

## Application of artificial intelligence for drug repositioning

Hiroaki Iwata

*Grad. Sch. Med., Kyoto Univ.*

"Drug repositioning" has been attracting attention as a drug discovery strategy to overcome the recent slowdown in new drug development. Drug repositioning is a technique for discovering new effects of known drugs and redeveloping them as new indications for other diseases. Known drugs have already been confirmed for human safety and pharmacokinetics, and information such as compound production methods can be reused. Therefore, the drug repositioning approach is expected to reduce developed time, risk, and expenditure. Today, pharmaceutical companies are increasing to reuse their own drugs for the drug repositioning approach.

In Life Intelligence Consortium (LINC), pharmaceutical companies, IT companies, and academia are developing together in more than 30 projects. In this talk, we will introduce the developed AI technology in one of the projects, "drug repositioning". In this project, the AI models that predict the target protein, drug efficacy, phenotype, etc. from the compound structure is constructed. The developed AI models can be expected to contribute to the target prediction of active compounds with unknown mechanisms of action, search for new drug discovery targets, and the new indication prediction by reprofiling known drugs.