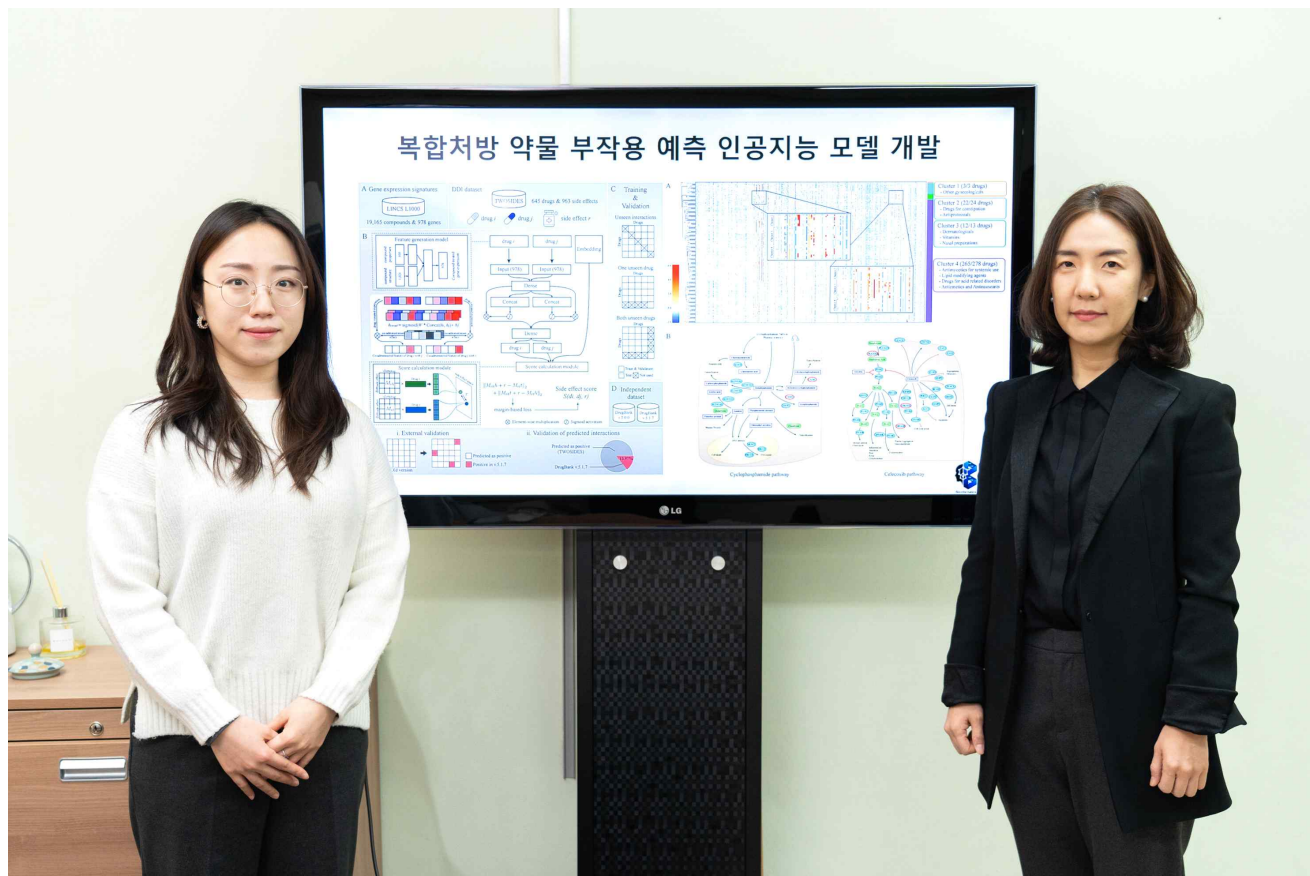


Development of technology for predicting side effects of complex prescription drugs

– Artificial intelligence model for predicting side effects due to drug-drug interactions



▲ From left: Student Eunyoung Kim (first author) and Professor Hojung Nam

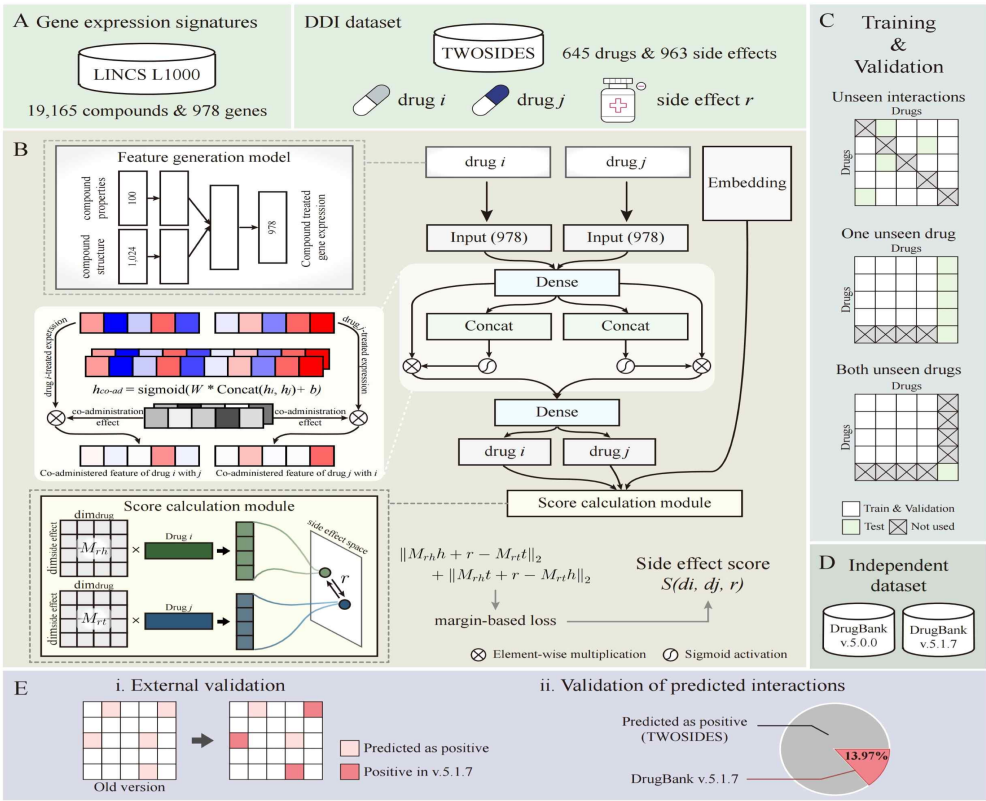
It is very common to receive a prescription for several drugs together for a quick therapeutic remedy, but it is necessary to be careful because side effects are more likely to occur if drug-drug interference caused by drug interaction has a large influence on each other.

GIST (Gwangju Institute of Science and Technology, President Kiseon Kim) School of Electrical Engineering and Computer Science Professor Hojung Nam's research team announced that they have developed an artificial intelligence technology that predicts side effects (DeSIDE-DDI: Interpretable prediction of drug-drug interactions using drug-induced gene expressions) caused by drug interactions based on gene expression data.

Considering that the main targets of complex drug prescriptions are the patient and the elderly, it is very important to predict side effects from drug-drug interactions in advance, which is difficult to identify in advance due to low frequency of observations in the new drug development stage.

To solve this problem, various computer-based side effect prediction models have been developed, but they cannot be applied to predict side effects between new drugs in the new drug development stage and commercially available drugs, and it is difficult to interpret the mechanism causing side effects.

The research team developed a DeSIDE-DDI artificial intelligence model to predict drug-drug interactions based on drug treatment gene expression data. Compared to existing related studies, it shows high prediction accuracy and has the advantage of being able to present genes related to drug-drug interactions, making it possible to interpret the cause of side effects.



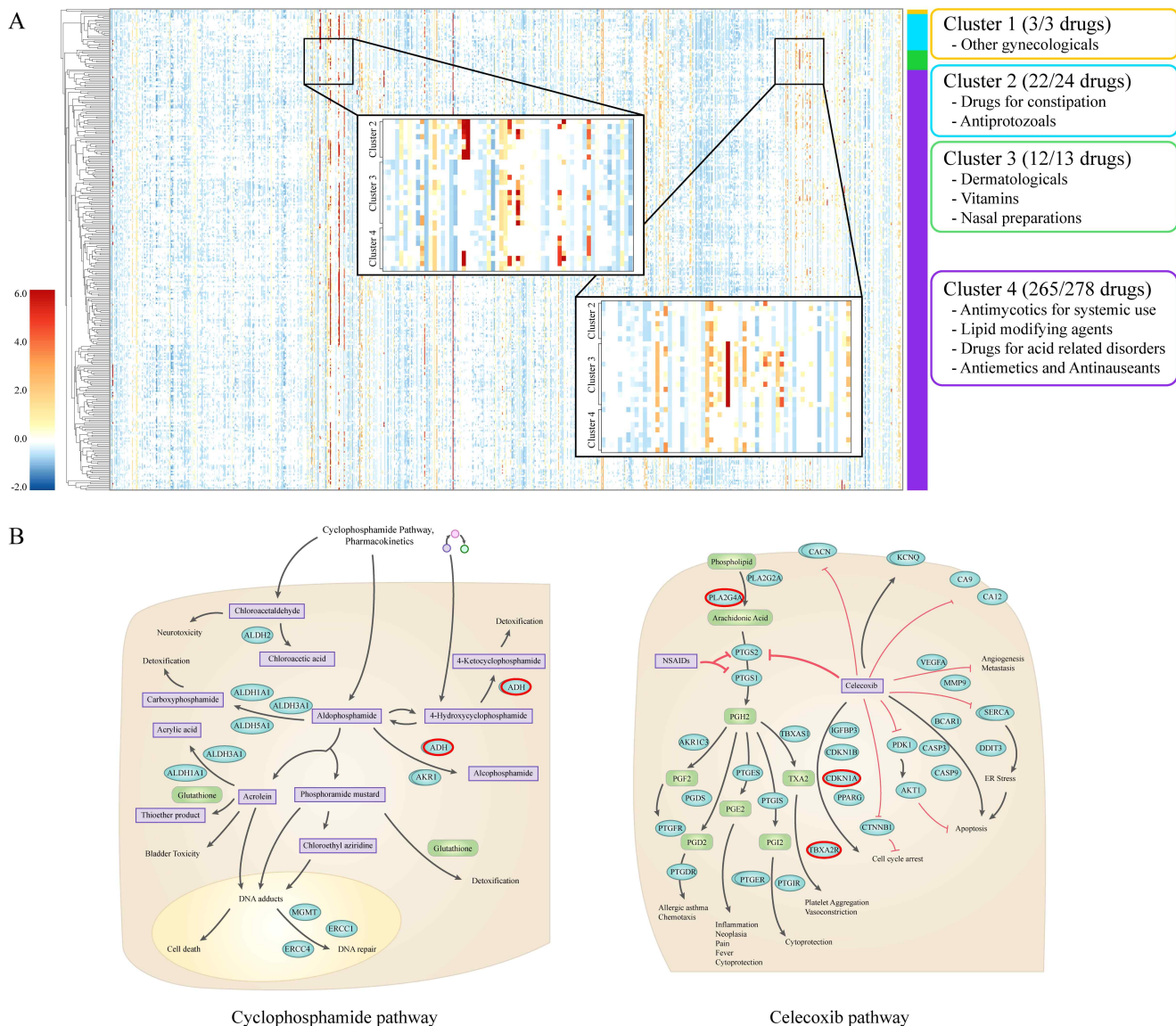
▲ DeSIDE-DDI model overview that comprehensively shows the data used in the model, the detailed structure of the model, and the evaluation and analysis methods.

This study consists of a model that generates drug treatment gene expression data to predict the side effects of various compounds in the drug development stage and a model that predicts drug-drug interactions.

The gene expression data generation model predicts gene expression data when cells are exposed to drugs from the structure and property information of the drug, and, through this, it is possible to predict side effects for drugs even without actual experimental information.

The generated data is used to predict drug-drug interactions, and the GLU (Gated Linear Unit) neural network unit is used to mimic the simultaneous dosing phenomenon within the artificial intelligence model, and, as a result, key gene extraction is also possible. Finally, the components (entities; drugs) and relationships (side effects) are converted into a low-dimensional vector space to predict the side effects of the corresponding drug pair.

The trained DeSIDE-DDI model showed high predictive performance that can be used to predict interactions with new drugs and has the feature of being able to identify highly related genes by weighted analysis of used gene expression data.



▲ A. Difference in gene expression due to combination with other drugs and B. major gene predicted by DeSIDE-DDI identified in the pathway of the drug (red). It can be seen that the GLU of the model reflects the simultaneous dosing information and gives a weight to the major genes.

Professor Hojung Nam said, "This research result is an important study that can be used as a drug stability monitoring system by predicting side effects according to complex drug interactions in advance." First author Eunyoung Kim said, "This can contribute to stability verification in the new drug development stage by explaining the mechanism when side effects occur due to interactions."

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