PRESS RELEASE

ULTIMATE 2.0 - INFINITY database: novel compounds for drug discovery

In the early stage of drug discovery, it is highly important for researchers to have access to a sufficient number of high quality drug-like compounds. The current number of so called "off-the-shelf" compounds provided for drug-discovery is estimated to be 10 million (10^7), while the number of so called "virtual" compounds that can be synthesized on demand is around 10 billion (10^{10}). By the combination of readily available building blocks, applying 1 or 2 consecutive reaction steps, the magnitude of virtual compounds can reach 10^{18}. The storage and curation of such a magnitude of data in databases would require a 10 million times larger storage capacity than the currently available ones, therefore these compounds are currently unavailable for drug discovery.

Mcule maintains a chemical marketplace that collects all available compounds and building blocks suitable for drug-discovery purposes in one place. In the ULTIMATE project, Mcule created a database of nearly 500 million novel drug-like compounds based on the available building blocks of 3 supplier partners. From this database the world's leading pharmaceutical companies and academic research groups can order novel drug-like compounds for fixed prices, which can be delivered in 2-6 weeks with a success rate of at least 80%. The synthesis of these compounds is performed by the supplier partners of Mcule, while Mcule prepares the final samples for experiments and delivers the product.

In the ULTIMATE 2.0 project, Mcule aims to elevate the number of commercially available virtual compounds to 1 trillion (100 times of the current number), thereby the ULTIMATE database would grow to 1,000 times of its current size.

The storage and searching of such large databases of compounds could only be performed via intelligent solutions that do not require the explicit enumeration of the whole database. The INFINITY storage and searching technology to be developed in this project, will provide a solution where the generation of only a part of the database that matches the searching criteria is necessary.

NATIONAL RESEARCH, DEVELOPMENT AND INNOVATION OFFICE HUNGARY

PROGRAM FINANCED FROM THE NRDI FUND

The development of ULTIMATE 2.0 involves the extension of the applied building blocks by integrating new supplier partners. This approach will not only ensure the growth of the database, but also will lead to very unique and diverse compounds if by mixing the supplier building blocks together.

The quality and number of new virtual compounds is highly depending on the applied chemical reactions – and chemoinformatic reaction rules based on them. Consequently, a minimum of 25 new, robust chemical reactions will be integrated to the system during the project.

In order to ensure the future extension of ULTIMATE with highly novel compounds, we are developing a platform that will allow the validation and market entry of novel, druglike structures developed by academic research groups. The aim of this platform is to investigate the possibility of transforming these novel structures to building blocks that can be used to continuously enlarge the numbers of unique, drug-like compounds for the ULTIMATE database.

NATIONAL RESEARCH, DEVELOPMENT AND INNOVATION OFFICE
HUNGARY

PROGRAM FINANCED FROM THE NRDI FUND