

## Course description

### **Hands-on Liquid Chromatography–Mass spectrometry course in the analysis of small molecules (phytochemicals, contaminants, primary metabolites)**

**ECTS credits: 8**

#### **Course parameters**

*Language:* English

*Level of course:* PhD course

*Semester/quarter:* Monday 12 June – Friday 23 June 2023

*Preparatory reading of textbook:* Approx. 40 hours.

*Hours per week during two weeks on-site work:* approx 45/per week. Monday 12 June – Friday 23 June: Long and intensive days, - part of the exercises will take place in the evening to assure that all participants have plenty of hands-on time.

*Report writing:* Approx. 100 hours

*Total hours workload:* 230

*Capacity limits:* 10

#### **Objectives of the course:**

Advanced tools such as liquid or gas chromatography coupled to mass spectrometry are necessary tool in the research into small molecules, either phytochemicals with defense or health properties, environmental contaminants such as pesticides or primary metabolites that can be affected by the presence of other bioactive compounds. The objective of the course is to teach the participant the theoretical background as well as the practical use of these tools for quantitative analysis as well as for identification. The course will take place in a well-equipped laboratory at Aarhus University, Research Centre Flakkebjerg, DK-4200 Slagelse, Denmark. LC-MSMS, LCMS-QTRAP, LC-TOF, GC-TOF instruments will be available for the students during the course and our experienced staff will provide instruction on the use of the equipment as well as practical techniques for the preparation of samples.

#### **Learning outcomes and competences:**

At the end of the course the student **is able to:**

- Use LCMSMS or GCMS equipment for quantitative and qualitative analysis of small molecules
- Give an account for the principles behind development of chromatographic methods for separation of small molecules
- Perform a basic method validation for quantitative analysis in LCMSMS
- Optimize the parameters for analysis of selected compounds
- Use LCMS-QTRAP or LC-QTOF in the identification of small molecules or their metabolization products

## **Compulsory programme:**

Entire course.

## **Course contents:**

The course is constructed as follows:

- ◆ Preparatory reading of selected chapters in an LC-MSMS textbook
- ◆ Approximately three days of practical exercises on basic LC-MSMS, quantitation methods, optimization of parameters for selected small molecules, preparation of samples, matrix effects, validation of the quantitative method
- ◆ Approximately three days of practical exercises chosen on the basis of each student's on-going PhD project
- ◆ Theoretical lessons on
  - ◆ Optimization of extraction methods
  - ◆ Method validation: LOD, LOQ, recovery, matrix interferences
  - ◆ ESI and APCI inlet systems
  - ◆ Use of an ion trap for analysis of small molecules
  - ◆ HPLC method development and optimization
  - ◆ Interpretation of mass spectra
  - ◆ Metabolomics
  - ◆ Representative sampling: plants, soil and water
  - ◆ Good Laboratory Practice
  - ◆ New developments in mass spectrometry
- ◆ Subsequent elaboration of a 30- to 40-page report on the practical exercises.

## **Prerequisites:**

The course is for PhD students (in special individual cases master students with already planned PhD projects can be given access)

## **Lecturers from Aarhus University**

Professor Inge S. Fomsgaard (course coordinator)

<https://pure.au.dk/portal/en/inge.fomsgaard@agro.au.dk>

Laboratory Technician Bente Laursen; PhD student Ida KL Andersen; postdoc Jawameer Hama.

## **Visiting lecturers**

Mass spectrometry specialist, Sciex; Chromatography specialist, Phenomenex,

**Type of course/teaching methods:** Lectures, practical exercises

**Literature:** Study material will be shipped to the participating students not later than May 15.

**Course homepage:** None

## **Course assessment:**

Elaboration of a 30- to 40-page report on the practical exercises. The report is assessed as "passed" or "not passed". Presence at a minimum of 90% of theoretical and practical lessons is required to obtain the course diploma.

**Provider:** Department of Agroecology, Aarhus University

**Special comments on this course:**

None

**Course venue**

The course venue is Research Centre Flakkebjerg, situated in Southwest Zealand, 10 km south of Slagelse (100 km west of Copenhagen). Complete address:

Department of Agroecology, Research Centre Flakkebjerg, Forsøgsvej 1,

DK-4200 Slagelse, Denmark, Telephone Inge S. Fomsgaard:+45 22 28 33 99.

[Inge.Fomsgaard@agro.au.dk](mailto:Inge.Fomsgaard@agro.au.dk).

**Accommodation**

Accommodation will be at OnlySleep, Trafikcenter Alle 2-4, DK-4200 Slagelse.

**Comments from participants in our 2022 course**

- ◆ The combination of introductory seminars with hands-on experiments from the very beginning of the course was a huge benefit and motivated participants a lot.
- ◆ What I find the most rewarding is definitely the establishment of a learning curve regarding LCMS work and optimization.
- ◆ The best and most important part of this course for me was the atmosphere. I am happy because everyone here was super nice to me and I was learning without feeling any pressure.
- ◆ The course was very well structured between lectures, lab- and instrument time, and every single topic/lecture felt like it had a use in the following lab/-instrument time slots.

**Time:** Monday 12 June – Friday 23 June 2023

**Place:** Aarhus University, Department of Agroecology, Forsøgsvej 1, DK-4200 Slagelse, Denmark

**Registration**

Deadline for registration and payment: 1 April, 2023. Maximum number of participants: 10. First come, first served. Please register at <https://www.conferencemanager.dk/hands-on-2023>

**Cancellation**

Registration is binding, but you may cancel your registration by sending an e-mail to Course Administrator [sonja.graugaard@agro.au.dk](mailto:sonja.graugaard@agro.au.dk) no later than 15 April 2023. If you cancel your registration later than 15 April, your registration fee will be forfeit, and your seat may be transferred to another person.

If you have any questions, please contact Course Administrator Sonja Graugaard, e-mail: [sonja.graugaard@agro.au.dk](mailto:sonja.graugaard@agro.au.dk)