

Building Robust and Predictive *in silico* Models in Pharmaceutical Industry using Machine Learning Approaches

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Today the pharmaceutical industry is facing the challenges of increasing efficiency in drug research by developing and using more innovative and effective research tools. Increasing problems related to toxicological effects as well as metabolic issues have also been added to the list of new challenges to be considered. Computer models describing biopharmaceutical properties, e.g. aqueous solubility and membrane permeability, with increasing predictive capabilities have successfully been developed both in academia as well as in industry during the last decade. The need for and utilisation of robust and predictive *in silico* models have become more and more important in early drug development. Machine learning techniques, such as rule-based ensemble or consensus models, have recently been introduced to achieve the objectives of reliability, predictive capability as well as robust behaviour for the developed computational models. Additionally, models deriving their information from different sources or descriptions have also started to be used as viable alternatives to traditional *in silico* modelling of structure-property relationships. The talk will give examples of how such models have been developed and are currently deployed at AstraZeneca R&D Södertälje as well as some practical issues to be taken into account when developing more general *in silico* screening models for web deployment.