The best online drug discovery platform, Building the Ultimate chemical database for drug discovery

Fact Sheet

Project Information

ULTIMATE

Grant agreement ID: 777828

Project website

DOI
10.3030/777828

Project closed

EC signature date
30 June 2017

Start date
1 August 2017

End date
31 July 2019

Funded under
INDUSTRIAL LEADERSHIP - Leadership in enabling and industrial technologies - Information and Communication Technologies (ICT)

Total cost
€ 2 011 662,50

EU contribution
€ 1 408 163,00

Coordinated by
MCULE.COM KFT
Hungary

Objective

Health and wellbeing are among the basic and most essential needs of humanity. Medicines have a major impact on the quality of life and are essential for treating various diseases. Despite the major achievements of the pharmaceutical industry, there are still diseases without effective treatment, such as different types of cancers and neurodegenerative diseases, including Alzheimer's disease. Pharmaceutical industry is continuously searching for new compounds that can become drug

candidates against such diseases. The first key stage of early-phase drug discovery is to select the most appropriate candidate molecules. However, researchers can typically select and order the starting compounds only from the 7-8 million molecules available “off-the-shelf” from suppliers. Our company, Mcule.com Ltd aims to provide the best web-based drug discovery platform for pharmaceutical researchers (big companies, contract research organisations and academics). Our solution, the Ultimate database will not only integrate all purchasable “off-the-shelf” compounds from multiple suppliers, but also includes virtual compounds, which are not yet synthesized, but predicted to be synthesizable with low effort for a reasonable price (https://mcule.com/ultimate-project/). To demonstrate the concept, in 2016 Mcule integrated the first set of virtual compounds and became the largest chemical web shop of the world offering 35 million purchasable compounds. In this project, we aim to create an easily searchable chemical database of 500 million purchasable compounds. Such a large chemical space would present a major advantage for pharmaceutical and biotech companies by increasing their chances to effectively identify novel compounds for diseases, reducing their costs and time losses. The ULTIMATE database will promote our growth by providing access to the database and web-based searching tools for a subscription fee and by increasing considerably our market share as a compound sourcing solution.

Fields of science (EuroSciVoc)

medical and health sciences > basic medicine > pharmacology and pharmacy > **drug discovery**

medical and health sciences > basic medicine > neurology > dementia > **alzheimer**

natural sciences > computer and information sciences > **databases**

medical and health sciences > clinical medicine > **oncology**

natural sciences > **chemical sciences**

Keywords

Drug discovery | cheminformatics | computational chemistry

Programme(s)

H2020-EU.2.1.1. - INDUSTRIAL LEADERSHIP - Leadership in enabling and industrial technologies - Information and Communication Technologies (ICT) MAIN PROGRAMME

H2020-EU.2.3.1. - Mainstreaming SME support, especially through a dedicated instrument

Topic(s)

SMEInst-01-2016-2017 - Open Disruptive Innovation Scheme

Call for proposal

H2020-SMEInst-2016-2017

See other projects for this call

Sub call

H2020-SMEINST-2-2016-2017

Funding Scheme

SME-2 - SME instrument phase 2

Coordinator

MCULE.COM KFT

Net EU contribution

€ 1 408 163,00

Total cost

€ 2 011 662,50

Address

BARTOK BELA UT 105-113
1115 Budapest
Hungary

SME

Yes

Region

Közép-Magyarország > Budapest > Budapest

Activity type

Private for-profit entities (excluding Higher or Secondary Education Establishments)

Links

Contact the organisation

Participation in EU R&I programmes

HORIZON collaboration network

Last update: 6 September 2024

Permalink: https://cordis.europa.eu/project/id/777828