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7TH MARCH 2017

NEXT SPARK EDUCATIONAL FORUM

LEAD OPTIMIZATION AND PHARMACOPHORE MODELING

5:00 – 7:00 PM

VIRCHOWWEG 6

CCO AUDITORIUM

DR. MARC NAZARÉ, FMP

HIT-TO-LEAD OPTIMIZATION IN MEDICINAL CHEMISTRY

The vast majority of marketed drugs underwent an extensive medicinal chemistry optimization prior entering clinical trials. The challenge is to carefully balance a multitude of parameters like activity, selectivity, metabolic stability and low toxicity in one single molecule. In this talk the principles for the selection of good hits as starting points for the chemical optimization, simple key descriptors of drug-likeness and the use of structure activity relationships as well as their underlying molecular recognition principles in protein ligand interactions will be discussed. Marc Nazare started his career as a medicinal chemist in pharmaceutical industry, and joined the Leibniz Institut fuer Molekulare Pharmakologie (FMP, Berlin) as a group leader in 2013.

PROF. GERHARD WOLBER, FU

3D PHARMACOPHORES AS STRATEGY FOR HIT IDENTIFICATION AND LEAD OPTIMIZATION

3D pharmacophores have become an established and consolidated method for in-silico drug discovery – mainly due to their ability to reflect the way of thinking of medicinal chemists in terms of hit identification, hit expansion and lead optimization. The simplicity and descriptive character of such a 3D pharmacophore model thus enables clear communication and rapid feedback cycles between modeling and synthesis teams. Despite the broad usage of the methodology, there are still several pitfalls and challenges for successful pharmacophore modeling – mainly related to the algorithmic challenge of flexibly fitting a molecule to a 3D pharmacophore model in a computationally efficient way. In this talk, several structure- and ligand-based 3D pharmacophore application studies will be presented and critically discussed in the context of virtual screening algorithms and overlay algorithms. Prof. Dr. Gerhard Wolber is a professor for Pharmaceutical Chemistry at the Institute of Pharmacy at the Freie Universitaet Berlin and a founder of Inte:Ligand, which successfully develops and markets computational drug development software.

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