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Supercomputer “K” opens the next generation of in silico drug discovery

スパコン「京」が拓く次世代インシリコ創薬

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The current state of the art in in-silico drug lead discovery is facing a serious problem with respect to prediction accuracy. For example, docking calculation, which is perhaps the most well-known method for virtual screening of leads, currently peaks out at a translational hit rate of a mere 5%, and the issue of how to improve prediction performance has been a problem for more than a decade. There are a multitude of reasons for why computational lead discovery has struggled to produce satisfactory prediction performance; one of main reasons is simply the lack of computational power.

Amidst the requirement to generate results in a realistic amount of time despite insufficient computational power, we have been required to resort to approximation algorithms which incur a loss in prediction performance. In response to this, hopes are high that the supercomputer “K” can resolve the problem of insufficient computational power and make a big contribution to in-silico drug discovery.

In this lecture, the representative of a consortium formed by 11 pharmaceutical and 2 IT companies for the use of the supercomputer “K” applied to in-silico drug discovery will introduce the said project, and discuss current and future directions for computational drug discovery.

Keywords : supercomputing, in silico drug discovery, chemoinformatics, molecular dynamics, machine learninghenotype, omics data, computational systems biology