LIGATEPROJECT.EU

LIGATE

The game changer in drug discovery

Major digital and computing advancements — including machine learning/artificial intelligence, extreme-scale computer simulations, and big-data analytics — have revolutionized the pharmaceutical industry and, by effectively harnessing these tools in a broader capacity for drug discovery, we have an excellent opportunity to reduce the time-to-patient and lower the investment risk.

We have to **accelerate drug discovery** and make it one million times faster to improve care for individual patients and impact the health of entire populations.

DEEP-TECH PROJECT LIGATE DEVELOPS AND VALIDATES A PORTABLE AND TUNABLE DRUG DISCOVERY SOLUTION IN HPC SYSTEMS UP TO EXASCALE LEVEL, READY FOR AN ENTIRE WORLD OF APPLICATIONS FOR PRECISION MEDICINE

OUTCOMES

LIGATE will bring the European structure-based computer-aided drug design (CADD) to a higher technological level both in terms of quality of results and with respect to the speed of response to public health emergencies.

The proposed solution, in a fully automated workflow, enables the result of the drug discovery campaign to be delivered in a predetermined amount of time and resources. This predictability will allow the silico drug discovery campaign to run fully in less than one day, and therefore respond promptly to worldwide challenges and reduce investment risks significantly.

In 3 years time we expect to deliver the following:

1. A portable and tunable drug discovery platform ready for Exascale HPC systems to respond promptly to worldwide pandemic crises.

2. A CADD solution to a novel problem of social interest, based on widespread experiment against immunoresistant targets.

3. Validated technologies introduced in CADD methods. Approach and software design will be easily applied to other industrial solutions with a similar structure, regardless of the industrial area.

LIGATE aims to improve analysis, efficiency, scalability, and portability in a unique leading solution.

THIS INTEGRATED SOLUTION WILL SIGNIFICANTLY BOOST THE DRUG DISCOVERY PLATFORM EXSCALATE DEVELOPED BY DOMPÉ, WHILE REDUCING THE EXECUTION TIME OF VIRTUAL SCREENING CAMPAIGNS AND IMPROVING DRUG DEVELOPMENT EFFECTIVENESS.

The overall purpose is the acceleration and automatization of the drug design process, which is currently performed with substantial human effort throughout the different phases of the process. AI-powered auto-tunable solutions allow for the intrinsic complexity of diseases to be addressed. A disease induces a significant perturbation of the physiological system and generates a pathological condition. Combining AI, data analytics, and computer vision, LIGATE will allow researchers to simulate more accurately and describe in greater detail the complexity of chemistry and physics in biological processes to revert perturbation.

The project plans to make the platform available and open to support the discovery of novel treatments in the fight against viral infections and multidrug-resistant bacteria.

Together with 10 outstanding European partners, **Dompé** aims to further strengthen the Exscalate platform at the service of the global scientific community.

Dompé

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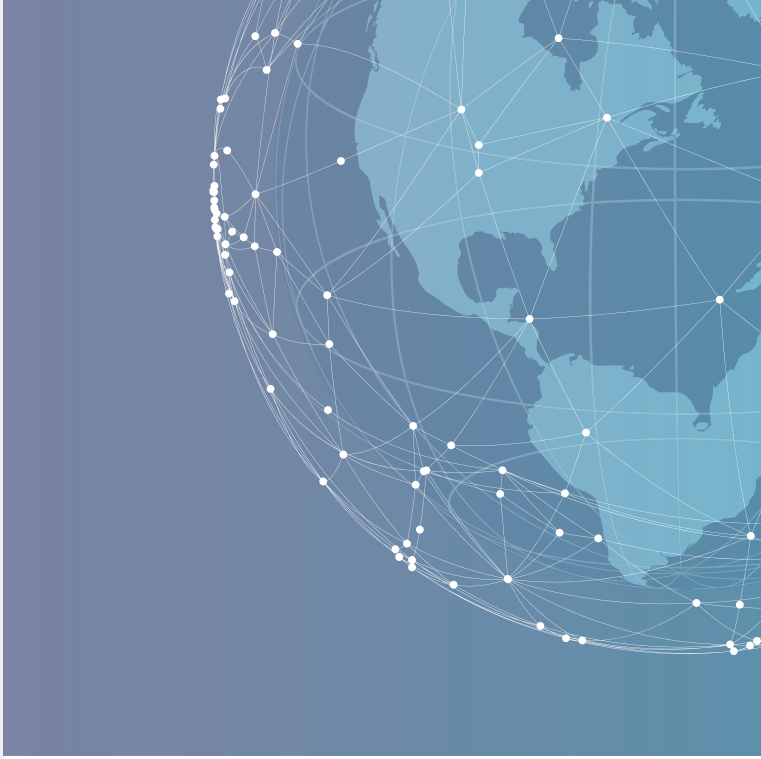

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European Commission

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