Institute of Molecular and Cell Biology
A*STAR

SEMINAR ANNOUNCEMENT

We would like to invite you to attend this seminar hosted by Dr Radoslaw Sobota:

Date: 19 September 2019, Thursday
Time: 10:00AM – 11:00AM
Venue: Level 3, IMCB Seminar Room 3-46, Proteos, Biopolis

Speaker: Prof. Jürgen Cox, Group Leader, Max Planck Institute for Biochemistry, Germany
Title: Computational proteomics enhancements in MaxQuant by (deep) machine learning and ion mobility awareness

Abstract
Machine learning has shown its great potential of improving identification and quantification in proteomics in many respects. We report on advances in the MaxQuant software for proteomics data analysis by the integration of conventional and deep learning algorithms. The prediction of MS/MS fragmentation spectra has reached accuracies that are only limited by the technical reproducibility of spectrum acquisition. The utility of these prediction models in conjunction with retention time prediction is illustrated by applying them to the analysis of both data-dependent and data-independent acquisition datasets. In the former case, we observe a q-value-dependent increase in the total number of peptide identifications. In the latter case, we confirm that the use of predicted tandem mass spectrometry spectra is nearly equivalent to the use of spectra from experimental libraries. We also describe the ion mobility aware MaxQuant software, which utilizes the data dimension added by ion mobility to LC-MS/MS data. A new matching between runs (MBR) algorithm that utilizes collisional cross section (CCS) values of MS1 features in the matching process significantly gains specificity from the extra dimension. Prerequisite for using CCS values in MBR is a relative alignment of the ion mobility values between the runs. The missing value problem in protein quantification over many samples is greatly reduced by CCS aware MBR.

Biography
Jürgen Cox studied physics in Aachen and received his PhD from the Massachusetts Institute of Technology, USA. After a Postdoc at the Technical University of Munich, he became a Senior Scientific Consultant for the bioinformatics company Genedata. In 2006, he joined the MPIB as a senior scientist and has been the independent leader of the research group “Computational Systems Biochemistry” since 2014. Cox was appointed as Honorary Professor of Proteomics at the University of Copenhagen, Denmark, in 2013. His work is focused on the development of computational approaches to analyze large scale data in the field of proteomics. Together with his team he developed the software platforms MaxQuant and Perseus. MaxQuant enables the analysis of large mass spectrometric data sets.

ALL ARE WELCOME *(No registration required)*

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