ULTIMATE 2.0 - INFINITY database: novel compounds for drug discovery

Mcule.com Kft. has been granted a fund of 120,726,122 HUF for the implementation of the proposal filed to the National Research, Development and Innovation Office titled ULTIMATE 2.0 – INFINITY database: new compounds in drug discovery (ID: 2020-1.1.2-PIACI-KFI-2020-00050). The implementation of the funded actions took place from January 1, 2021 to December 31, 2022. The total cost of the applied research and development project related to health care is 176,047,444 HUF.

Mcule operates a chemical marketplace which collects all compounds and building blocks suitable for drug discovery purposes and available on the market from all over the world. Within the ULTIMATE project, utilizing the building blocks of 3 chemical suppliers, Mcule has already established a database consisting of nearly 500 million virtual compounds which the leading drug discovery companies and academic research centers of the world may choose from and purchase at a fixed price. Assisted by its chemical partners, Mcule produces these compounds, prepares them to be suitable for experimental measurements and delivers them.

In this ULTIMATE 2.0 project, Mcule has developed the INFINITY database storage and searching technology which allows that only the part of the database corresponding to the relevant searching parameters is generated. In addition, by this technology, the number of compounds available in the ULTIMATE database has increased to the scale of billions and the issue of the supply of new building blocks has been resolved. Thus, in the frame of the ULTIMATE 2.0 project, the development of the INFINITY technology has been implemented which enables billions of new compounds (products) to be utilized in drug discovery to become available on the market. A platform called NEWS has also been established during the project. NEWS supports the development of, for example, academic, new building blocks and this way enhances the more efficient development of compounds to be used for drug discovery (new products) and together with that, the extension of the range of products available in ULTIMATE.