A U S H A N G

FREIE UNIVERSITÄT BERLIN
Fachbereich Mathematik und Informatik

Promotionsbüro, Arnimallee 14, 14195 Berlin

D I S P U T A T I O N

Montag, 30. September 2013, 10.00 Uhr

Ort: Arnimallee 6 (Pi-Gebäude)
14195 Berlin, Raum 108/109

Disputation über die Doktorarbeit von

Herrn Stephan Aiche

Thema der Dissertation:
Inferring Proteolytic Processes form Mass Spectrometry Time Series Data

Thema der Disputation:
Optimal de novo design of SRM experiments

Die Arbeit wurde unter der Betreuung von **Prof. Dr. Chr. Schütte** durchgeführt.

Abstract: Targeted proteomics approaches like SRM (selected reaction monitoring) have shown to be superior in terms of sensitivity, dynamic range, and reproducibility when compared to regular label-free proteomics approaches. However, SRM requires an a priori selection of proteins that should be quantified. More precisely so called transitions have to be selected that identify a proteotypic peptide of the target protein. As the number of transitions that can be monitored is limited the optimal selection of transitions that yield a maximal number of quantified proteins is of great interest for the proteomics community.

In this talk I will present an in silico approach for optimal SRM design [1], that is based on a combination of machine learning approaches and combinatorial optimization. Machine learning is applied to predict relevant features of peptides to generate a list of suitable transitions. Based on this input the scheduling problem is formulated that optimizes the measurement schedule and transition selection with respect to the number of quantified proteins and an optimal use of the instruments measurement time.

[1] Nahnsen S, Kohlbacher O. In silico design of targeted SRM-based experiments. BMC Bioinformatics. 2012;13 Suppl 16:S8. doi: 10.1186/1471-2105-13-S16-S8. Epub 2012 Nov 5

Die Disputation besteht aus dem o. g. Vortrag, danach der Vorstellung der Dissertation einschließlich jeweils anschließenden Aussprachen.

Interessierte werden hiermit herzlich eingeladen

Der Vorsitzende der Promotionskommission
Prof. Dr. Chr. Schütte