

Deep learning predicts drug-drug and drug-food interactions

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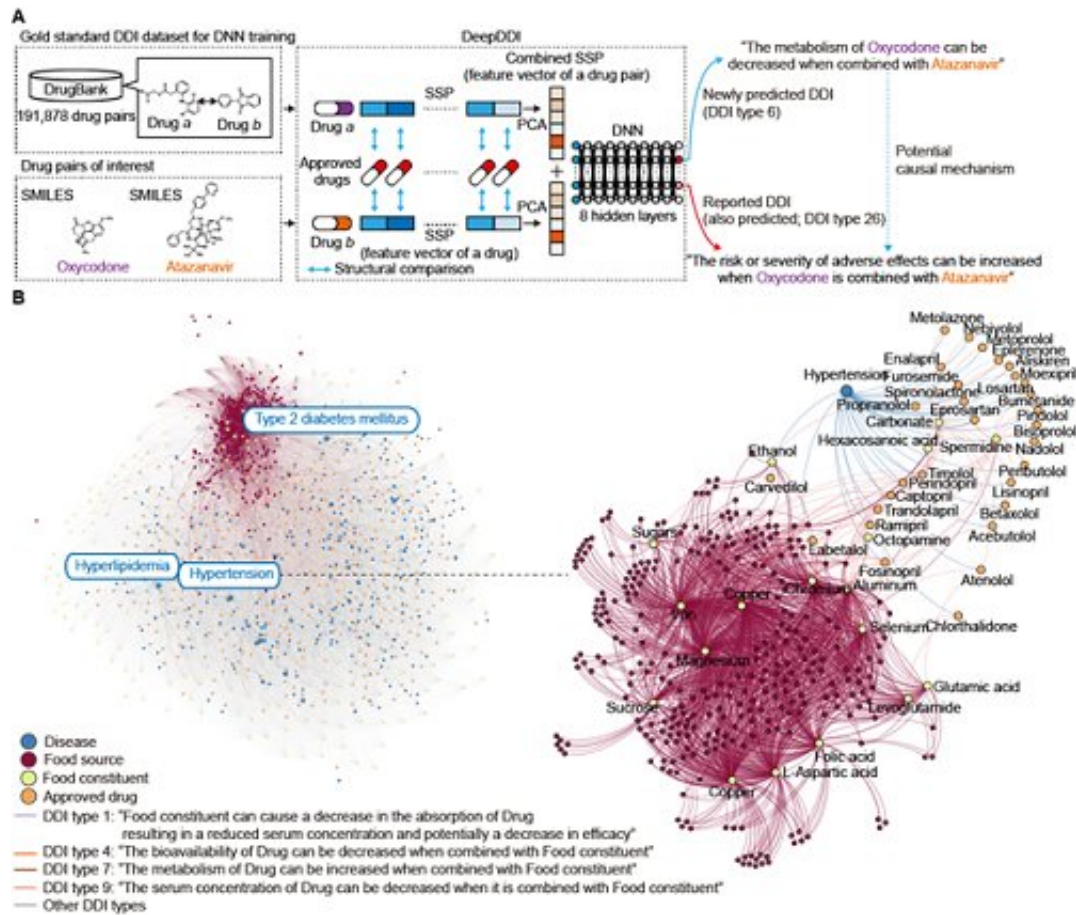


Figure 1. Overall scheme of Deep DDDI and prediction of food constituents that reduce the in vivo concentration of approved drugs. Credit: Korea Advanced Institute of Science and Technology

Drug interactions, including drug-drug interactions (DDIs) and drug-

food constituent interactions (DFIs), can trigger unexpected pharmacological effects, including adverse drug events (ADEs), with causal mechanisms often unknown. However, current prediction methods do not provide sufficient details beyond the chance of DDI occurrence, or require detailed drug information often unavailable for DDI prediction.

To tackle this problem, Dr. Jae Yong Ryu, Assistant Professor Hyun Uk Kim and Distinguished Professor Sang Yup Lee, all from the Department of Chemical and Biomolecular Engineering at Korea Advanced Institute of Science and Technology (KAIST), developed a computational framework, named DeepDDI, that accurately predicts 86 DDI types for a given drug pair. The research results were published online in *Proceedings of the National Academy of Sciences (PNAS)* on April 16, 2018, which is titled "Deep learning improves prediction of drug-drug and drug-food interactions."

DeepDDI takes structural information and names of two drugs in pair as inputs, and predicts relevant DDI types for the input drug pair. DeepDDI uses deep neural network to predict 86 DDI types with a mean accuracy of 92.4% using the DrugBank gold standard DDI dataset covering 192,284 DDIs contributed by 191,878 drug pairs. Very importantly, DDI types predicted by DeepDDI are generated in the form of human-readable sentences as outputs, which describe changes in pharmacological effects and/or the risk of ADEs as a result of the interaction between two drugs in pair. For example, DeepDDI output sentences describing potential interactions between oxycodone (opioid pain medication) and atazanavir (antiretroviral medication) were generated as follows: "The metabolism of Oxycodone can be decreased when combined with Atazanavir"; and "The risk or severity of adverse effects can be increased when Oxycodone is combined with Atazanavir". By doing this, DeepDDI can provide more specific information on [drug interactions](#) beyond the occurrence chance of DDIs or ADEs typically

reported to date.

DeepDDI was first used to predict DDI types of 2,329,561 drug pairs from all possible combinations of 2,159 approved drugs, from which DDI types of 487,632 drug pairs were newly predicted. Also, DeepDDI can be used to suggest which drug or food to avoid during medication in order to minimize the chance of [adverse drug events](#) or optimize the drug efficacy. To this end, DeepDDI was used to suggest potential causal mechanisms for the reported ADEs of 9,284 drug pairs, and also predict alternative drug candidates for 62,707 [drug pairs](#) having negative health effects to keep only the beneficial effects. Furthermore, DeepDDI was applied to 3,288,157 drug-food constituent pairs (2,159 approved drugs and 1,523 well-characterized food constituents) to predict DFIs. The effects of 256 food constituents on pharmacological effects of interacting drugs and bioactivities of 149 food constituents were also finally predicted. All these prediction results can be useful if an individual is taking medications for a specific (chronic) disease such as hypertension or diabetes mellitus type 2.

Distinguished Professor Sang Yup Lee said, "We have developed a platform technology DeepDDI that will allow precision medicine in the era of Fourth Industrial Revolution. DeepDDI can serve to provide important information on [drug](#) prescription and dietary suggestions while taking certain drugs to maximize health benefits and ultimately help maintain a healthy life in this aging society."

More information: Deep learning improves prediction of drug–drug and drug–food interactions, *Proceedings of the National Academy of Sciences* (2018). [10.1073/pnas.1803294115](https://doi.org/10.1073/pnas.1803294115)

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(KAIST)

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