Universität Basel

Research Project

Entwicklung einer in silico Plattform zur Früherkennung von Nebenwirkungen

Third-party funded project

Project title Entwicklung einer in silico Plattform zur Früherkennung von Nebenwirkungen
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Organisation / Research unit
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Department
Project start 01.01.2020
Probable end 31.12.2022
Status Completed

Modern society needs new chemical compounds like pharmaceuticals, cosmetics, agrochemicals, food additives, as well as natural compounds to maintain and further improve the standard of living. According to regulations, all chemicals that may come to contact with humans have to be fully characterised, including information about their possible harmful effects. Such a detailed characterisation is not only resource intensive, but also results in extensive animal testing.
Fortunately, in silico methods offer a cost-effective and ethical alternative. Ever increasing computational power in combination with the latest knowledge from multiple disciplines allow us to perform virtual experiments by means of computer simulation. Thus, we can learn about the nature of the chemical compound without need to have it physically synthesized and tested on animals. This means, that the extent of animal testing can be effectively reduced – it is performed only using the safest, computationally pre-evaluated compounds. Increased expected safety translates to animal testing reduced to inevitable minimum required for the regulatory approval.
The goal of this grant proposal is to develop and maintain a modular in silico screening platform which could be used to effectively identify possible harmful interference of chemicals with human proteins termed “anti-targets”, as any interaction with them is undesired. Using the most advanced simulations and modeling methods we would actively search for so-called molecular initiating events. These events are the first step in a complex cascade of processes eventually leading to an adverse outcome.
With this approach, we present a cost and resource effective alternative to conventional chemical risk assessment.

Keywords off-target bining, anti-target binding, in silico, toxicity, prediction
Financed by
Foundations and Associations

Add publication

Add documents

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