[P18] IDAAPM: integrated database of ADMET and adverse effects of predictive modeling based on FDA approved drug data

Ashenafi Legehar[1], Henri Xhaard[12], Leo Ghemtio[2]

[1] *Division of Pharmaceutical Chemistry, Faculty of Pharmacy, University of Helsinki, P.O.Box 56, 00014 Helsinki, Finland*

Absorption, Distribution, Metabolism, Excretion, Toxicity (ADMET) properties and adverse effect, critically affects late stage failure of drug candidates. Computation prediction of ADMET and adverse effects are effective approaches to minimize the risk of late-stage attrition. However, the availability of approved drugs data from single source, the quality and the size of the data are still a major problem.

Here, we have built a relational database (IDAAPM) to link FDA-approved drugs properties to known druggable/toxic targets and ADMET and adverse effect data. We coupled the database with a data analytic platform to allow analysis and predictive modeling. This database has a unique resource that provides information on FDA approved drugs including their ADMET properties and adverse effects, the corresponding targets with bioactivity data and coupled with a data analytic platform. IDAAPM can be accessed through web application (http://idaapm.helsinki.fi) or KNIME workflow which is connected to the database.

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