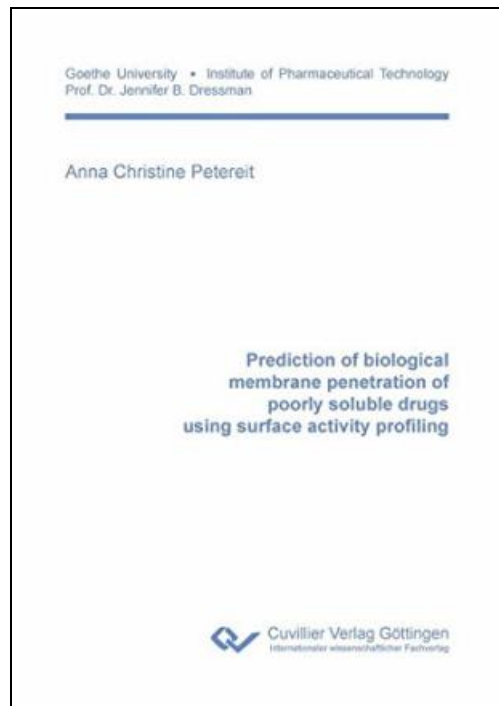


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PREDICTION OF BIOLOGICAL MEMBRANE PENETRATION OF POORLY SOLUBLE DRUGS USING SURFACE ACTIVITY PROFILING



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Cuvillier Verlag Aug 2012, 2012. Taschenbuch. Condition: Neu. Neuware - Since combinatorial chemistry and high throughput screening have become a common technique in the drug discovery phase the number of compounds being considered has increased frequently. These structures are often characterized by high molecular weight, high lipophilicity and low solubility in aqueous and physiological media. Due to the generally poor bioavailability, new in vitro techniques were needed for screening of pharmacokinetic properties. An important parameter for these screening methods is the implementation at an early state of drug discovery phase, to find potential lead structures, before investment costs become significant. The established in vitro methods for the prediction of membrane interaction are not reliable especially for poorly soluble compounds. A new method that is fast and easy to use, requires only small amounts of NCE and which can provide more reliable predictions is needed. In this study, a new screening technique based on surface activity profiling for the prediction of oral drug absorption was evaluated with special emphasis on the predictability of biological membrane interaction of poorly soluble drug compounds. It was demonstrated that drug absorption through a bilayer membrane can be modeled by the orientation of compounds at the air/water interface. Thus amphiphilicity of a drug is generally related to both oral absorption and blood brain barrier penetration. In turn, amphiphilicity is influenced by the lipophilicity, size and charge distribution of a drug. Surface activity profiling was determined by analysis of surface pressure profiles using the Gibbs adsorption isotherm. The surface activity measurements were carried out using a multichannel tensiometer Delta 8, which was developed by Kibron to be utilized in conjugation high throughput screening in early drug discovery processes. For this study two test sets were analyzed, one for the prediction of gastrointestinal wall interaction and the second for the prediction of...



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