The Doctoral Program **ION CHANNELS AND TRANSPORTERS AS MOLECULAR DRUG TARGETS** („MolTag“)

is pleased to invite you to the following **ONLINE** lecture

"Computational Methods for Active Compound Design and Risk Assessment”

by Ass.Prof.Dr. Andrea VOLKAMER

Institute of Physiology, Charité Universitätsmedizin Berlin

on: Tuesday, January 26, 2021, 16:00.

Host: Prof. Dr. Gerhard ECKER, UniVie

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ABSTRACT*:* Due to the ever-growing amount of available structural protein and compound data - from experimental sources or modeling approaches - computational methods to collect the data and put it to practical use are becoming more and more important. Thus**,** learning from the large pool of available data and using this knowledge for *in silico* predictions is of high practical value**. In this presentation, structural bioinformatics and cheminformatics methods will be introduced which can be applied in translational projects** to guide the design of more active, selective and/or less toxic compounds.

Professional Career Andrea Volkamer:

July 2016 – Present; Charité Berlin, Assistant professor; Field of research: In-silico toxicology predictions and structural bioinformatics

Sept 2013 – June 2016; BioMed X GmbH, Heidelberg: PostDoc Researcher; Field of research: Selective kinase inhibitor design

Feb 2013 – Aug 2013; University of Hamburg, Center for Bioinformatics, Pro Exzellenzia PostDoc Fellow in the group of Prof. Dr. Matthias Rarey

June 2008 – Sept 2012; University of Hamburg, Center for Bioinformatics, group of Prof. Dr. Matthias Rarey; Research scientist and coordinator of the project "COMPASITES: Computeraided active site analysis of protein structures". The project was part of the Biocatalysis 2021 cluster, funded by the BMBF with the industrial cooperation partners Merck KGaA, Darmstadt, and BioSolveIT GmbH.

April 2007 – May 2008: Purdue University (West Lafayette, USA), Scientific Researcher/Visiting Scholar in the group of Assistant Prof. Markus Lill, Ph.D.

Education: University of Hamburg Dr. rer. nat., Computational Biology (2008 - 2013), Universität des Saarlandes M.Sc., Bioinformatik (2005 – 2007)

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Der Wissenschaftsfonds.