CS02-4 Informatic Approaches to Predicting Oral Bioavailability of Drugs

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In silico method is an essential technology to accelerate drug discovery and development. With rapid progress of information technology, various techniques aimed for management of screening data or rational design of active drugs and formulations have been presented. Oral bioavailability is one of critical issues to determine the success of clinical drug development, and many studies have been done with development of prediction models for assessing the drug property. A physiologically-based kinetic model attempts to develop a systematic understanding of oral drug absorption comprising various kinetic processes, and a structure/activity relationship (SAR) model attempts to predict kinetic properties from chemical structure for effective drug designs. It is an important issue to improve accuracy of each type of the models and seamlessly integrate them together. We proposed SAR modeling methods by the use of machine learning techniques such as artificial neural network, genetic algorithm, and therefore developed in silico prediction models for oral bioavailability-related kinetic processes. We presented large-scale visualization techniques for evaluating drug likeness effectively. In this presentation, in silico methods for predicting and evaluating oral drug absorption will be reviewed, including the introduction of our approaches.