

This talk was presented by Dr Alexey Zakharov at the American Chemical Society 2012 Fall Meeting in Philadelphia.

Abstract

The most important factor affecting metabolic excretion of compounds from the body is their half-life time. This provides an indication of compound stability of, e.g., drug molecules. We report on our efforts to develop QSAR models for metabolic stability of compounds, based on in vitro half-life assay data measured in human liver microsomes (HLM), taken from literature and several commercial or free databases. A variety of QSAR models generated using different statistical methods and descriptor sets implemented in both open-source and commercial programs were analyzed. The models obtained were compared using several external validation sets from public and commercial data sources. We also report on our use of the most predictive ones among the models for calculating the HLM half-life time as a predictor of the metabolic stability for about 250,000 compounds from the publicly available Open NCI database. These predictions are being made available freely to the scientific community.

You can download the slides as a [PDF](#) .