser:  
The *chemometrics* package in *R* - applications in multivariate calibration and classification
- 12:40 - 12:55 Discussion