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An alle Interessierten

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Einladung zum Vortrag im Rahmen der BioStruct Lecture Series

Dr. Olivier Sperandio
Inserm UMR-S973/MTi. Université Paris Diderot

Düsseldorf, 10.12.2012

What compounds for what PPI target?

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Protein-protein interactions (PPI) are involved in vital cellular processes and are therefore associated to a growing number of diseases. But working with them as therapeutic targets comes with some major hurdles that require substantial mutations from our way to design drugs on historical targets such as enzymes and G-Protein Coupled Receptor (GPCR). Among the numerous ways we could improve our methodologies to maximize the potential of developing new chemical entities on PPI targets, is the fundamental question of what type of compounds should we use to identify the first hits and among which chemical space should we navigate to optimize them to the drug candidate stage.

In this presentation, I will describe our new iPPI-DB database that contains more than 1600 inhibitors of protein-protein interactions (iPPI) on about 15 classes of PPI targets. Those compounds were manually retrieved by medicinal chemists from the literature including peer-reviewed articles and world patents. Information contained in iPPI-DB includes pharmacological activities, physico-chemical properties for the compounds, and biological information about the PPI targets such as protein domain, function and associated diseases. The database was used to get some insight into the chemical space of iPPI and to describe not only the specificity of those compounds with respect to existing drugs but also the specificity that seems to characterize given subsets of PPI targets. This type of approach will certainly help the chemist and the biologist to select existing compounds from chemical libraries or to prioritize chemical synthesis in order to maximize the chances of obtaining chemical probes on PPI targets.

Ort: Hörsaal 6D

Zeit: Donnerstag, 24. Januar 2013, 17:00 Uhr s.t.

Gäste sind herzlich willkommen.