

## **EDA-EMERGE SUMMER SCHOOL**

Venue: Helmholtz-Centre for Environmental Research – UFZ, Leipzig, Germany

Organizer: Dr. Werner Brack, Dr. Selvan Govender

Date: 25.06 to 29.06.2012

Time: 9h00 – 18h00

### **Course description:**

The goal of the summer school was to create a common platform for all ESR fellows and partners to meet as early into the project as possible in order to highlight the basis for the start of successful PhD projects, achievement of EDA-EMERGE goals and by virtue of lectures and training courses, also cover a broad range of topics from bio-diagnosis, fractionation and structure elucidation to regulatory issues. As such ESR fellows and other more experienced PhD fellows from the partner and network institutes were invited to attend lectures and courses by internal EDA-EMERGE consortium members and external experts for 1 week during 25-29 Jun 2012 in Leipzig, Germany.

The summer school programme consisted of lectures, a poster session, a hands-on chemical structure elucidation workshop, laboratory tours and project meetings. The academic programme was supplemented with an excursion to the regenerated and rehabilitated Mulder river valley area in the German state of Saxony together with evening social activities such as a common dinner, daily common lunch and tea breaks and city tour, which afforded the fellows more intensive one on one discussions with presenters, co-supervisors and EDA-EMERGE scientists.

**AGENDA**

**EDA-EMERGE SUMMER SCHOOL**

25 - 29 June 2012, Leipzig, Germany

General	European Regulatory Framework	EDA & Sample Preparation	Chemical analysis & Structure Elucidation	Separation & Fractionation	Biodiagnostic Tools	PC based workshop
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Time	Monday 25 June 2012	Tuesday 26 June 2012	Wednesday 27 June 2012	Thursday 28 June 2012	Friday 29 June 2012
9:00	<b>Arrival</b>	W. Brack: EDA concepts and approaches	J. Hollender: Liquid chromatography-mass spectrometry (LC-MS)	K.E. Tollefsen: "omics" techniques and effect assessments	A. Tindall: Innovative vertebrate tools
10:00		K. van Leeuwen: Water pollution and drinking water	R. Altenburger: Mixture toxicity assessment and prediction, application in EDA	P. Leonards: Gas chromatography-mass spectrometry (GC-MS), GCxGC	M. Carere: WFD Monitoring: present approach and future perspectives
11:00		<b>Coffee Break (KUBUS Foyer)</b>			
11:15		M. Ahel: Theoretical background of chromatography	M. Wirtz: Multivariate statistics for evaluation of large datasets	T. Schulze: Sampling	R. Burgess: Water quality assessment and toxicant identification in the U.S
12:15	<b>Registration (KUBUS Foyer)</b>	M. Lamoree: GC- and LC-based analytical and preparative separation	H. Hollert: Integrative and mode-of-action based toxicological endpoints	M. Krauss: Structure elucidation	M. Hewitt: Water quality assessment and toxicant identification in Canada
13:15	<b>Lunch time (KUBUS Foyer)</b>				
14:00	W. Brack: Welcome to the EDA-EMERGE Summer-school, Organisational issues	<b>EDA-EMERGE Project Meeting</b>	Excursion to Wechselburg	Virtual Case Studies	<b>Advisory Board Meeting</b>
15:00	B. Gawlik: Pollutant prioritisation for WFD monitoring and assessment			M. Krauss: Structure Elucidation Workshop	Lab Tour
16:00	Poster Session			Venue: KUBUS PC Room	Departure
17:00	Poster presentations by ESR fellows				
		19h00: Common Dinner (Ratskeller Leipzig)	18h00: Drinks and Dinner in Landgasthof Sörnzig		

## Lectures

The summer school featured 18 lectures of 60 min each (allowing for a 10 min discussion or question session). Details of the speakers and titles of the talks are as follows:

Speaker	Affiliation	Thematic area and Talk Title
Werner Brack	UFZ, Germany	Effect-Directed Analysis (EDA) to Identify Toxicants
Bernd Gawlik	JRC, Italy	Pollutant Prioritization in the context of the Water Framework Directive
Keeus van Leeuwen	KWR, Netherlands	Water pollution and drinking water
Marijan Ahel	IRB, Croatia	Theoretical background of chromatography
Marja Lamoree	VU IVM, Netherlands	GC and LC based analytical and preparative fractioning
Juliane Hollender	EAWAG; Switzerland	LC-MS
Rolf Altenburger	UFZ; Germany	Mixture toxicity assessment and prediction – application in EDA
Monika H-Witz	Gaiac, Germany	Multivariate statistics for evaluation of large datasets.
Henner Hollert	RWTH, Aachen	Integrated and mode of action based toxicological endpoints
Knut-Erik Tollefsen	NIVA, Norway	OMICS techniques and effect assessment
Pim Leonards	VU IVM, Netherlands	GC-mass spectrometry and GCxGC
Tobias Schulze	ISS, Italy	Sampling
Martin Krauss	UFZ	Structure elucidation by GC-MS and LC-HRMS
Andrew Tindall	Watchfrog, France	Smart Sensors
Mario Carere	ISS; Italy	WFD Monitoring: present approaches and future perspectives
Rob Burgess	US EPA; USA	An overview of water quality assessment and toxicant identification in the US
Mark Hewitt	Environment, Canada	Water Quality assessment and toxicant identification in Canada



### **Workshop**

Using an adjoining computer facility at the conference venue, Dr. Martin Krauss delivered a hands on workshop for the PhD fellows on the use of computational tools for chemical structure elucidation. Students were organized in pairs of two to identify environmentally relevant example compounds based on their GC-MS and LC-HRMS mass spectra. To this end, the students were guided through workflows utilizing manual spectra interpretation as well as freely available, web-based software tools.

### **Poster Session**

The poster session (25 June) was used to give each PhD fellow 5-10 min to introduce themselves and provide a short background about their current research, publications and recent achievements.

### **Excursions and social activities**

A communal dinner was organized in the city centre in the evening of 26 June after the project meeting, allowing for enough time to socialise and tour the city centre.

Half a day was also used for an excursion (28 June) to the Wechselburg region of Saxony. Here the group visited a medieval monastery and then hiked from Wechselburg to Sörnzig along the Mulder river valley. The Mulder river valley is an example of a regenerated ecosystem which is recovering from the pollutant effects of the former mining industry. In Sörnzig the group had dinner and drinks together with informal discussions.