

**AARHUS UNIVERSITY**  
**EXTERNAL SEMINAR**  
**DEPARTMENT OF ENVIRONMENTAL SCIENCE**  
**Frederiksborgvej 399, 4000 Roskilde**  
**7 June 2019, 13:00 – 14:00**  
**Venue: C2.05 at Risø Campus in Roskilde, AU**



**Title: Deciphering Complex Metabolite Mixtures in the Omics Era**

**Speaker: Madeleine Ernst, Postdoctoral Scholar**, Dorrestein Lab, Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA, USA

**Abstract:** Untargeted mass spectrometry-based metabolomics has become a method of choice to evaluate differences and similarities in metabolite profiles of diverse sample types and within a broad range of applications. Furthermore, recent advances in computational mass spectral metabolomics tools, such as mass spectral molecular networking through the Global Natural Products Social Molecular Networking platform or unsupervised substructure discovery through MS2LDA have enabled rapid and high-throughput metabolome mining and chemical characterization of thousands of samples. Nevertheless, the unambiguous identification of a chemical structure still represents a significant bottleneck. Here, I will present recent advances for the integration of existing metabolome mining and annotation tools maximizing chemical structural information retrieved in a metabolomics experiment. Furthermore, I will highlight advances in metabolomics data analysis and interpretation by introducing two chemically informed distance metrics. Conventional distance metrics used to measure pairwise dissimilarities across samples ignore the chemical structural relatedness between molecules. Thus, whilst two samples could contain chemically similar yet distinct molecules, they would be regarded as very different. Using datasets from diverse sources, I will show how these metrics can improve multivariate statistics and subsequent data interpretation.

**Host: Martin Hansen**, Senior Researcher, Section of Environmental Chemistry and Toxicology, Department of Environmental Science, Aarhus University

**External Guests** interested in attending the presentation should e-mail Department Secretary Christel Ege-Johansen, [cej@envs.au.dk](mailto:cej@envs.au.dk)

