

# CLS /CCI Spring 2009 Seminar Series

4/30/2009

4:00pm

**Andreas Bender**

Leiden/Amsterdam Center for Drug Research

Location: 1462 Clifton Road (Dental School Building), Room 230

**“How can computers support drug discovery? In silico approaches for compound profiling, predicting targets, and predicting ligand activity against particular protein mutants”**

**Abstract:**

Today, a vast number of associations (hundreds of thousands to millions) between small molecule structures and their respective target affinities are known. Those associations are exploited here for the prediction of on-target as well as off-target effects of novel compounds, and to analyze factors contributing to promiscuity of new structures. Namely, we describe the development of in silico models to predict targets of compounds, such as those contained in common safety profiling panels<sup>1</sup>, to prioritize targets to be screened in safety evaluations. For the analysis of compound promiscuity, a usually undesired feature of active ingredients, we present computational models which firstly provide estimates for compound promiscuity, and secondly give insight into features frequently associated with promiscuous compounds.<sup>2</sup> Finally, we will discuss ideas how phenotypic profiling of compounds can be integrated with in silico techniques to derive a comprehensive assessment of the biomodulatory capabilities of a compound.<sup>3</sup> Applications will in particular be presented on the prediction of compound activity against particular mutants of HIV Reverse Transcriptase, using so-called proteochemometric modeling approaches.



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