

# FUNDING PROGRAM FOR NEXT GENERATION WORLD-LEADING RESEARCHERS

**Project Title:** Computational drug design technologies to innovate pharmaceutical development

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## 1. Background of research

The pharmaceutical industry is facing a serious problem due to the ongoing continual reduction of the number of approved novel medicines. It therefore follows that efficient creation of new medicinal agents is a critical aspect of research.

However, the number of candidate molecules to be evaluated as drugs (chemical space) has an infinite variety of structures available, and it is consequently impossible to create and validate the efficiency of each and every candidate. Adding to the difficulty of the situation is that there is no fundamental approach established for an efficient drug candidate creation and discovery process.

## 2. Research objectives

Given the impetus described above, the objective of this research is to apply computers and develop computational methods for the automatic design of molecules that can serve as candidate medicines which interact with proteins correlated to illnesses.

## 3. Research characteristics (incl. originality and creativity)

What makes this research approach unique is its ability to incorporate artificial intelligence and other state-of-the-art information technologies in order to create a system that can selectively design (predict) potential medicinal molecules amongst the infinite variety of molecules possible.

This project is also special in that it aims to establish a fundamental set of technologies for improved efficiency in designing novel drug molecules.

## 4. Anticipated effects and future applications of research

Through the application of the computational techniques developed in this research project, it is expected that the speed in which medicinal products are developed will be drastically increased, and as a result, new medicines will be developed and made available to patients requiring them more rapidly than in the past.

The resulting contribution of the pharmaceutical industry to the economy is also expected to be significant.