in silico Prediction of Xenobiotics ADME-Toxicity for Drug Discovery

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In the last decade, the technology for New Drug Discovery (NDD) changes rapidly due to the increase of biological information, the development of High Throughput Experiment (THE) technologies, and the increase of computing power.

Despite the technological advances (e.g., combinatorial chemistry, high-throughput screening, functional genomics and proteomics) made in discovering and developing new drugs and an increased spending on research and development [estimated to be over 800 million US Dollars for each new molecular entity (NME)] during the last decade, the rate of drug attrition has not decreased. A significant bottleneck in the drug discovery process in the later stages of lead discovery is the analysis of the ADME and overt toxicity properties of drug compounds. ADME/Tox deficiencies account for 50-60% of the compound failures during development.

The discovery and development phases are governed by clear "go" or "no go" decisions throughout the non-clinical and clinical development of drugs. Therefore it is important to have in vitro and in silico tools for "go" or "no go" decision of chemicals to next stage.

In the presentation, the trends in in silico PK and Toxicity prediction and the S/W developed by BMD for A/M/Tox prediction will be introduced.