



SECOND WORKSHOP

Ph.D. course: Mass Spectrometry
Coupled to Separation Techniques
in Bioanalytical Chemistry

07th - 11th January 2019 - University of Copenhagen - Denmark

Day I - Monday 7th January 2019 - Introduction, basic concepts, ionization techniques and mass analyzers

- 09.00-09.45 **Introduction, generally about interpretation of spectra, basic concepts**
Christian Skonberg, H. Lundbeck A/S - Denmark
- 09.50-10.35 **Basic concepts continued**
Christian Skonberg, H. Lundbeck A/S - Denmark
- 10.35-11.00 *Coffee break*
- 11.00-11.45 **Basic concepts continued**
Christian Skonberg, H. Lundbeck A/S - Denmark
- 11.45-12.30 *Lunch*
- 12.30-13.15 **Ionization techniques I: Overview of common ionization methods, EI, CI, MALDI**
Christian Janfelt, Dept. of Pharmacy, KU - Denmark
- 13.20-14.05 **Ionization techniques II: Methods used in coupling with LC and CE. ESI (incl. nanospray), APCI and APPI**
Andreas Kretschmann, Dept. of Pharmacy, KU - Denmark
- 14.05-14.25 *Coffee break*
- 14.25-15.10 **Mass analysers I: Basic concepts, Sector field instruments, the quadrupole mass filter and the ion trap**
Christian Janfelt, Dept. of Pharmacy, KU - Denmark
- 15.15-16.00 **Mass analysers I, continued**
Christian Janfelt, Dept. of Pharmacy, KU - Denmark

Day II - Tuesday 8th January 2019 - Mass analysers, types of instruments

- 09.00-09.45 **Mass analysers II: The FT-ICR, the Orbitrap and hyphenated instruments**
Christian Janfelt, Dept. of Pharmacy, KU - Denmark
- 09.50-10.35 **Mass analysers III: TOF and Ion mobility spectroscopy**
Kasper Dyrberg Rand, Dept. of Pharmacy, KU - Denmark
- 10.35-11.00 *Coffee break*
- 11.00- 11.45 **Ionization techniques III: ICP-MS**
Stefan Stürup, Dept. of Pharmacy, KU - Denmark
- 11.45-12.30 *Lunch*
- 12.30-13.15 **Coupled techniques I: GC-MS**
Asger W. Nørgaard, Novo Nordisk A/S - Denmark
- 13.20-14.05 **The MS market - commercial instruments**
Christian Janfelt, Dept. of Pharmacy, KU - Denmark
- 14.05-14.25 *Coffee break*
- 14.25-15.25 **Mass spectrometry in use – participants' presentations**
Christian Janfelt, Dept. of Pharmacy, KU - Denmark
- 15.30-16.00 **Mass spectrometry in use – participants' presentations**
Christian Janfelt, Dept. of Pharmacy, KU - Denmark





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Day III - Wednesday 9th January 2019 - Interpretation of MS spectra and HPLC-MS

- 09.00-09.45 **Interpretation of MS spectra. Exact mass determination, isotopic composition (isotopes and isotope peaks, isotope patterns for larger molecules)**
Line Rørbæk Olsen, H. Lundbeck A/S - Denmark
- 09.50-10.35 **Computer exercise: Interpretation of MS spectra**
Line Rørbæk Olsen, H. Lundbeck A/S - Denmark
- 10.35-11.00 *Coffee break*
- 11.00-11.45 **Computer exercise, Interpretation of MS spectra; continued.**
Line Rørbæk Olsen, H. Lundbeck A/S - Denmark
- 11.45-12.30 *Lunch*
- 12.30-13.15 **Coupled techniques I: LC-MS. HPLC-hardware, columns, separation principles, and method development**
Andreas Kretschmann, Dept. of Pharmacy, KU - Denmark
- 13.20-14.05 **Coupled techniques I: Coupling between LC and MS**
Andreas Kretschmann, Dept. of Pharmacy, KU - Denmark
- 14.05-14.25 *Coffee break*
- 14.25-15.10 **Coupled techniques I: LC-MS method optimization**
Andreas Kretschmann, Dept. of Pharmacy, KU - Denmark
- 15.15-16.00 **Coupled techniques I: LC-MS method optimization**
Andreas Kretschmann, Dept. of Pharmacy, KU - Denmark

Day IV - Thursday 10th January 2019 - Protein analysis and examples of use

- 09.00-09.45 **Proteins and peptides, basic concepts**
Kasper Dyrberg Rand, Dept. of Pharmacy, KU - Denmark
- 09.50-10.35 **Proteins and peptides, examples**
Kasper Dyrberg Rand, Dept. of Pharmacy, KU - Denmark
- 10.35-11.00 *Coffee break*
- 11.00-11.45 **Analysis of protein conformation by MS: Hydrogen-deuterium exchange MS (HX-MS)**
Kasper Dyrberg Rand, Dept. of Pharmacy, KU - Denmark
- 11.45-12.30 *Lunch*
- 12.30-13.15 **Mass spectrometry in forensic science**
Petur Weihe Dalsgaard, Dept. of Forensic Medicine, KU - Denmark
- 13.20-14.05 **Work on MS problems**
Christian Janfelt, Dept. of Pharmacy, KU - Denmark
- 14.05-14.25 *Coffee break*
- 14.25-15.10 **Coupled techniques III: CE-MS (p. 228)**
Nickolaj J. Petersen, Dept. of Pharmacy, KU - Denmark
- 15.15-16.00 **Metabolite identification and characterization in drug development**
Lars Bendahl, H. Lundbeck A/S - Denmark





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Day V - Friday 11th January 2019 - Quantitation and examples of use

- 09.00-09.45 **Quantitative analysis, basic concepts, Isotope labeling, suppression, Limits of detection**
Lars Ynddal, Gubra - Denmark
- 09.50-10.35 **High throughput Screening (HTPS), Pharmacokinetic studies**
Lars Ynddal, Gubra - Denmark
- 10.35-11.00 *Coffee break*
- 11.00-11.45 **Quantitative analysis of biomacromolecules**
Carsten Boye Knudsen, Zealand Pharma A/S - Denmark
- 11.45-12.30 *Lunch*
- 12.30-13.15 **Mass spectrometry imaging**
Christian Janfelt, Dept. of Pharmacy, KU - Denmark
- 13.20-14.05 **Work on MS problems**
Christian Janfelt, Dept. of Pharmacy, KU - Denmark
- 14.05-14.25 *Coffee break*
- 14.25-15.10 **Mass spectrometry-based proteomics**
Michael Lund Nielsen, The Novo Nordisk Foundation Center for Protein Research, KU - Denmark
- 15.15-16.00 **Course evaluation and MS Lab tour at Department of Pharmacy, KU**
Christian Janfelt, Dept. of Pharmacy, KU - Denmark

