Deep learning for prediction of drug-drug and drug-food interactions

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Drug interactions, including drug-drug interactions (DDIs) and drug-food constituent interactions (DFIs), can cause unexpected pharmacological effects such as adverse drug events. Here, we report development of a computational framework DeepDDI that takes structural information and names of two drugs in pair as inputs, and predicts relevant DDI types as outputs. DeepDDI uses deep neural network with its optimized prediction performance and predicts 86 DDI types with a mean accuracy of 92.4% using the DrugBank gold standard DDI dataset covering 192,284 DDIs. Furthermore, DeepDDI is applied to drug-food constituent pairs to predict DFIs. DeepDDI can provide important information on drug prescription and even dietary suggestions to improve healthcare. [This work was supported by the Technology Development Program to Solve Climate Changes on Systems Metabolic Engineering for Biorefineries (Grants NRF-2012M1A2A2026556 and NRF-2012M1A2A2026557) from the Ministry of Science and ICT through the National Research Foundation (NRF) of Korea. This work was also supported by the Fourth Industrial Revolution AI Flagship initiative from the Korean Advanced Institute of Science and Technology.]