

## nformatik-Kolloquium

Der Fachbereich Informatik der Johannes Kepler Universität Linz<sup>1</sup> lädt in Zusammenarbeit mit der Österreichischen Gesellschaft für Informatik (ÖGI) zu folgendem Vortrag ein:

**Thomas Unterthiner**

JKU

### **Toxicity Prediction using Deep Learning**

**Thursday, April 23, 5:15 pm,  
Room JKU S3-055 in Science Park 3,**

**Abstract:** Everyday we are exposed to various chemicals via food additives, cleaning and cosmetic products and medicines -- and some of them might be toxic. However testing the toxicity of all existing compounds by biological experiments is neither financially nor logistically feasible. Therefore the government agencies NIH, EPA and FDA launched the Tox21 Data Challenge within the "Toxicology in the 21st Century" (Tox21) initiative. The goal of this challenge was to assess the performance of computational methods in predicting the toxicity of chemical compounds. State of the art toxicity prediction methods build upon specifically-designed chemical descriptors developed over decades. Though Deep Learning is new to the field and was never applied to toxicity prediction before, it clearly outperformed all other participating methods. In this talk we will look behind the curtains of the winning method, and show how deep nets automatically learn to recognize features resembling well-established toxicological properties of chemical compounds. In total, our Deep Learning approach won both of the panel-challenges (nuclear receptors and stress response) as well as the overall Grand Challenge, and thereby sets a new standard in toxicology prediction.

**Short Bio:** Thomas Unterthiner has a BSc in Computer Science and an MSc in Bioinformatics from the Johannes Kepler University Linz (JKU). He is currently working towards a PhD under the supervision of Prof. Sepp Hochreiter. His research focuses on the theory and application of Machine Learning techniques on biological data, mostly involving Deep Learning and Neural Networks. Recently, he was part of the research team that won the prestigious Tox21 Data Challenge.

*Univ.-Prof. Dr. Volker Strumpfen  
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<sup>1</sup> Der Fachbereich (<http://informatik.jku.at>) besteht aus folgenden Instituten:

Application Oriented Knowledge Processing (FAW), Bioinformatics, Computational Perception, Computer Architecture, Applied Systems Research and Statistics, Computer Graphics, Formal Models and Verification, Networks and Security, Integrated Circuits, Pervasive Computing, Software Systems Engineering, System Software, Telecooperation, Signal Processing