

FREIE UNIVERSITÄT BERLIN Fachbereich Mathematik und Informatik

Promotionsbüro, Arnimallee 14, 14195 Berlin

DISPUTATION

Montag, 9. Juli 2018, 10.00 Uhr

Ort: Raum 108/109, Arnimallee 6, 14195 Berlin

Disputation über die Doktorarbeit von

Frau Borong Shao

**Thema der Dissertation:
Phenotype Relevant Network-Based Biomarker Discovery
Integrating Multiple Omics Data –
EMT Network-Based Lung Cancer Prognosis Prediction**

**Thema der Disputation:
An overview of computational approaches in peptide –
MHC binding prediction**

Die Arbeit wurde unter der Betreuung von **Prof. Dr. T. Conrad** durchgeführt.

Abstract: The immune system protects us against diseases by detecting a wide variety of pathogens and eliminating them. One fundamental mechanism is cellular immunity, where infected or tumoral cells are recognized and killed by T cells. This can only happen when the antigens are processed and presented on the cell surface by MHC (major histocompatibility complex) molecules. The binding of antigen-derived peptides with MHC is the single most selective step in antigen presentation. The capability to predict whether a peptide binds to certain MHC molecules has great value in the areas of transplantation, vaccine development and cancer immunotherapy [1].

This talk will begin with an introduction of the biological background. Then two major approaches for binding prediction: position-specific scoring matrix [2,3] and neural networks [4,5] will be explained. This is followed by their application in cancer immunotherapy [6]. Further, molecular docking approach [7] is shown to address the physics of binding which could be important for the immunogenicity. At last, we summarize that by taking a holistic view of cancer immunotherapy, we can better incorporate the complexities into computational models to aid in rational therapy design [8].

Reference

- [1] Schumacher, Ton N., and Robert D. Schreiber. "Neoantigens in cancer immunotherapy." *Science* 348.6230 (2015): 69-74.
- [2] Reche, Pedro A., John-Paul Glutting, and Ellis L. Reinherz. "Prediction of MHC class I binding peptides using profile motifs." *Human immunology* 63.9 (2002): 701-709.
- [3] Andreatta, Massimo, Ole Lund, and Morten Nielsen. "Simultaneous alignment and clustering of peptide data using a Gibbs sampling approach." *Bioinformatics* 29.1 (2012): 8-14.
- [4] Nielsen, Morten, and Massimo Andreatta. "NetMHCpan-3.0; improved prediction of binding to MHC class I molecules integrating information from multiple receptor and peptide length datasets." *Genome medicine* 8.1 (2016): 33.
- [5] Han, Youngmahn, and Dongsup Kim. "Deep convolutional neural networks for pan-specific peptide-MHC class I binding prediction." *BMC bioinformatics* 18.1 (2017): 585.
- [6] Sahin, Ugur, et al. "Personalized RNA mutanome vaccines mobilize poly-specific therapeutic immunity against cancer." *Nature* 547.7662 (2017): 222.
- [7] Antunes, Dinler A., et al. "General Prediction of Peptide-MHC Binding Modes Using Incremental Docking: A Proof of Concept." *Scientific reports* 8.1 (2018): 4327.
- [8] Konstorum, Anna, et al. "Addressing current challenges in cancer immunotherapy with mathematical and computational modelling." *Journal of The Royal Society Interface* 14.131 (2017): 20170150.

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. T. Conrad