

## **EDA-EMERGE Specialized Course 1:**

### **“Advanced course on preparative and analytical chromatography in effect-directed analysis”**

Venue: Rudjer Boskovic Institute (IRB), Zagreb, Croatia

Organizer: Dr. Marijan Ahel (IRB)

Date: 02.07 to 03.07.2014

Time: 8h30 – 20h00, 8h30 – 12h30

#### **Course description:**

The SC1 was a 2 day EDA-EMERGE training course on preparative and analytical chromatography in effect-directed analysis.

Building on the theoretical knowledge provided by the summer school this course focused on the practical demonstration of EDA including sample extraction, tier 1 and higher tier fractionation and methods for the final chemical and bioassay characterization. Different separation techniques based on complementary chromatographic mechanisms were demonstrated. Furthermore, specific requirements for the GC- and LC-analysis of environmental samples were discussed.

This amounted to a minimum total academic involvement of 15 hours and equivalent to 0.5 ECTS points for the participants.

## AGENDA

Wednesday, 02.07.2014		
Time	Title	Lecturer
8:30-8:45	Brief introduction to the course	
8:45-10:30	Demonstration of 2 enrichment protocols for EDA	Sanja Koprivica Dr. Marijan Ahel
10:30-10:45	Coffee break	
10:45-11:45	Extraction and fractionation of environmental samples for effect-directed analysis	Dr. Marijan Ahel
11:45-12:45	Identification of biologically active substances in complex environmental samples – ecotoxicological considerations	Dr. Tvrtko Smital
13:00-13:45	Lunch	
13:45-15:45	Tier 1 (simplified) fractionation protocols for EDA analysis	Sanja Koprivica Dr. Ivan Senta Dr. Marijan Ahel
15:45-16:00	Coffee break	
16:00-19:00	Higher tier fractionation using preparative HPLC. Combination of different chromatographic principles for final fractionation.	Dr. Ivan Senta Sanja Koprivica Dr. Marijan Ahel
19:00-	Comprehensive analysis of fractionated extracts using UPLC/Q-ToF and GC/MS	Sanja Koprivica Dr. Senka Terzić Dr. Marijan Ahel

Thursday, 03.07.2014		
Time	Title	Lecturer
8:30-10:30	Evaluation of the UPLC/Q-ToF analyses	Sanja Koprivica Dr. Senka Terzić Dr. Marijan Ahel
10:30-10:45	Coffee break	
10:45-11:45	Evaluation of GC/MS analyses	Dr. Marijan Ahel
11:45-12:30	Summary discussion	Dr. Marijan Ahel

## COURSE CONTENT

The course covered the following topics:

- A demonstration of two different enrichment protocols for EDA
  - Mixed SPE sorbent bed (HR-X+HR-XAW+HR-XCW)
  - Serially coupled single-sorbent beds – 1) HR-X 2) HR-XAW 3) HR-XCW (EDP procedure = sequential extraction)
- The extraction and fractionation of environmental samples for EDA
- Tier 1 (simplified) fractionation protocols for EDA analysis
- Higher tier fractionation using preparative HPLC
- Analysis of fractionated extracts using UPLC/Q-ToF and GC/MS and instrumental conditions
- The combination of different chromatographic principles for final fractionation
- The evaluation of the UPLC/Q-ToF and GC/MS analyses
- Comprehensive Schemes for Suspect and Non-target Screening of Environmental Contaminants and their Application in Effect-directed Analysis
- The identification of biologically active substances in complex environmental samples as well as ecotoxicological considerations
  - Effect-directed analysis (scheme, phases, prerequisites)
  - Challenges and optimal approaches for sample collection and preparation
  - High resolution chemical analysis
  - High-Throughput Screening (HTS) bioassays
  - Toolbox of bioassays within EDA
  - Case studies addressing (i) problems of mixture, (ii) lack of pure standards for confirmation, (iii) biologically active substances, (iv) world of toxic cyanobacteria