

## Programme of 1st Winter School of ECO

MONDAY, 21.FEB.		
09:00 - 09:15	<b>Welcome by the organisator and the projectmanager</b>	HS A_E.01
<b>Practical Lessons</b>		
09:15 - 12:30	Training in PLS methods <i>Dr. Frank Westad, CAMO Software AS, Norway</i> <ul style="list-style-type: none"> <li>· Introduction: Science, validation, significance vs. relevance</li> <li>· Visualising data – the basic tools</li> <li>· The mother of all multivariate methods: Principal Component Analysis (PCA) - theory and examples</li> <li>· Outlier detection in PCA</li> </ul>	CR A_2.01
12:30 - 13:00	Lunch Break	Cafeteria
13:00 - 17:00	Training in PLS methods <i>Dr. Frank Westad, CAMO Software AS, Norway</i> <ul style="list-style-type: none"> <li>· Hands-on exercise, PCA</li> <li>· Multivariate regression – theory and examples               <ul style="list-style-type: none"> <li>- Multiple Linear Regression (MLR)</li> <li>- Principal Component Regression (PCR)</li> <li>- Partial Least Squares Regression (PLSR)</li> </ul> </li> <li>· Hands-on exercise, regression</li> <li>· Prediction</li> <li>· Summary: Steps in multivariate regression</li> </ul>	CR A_2.01
17:00	End	
TUESDAY, 22.FEB.		
<b>Practical Lessons</b>		
08:30 - 12:30	Training in PLS methods <i>Dr. Frank Westad, CAMO Software AS, Norway</i> <ul style="list-style-type: none"> <li>· Variable selection</li> <li>· Multivariate regression: More hands-on               <ol style="list-style-type: none"> <li>1. Choosing validation scheme</li> <li>2. Decide on transformation of the original data</li> <li>3. Modelling</li> <li>4. Outlier detection</li> <li>5. Prediction</li> </ol> </li> <li>· When do we need non-linear methods?</li> <li>· Introduction to supervised classification methods               <ol style="list-style-type: none"> <li>1. PCA as a classification method</li> <li>2. PLS Discriminant Analysis (PLS-DA)</li> <li>3. Support Vector Machines</li> </ol> </li> <li>· Summary, questions and answers (30 mins)</li> </ul>	CR A_2.01
12:30 - 13:00	Lunch Break	Cafeteria
<b>Theoretical Lessons</b>		
13:00 - 15:00	Introduction to sampling on Wednesday and analytical exercises on Thursday <i>Prof. Thomas Knepper, Hochschule Fresenius, Idstein</i>	HS A_E.01
<b>Practical Lessons</b>		
15:00 - 18:00	Advanced training in OCHEM <i>Dr. Igor Tetko, Helmholtz-Zentrum München</i>	CR A_2.01
18:00	End	
18:30 - 23:00	Fellows meeting at "Brauhaus Idstein" <i>only for fellows</i>	
WEDNESDAY, 23.FEB.		
<b>Excursion</b>		
09:15 - 10:00	Bus ride to Schierstein	Meeting Point ZOB
10:00 - 14:00	Visit of Wasserwerk Schierstein including sampling	
11:00 - 13:00	Systematic monitoring of pesticide transport and fate in water and soil systems, <i>Prof. Thomas Knepper, Hochschule Fresenius, Idstein</i>	
15:00	Arrival in Nieder-Walluf	
15:00 - 16:00	Joint lunch at "Bug's Weinschänke" in Nieder-Walluf	
16:00	Departure Nieder-Walluf	Meeting Point KD
16:45	Arrival at Idstein	

**THURSDAY, 24.FEB.****Practical Lessons**

- Determination of pharmaceuticals with Liquid chromatography tandem mass spectrometry (LC-MS/MS) after solid phase extraction
- 09:00 - 12:30 Extraction of selected pharmaceuticals by solid phase extraction (SPE),  
Prof. Thomas Knepper and team, Hochschule Fresenius, Idstein
- Selected pharmaceuticals:
- Antibiotics sulfamethoxazole and trimethoprim,
  - Betablockers metoprolol and propranolol,
  - Antiepileptic drug carbamazepine,
  - Painkiller phenazon,
- SPE:
- Filtration of surface water samples
  - Adding internal standard
  - Conditioning the SPE cartridges
  - Extraction
  - Drying the SPE cartridges
  - Elution
  - Evaporation of the extracts

Laboratories

12:30 - 13:00

Lunch Break

Cafeteria

**Practical Lessons**

- 13:00 - 17:45 Analysis with LC-MS/MS, *Prof. Thomas Knepper, Hochschule Fresenius, Idstein*
- Instrument: 3200 Q Trap® LC/MS/MS (Applied Biosystems, Foster City, USA)
- LC-MS/MS method development:
- Infusion of one selected pharmaceutical via syringe pump
  - Optimisation of instrumental parameters (declustering potential, entrance potential, collision energy, collision cell entrance/exit potential) by continuous flow injection.
  - Discussion of fragmentation routes during collisional-induced dissociation (CID)
  - Development of a multiple reaction monitoring (MRM) method for all selected pharmaceuticals
  - Measuring the samples in MRM mode overnight.

17:45 - 18:00

Evaluation of Passive Sampling with SBSE (Autumn School) *Prof. Karl-Werner Schramm, Helmholtz-Zentrum München*

18:00 - 20:00

General Assembly *only for Project leaders and -manager*

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Laboratories

**FRIDAY, 25.FEB.****Practical Lessons**

- 09:00 - 12:30 Analysis with LC-MS/MS, *Prof. Thomas Knepper, Hochschule Fresenius, Idstein*
- Calibration
  - Quantification
  - Validation

Laboratories

12:30 - 13:30

Lunch Break

Cafeteria

**Theoretical Lessons**

- 13:30 - 15:00 Scientific discussion round of fellows *Dr. Eva Schlosser, Helmholtz-Zentrum München*
- 15:00 - 16:00 Scientific project management *Dr. Eva Schlosser, Helmholtz-Zentrum München*
- 16:00 - 17:00 Come together / Farewell
- 17:00 **Departure**

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