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2019.06.18

Professor Hojung Nam's research team develops an artificial intelligence model to identify drug-target protein interaction

- GIST (President Kiseon Kim) School of Electrical Engineering and Computer Science Professor Hojung Nam's research team presented a methodology for performing drug-target protein interaction * identification at the early stage of drug development using an artificial intelligence model.

* Drug-target protein interaction: The drug target is the native protein in the body whose activity is modified by a drug resulting in a desirable therapeutic effect.

- The research team predicted drug-target protein interaction, which was previously performed experimentally, by using synthetic multiplication neural network (Convolutional Neural Network) AI model.
- In the early stages of drug development, target proteins that are believed to be involved in the disease are selected and then compounds that interact with the target protein are screened. Performing drug-target protein interaction experiments is time consuming and costly. In addition, because determining experimental drug-target protein

interactions is performed on random compounds in a given compound library *, the rate of finding actual interacting compounds is very low.

* Compound library: a collection of stored chemicals used for drug discovery, drug screening, drug target identification, and other pharmaceutical-related applications

- Not all sequences of proteins are involved in drug interaction. However, computer models use all sequences of expressed proteins and their physico-chemical properties. Thus, in this study, the researchers used a Convolutional Neural Network (CNN) * to extract local sequence patterns interacting with drugs and use it to predict drug-target protein interactions.

* Convolutional Neural Network: a deep-learning algorithm which can take in an input image, assign importance (learnable weights and biases) to various aspects/objects in the image and be able to differentiate one from the other

- Tests of more than 24,000 drug-targeted protein data showed an accuracy of about 80%. In addition, the results of the synthetic fiber network could be interpreted to confirm that the extracted region sequence pattern was actually part of the drug-target protein interaction.

- Professor Hojung Nam is currently carrying out a project to establish new drug development platform based on artificial intelligence with the Ministry of Science and ICT, and Professor Yong-Chul Kim of the School of Life Sciences and Professor Jin Hee Ahn of the School of Physics and Chemistry carried out actual screening experiments on compounds presented through the artificial intelligence model, and the results showed that the hit * in single-white groups such as kinase, ion channel, G-protein coupled receptor (GPCR) increased by 10-20 times.

* hit: Hit identification is the first committed step for a successful drug discovery project. In this process, the right small molecules, also called hits, which binding to the target and modifying its function are identified.

- Professor Hojung Nam said, "This study was carried out using artificial intelligence to identify drug-target interactions in the early

stages of drug development. Experiments on candidates predicted through artificial intelligence, rather than the conventional random screening method, can greatly improve the time and cost efficiency of drug development."

- The currently developed artificial intelligence model will be officially applied to the new drug development platform under joint development with researchers from the Korea Research Institute of Chemical Technology and will start service later this year by using specific proteins in a compound library.
- This research was led by GIST School of Electrical Engineering and Computer Science Professor Hojung Nam (corresponding author) and researchers Ingoo Lee and Jongsoo Keum as the co-first authors with support from the Bio-Synergy Research Center, and the results of the research were published on June 14, 2019, in *PLoS Computational Biology* (IF 3.95).